Full wwPDB EM Validation Report ⓘ

Mar 10, 2026 – 02:21 AM UTC

PDB ID	:	7PIW / pdb_00007piw
EMDB ID	:	EMD-13455
Title	:	Stacked stretched Dunaliella PSII
Authors	:	Caspy, I.; Fadeeva, M.; Mazor, Y.; Nelson, N.
Deposited on	:	2021-08-23
Resolution	:	4.00 Å(reported)
Based on initial model	:	6KAC

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:

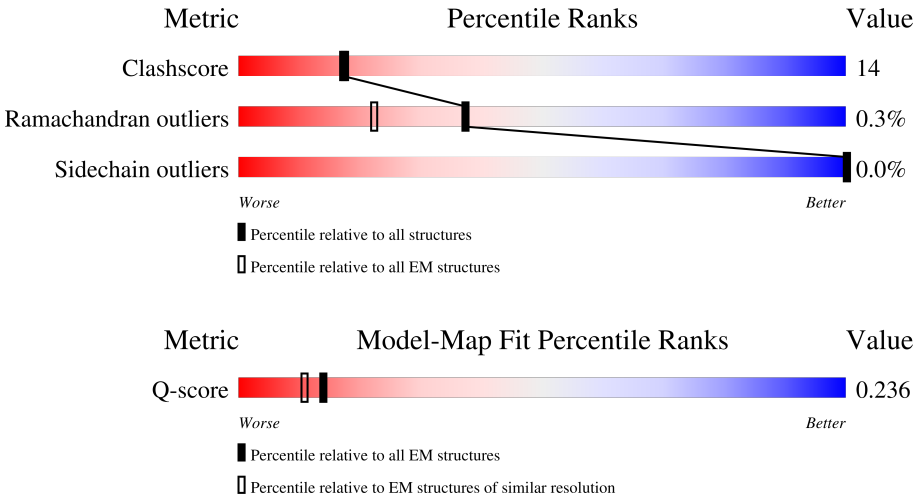
EMDB validation analysis	:	0.0.1.dev132
Mogul	:	2022.3.0, CSD as543be (2022)
MolProbity	:	4-5-2 with Phenix2.0
Buster-report	:	wwPDB partial adaption of 1.1.7 (2018)
Percentile statistics	:	20250101.v01 (using entries in the PDB archive January 1st 2025)
EM percentile statistics	:	202505.v01 (Using data 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 4.00 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	7587 (3.50 - 4.50)

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

Mol	Chain	Length	Quality of chain
1	A	336	31% 74% 26%
1	A1	336	16% 61% 39%
1	a	336	37% 68% 32%
1	a1	336	42% 63% 37%

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Mol	Chain	Length	Quality of chain
2	B	484	53% 77% 23%
2	B1	484	16% 66% 34%
2	b	484	56% 74% 26%
2	b1	484	33% 69% 31%
3	V	32	59% 88% 12%
3	V1	32	28% 72% 28%
3	v	32	84% 69% 31%
3	v1	32	66% 88% 12%
4	C	449	28% 72% 27%
4	C1	449	11% 69% 31%
4	c	449	46% 64% 36%
4	c1	449	36% 70% 30%
5	D	348	41% 72% 28%
5	D1	348	18% 66% 34%
5	d	348	41% 70% 29%
5	d1	348	43% 68% 32%
6	E	76	58% 84% 16%
6	E1	76	12% 75% 25%
6	e	76	75% 79% 21%
6	e1	76	45% 82% 18%
7	F	31	45% 77% 23%
7	F1	31	68% 32%
7	f	31	65% 61% 39%
7	f1	31	29% 77% 23%
8	H	67	70% 76% 22%

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Mol	Chain	Length	Quality of chain
8	H1	67	34% 64% 36%
8	h	67	78% 73% 27%
8	h1	67	46% 60% 40%
9	I	35	40% 74% 26%
9	I1	35	20% 66% 34%
9	i	35	37% 60% 40%
9	i1	35	46% 80% 20%
10	J	36	39% 86% 14%
10	J1	36	36% 83% 17%
10	j	36	72% 78% 22%
10	j1	36	47% 92% 8%
11	K	37	51% 70% 27%
11	K1	37	19% 49% 51%
11	k	37	57% 57% 43%
11	k1	37	46% 68% 32%
12	L	38	53% 61% 39%
12	L1	38	39% 68% 32%
12	l	38	50% 82% 18%
13	M	32	62% 75% 25%
13	m	32	84% 72% 28%
14	O	238	79% 74% 26%
14	O1	238	24% 70% 30%
14	o	238	82% 67% 32%
14	o1	238	33% 78% 22%
15	P	187	100% 82% 18%

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Mol	Chain	Length	Quality of chain
15	P1	187	94% 77% 23%
15	p	187	100% 87% 13%
15	p1	187	93% 82% 18%
16	T	30	53% 87% 13%
16	T1	30	40% 77% 23%
16	t	30	53% 70% 30%
16	t1	30	63% 70% 30%
17	W	44	68% 84% 16%
17	W1	44	14% 68% 32%
17	w	44	59% 91% 9%
17	w1	44	41% 84% 16%
18	X	30	73% 83% 17%
18	X1	30	20% 83% 17%
18	x	30	73% 83% 17%
18	x1	30	60% 97%
19	Z	61	75% 82% 18%
19	Z1	61	15% 97%
19	z	61	92% 79% 21%
19	z1	61	46% 97%
20	N	222	65% 73% 26%
20	N1	222	9% 78% 22%
20	n	222	88% 73% 26%
20	n1	222	26% 80% 20%
21	G	221	83% 75% 25%
21	G1	221	10% 78% 22%

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Mol	Chain	Length	Quality of chain
21	g	221	89% 74% 26%
21	g1	221	23% 78% 22%
22	R	202	97% 81% 19%
22	r	202	94% 78% 22%
23	S	243	77% 82% 17%
23	S1	243	9% 83% 17%
23	s	243	87% 78% 22%
23	s1	243	44% 81% 19%
24	Y	222	56% 75% 24%
24	Y1	222	11% 77% 23%
24	y	222	64% 81% 19%
24	y1	222	27% 78% 22%
25	U	27	89% 85% 15%
25	U1	27	41% 74% 26%
25	u	27	78% 70% 30%
25	u1	27	52% 74% 22%
26	M1	31	65% 58% 42%
26	m1	31	55% 65% 35%
27	R1	202	39% 83% 14%
27	r1	202	41% 80% 16%

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
31	CLA	A	405	X	-	-	-
31	CLA	A	406	X	-	-	-
31	CLA	A	407	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	A	410	X	-	-	-
31	CLA	A1	405	X	-	-	-
31	CLA	A1	406	X	-	-	-
31	CLA	A1	407	X	-	-	-
31	CLA	A1	410	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	-	-	-
31	CLA	B1	602	X	-	-	-
31	CLA	B1	603	X	-	-	-
31	CLA	B1	604	X	-	-	-
31	CLA	B1	605	X	-	-	-
31	CLA	B1	606	X	-	-	-
31	CLA	B1	607	X	-	-	-
31	CLA	B1	608	X	-	-	-
31	CLA	B1	609	X	-	-	-
31	CLA	B1	610	X	-	-	-
31	CLA	B1	611	X	-	-	-
31	CLA	B1	612	X	-	-	-
31	CLA	B1	613	X	-	-	-
31	CLA	B1	614	X	-	-	-
31	CLA	B1	615	X	-	-	-
31	CLA	B1	616	X	-	-	-
31	CLA	B1	617	X	-	-	-
31	CLA	C	501	X	-	-	-
31	CLA	C	502	X	-	-	-
31	CLA	C	503	X	-	-	-
31	CLA	C	504	X	-	-	-
31	CLA	C	505	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	C	506	X	-	-	-
31	CLA	C	507	X	-	-	-
31	CLA	C	508	X	-	-	-
31	CLA	C	509	X	-	-	-
31	CLA	C	510	X	-	-	-
31	CLA	C	511	X	-	-	-
31	CLA	C	512	X	-	-	-
31	CLA	C	513	X	-	-	-
31	CLA	C1	501	X	-	-	-
31	CLA	C1	502	X	-	-	-
31	CLA	C1	503	X	-	-	-
31	CLA	C1	504	X	-	-	-
31	CLA	C1	505	X	-	-	-
31	CLA	C1	506	X	-	-	-
31	CLA	C1	507	X	-	-	-
31	CLA	C1	508	X	-	-	-
31	CLA	C1	509	X	-	-	-
31	CLA	C1	510	X	-	-	-
31	CLA	C1	511	X	-	-	-
31	CLA	C1	512	X	-	-	-
31	CLA	C1	513	X	-	-	-
31	CLA	D	402	X	-	-	-
31	CLA	D	403	X	-	-	-
31	CLA	D1	402	X	-	-	-
31	CLA	D1	403	X	-	-	-
31	CLA	G	602	X	-	-	-
31	CLA	G	603	X	-	-	-
31	CLA	G	604	X	-	-	-
31	CLA	G	610	X	-	-	-
31	CLA	G	611	X	-	-	-
31	CLA	G	612	X	-	-	-
31	CLA	G	613	X	-	-	-
31	CLA	G	614	X	-	-	-
31	CLA	G1	602	X	-	-	-
31	CLA	G1	603	X	-	-	-
31	CLA	G1	604	X	-	-	-
31	CLA	G1	610	X	-	-	-
31	CLA	G1	611	X	-	-	-
31	CLA	G1	612	X	-	-	-
31	CLA	G1	613	X	-	-	-
31	CLA	G1	614	X	-	-	-
31	CLA	N	602	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	N	603	X	-	-	-
31	CLA	N	604	X	-	-	-
31	CLA	N	610	X	-	-	-
31	CLA	N	611	X	-	-	-
31	CLA	N	612	X	-	-	-
31	CLA	N	613	X	-	-	-
31	CLA	N	614	X	-	-	-
31	CLA	N1	602	X	-	-	-
31	CLA	N1	603	X	-	-	-
31	CLA	N1	604	X	-	-	-
31	CLA	N1	610	X	-	-	-
31	CLA	N1	611	X	-	-	-
31	CLA	N1	612	X	-	-	-
31	CLA	N1	613	X	-	-	-
31	CLA	N1	614	X	-	-	-
31	CLA	R	602	X	-	-	-
31	CLA	R	603	X	-	-	-
31	CLA	R	604	X	-	-	-
31	CLA	R	608	X	-	-	-
31	CLA	R	609	X	-	-	-
31	CLA	R	610	X	-	-	-
31	CLA	R	611	X	-	-	-
31	CLA	R	612	X	-	-	-
31	CLA	R	613	X	-	-	-
31	CLA	R1	602	X	-	-	-
31	CLA	R1	603	X	-	-	-
31	CLA	R1	604	X	-	-	-
31	CLA	R1	608	X	-	-	-
31	CLA	R1	609	X	-	-	-
31	CLA	R1	610	X	-	-	-
31	CLA	R1	612	X	-	-	-
31	CLA	S	602	X	-	-	-
31	CLA	S	603	X	-	-	-
31	CLA	S	604	X	-	-	-
31	CLA	S	605	X	-	-	-
31	CLA	S	609	X	-	-	-
31	CLA	S	610	X	-	-	-
31	CLA	S	611	X	-	-	-
31	CLA	S	612	X	-	-	-
31	CLA	S	613	X	-	-	-
31	CLA	S	614	X	-	-	-
31	CLA	S	617	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	S1	602	X	-	-	-
31	CLA	S1	603	X	-	-	-
31	CLA	S1	604	X	-	-	-
31	CLA	S1	605	X	-	-	-
31	CLA	S1	609	X	-	-	-
31	CLA	S1	610	X	-	-	-
31	CLA	S1	611	X	-	-	-
31	CLA	S1	612	X	-	-	-
31	CLA	S1	613	X	-	-	-
31	CLA	S1	614	X	-	-	-
31	CLA	S1	617	X	-	-	-
31	CLA	Y	602	X	-	-	-
31	CLA	Y	603	X	-	-	-
31	CLA	Y	604	X	-	-	-
31	CLA	Y	608	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	Y1	602	X	-	-	-
31	CLA	Y1	603	X	-	-	-
31	CLA	Y1	604	X	-	-	-
31	CLA	Y1	608	X	-	-	-
31	CLA	Y1	610	X	-	-	-
31	CLA	Y1	611	X	-	-	-
31	CLA	Y1	612	X	-	-	-
31	CLA	Y1	613	X	-	-	-
31	CLA	Y1	614	X	-	-	-
31	CLA	a	405	X	-	-	-
31	CLA	a	406	X	-	-	-
31	CLA	a	407	X	-	-	-
31	CLA	a	410	X	-	-	-
31	CLA	a1	405	X	-	-	-
31	CLA	a1	406	X	-	-	-
31	CLA	a1	407	X	-	-	-
31	CLA	a1	410	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	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
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	-	-	-
31	CLA	b1	602	X	-	-	-
31	CLA	b1	603	X	-	-	-
31	CLA	b1	604	X	-	-	-
31	CLA	b1	605	X	-	-	-
31	CLA	b1	606	X	-	-	-
31	CLA	b1	607	X	-	-	-
31	CLA	b1	608	X	-	-	-
31	CLA	b1	609	X	-	-	-
31	CLA	b1	610	X	-	-	-
31	CLA	b1	611	X	-	-	-
31	CLA	b1	612	X	-	-	-
31	CLA	b1	613	X	-	-	-
31	CLA	b1	614	X	-	-	-
31	CLA	b1	615	X	-	-	-
31	CLA	b1	616	X	-	-	-
31	CLA	b1	617	X	-	-	-
31	CLA	c	501	X	-	-	-
31	CLA	c	502	X	-	-	-
31	CLA	c	503	X	-	-	-
31	CLA	c	504	X	-	-	-
31	CLA	c	505	X	-	-	-
31	CLA	c	506	X	-	-	-
31	CLA	c	507	X	-	-	-
31	CLA	c	508	X	-	-	-
31	CLA	c	509	X	-	-	-
31	CLA	c	510	X	-	-	-
31	CLA	c	511	X	-	-	-
31	CLA	c	512	X	-	-	-
31	CLA	c	513	X	-	-	-
31	CLA	c1	501	X	-	-	-
31	CLA	c1	502	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	c1	503	X	-	-	-
31	CLA	c1	504	X	-	-	-
31	CLA	c1	505	X	-	-	-
31	CLA	c1	506	X	-	-	-
31	CLA	c1	507	X	-	-	-
31	CLA	c1	508	X	-	-	-
31	CLA	c1	509	X	-	-	-
31	CLA	c1	510	X	-	-	-
31	CLA	c1	511	X	-	-	-
31	CLA	c1	512	X	-	-	-
31	CLA	c1	513	X	-	-	-
31	CLA	d	402	X	-	-	-
31	CLA	d	403	X	-	-	-
31	CLA	d1	402	X	-	-	-
31	CLA	d1	403	X	-	-	-
31	CLA	g	602	X	-	-	-
31	CLA	g	603	X	-	-	-
31	CLA	g	604	X	-	-	-
31	CLA	g	610	X	-	-	-
31	CLA	g	611	X	-	-	-
31	CLA	g	612	X	-	-	-
31	CLA	g	613	X	-	-	-
31	CLA	g	614	X	-	-	-
31	CLA	g1	602	X	-	-	-
31	CLA	g1	603	X	-	-	-
31	CLA	g1	604	X	-	-	-
31	CLA	g1	610	X	-	-	-
31	CLA	g1	611	X	-	-	-
31	CLA	g1	612	X	-	-	-
31	CLA	g1	613	X	-	-	-
31	CLA	g1	614	X	-	-	-
31	CLA	n	602	X	-	-	-
31	CLA	n	603	X	-	-	-
31	CLA	n	604	X	-	-	-
31	CLA	n	610	X	-	-	-
31	CLA	n	611	X	-	-	-
31	CLA	n	612	X	-	-	-
31	CLA	n	613	X	-	-	-
31	CLA	n	614	X	-	-	-
31	CLA	n1	602	X	-	-	-
31	CLA	n1	603	X	-	-	-
31	CLA	n1	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	n1	610	X	-	-	-
31	CLA	n1	611	X	-	-	-
31	CLA	n1	612	X	-	-	-
31	CLA	n1	613	X	-	-	-
31	CLA	n1	614	X	-	-	-
31	CLA	r	602	X	-	-	-
31	CLA	r	603	X	-	-	-
31	CLA	r	604	X	-	-	-
31	CLA	r	608	X	-	-	-
31	CLA	r	609	X	-	-	-
31	CLA	r	610	X	-	-	-
31	CLA	r	611	X	-	-	-
31	CLA	r	612	X	-	-	-
31	CLA	r	613	X	-	-	-
31	CLA	r1	602	X	-	-	-
31	CLA	r1	603	X	-	-	-
31	CLA	r1	604	X	-	-	-
31	CLA	r1	608	X	-	-	-
31	CLA	r1	609	X	-	-	-
31	CLA	r1	610	X	-	-	-
31	CLA	r1	612	X	-	-	-
31	CLA	s	602	X	-	-	-
31	CLA	s	603	X	-	-	-
31	CLA	s	604	X	-	-	-
31	CLA	s	605	X	-	-	-
31	CLA	s	609	X	-	-	-
31	CLA	s	610	X	-	-	-
31	CLA	s	611	X	-	-	-
31	CLA	s	612	X	-	-	-
31	CLA	s	613	X	-	-	-
31	CLA	s	614	X	-	-	-
31	CLA	s	617	X	-	-	-
31	CLA	s1	602	X	-	-	-
31	CLA	s1	603	X	-	-	-
31	CLA	s1	604	X	-	-	-
31	CLA	s1	605	X	-	-	-
31	CLA	s1	609	X	-	-	-
31	CLA	s1	610	X	-	-	-
31	CLA	s1	611	X	-	-	-
31	CLA	s1	612	X	-	-	-
31	CLA	s1	613	X	-	-	-
31	CLA	s1	614	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
31	CLA	s1	617	X	-	-	-
31	CLA	y	602	X	-	-	-
31	CLA	y	603	X	-	-	-
31	CLA	y	604	X	-	-	-
31	CLA	y	608	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	y1	602	X	-	-	-
31	CLA	y1	603	X	-	-	-
31	CLA	y1	604	X	-	-	-
31	CLA	y1	608	X	-	-	-
31	CLA	y1	610	X	-	-	-
31	CLA	y1	611	X	-	-	-
31	CLA	y1	612	X	-	-	-
31	CLA	y1	613	X	-	-	-
31	CLA	y1	614	X	-	-	-
37	C7Z	B	620	X	-	-	-
37	C7Z	B1	620	X	-	-	-
37	C7Z	b	620	X	-	-	-
37	C7Z	b1	620	X	-	-	-
42	LMK	C	527	X	-	-	-
42	LMK	C1	527	X	-	-	-
42	LMK	c	627	X	-	-	-
42	LMK	c1	527	X	-	-	-
46	RRX	H	101	X	-	X	-
46	RRX	H1	101	X	-	-	-
46	RRX	h	101	X	-	-	-
46	RRX	h1	101	X	-	-	-
47	CHL	G	601	X	-	-	-
47	CHL	G	605	X	-	-	-
47	CHL	G	606	X	-	-	-
47	CHL	G	607	X	-	-	-
47	CHL	G	608	X	-	-	-
47	CHL	G	609	X	-	-	-
47	CHL	G1	601	X	-	-	-
47	CHL	G1	605	X	-	-	-
47	CHL	G1	606	X	-	-	-
47	CHL	G1	607	X	-	-	-
47	CHL	G1	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
47	CHL	G1	609	X	-	-	-
47	CHL	N	601	X	-	-	-
47	CHL	N	605	X	-	-	-
47	CHL	N	606	X	-	-	-
47	CHL	N	607	X	-	-	-
47	CHL	N	608	X	-	-	-
47	CHL	N	609	X	-	-	-
47	CHL	N1	601	X	-	-	-
47	CHL	N1	605	X	-	-	-
47	CHL	N1	606	X	-	-	-
47	CHL	N1	607	X	-	-	-
47	CHL	N1	608	X	-	-	-
47	CHL	N1	609	X	-	-	-
47	CHL	R	606	X	-	-	-
47	CHL	R	607	X	-	-	-
47	CHL	R1	606	X	-	-	-
47	CHL	R1	607	X	-	-	-
47	CHL	S	601	X	-	-	-
47	CHL	S	606	X	-	-	-
47	CHL	S	607	X	-	-	-
47	CHL	S	608	X	-	-	-
47	CHL	S1	601	X	-	-	-
47	CHL	S1	606	X	-	-	-
47	CHL	S1	607	X	-	-	-
47	CHL	S1	608	X	-	-	-
47	CHL	Y	601	X	-	-	-
47	CHL	Y	605	X	-	-	-
47	CHL	Y	606	X	-	-	-
47	CHL	Y	607	X	-	-	-
47	CHL	Y	609	X	-	-	-
47	CHL	Y1	601	X	-	-	-
47	CHL	Y1	605	X	-	-	-
47	CHL	Y1	606	X	-	-	-
47	CHL	Y1	607	X	-	-	-
47	CHL	Y1	609	X	-	-	-
47	CHL	g	601	X	-	-	-
47	CHL	g	605	X	-	-	-
47	CHL	g	606	X	-	-	-
47	CHL	g	607	X	-	-	-
47	CHL	g	608	X	-	-	-
47	CHL	g	609	X	-	-	-
47	CHL	g1	601	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
47	CHL	g1	605	X	-	-	-
47	CHL	g1	606	X	-	-	-
47	CHL	g1	607	X	-	-	-
47	CHL	g1	608	X	-	-	-
47	CHL	g1	609	X	-	-	-
47	CHL	n	601	X	-	-	-
47	CHL	n	605	X	-	-	-
47	CHL	n	606	X	-	-	-
47	CHL	n	607	X	-	-	-
47	CHL	n	608	X	-	-	-
47	CHL	n	609	X	-	-	-
47	CHL	n1	601	X	-	-	-
47	CHL	n1	605	X	-	-	-
47	CHL	n1	606	X	-	-	-
47	CHL	n1	607	X	-	-	-
47	CHL	n1	608	X	-	-	-
47	CHL	n1	609	X	-	-	-
47	CHL	r	606	X	-	-	-
47	CHL	r	607	X	-	-	-
47	CHL	r1	606	X	-	-	-
47	CHL	r1	607	X	-	-	-
47	CHL	s	601	X	-	-	-
47	CHL	s	606	X	-	-	-
47	CHL	s	607	X	-	-	-
47	CHL	s	608	X	-	-	-
47	CHL	s1	601	X	-	-	-
47	CHL	s1	606	X	-	-	-
47	CHL	s1	607	X	-	-	-
47	CHL	s1	608	X	-	-	-
47	CHL	y	601	X	-	-	-
47	CHL	y	605	X	-	-	-
47	CHL	y	606	X	-	-	-
47	CHL	y	607	X	-	-	-
47	CHL	y	609	X	-	-	-
47	CHL	y1	601	X	-	-	-
47	CHL	y1	605	X	-	-	-
47	CHL	y1	606	X	-	-	-
47	CHL	y1	607	X	-	-	-
47	CHL	y1	609	X	-	-	-
48	LUT	G	621	X	-	-	-
48	LUT	R1	620	X	-	-	-
48	LUT	S	620	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
48	LUT	Y	621	X	-	-	-
48	LUT	g1	621	X	-	-	-
48	LUT	n	621	X	-	-	-
48	LUT	s	620	X	-	-	-
49	XAT	G	622	X	-	-	-
49	XAT	G1	622	X	-	-	-
49	XAT	N	622	X	-	-	-
49	XAT	N1	622	X	-	-	-
49	XAT	R	621	X	-	-	-
49	XAT	Y	622	X	-	-	-
49	XAT	Y1	622	X	-	-	-
49	XAT	g	622	X	-	-	-
49	XAT	g1	622	X	-	-	-
49	XAT	n1	622	X	-	-	-
49	XAT	r	622	X	-	-	-
49	XAT	r1	621	X	-	-	-
56	ERG	R1	626	X	-	-	-
56	ERG	r1	626	X	-	-	-

2 Entry composition (i)

There are 57 unique types of molecules in this entry. The entry contains 151508 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Photosystem II protein D1.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	A	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		
1	a	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		
1	A1	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		
1	a1	336	Total	C	N	O	S	1	0
			2638	1721	432	468	17		

- Molecule 2 is a protein called Photosystem II CP47 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
2	B	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		
2	b	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		
2	B1	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		
2	b1	484	Total	C	N	O	S	0	0
			3783	2480	630	663	10		

There are 8 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
B	298	VAL	LEU	variant	UNP D0FY05
B	415	SER	LEU	variant	UNP D0FY05
b	298	VAL	LEU	variant	UNP D0FY05
b	415	SER	LEU	variant	UNP D0FY05
B1	298	VAL	LEU	variant	UNP D0FY05
B1	415	SER	LEU	variant	UNP D0FY05
b1	298	VAL	LEU	variant	UNP D0FY05
b1	415	SER	LEU	variant	UNP D0FY05

- Molecule 3 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms				AltConf	Trace
3	V	32	Total 227	C 152	N 37	O 38	0	0
3	v	32	Total 227	C 152	N 37	O 38	0	0
3	V1	32	Total 227	C 152	N 37	O 38	0	0
3	v1	32	Total 227	C 152	N 37	O 38	0	0

- Molecule 4 is a protein called Photosystem II CP43 reaction center protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
4	C	449	Total 3483	C 2282	N 581	O 607	S 13	0	0
4	c	449	Total 3483	C 2282	N 581	O 607	S 13	0	0
4	C1	449	Total 3483	C 2282	N 581	O 607	S 13	0	0
4	c1	449	Total 3483	C 2282	N 581	O 607	S 13	0	0

- Molecule 5 is a protein called Photosystem II D2 protein.

Mol	Chain	Residues	Atoms					AltConf	Trace
5	D	348	Total 2766	C 1824	N 454	O 477	S 11	0	0
5	d	348	Total 2766	C 1824	N 454	O 477	S 11	0	0
5	D1	348	Total 2766	C 1824	N 454	O 477	S 11	0	0
5	d1	348	Total 2766	C 1824	N 454	O 477	S 11	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
D	319	ILE	LEU	variant	UNP D0FXW8
d	319	ILE	LEU	variant	UNP D0FXW8
D1	319	ILE	LEU	variant	UNP D0FXW8
d1	319	ILE	LEU	variant	UNP D0FXW8

- Molecule 6 is a protein called Cytochrome b559 subunit alpha.

Mol	Chain	Residues	Atoms				AltConf	Trace
6	E	76	Total 621	C 404	N 102	O 115	0	0
6	e	76	Total 621	C 404	N 102	O 115	0	0
6	E1	76	Total 621	C 404	N 102	O 115	0	0
6	e1	76	Total 621	C 404	N 102	O 115	0	0

- Molecule 7 is a protein called Cytochrome b559 subunit beta.

Mol	Chain	Residues	Atoms					AltConf	Trace
7	F	31	Total 252	C 172	N 42	O 37	S 1	0	0
7	f	31	Total 252	C 172	N 42	O 37	S 1	0	0
7	F1	31	Total 252	C 172	N 42	O 37	S 1	0	0
7	f1	31	Total 252	C 172	N 42	O 37	S 1	0	0

- Molecule 8 is a protein called Photosystem II reaction center protein H.

Mol	Chain	Residues	Atoms					AltConf	Trace
8	H	67	Total 503	C 334	N 76	O 92	S 1	0	0
8	h	67	Total 503	C 334	N 76	O 92	S 1	0	0
8	H1	67	Total 503	C 334	N 76	O 92	S 1	0	0
8	h1	67	Total 503	C 334	N 76	O 92	S 1	0	0

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
H	85	ALA	SER	variant	UNP D0FY02
h	85	ALA	SER	variant	UNP D0FY02
H1	85	ALA	SER	variant	UNP D0FY02
h1	85	ALA	SER	variant	UNP D0FY02

- Molecule 9 is a protein called Photosystem II reaction center protein I.

Mol	Chain	Residues	Atoms					AltConf	Trace
9	I	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	i	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	I1	35	Total	C	N	O	S	0	0
			279	190	42	46	1		
9	i1	35	Total	C	N	O	S	0	0
			279	190	42	46	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
10	J	36	Total	C	N	O	0	0
			266	183	40	43		
10	j	36	Total	C	N	O	0	0
			266	183	40	43		
10	J1	36	Total	C	N	O	0	0
			266	183	40	43		
10	j1	36	Total	C	N	O	0	0
			266	183	40	43		

There are 12 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
J	7	ILE	THR	variant	UNP D0FXW2
J	28	ALA	GLY	variant	UNP D0FXW2
J	42	LEU	GLN	variant	UNP D0FXW2
j	7	ILE	THR	variant	UNP D0FXW2
j	28	ALA	GLY	variant	UNP D0FXW2
j	42	LEU	GLN	variant	UNP D0FXW2
J1	7	ILE	THR	variant	UNP D0FXW2
J1	28	ALA	GLY	variant	UNP D0FXW2
J1	42	LEU	GLN	variant	UNP D0FXW2
j1	7	ILE	THR	variant	UNP D0FXW2
j1	28	ALA	GLY	variant	UNP D0FXW2
j1	42	LEU	GLN	variant	UNP D0FXW2

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

Mol	Chain	Residues	Atoms				AltConf	Trace
11	K	37	Total	C	N	O	0	0
			297	207	43	47		

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Mol	Chain	Residues	Atoms				AltConf	Trace
11	k	37	Total 297	C 207	N 43	O 47	0	0
11	K1	37	Total 297	C 207	N 43	O 47	0	0
11	k1	37	Total 297	C 207	N 43	O 47	0	0

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

Mol	Chain	Residues	Atoms					AltConf	Trace
12	L	38	Total 313	C 209	N 51	O 52	S 1	0	0
12	l	38	Total 313	C 209	N 51	O 52	S 1	0	0
12	L1	38	Total 313	C 209	N 51	O 52	S 1	0	0

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	M	32	Total 243	C 164	N 34	O 45	0	0
13	m	32	Total 243	C 164	N 34	O 45	0	0

There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M	9	THR	ILE	variant	UNP D0FXZ3
m	9	THR	ILE	variant	UNP D0FXZ3

- Molecule 14 is a protein called PsbO.

Mol	Chain	Residues	Atoms					AltConf	Trace
14	O	238	Total 1820	C 1149	N 295	O 370	S 6	0	0
14	o	238	Total 1820	C 1149	N 295	O 370	S 6	0	0
14	O1	238	Total 1820	C 1149	N 295	O 370	S 6	0	0
14	o1	238	Total 1820	C 1149	N 295	O 370	S 6	0	0

- Molecule 15 is a protein called PsbP.

Mol	Chain	Residues	Atoms					AltConf	Trace
15	P	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	p	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	P1	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		
15	p1	187	Total	C	N	O	S	0	0
			1444	916	242	285	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	T	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	t	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	T1	30	Total	C	N	O	S	0	0
			247	171	36	39	1		
16	t1	30	Total	C	N	O	S	0	0
			247	171	36	39	1		

- Molecule 17 is a protein called PsbW.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	W	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	w	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	W1	44	Total	C	N	O	S	0	0
			332	215	53	63	1		
17	w1	44	Total	C	N	O	S	0	0
			332	215	53	63	1		

- Molecule 18 is a protein called PsbX.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	X	30	Total	C	N	O	0	0
			201	132	32	37		
18	x	30	Total	C	N	O	0	0
			201	132	32	37		
18	X1	30	Total	C	N	O	0	0
			201	132	32	37		

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Mol	Chain	Residues	Atoms				AltConf	Trace
18	x1	30	Total 201	C 132	N 32	O 37	0	0

- Molecule 19 is a protein called PsbZ.

Mol	Chain	Residues	Atoms					AltConf	Trace
19	Z	61	Total 457	C 312	N 68	O 76	S 1	0	0
19	z	61	Total 457	C 312	N 68	O 76	S 1	0	0
19	Z1	61	Total 457	C 312	N 68	O 76	S 1	0	0
19	z1	61	Total 457	C 312	N 68	O 76	S 1	0	0

- Molecule 20 is a protein called LHCII M3.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	N	222	Total 1703	C 1100	N 277	O 321	S 5	0	0
20	n	222	Total 1703	C 1100	N 277	O 321	S 5	0	0
20	N1	222	Total 1703	C 1100	N 277	O 321	S 5	0	0
20	n1	222	Total 1703	C 1100	N 277	O 321	S 5	0	0

- Molecule 21 is a protein called LHCII M2.

Mol	Chain	Residues	Atoms					AltConf	Trace
21	G	221	Total 1680	C 1085	N 271	O 321	S 3	0	0
21	g	221	Total 1680	C 1085	N 271	O 321	S 3	0	0
21	G1	221	Total 1680	C 1085	N 271	O 321	S 3	0	0
21	g1	221	Total 1680	C 1085	N 271	O 321	S 3	0	0

- Molecule 22 is a protein called CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
22	R	202	Total	C	N	O	S	0	0
			1533	974	258	298	3		
22	r	202	Total	C	N	O	S	0	0
			1533	974	258	298	3		

- Molecule 23 is a protein called CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	242	Total	C	N	O	S	0	0
			1849	1195	297	354	3		
23	s	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	S1	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		
23	s1	243	Total	C	N	O	S	0	0
			1856	1200	298	355	3		

- Molecule 24 is a protein called LHCII M1.

Mol	Chain	Residues	Atoms					AltConf	Trace
24	Y	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	y	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	Y1	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		
24	y1	222	Total	C	N	O	S	0	0
			1667	1080	272	312	3		

- Molecule 25 is a protein called PsbU.

Mol	Chain	Residues	Atoms					AltConf	Trace
25	U	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
25	u	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
25	U1	27	Total	C	N	O	S	0	0
			224	134	42	47	1		
25	u1	27	Total	C	N	O	S	0	0
			224	134	42	47	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
26	M1	31	Total 234	C 159	N 33	O 42	0	0
26	m1	31	Total 234	C 159	N 33	O 42	0	0

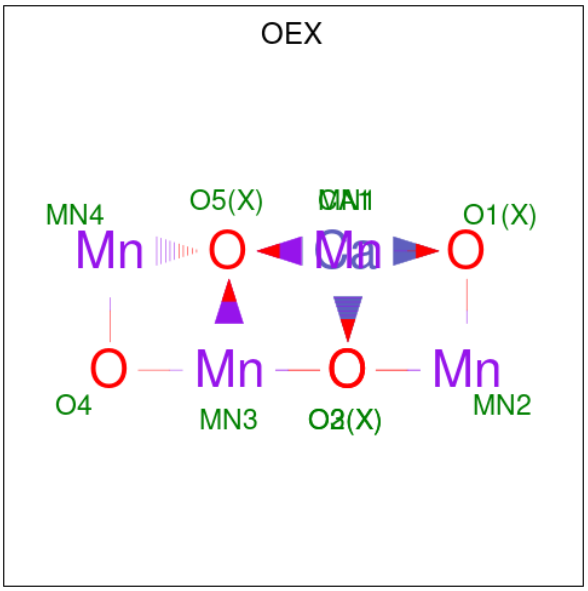
There are 2 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
M1	9	THR	ILE	variant	UNP D0FXZ3
m1	9	THR	ILE	variant	UNP D0FXZ3

- Molecule 27 is a protein called CP29.

Mol	Chain	Residues	Atoms						AltConf	Trace
27	R1	196	Total 1490	C 943	N 251	O 292	P 1	S 3	0	0
27	r1	196	Total 1490	C 943	N 251	O 292	P 1	S 3	0	0

- Molecule 28 is CA-MN4-O5 CLUSTER (CCD ID: OEX) (formula: $CaMn_4O_5$).



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

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Mol	Chain	Residues	Atoms				AltConf
28	A1	1	Total 10	Ca 1	Mn 4	O 5	0
28	a1	1	Total 10	Ca 1	Mn 4	O 5	0

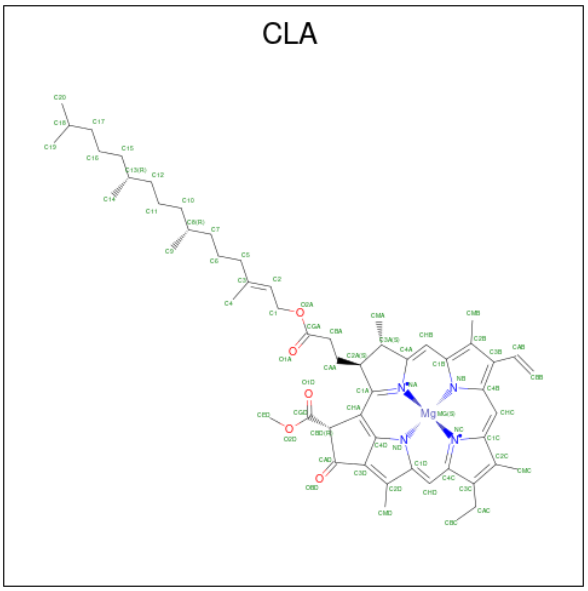
- Molecule 29 is FE (II) ION (CCD ID: FE2) (formula: Fe).

Mol	Chain	Residues	Atoms		AltConf
29	A	1	Total 1	Fe 1	0
29	a	1	Total 1	Fe 1	0
29	A1	1	Total 1	Fe 1	0
29	a1	1	Total 1	Fe 1	0

- Molecule 30 is CHLORIDE ION (CCD ID: CL) (formula: Cl).

Mol	Chain	Residues	Atoms		AltConf
30	A	2	Total 2	Cl 2	0
30	a	2	Total 2	Cl 2	0
30	A1	2	Total 2	Cl 2	0
30	a1	2	Total 2	Cl 2	0

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



Mol	Chain	Residues	Atoms					AltConf
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	
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	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
			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
			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	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	

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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
			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
			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	G	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
			49	39	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
			45	35	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	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
			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	

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Mol	Chain	Residues	Atoms					AltConf
31	R	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	R	1	Total	C	Mg	N	O	0
			46	36	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
			46	36	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
			55	45	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
			45	35	1	4	5	
31	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	S	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	S	1	Total	C	Mg	N	O	0
			50	40	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
			50	40	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
			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
			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	
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	

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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	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
			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
			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	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
			65	55	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
			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	g	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
			49	39	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
			45	35	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	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
			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
			60	50	1	4	5	
31	r	1	Total	C	Mg	N	O	0
			46	36	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
			46	36	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
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
			55	45	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
			45	35	1	4	5	
31	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	s	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	s	1	Total	C	Mg	N	O	0
			50	40	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
			50	40	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	A1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	A1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	A1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	A1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	B1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	C1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	D1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	D1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	N1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	N1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	N1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	N1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	N1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	N1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	N1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	N1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	G1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	G1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	G1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	G1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	G1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	G1	1	Total	C	Mg	N	O	0
			43	35	1	4	3	
31	G1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	G1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	R1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	R1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	R1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	R1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	R1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	R1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	R1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	S1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	S1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	S1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	S1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	S1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	S1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	S1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	S1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	S1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	S1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	S1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	Y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	Y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	Y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	Y1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	Y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	Y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	Y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	Y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	Y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	a1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	a1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	a1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	a1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	b1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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Mol	Chain	Residues	Atoms					AltConf
31	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	c1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	d1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	d1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	n1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	n1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	n1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	n1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	n1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	n1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	n1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	n1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	g1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	g1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	g1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	g1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	g1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	g1	1	Total	C	Mg	N	O	0
			43	35	1	4	3	

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Mol	Chain	Residues	Atoms					AltConf
31	g1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	g1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	r1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	r1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	r1	1	Total	C	Mg	N	O	0
			49	39	1	4	5	
31	r1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	r1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	r1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	r1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	s1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	s1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	s1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	s1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	s1	1	Total	C	Mg	N	O	0
			60	50	1	4	5	
31	s1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	s1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	s1	1	Total	C	Mg	N	O	0
			45	35	1	4	5	
31	s1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	s1	1	Total	C	Mg	N	O	0
			55	45	1	4	5	
31	s1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

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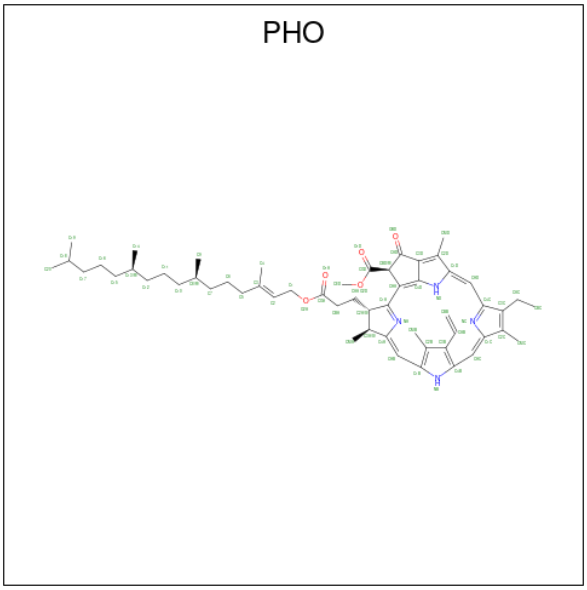
Mol	Chain	Residues	Atoms					AltConf
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			50	40	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	
31	y1	1	Total	C	Mg	N	O	0
			65	55	1	4	5	

- Molecule 32 is PHEOPHYTIN A (CCD ID: PHO) (formula: $C_{55}H_{74}N_4O_5$).



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

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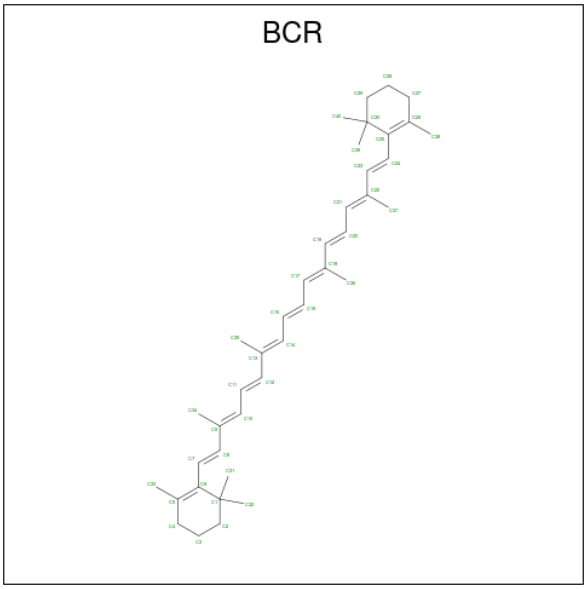
Mol	Chain	Residues	Atoms	AltConf
32	a	1	Total C N O 64 55 4 5	0
32	A1	1	Total C N O 64 55 4 5	0
32	A1	1	Total C N O 64 55 4 5	0
32	a1	1	Total C N O 64 55 4 5	0
32	a1	1	Total C N O 64 55 4 5	0

- Molecule 33 is BETA-CAROTENE (CCD ID: BCR) (formula: $C_{40}H_{56}$).



Mol	Chain	Residues	Atoms	AltConf
33	A	1	Total C 40 40	0
33	B	1	Total C 40 40	0
33	B	1	Total C 40 40	0
33	C	1	Total C 40 40	0
33	C	1	Total C 40 40	0
33	C	1	Total C 40 40	0

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Mol	Chain	Residues	Atoms	AltConf
33	C	1	Total C 40 40	0
33	D	1	Total C 40 40	0
33	a	1	Total C 40 40	0
33	b	1	Total C 40 40	0
33	b	1	Total C 40 40	0
33	c	1	Total C 40 40	0
33	c	1	Total C 40 40	0
33	c	1	Total C 40 40	0
33	c	1	Total C 40 40	0
33	d	1	Total C 40 40	0
33	A1	1	Total C 40 40	0
33	B1	1	Total C 40 40	0
33	B1	1	Total C 40 40	0
33	C1	1	Total C 40 40	0
33	C1	1	Total C 40 40	0
33	C1	1	Total C 40 40	0
33	C1	1	Total C 40 40	0
33	D1	1	Total C 40 40	0
33	a1	1	Total C 40 40	0
33	b1	1	Total C 40 40	0
33	b1	1	Total C 40 40	0

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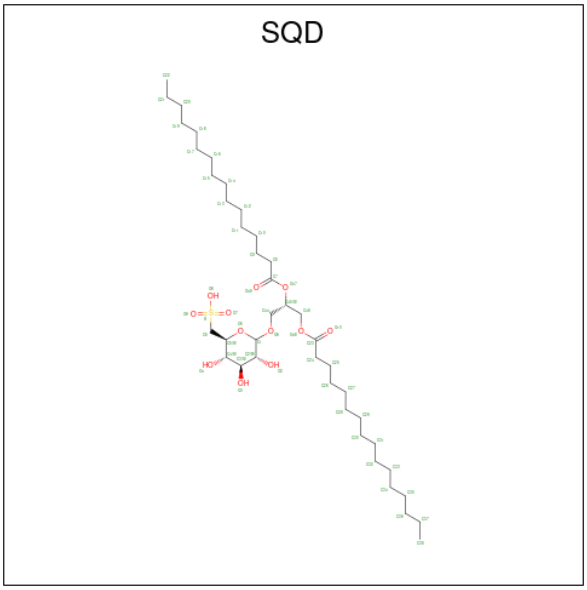
Mol	Chain	Residues	Atoms	AltConf
33	c1	1	Total C 40 40	0
33	c1	1	Total C 40 40	0
33	c1	1	Total C 40 40	0
33	c1	1	Total C 40 40	0
33	d1	1	Total C 40 40	0

- Molecule 34 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (CCD ID: SQD) (formula: $C_{41}H_{78}O_{12}S$).



Mol	Chain	Residues	Atoms	AltConf
34	A	1	Total C O S 51 38 12 1	0
34	B	1	Total C O S 54 41 12 1	0
34	C	1	Total C O S 54 41 12 1	0
34	a	1	Total C O S 51 38 12 1	0
34	b	1	Total C O S 54 41 12 1	0
34	c	1	Total C O S 54 41 12 1	0

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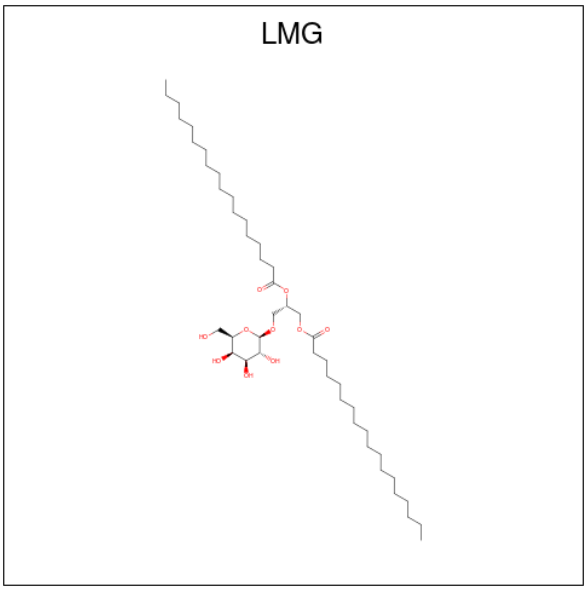
Mol	Chain	Residues	Atoms				AltConf
34	A1	1	Total	C	O	S	0
			51	38	12	1	
34	B1	1	Total	C	O	S	0
			42	29	12	1	
34	B1	1	Total	C	O	S	0
			54	41	12	1	
34	C1	1	Total	C	O	S	0
			54	41	12	1	
34	M1	1	Total	C	O	S	0
			42	29	12	1	
34	a1	1	Total	C	O	S	0
			51	38	12	1	
34	b1	1	Total	C	O	S	0
			42	29	12	1	
34	b1	1	Total	C	O	S	0
			54	41	12	1	
34	c1	1	Total	C	O	S	0
			54	41	12	1	
34	m1	1	Total	C	O	S	0
			42	29	12	1	

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



Mol	Chain	Residues	Atoms			AltConf
35	A	1	Total	C	O	0
			48	38	10	

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Mol	Chain	Residues	Atoms			AltConf
35	B	1	Total	C	O	0
			44	34	10	
35	C	1	Total	C	O	0
			51	41	10	
35	D	1	Total	C	O	0
			46	36	10	
35	H	1	Total	C	O	0
			48	38	10	
35	J	1	Total	C	O	0
			45	35	10	
35	a	1	Total	C	O	0
			48	38	10	
35	b	1	Total	C	O	0
			44	34	10	
35	c	1	Total	C	O	0
			51	41	10	
35	d	1	Total	C	O	0
			46	36	10	
35	h	1	Total	C	O	0
			48	38	10	
35	j	1	Total	C	O	0
			45	35	10	
35	A1	1	Total	C	O	0
			48	38	10	
35	B1	1	Total	C	O	0
			44	34	10	
35	C1	1	Total	C	O	0
			51	41	10	
35	C1	1	Total	C	O	0
			55	45	10	
35	D1	1	Total	C	O	0
			46	36	10	
35	H1	1	Total	C	O	0
			48	38	10	
35	W1	1	Total	C	O	0
			39	29	10	
35	a1	1	Total	C	O	0
			48	38	10	
35	b1	1	Total	C	O	0
			44	34	10	
35	c1	1	Total	C	O	0
			51	41	10	

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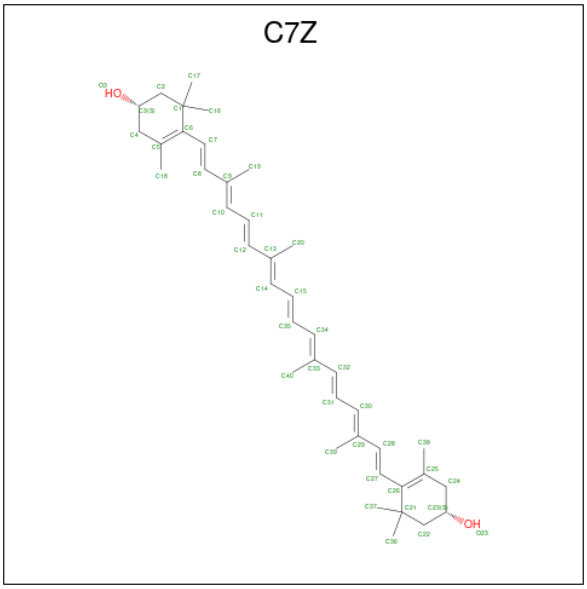
Mol	Chain	Residues	Atoms	AltConf
35	c1	1	Total C O 55 45 10	0
35	d1	1	Total C O 46 36 10	0
35	h1	1	Total C O 48 38 10	0
35	w1	1	Total C O 39 29 10	0

- Molecule 36 is SODIUM ION (CCD ID: NA) (formula: Na).

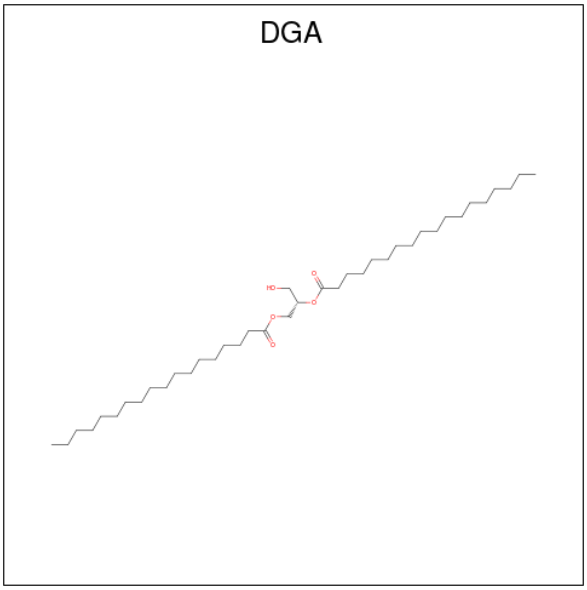
Mol	Chain	Residues	Atoms	AltConf
36	A	1	Total Na 1 1	0
36	a	1	Total Na 1 1	0
36	A1	1	Total Na 1 1	0
36	a1	1	Total Na 1 1	0

- Molecule 37 is (1 {S})-3,5,5-trimethyl-4-[(1 {E},3 {E},5 {E},7 {E},9 {E},11 {E},13 {E},15 {E},17 {E})-3,7,12,16-tetramethyl-18-[(4 {S})-2,6,6-trimethyl-4-oxidanyl-cyclohexen-1-yl]octadeca-1,3,5,7,9,11,13,15,17-nonaenyl]cyclohex-3-en-1-ol (CCD ID: C7Z) (formula: $C_{40}H_{56}O_2$).



Mol	Chain	Residues	Atoms			AltConf
37	B	1	Total	C	O	0
			42	40	2	
37	b	1	Total	C	O	0
			42	40	2	
37	B1	1	Total	C	O	0
			42	40	2	
37	b1	1	Total	C	O	0
			42	40	2	

- Molecule 38 is DIACYL GLYCEROL (CCD ID: DGA) (formula: $C_{39}H_{76}O_5$).



Mol	Chain	Residues	Atoms			AltConf
38	B	1	Total	C	O	0
			44	39	5	
38	C	1	Total	C	O	0
			44	39	5	
38	b	1	Total	C	O	0
			44	39	5	
38	c	1	Total	C	O	0
			44	39	5	
38	B1	1	Total	C	O	0
			44	39	5	
38	C1	1	Total	C	O	0
			44	39	5	
38	J1	1	Total	C	O	0
			29	24	5	
38	b1	1	Total	C	O	0
			44	39	5	

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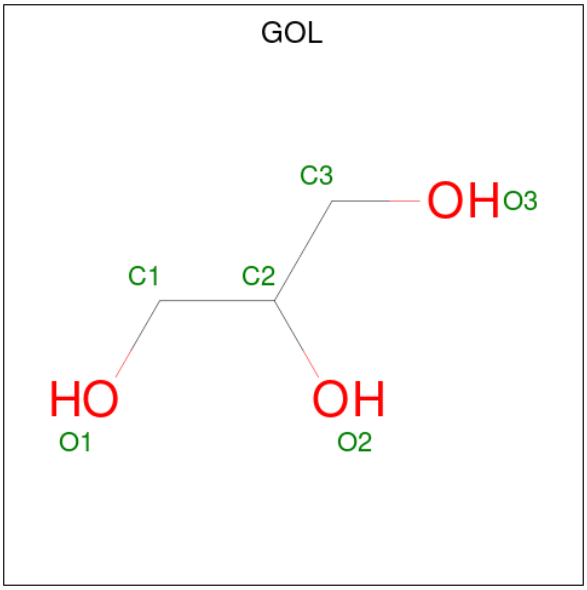
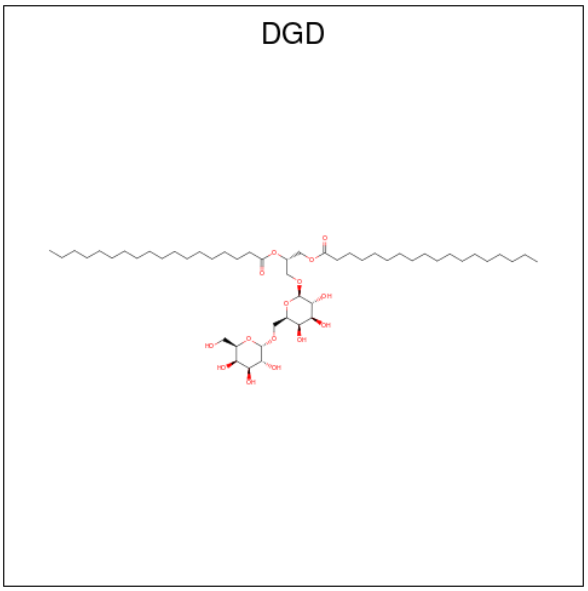
Mol	Chain	Residues	Atoms	AltConf
38	c1	1	Total C O 44 39 5	0
38	j1	1	Total C O 29 24 5	0

- Molecule 39 is GLYCEROL (CCD ID: GOL) (formula: $C_3H_8O_3$).



Mol	Chain	Residues	Atoms	AltConf
39	B	1	Total C O 6 3 3	0
39	b	1	Total C O 6 3 3	0
39	b	1	Total C O 6 3 3	0
39	y	1	Total C O 6 3 3	0
39	I1	1	Total C O 6 3 3	0

- Molecule 40 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (CCD ID: DGD) (formula: $C_{51}H_{96}O_{15}$).



Mol	Chain	Residues	Atoms			AltConf
40	C	1	Total	C	O	0
			55	40	15	
40	C	1	Total	C	O	0
			62	47	15	
40	C	1	Total	C	O	0
			59	44	15	
40	C	1	Total	C	O	0
			66	51	15	
40	c	1	Total	C	O	0
			55	40	15	
40	c	1	Total	C	O	0
			62	47	15	
40	c	1	Total	C	O	0
			59	44	15	
40	c	1	Total	C	O	0
			66	51	15	
40	B1	1	Total	C	O	0
			43	28	15	
40	C1	1	Total	C	O	0
			55	40	15	
40	C1	1	Total	C	O	0
			62	47	15	
40	C1	1	Total	C	O	0
			59	44	15	
40	b1	1	Total	C	O	0
			43	28	15	
40	c1	1	Total	C	O	0
			55	40	15	

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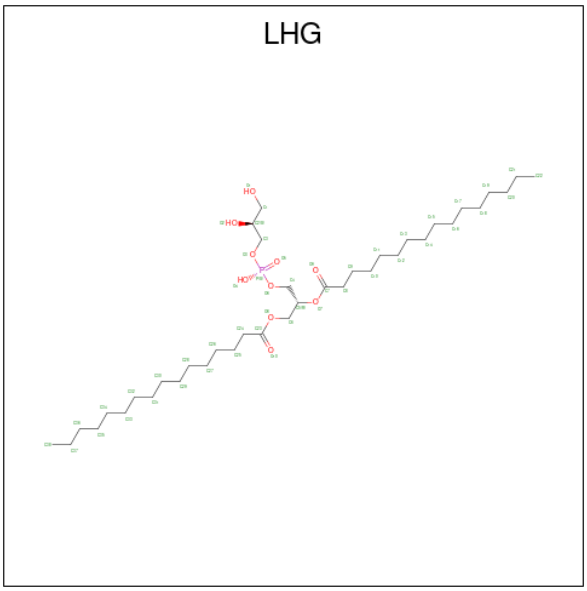
Mol	Chain	Residues	Atoms	AltConf
40	c1	1	Total C O 62 47 15	0
40	c1	1	Total C O 59 44 15	0

- Molecule 41 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (CCD ID: LHG) (formula: $C_{38}H_{75}O_{10}P$).



Mol	Chain	Residues	Atoms	AltConf
41	C	1	Total C O P 47 36 10 1	0
41	D	1	Total C O P 44 33 10 1	0
41	D	1	Total C O P 49 38 10 1	0
41	D	1	Total C O P 39 28 10 1	0
41	L	1	Total C O P 49 38 10 1	0
41	N	1	Total C O P 49 38 10 1	0
41	G	1	Total C O P 49 38 10 1	0
41	S	1	Total C O P 45 34 10 1	0
41	Y	1	Total C O P 49 38 10 1	0

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Mol	Chain	Residues	Atoms				AltConf
41	c	1	Total	C	O	P	0
			47	36	10	1	
41	d	1	Total	C	O	P	0
			44	33	10	1	
41	d	1	Total	C	O	P	0
			49	38	10	1	
41	d	1	Total	C	O	P	0
			39	28	10	1	
41	l	1	Total	C	O	P	0
			49	38	10	1	
41	n	1	Total	C	O	P	0
			49	38	10	1	
41	g	1	Total	C	O	P	0
			49	38	10	1	
41	s	1	Total	C	O	P	0
			45	34	10	1	
41	y	1	Total	C	O	P	0
			49	38	10	1	
41	C1	1	Total	C	O	P	0
			47	36	10	1	
41	D1	1	Total	C	O	P	0
			44	33	10	1	
41	D1	1	Total	C	O	P	0
			49	38	10	1	
41	D1	1	Total	C	O	P	0
			39	28	10	1	
41	L1	1	Total	C	O	P	0
			49	38	10	1	
41	N1	1	Total	C	O	P	0
			49	38	10	1	
41	G1	1	Total	C	O	P	0
			49	38	10	1	
41	S1	1	Total	C	O	P	0
			45	34	10	1	
41	Y1	1	Total	C	O	P	0
			49	38	10	1	
41	c1	1	Total	C	O	P	0
			47	36	10	1	
41	d1	1	Total	C	O	P	0
			44	33	10	1	
41	d1	1	Total	C	O	P	0
			49	38	10	1	

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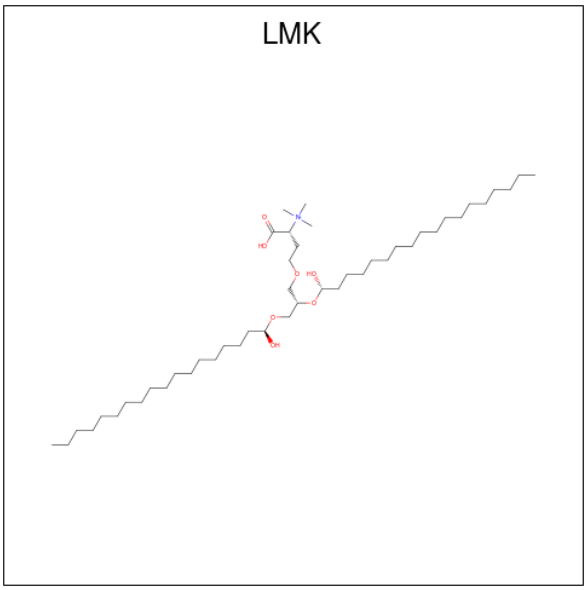
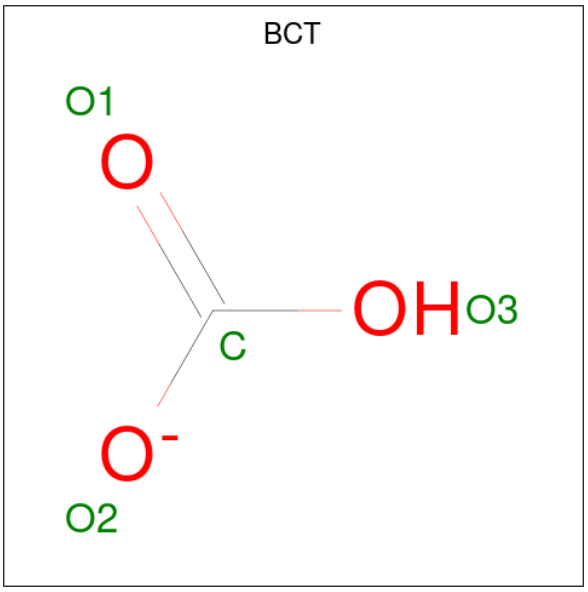
Mol	Chain	Residues	Atoms				AltConf
41	d1	1	Total	C	O	P	0
			39	28	10	1	
41	n1	1	Total	C	O	P	0
			49	38	10	1	
41	g1	1	Total	C	O	P	0
			49	38	10	1	
41	s1	1	Total	C	O	P	0
			45	34	10	1	
41	y1	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 42 is trimethyl-[(2 {R})-1-oxidanyl-1-oxidanylidene-4-[(2 {S})-2-[(1 {S})-1-oxidanyloctadecoxy]-3-[(1 {R})-1-oxidanyloctadecoxy]propoxy]butan-2-yl]azanium (CCD ID: LMK) (formula: $C_{46}H_{94}NO_7$).



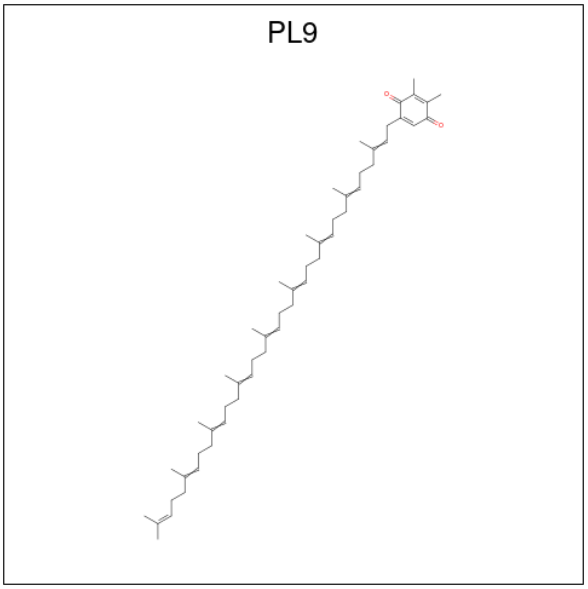
Mol	Chain	Residues	Atoms				AltConf
42	C	1	Total	C	N	O	0
			40	32	1	7	
42	c	1	Total	C	N	O	0
			40	32	1	7	
42	C1	1	Total	C	N	O	0
			40	32	1	7	
42	c1	1	Total	C	N	O	0
			40	32	1	7	

- Molecule 43 is BICARBONATE ION (CCD ID: BCT) (formula: CHO_3).



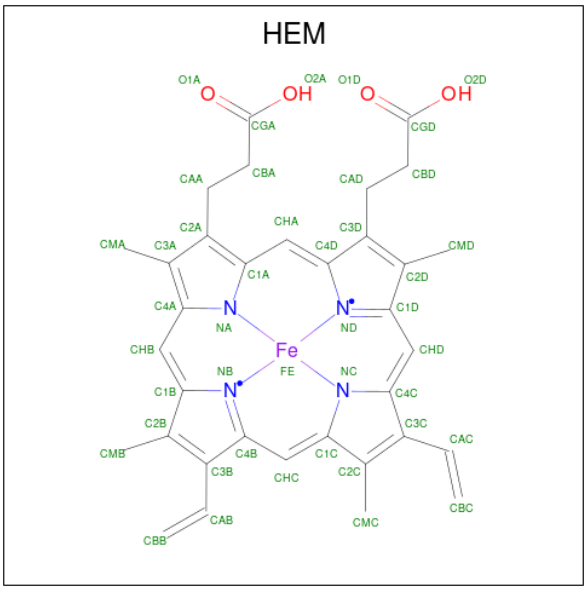
Mol	Chain	Residues	Atoms			AltConf
43	D	1	Total	C	O	0
			4	1	3	
43	d	1	Total	C	O	0
			4	1	3	
43	D1	1	Total	C	O	0
			4	1	3	
43	d1	1	Total	C	O	0
			4	1	3	

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



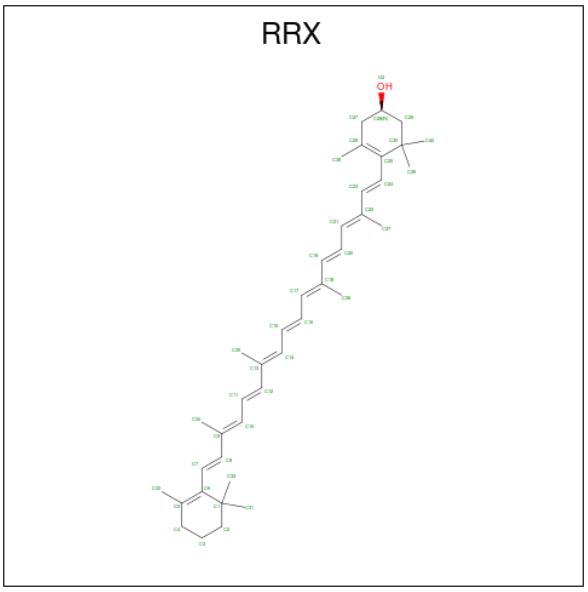
Mol	Chain	Residues	Atoms			AltConf
44	D	1	Total	C	O	0
			55	53	2	
44	d	1	Total	C	O	0
			55	53	2	
44	D1	1	Total	C	O	0
			55	53	2	
44	d1	1	Total	C	O	0
			55	53	2	

- Molecule 45 is PROTOPORPHYRIN IX CONTAINING FE (CCD ID: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



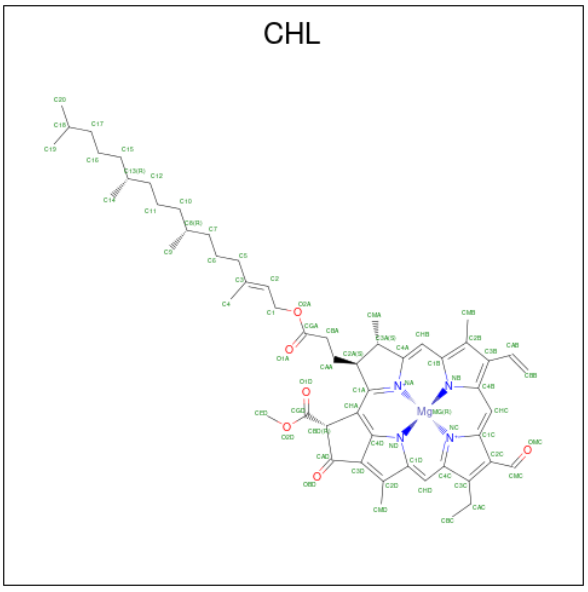
Mol	Chain	Residues	Atoms					AltConf
45	F	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
45	f	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
45	F1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	
45	f1	1	Total	C	Fe	N	O	0
			43	34	1	4	4	

- Molecule 46 is (3R)-beta,beta-caroten-3-ol (CCD ID: RRX) (formula: $C_{40}H_{56}O$).



Mol	Chain	Residues	Atoms	AltConf
46	H	1	Total C O 41 40 1	0
46	h	1	Total C O 41 40 1	0
46	H1	1	Total C O 41 40 1	0
46	h1	1	Total C O 41 40 1	0

- Molecule 47 is CHLOROPHYLL B (CCD ID: CHL) (formula: $C_{55}H_{70}MgN_4O_6$).



Mol	Chain	Residues	Atoms					AltConf
47	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	N	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
47	N	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	G	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
47	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
47	G	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
47	G	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
47	G	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	R	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
47	R	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
47	S	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
47	S	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
47	S	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
47	S	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
47	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	Y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
47	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
47	Y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	n	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
47	n	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	g	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
47	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
47	g	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
47	g	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
47	g	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	r	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
47	r	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
47	s	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
47	s	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
47	s	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
47	s	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
47	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	y	1	Total	C	Mg	N	O	0
			46	35	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
47	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	y	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	N1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	N1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	N1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	N1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	N1	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
47	N1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	G1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	G1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
47	G1	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
47	G1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	G1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
47	G1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	R1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
47	R1	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
47	S1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
47	S1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
47	S1	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
47	S1	1	Total	C	Mg	N	O	0
			61	50	1	4	6	

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Mol	Chain	Residues	Atoms					AltConf
47	Y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	Y1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
47	Y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	Y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	Y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	n1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	n1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	n1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	n1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	n1	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
47	n1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	g1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	g1	1	Total	C	Mg	N	O	0
			48	37	1	4	6	
47	g1	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
47	g1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	g1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
47	g1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	r1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	
47	r1	1	Total	C	Mg	N	O	0
			50	39	1	4	6	
47	s1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
47	s1	1	Total	C	Mg	N	O	0
			44	35	1	4	4	

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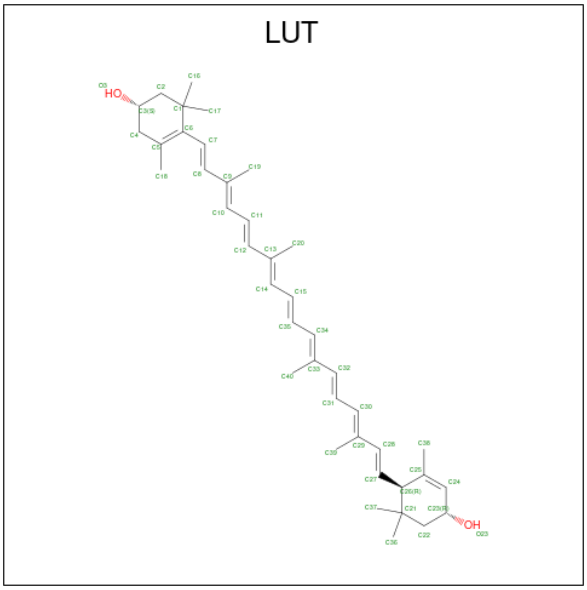
Mol	Chain	Residues	Atoms					AltConf
47	s1	1	Total	C	Mg	N	O	0
			43	34	1	4	4	
47	s1	1	Total	C	Mg	N	O	0
			61	50	1	4	6	
47	y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	y1	1	Total	C	Mg	N	O	0
			46	35	1	4	6	
47	y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	
47	y1	1	Total	C	Mg	N	O	0
			66	55	1	4	6	

- Molecule 48 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
48	N	1	Total	C	O	0
			42	40	2	
48	N	1	Total	C	O	0
			42	40	2	
48	G	1	Total	C	O	0
			42	40	2	
48	G	1	Total	C	O	0
			42	40	2	

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Mol	Chain	Residues	Atoms			AltConf
48	R	1	Total	C	O	0
			42	40	2	
48	S	1	Total	C	O	0
			42	40	2	
48	S	1	Total	C	O	0
			42	40	2	
48	Y	1	Total	C	O	0
			42	40	2	
48	Y	1	Total	C	O	0
			42	40	2	
48	n	1	Total	C	O	0
			42	40	2	
48	n	1	Total	C	O	0
			42	40	2	
48	g	1	Total	C	O	0
			42	40	2	
48	g	1	Total	C	O	0
			42	40	2	
48	r	1	Total	C	O	0
			42	40	2	
48	s	1	Total	C	O	0
			42	40	2	
48	s	1	Total	C	O	0
			42	40	2	
48	y	1	Total	C	O	0
			42	40	2	
48	y	1	Total	C	O	0
			42	40	2	
48	N1	1	Total	C	O	0
			42	40	2	
48	N1	1	Total	C	O	0
			42	40	2	
48	G1	1	Total	C	O	0
			42	40	2	
48	G1	1	Total	C	O	0
			42	40	2	
48	R1	1	Total	C	O	0
			42	40	2	
48	S1	1	Total	C	O	0
			42	40	2	
48	S1	1	Total	C	O	0
			42	40	2	

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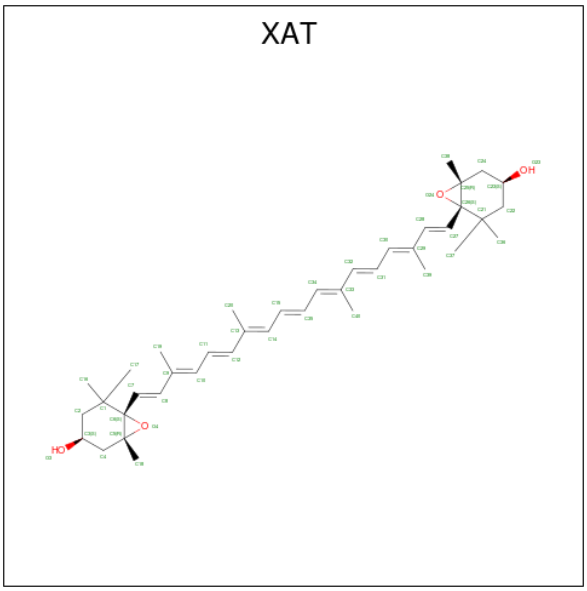
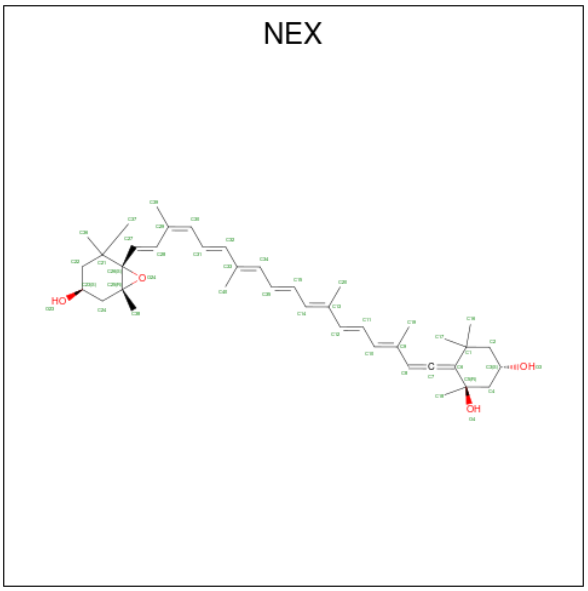
Mol	Chain	Residues	Atoms			AltConf
48	Y1	1	Total	C	O	0
			42	40	2	
48	Y1	1	Total	C	O	0
			42	40	2	
48	n1	1	Total	C	O	0
			42	40	2	
48	n1	1	Total	C	O	0
			42	40	2	
48	g1	1	Total	C	O	0
			42	40	2	
48	g1	1	Total	C	O	0
			42	40	2	
48	r1	1	Total	C	O	0
			42	40	2	
48	s1	1	Total	C	O	0
			42	40	2	
48	s1	1	Total	C	O	0
			42	40	2	
48	y1	1	Total	C	O	0
			42	40	2	
48	y1	1	Total	C	O	0
			42	40	2	

- Molecule 49 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
49	N	1	Total	C	O	0
			44	40	4	
49	G	1	Total	C	O	0
			44	40	4	
49	R	1	Total	C	O	0
			44	40	4	
49	Y	1	Total	C	O	0
			44	40	4	
49	n	1	Total	C	O	0
			44	40	4	
49	g	1	Total	C	O	0
			44	40	4	
49	r	1	Total	C	O	0
			44	40	4	
49	y	1	Total	C	O	0
			44	40	4	
49	N1	1	Total	C	O	0
			44	40	4	
49	G1	1	Total	C	O	0
			44	40	4	
49	R1	1	Total	C	O	0
			44	40	4	
49	Y1	1	Total	C	O	0
			44	40	4	
49	n1	1	Total	C	O	0
			44	40	4	
49	g1	1	Total	C	O	0
			44	40	4	
49	r1	1	Total	C	O	0
			44	40	4	
49	y1	1	Total	C	O	0
			44	40	4	

- Molecule 50 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
50	N	1	Total C O 44 40 4	0
50	G	1	Total C O 44 40 4	0
50	R	1	Total C O 44 40 4	0
50	S	1	Total C O 44 40 4	0
50	Y	1	Total C O 44 40 4	0
50	n	1	Total C O 44 40 4	0
50	g	1	Total C O 44 40 4	0
50	r	1	Total C O 44 40 4	0
50	s	1	Total C O 44 40 4	0
50	y	1	Total C O 44 40 4	0
50	N1	1	Total C O 44 40 4	0
50	G1	1	Total C O 44 40 4	0
50	R1	1	Total C O 44 40 4	0
50	S1	1	Total C O 44 40 4	0

Continued on next page...

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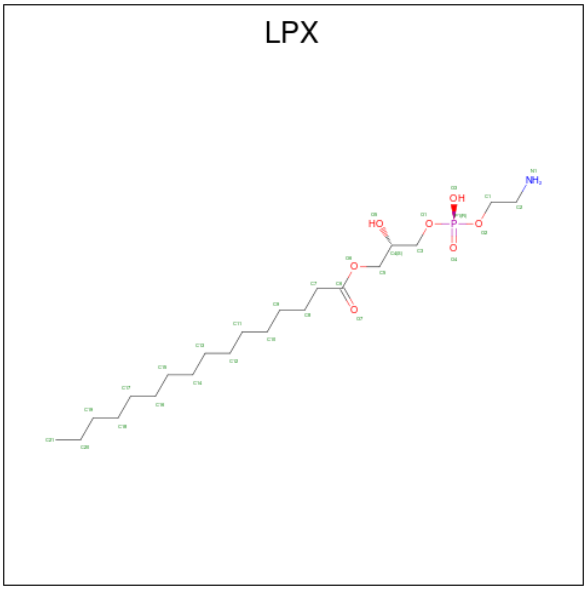
Mol	Chain	Residues	Atoms			AltConf
50	Y1	1	Total	C	O	0
			44	40	4	
50	n1	1	Total	C	O	0
			44	40	4	
50	g1	1	Total	C	O	0
			44	40	4	
50	r1	1	Total	C	O	0
			44	40	4	
50	s1	1	Total	C	O	0
			44	40	4	
50	y1	1	Total	C	O	0
			44	40	4	

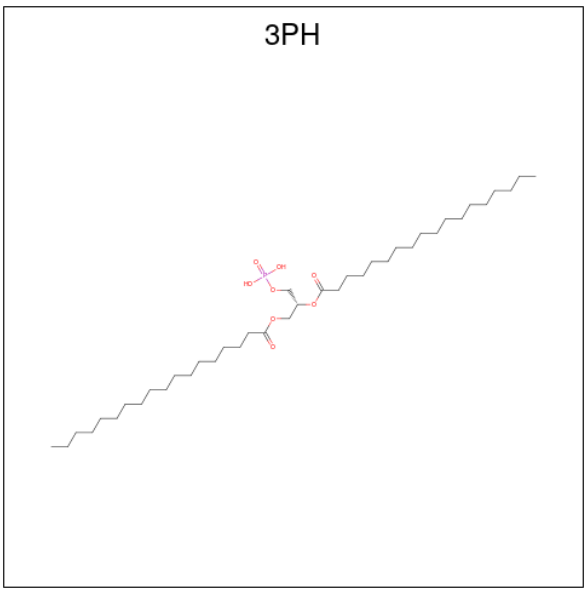
- Molecule 51 is (2S)-3-{[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (CCD ID: LPX) (formula: $C_{21}H_{44}NO_7P$).



Mol	Chain	Residues	Atoms					AltConf
51	S	1	Total	C	N	O	P	0
			30	21	1	7	1	
51	s	1	Total	C	N	O	P	0
			30	21	1	7	1	
51	S1	1	Total	C	N	O	P	0
			30	21	1	7	1	
51	s1	1	Total	C	N	O	P	0
			30	21	1	7	1	

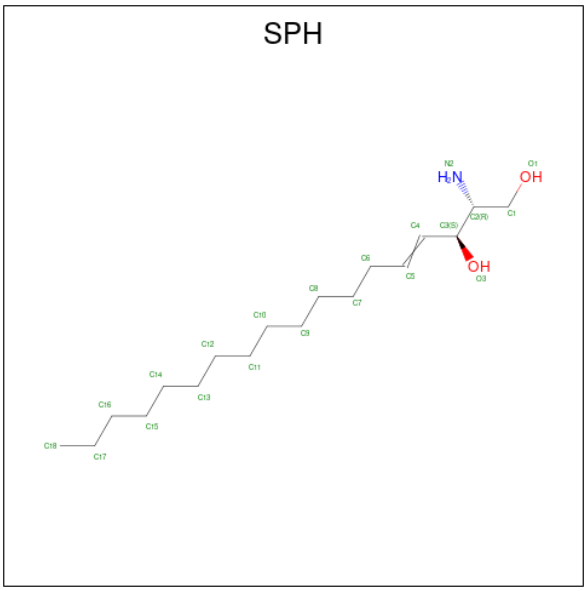
- Molecule 52 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (CCD ID: 3PH) (formula:

$C_{39}H_{77}O_8P$).



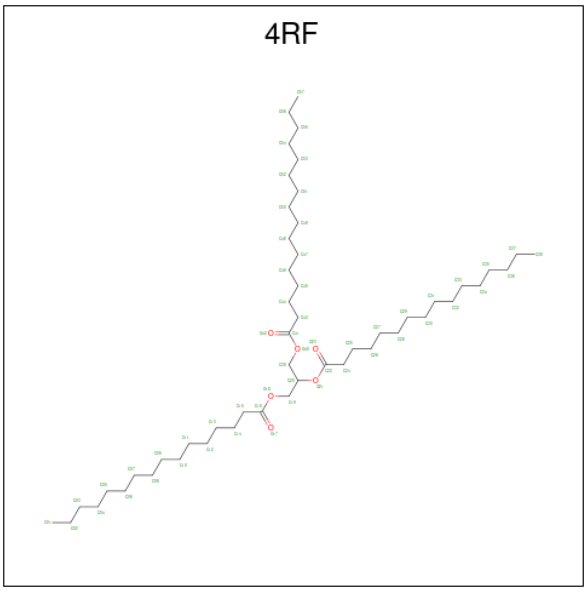
Mol	Chain	Residues	Atoms				AltConf
52	S	1	Total	C	O	P	0
			48	39	8	1	
52	i	1	Total	C	O	P	0
			48	39	8	1	
52	s	1	Total	C	O	P	0
			48	39	8	1	
52	B1	1	Total	C	O	P	0
			48	39	8	1	
52	T1	1	Total	C	O	P	0
			48	39	8	1	
52	S1	1	Total	C	O	P	0
			48	39	8	1	
52	b1	1	Total	C	O	P	0
			48	39	8	1	
52	t1	1	Total	C	O	P	0
			48	39	8	1	
52	s1	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 53 is SPHINGOSINE (CCD ID: SPH) (formula: $C_{18}H_{37}NO_2$).



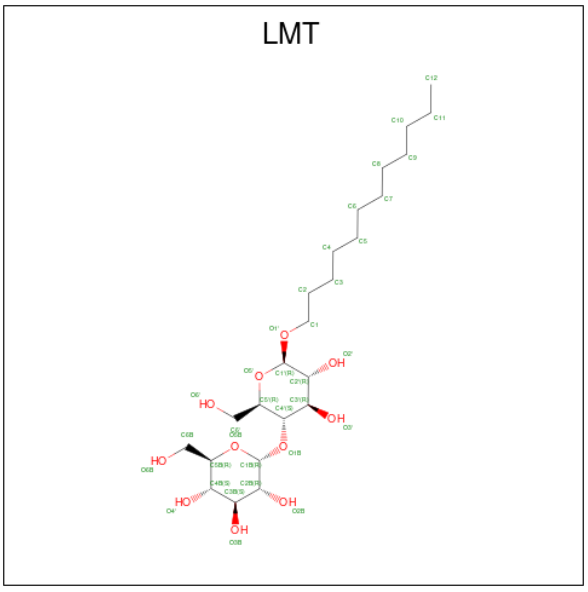
Mol	Chain	Residues	Atoms				AltConf
53	Y	1	Total	C	N	O	0
			21	18	1	2	
53	y	1	Total	C	N	O	0
			21	18	1	2	
53	A1	1	Total	C	N	O	0
			21	18	1	2	
53	Y1	1	Total	C	N	O	0
			21	18	1	2	
53	a1	1	Total	C	N	O	0
			21	18	1	2	
53	y1	1	Total	C	N	O	0
			21	18	1	2	

- Molecule 54 is Tripalmitoylglycerol (CCD ID: 4RF) (formula: $C_{51}H_{98}O_6$).



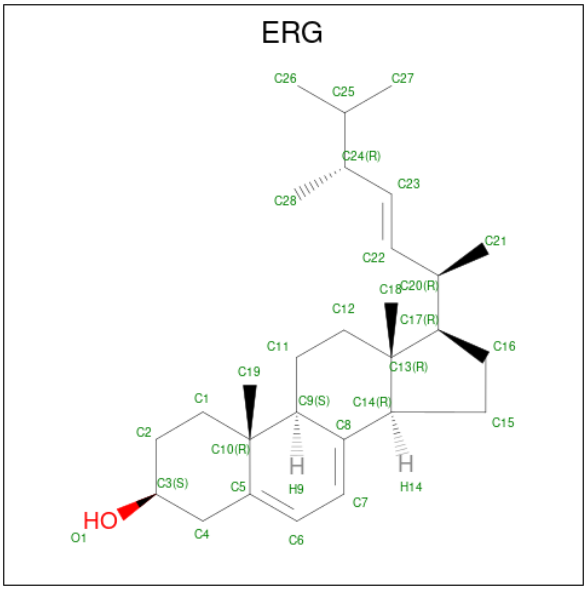
Mol	Chain	Residues	Atoms	AltConf
54	I1	1	Total C O 57 51 6	0
54	K1	1	Total C O 57 51 6	0
54	i1	1	Total C O 57 51 6	0
54	k1	1	Total C O 57 51 6	0

- Molecule 55 is DODECYL-BETA-D-MALTOSIDE (CCD ID: LMT) (formula: $C_{24}H_{46}O_{11}$).



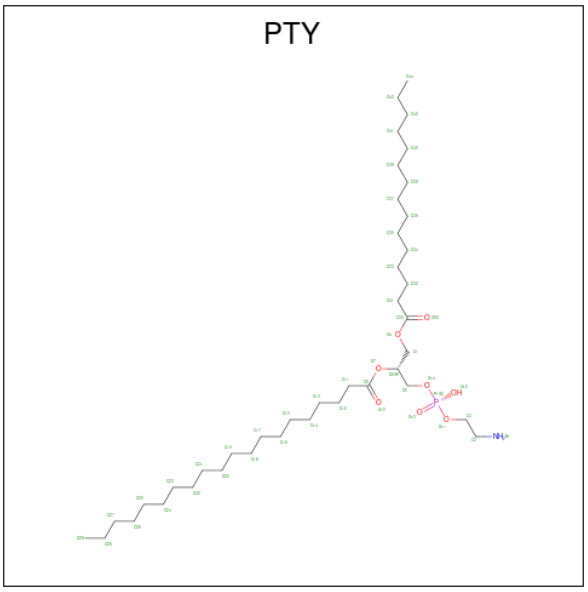
Mol	Chain	Residues	Atoms	AltConf
55	R1	1	Total C O 35 24 11	0
55	r1	1	Total C O 35 24 11	0

- Molecule 56 is ERGOSTEROL (CCD ID: ERG) (formula: $C_{28}H_{44}O$).



Mol	Chain	Residues	Atoms	AltConf
56	R1	1	Total C O 29 28 1	0
56	r1	1	Total C O 29 28 1	0

- Molecule 57 is PHOSPHATIDYLETHANOLAMINE (CCD ID: PTY) (formula: $C_{40}H_{80}NO_8P$).



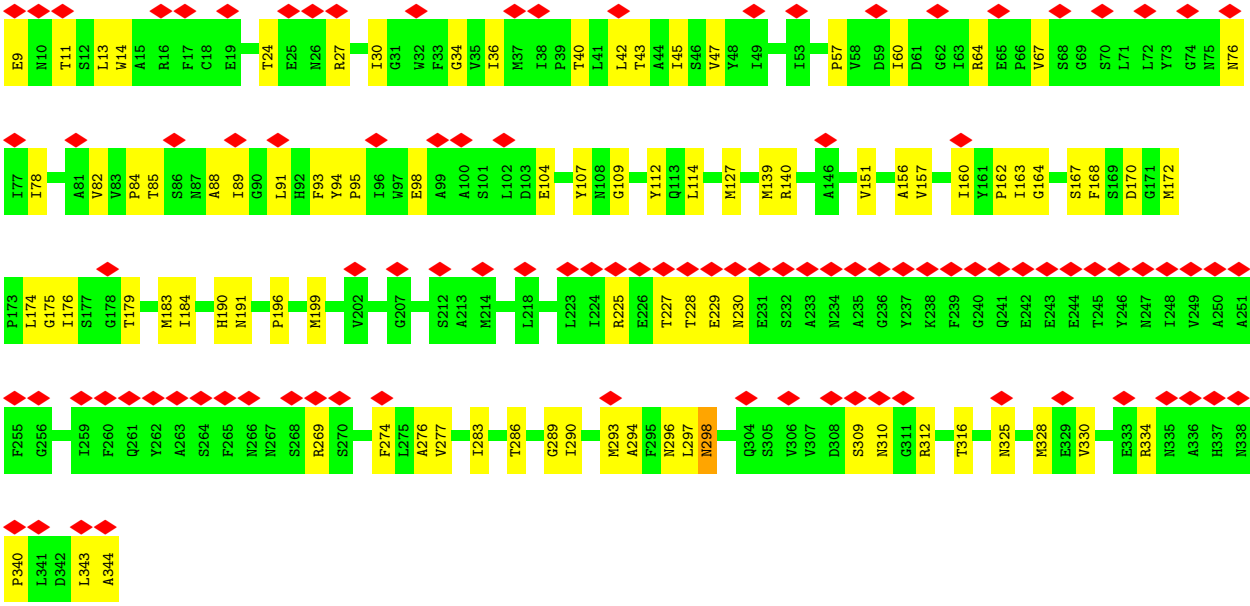
Mol	Chain	Residues	Atoms					AltConf
57	Y1	1	Total	C	N	O	P	0
			50	40	1	8	1	
57	Y1	1	Total	C	N	O	P	0
			19	9	1	8	1	
57	y1	1	Total	C	N	O	P	0
			50	40	1	8	1	
57	y1	1	Total	C	N	O	P	0
			19	9	1	8	1	

3 Residue-property plots (i)

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

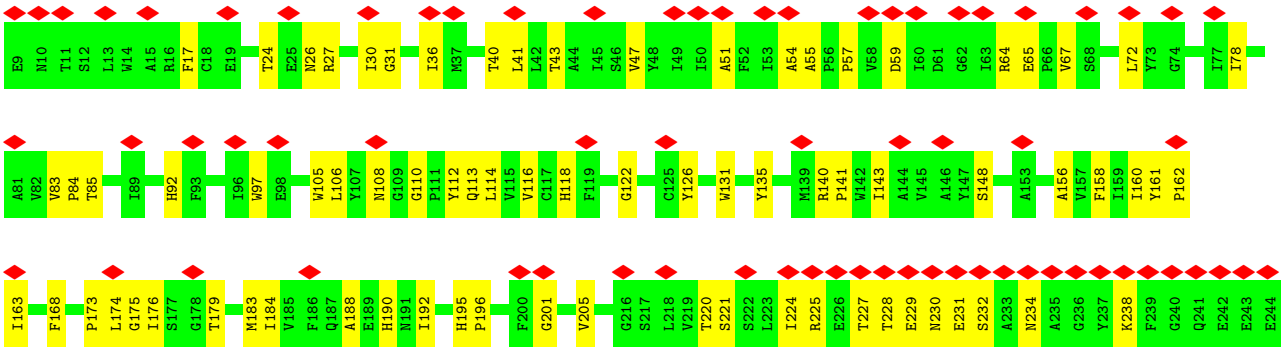
• Molecule 1: Photosystem II protein D1

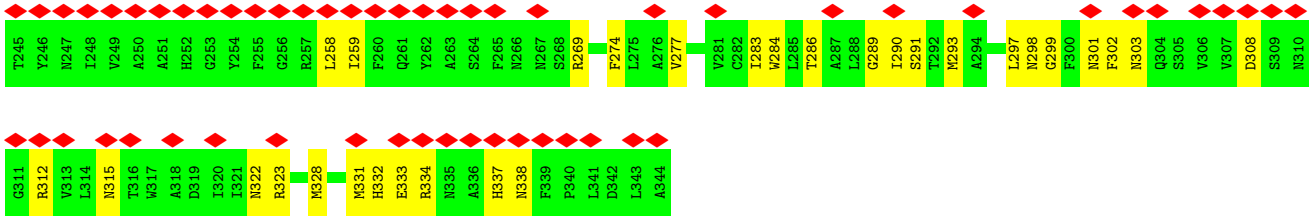
Chain A:



• Molecule 1: Photosystem II protein D1

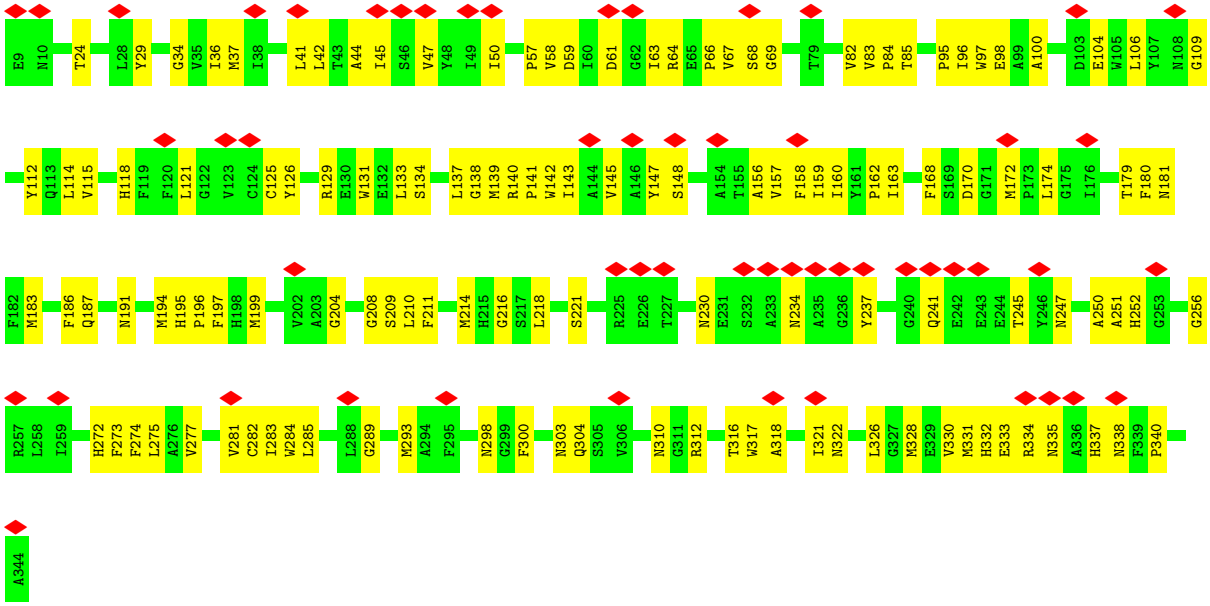
Chain a:





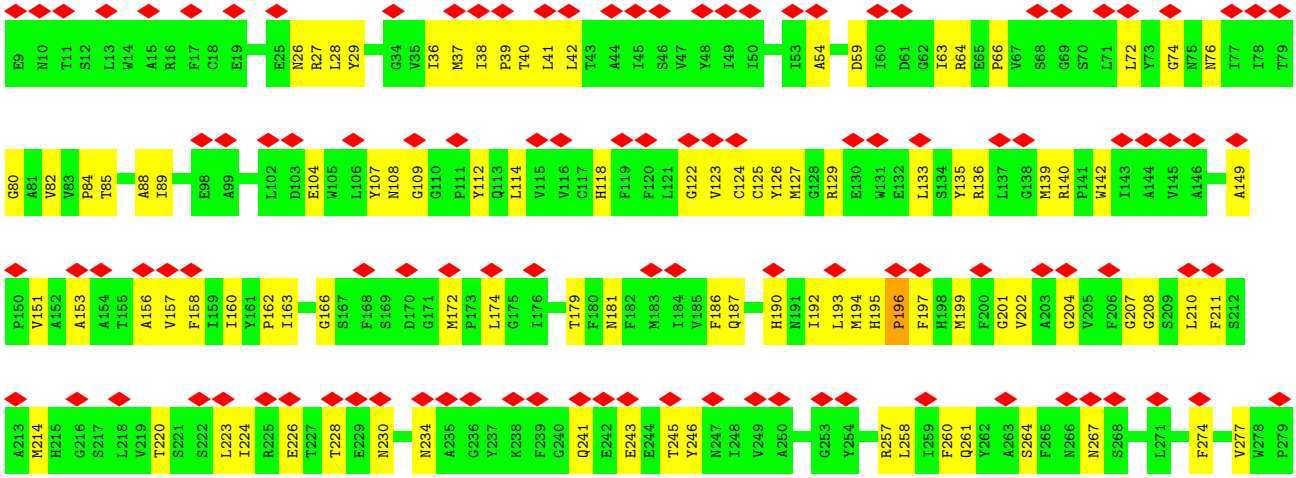
• Molecule 1: Photosystem II protein D1

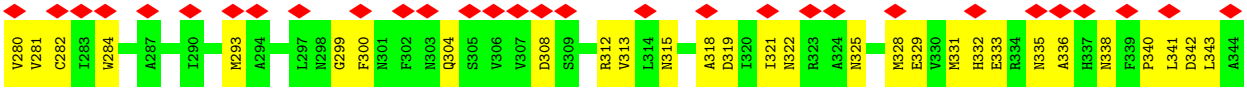
Chain A1:



• Molecule 1: Photosystem II protein D1

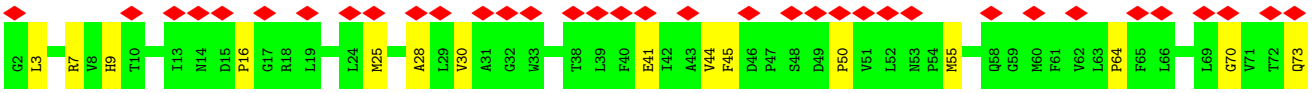
Chain a1:

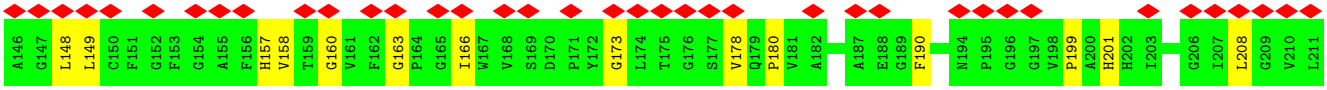


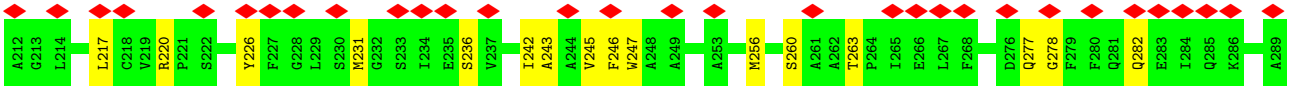


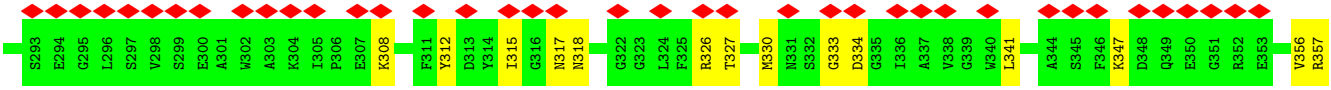
• Molecule 2: Photosystem II CP47 reaction center protein

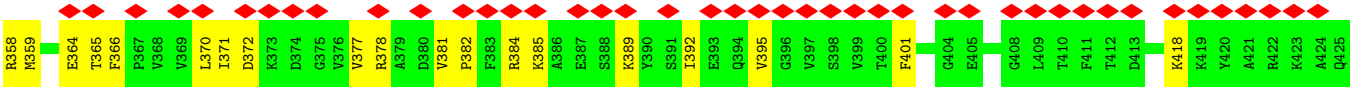
Chain B:

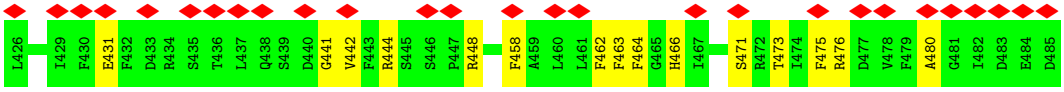






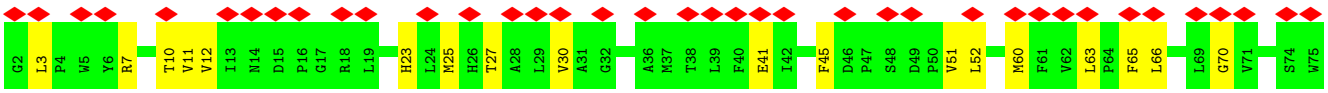


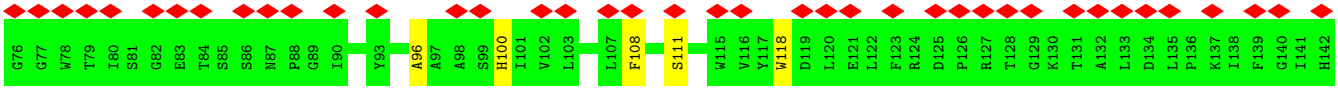


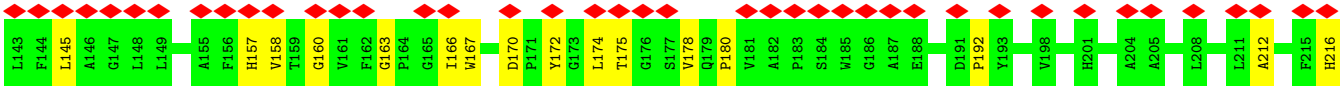


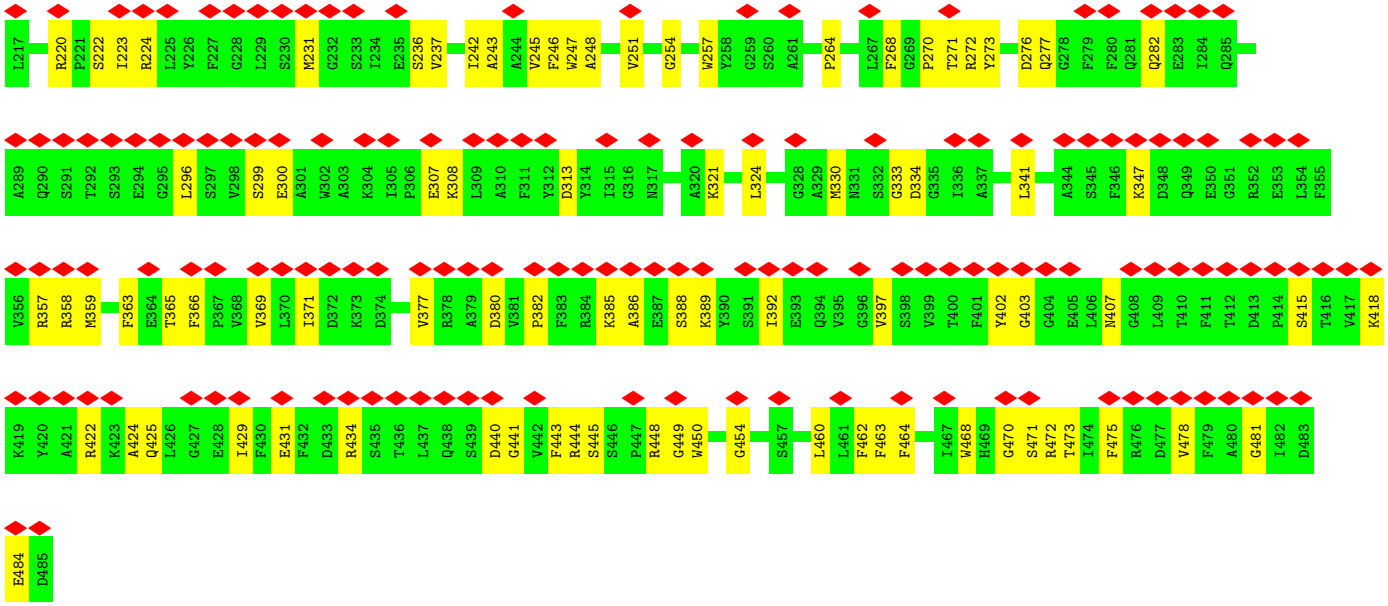
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b:



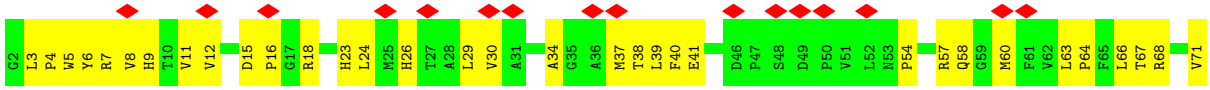


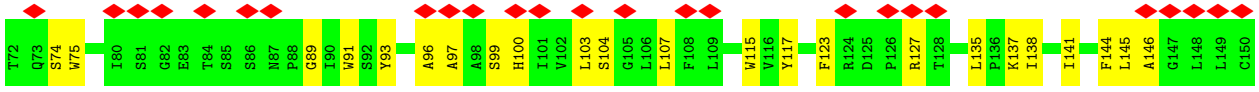


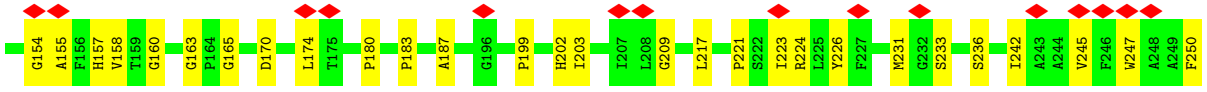


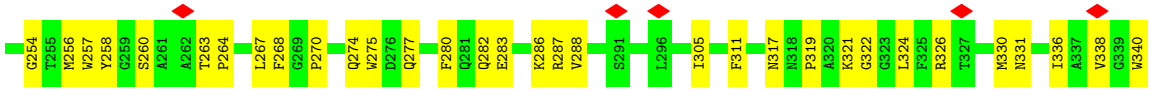
• Molecule 2: Photosystem II CP47 reaction center protein

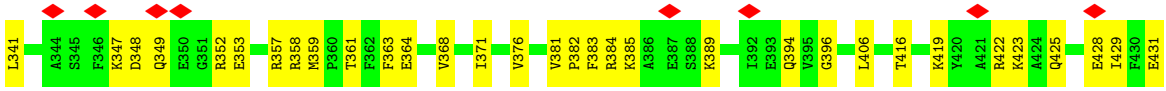
Chain B1:

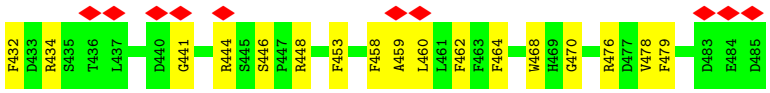






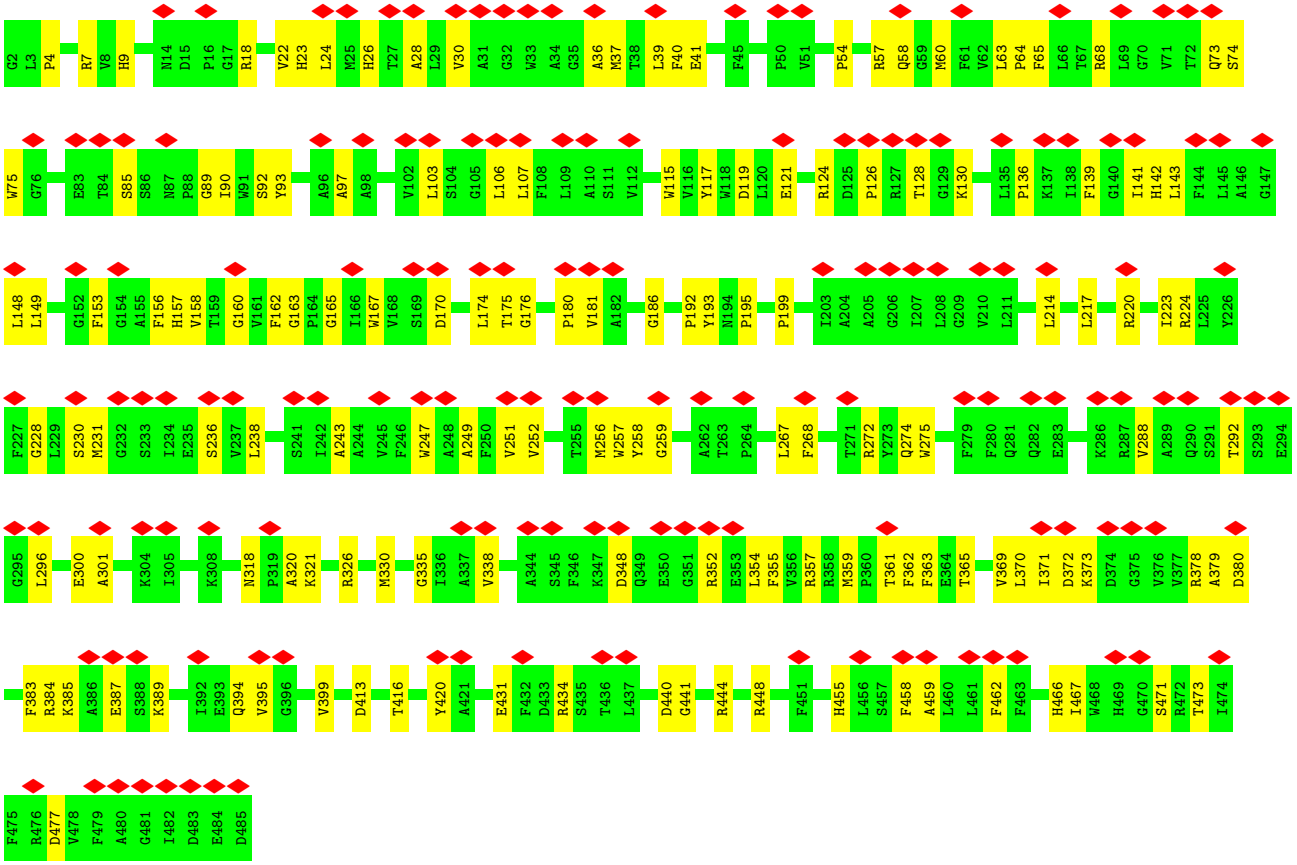






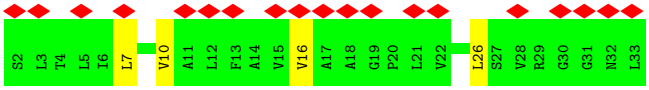
• Molecule 2: Photosystem II CP47 reaction center protein

Chain b1:



• Molecule 3: Photosystem II reaction center protein Ycf12

Chain V:

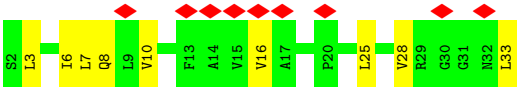


• Molecule 3: Photosystem II reaction center protein Ycf12

Chain v:

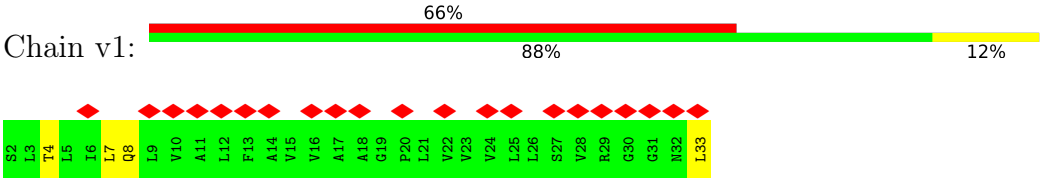
• Molecule 3: Photosystem II reaction center protein Ycf12

Chain V1:



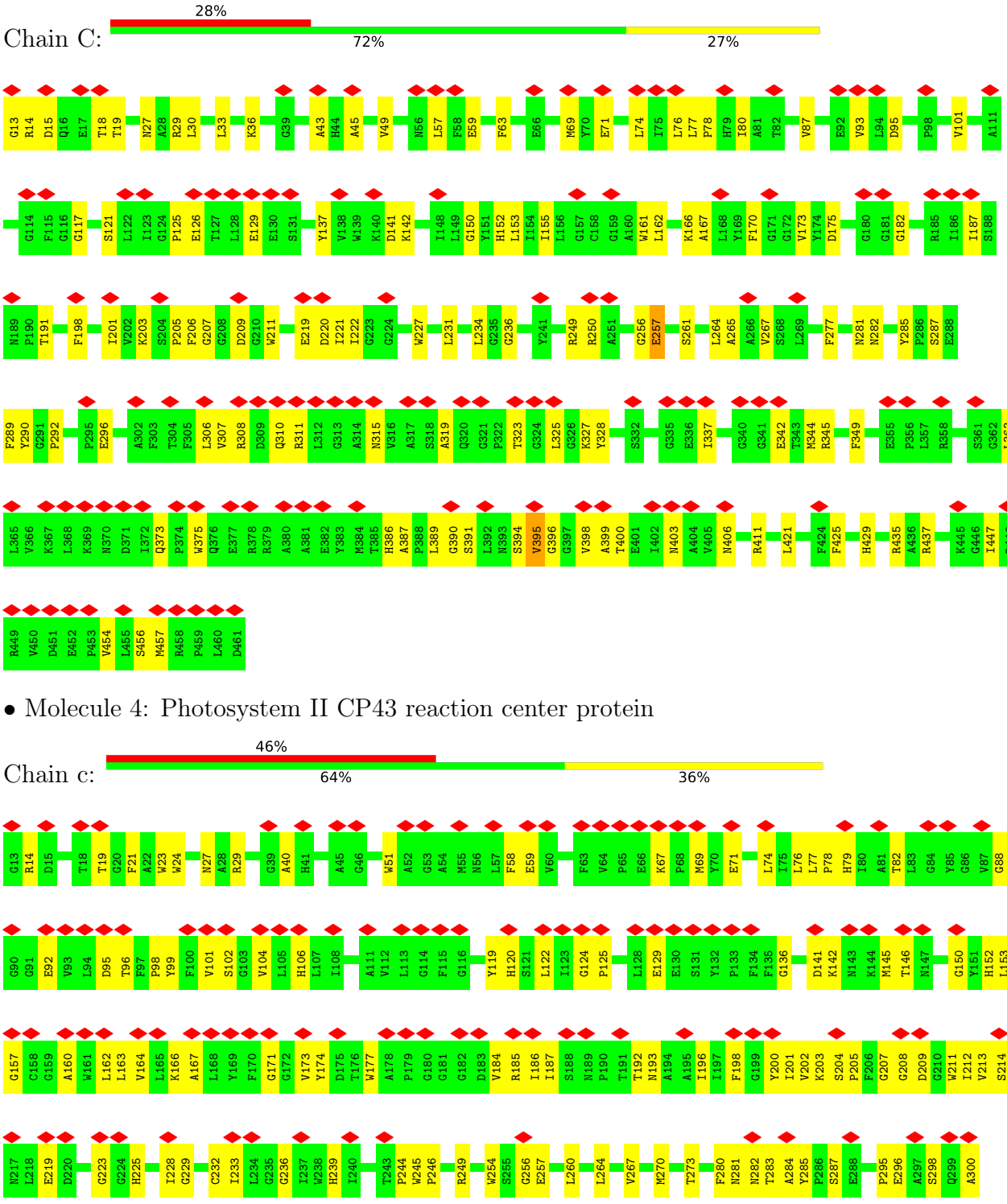
• Molecule 3: Photosystem II reaction center protein Ycf12

Chain v1:



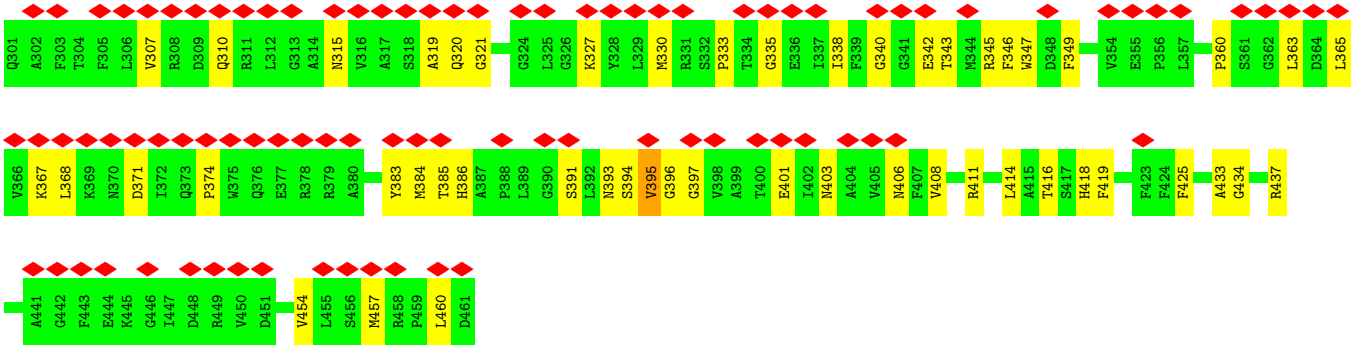
• Molecule 4: Photosystem II CP43 reaction center protein

Chain C:



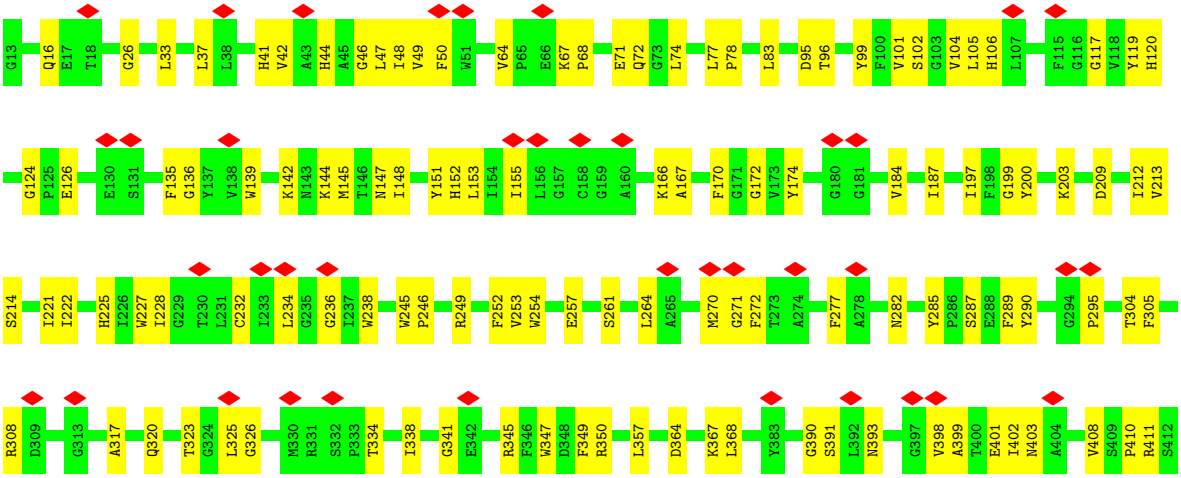
• Molecule 4: Photosystem II CP43 reaction center protein

Chain c:



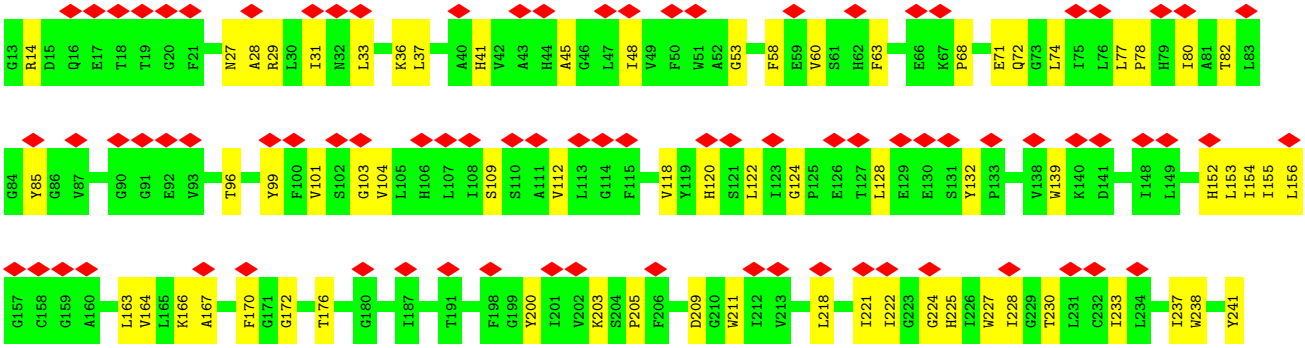
• Molecule 4: Photosystem II CP43 reaction center protein

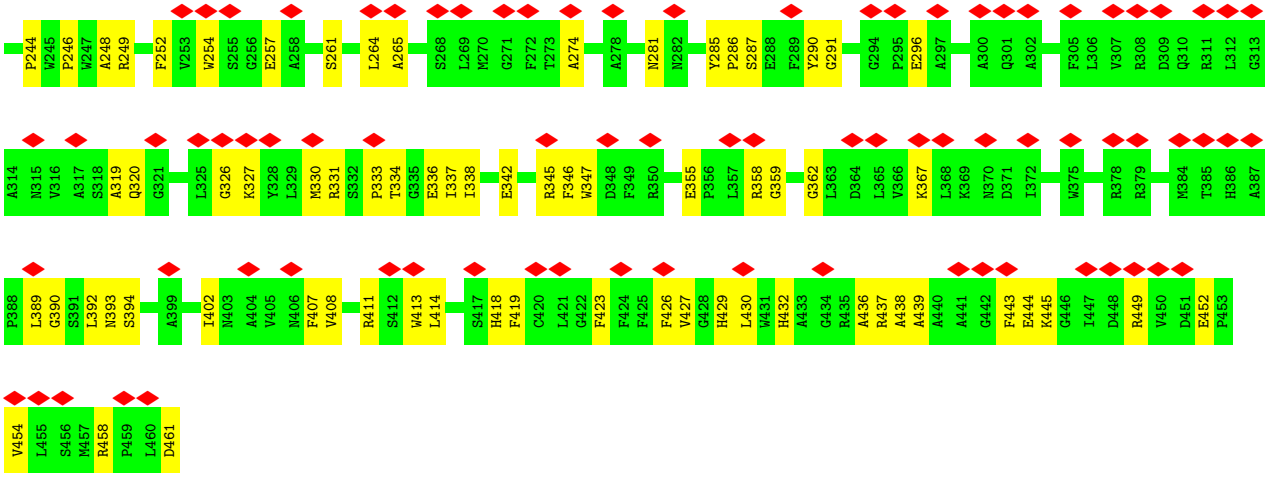
Chain C1:



• Molecule 4: Photosystem II CP43 reaction center protein

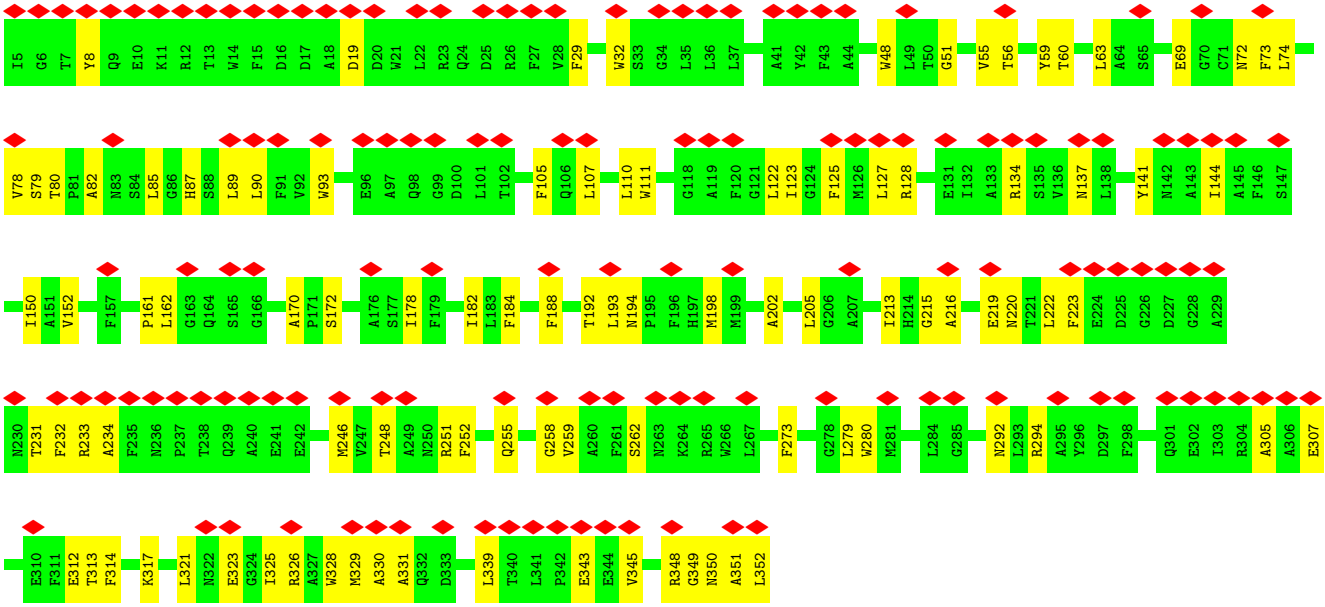
Chain c1:





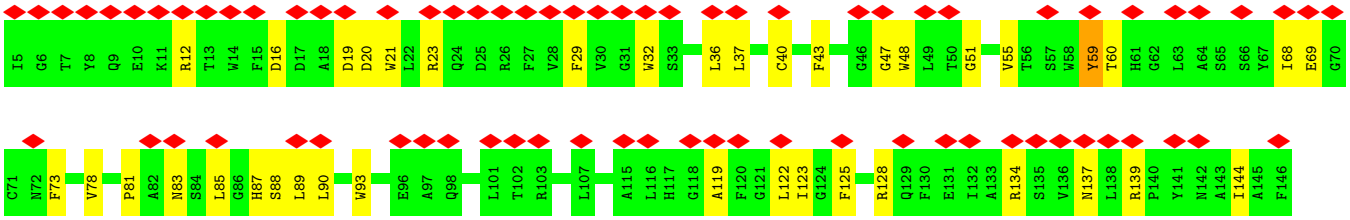
• Molecule 5: Photosystem II D2 protein

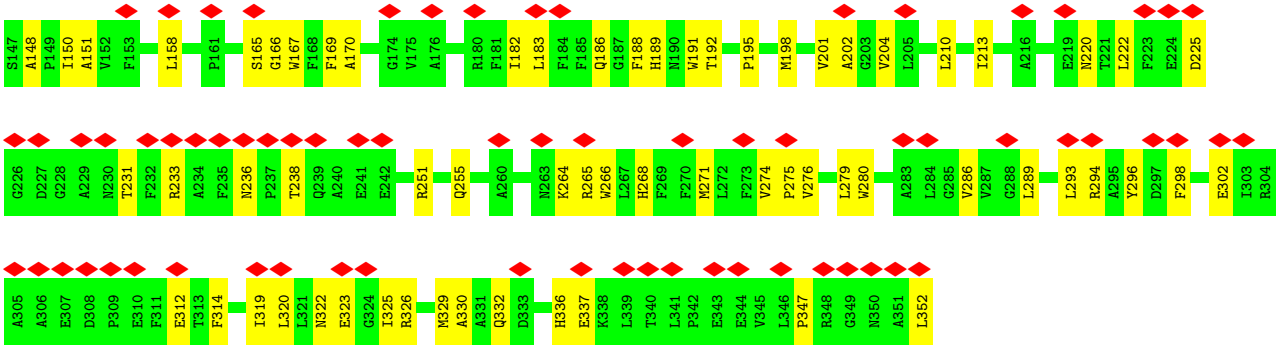
Chain D:



• Molecule 5: Photosystem II D2 protein

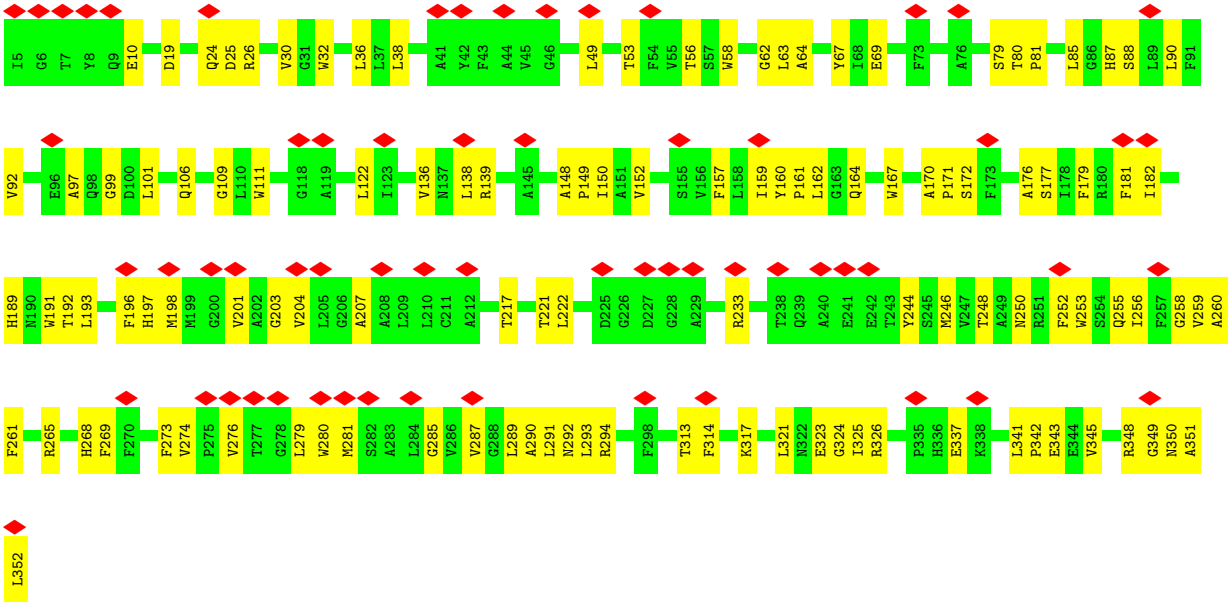
Chain d:





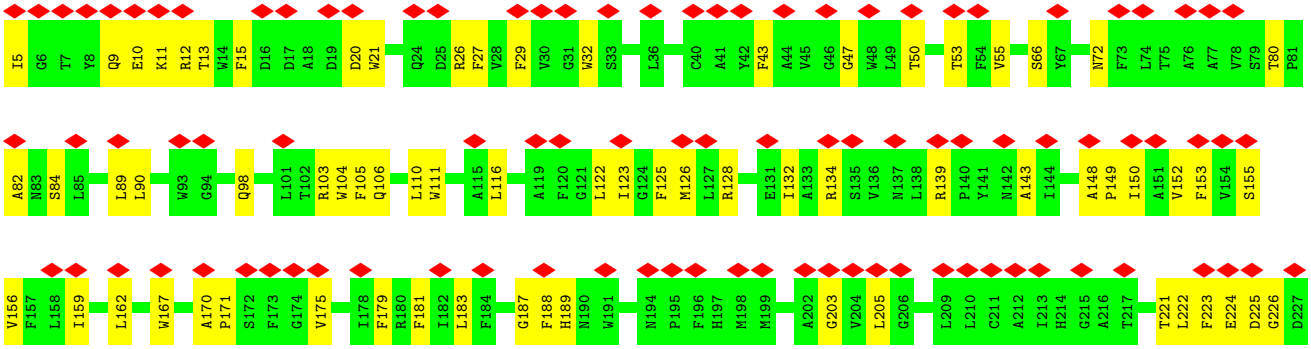
• Molecule 5: Photosystem II D2 protein

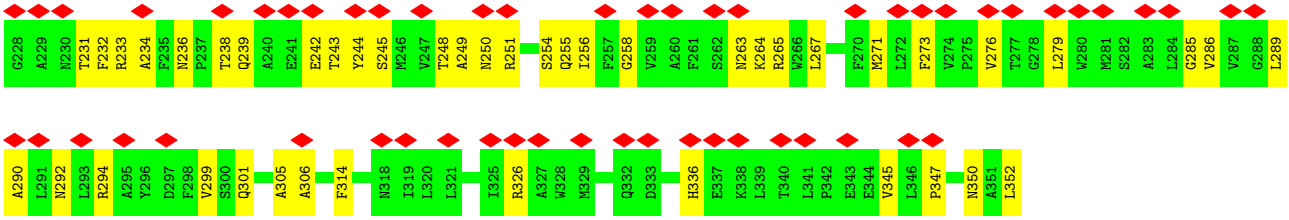
Chain D1:



• Molecule 5: Photosystem II D2 protein

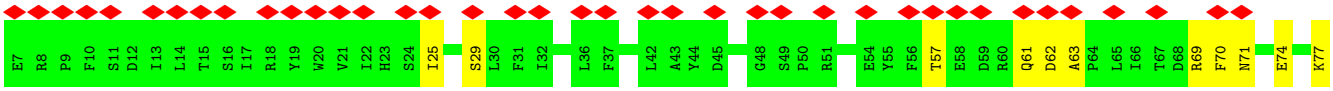
Chain d1:

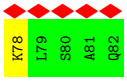




• Molecule 6: Cytochrome b559 subunit alpha

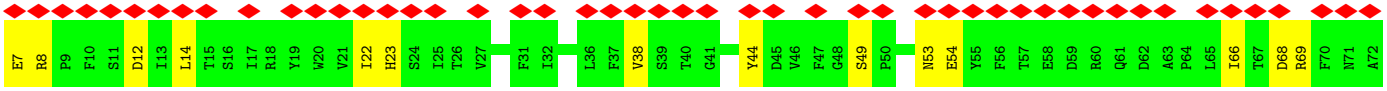
Chain E:

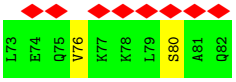




• Molecule 6: Cytochrome b559 subunit alpha

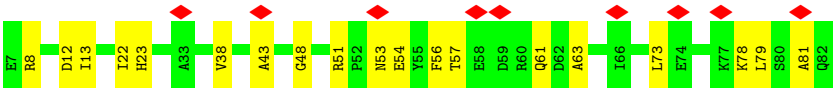
Chain e:





• Molecule 6: Cytochrome b559 subunit alpha

Chain E1:

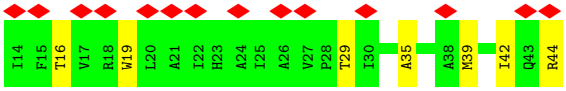


• Molecule 6: Cytochrome b559 subunit alpha

Chain e1:

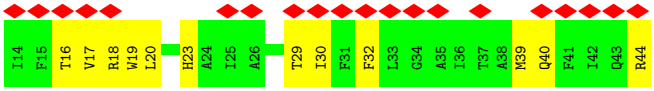
• Molecule 7: Cytochrome b559 subunit beta

Chain F:



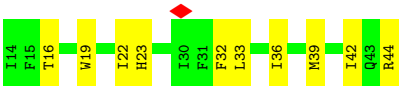
• Molecule 7: Cytochrome b559 subunit beta

Chain f:



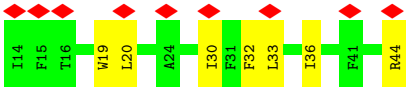
• Molecule 7: Cytochrome b559 subunit beta

Chain F1:



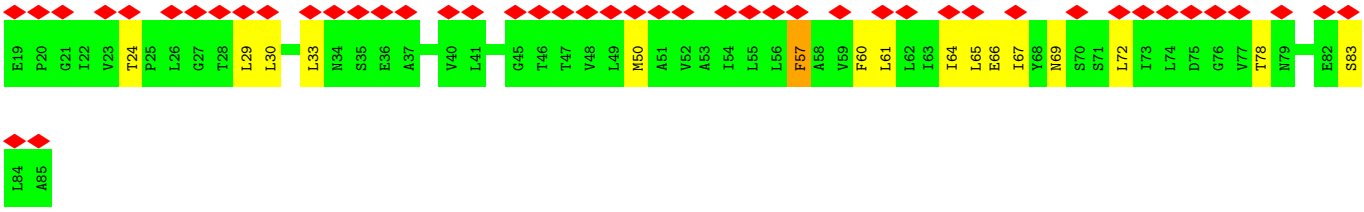
• Molecule 7: Cytochrome b559 subunit beta

Chain f1:



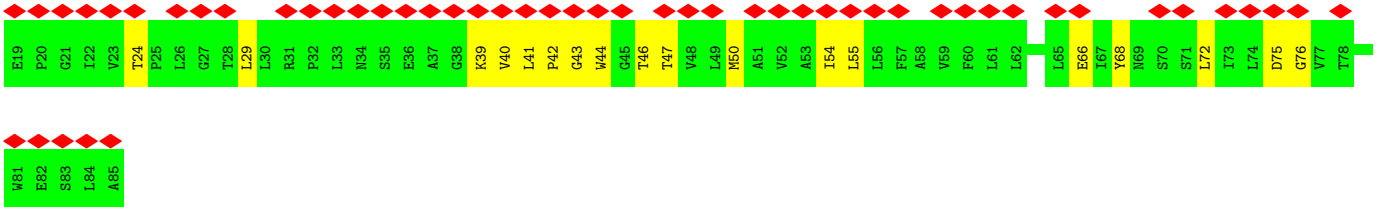
• Molecule 8: Photosystem II reaction center protein H

Chain H:



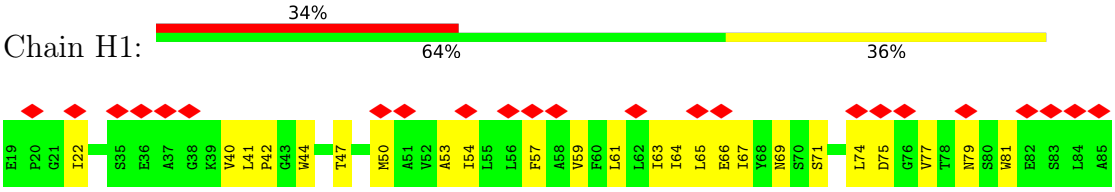
• Molecule 8: Photosystem II reaction center protein H

Chain h:



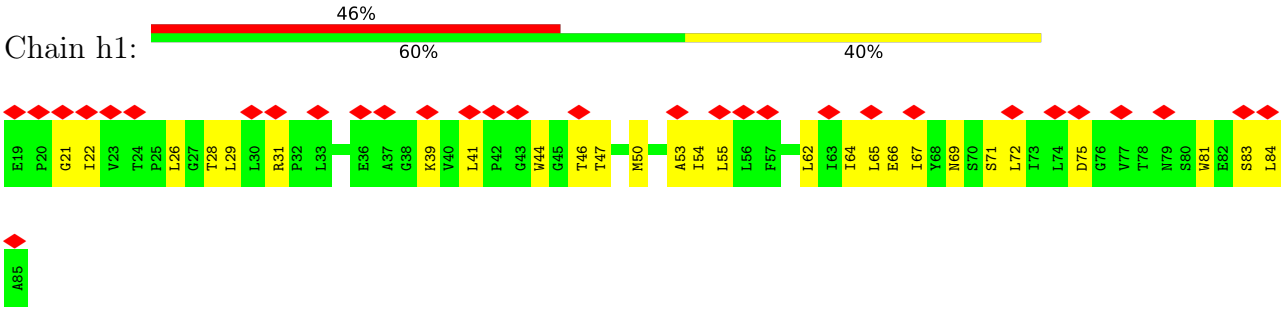
• Molecule 8: Photosystem II reaction center protein H

Chain H1:



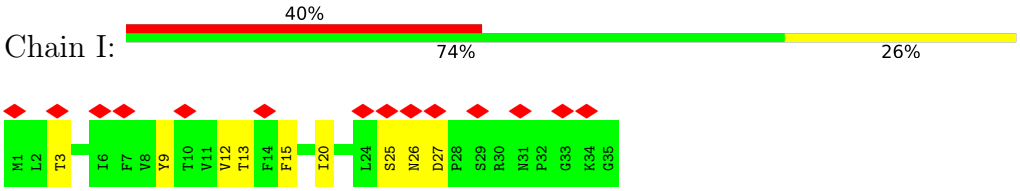
• Molecule 8: Photosystem II reaction center protein H

Chain h1:



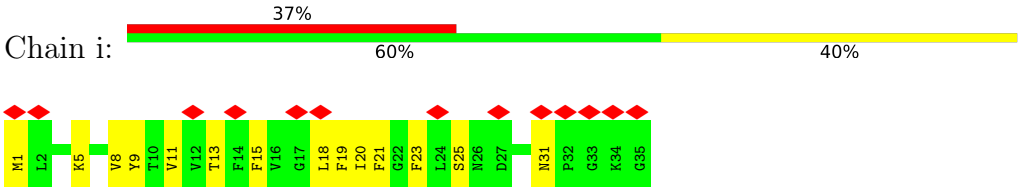
• Molecule 9: Photosystem II reaction center protein I

Chain I:



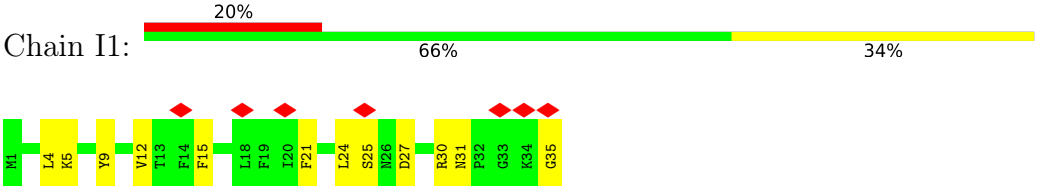
• Molecule 9: Photosystem II reaction center protein I

Chain i:



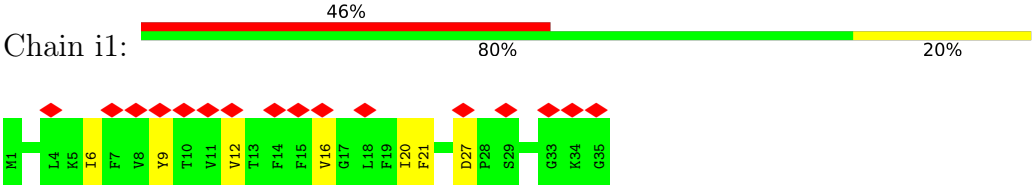
• Molecule 9: Photosystem II reaction center protein I

Chain I1:



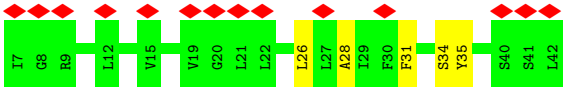
• Molecule 9: Photosystem II reaction center protein I

Chain i1:

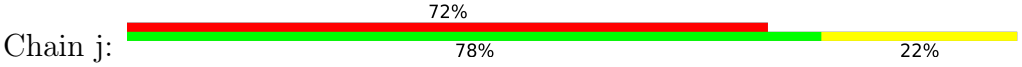


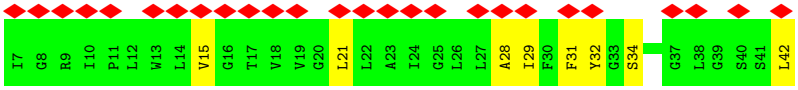
• Molecule 10: Photosystem II reaction center protein J

Chain J:

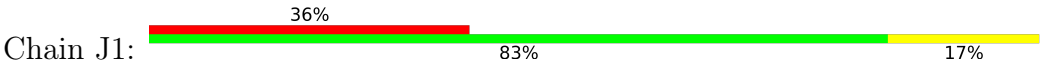


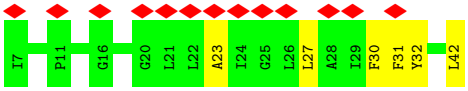
• Molecule 10: Photosystem II reaction center protein J



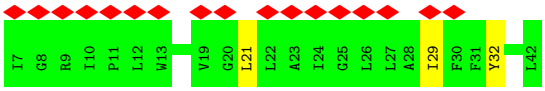


• Molecule 10: Photosystem II reaction center protein J





• Molecule 10: Photosystem II reaction center protein J



• Molecule 11: Photosystem II reaction center protein K

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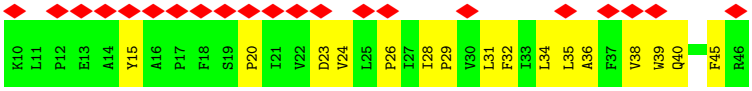
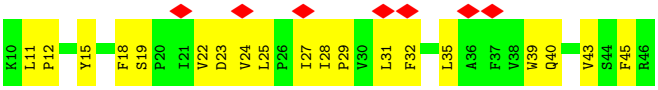
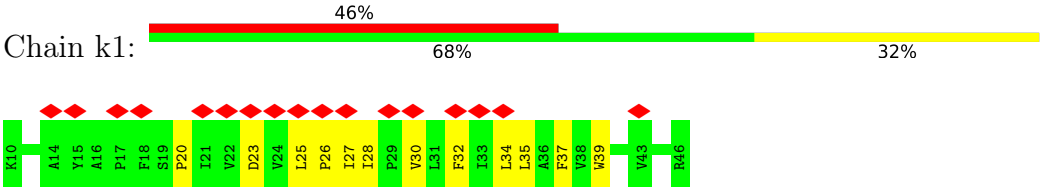


• Molecule 11: Photosystem II reaction center protein K



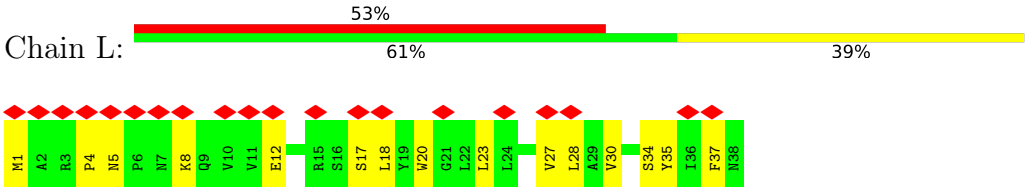
• Molecule 11: Photosystem II reaction center protein K

Chain k1:



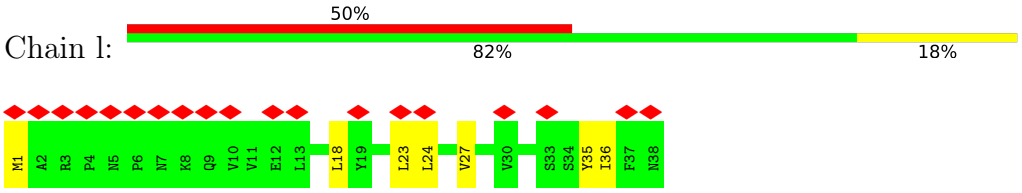
• Molecule 12: Photosystem II reaction center protein L

Chain L:



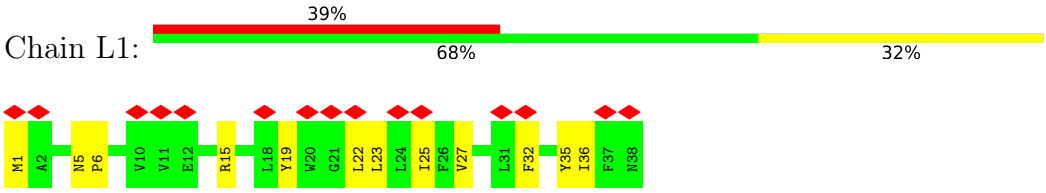
• Molecule 12: Photosystem II reaction center protein L

Chain l:



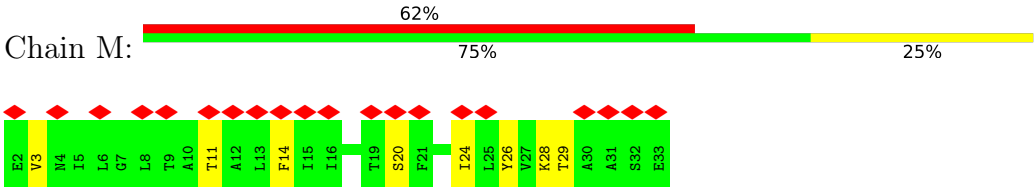
• Molecule 12: Photosystem II reaction center protein L

Chain L1:



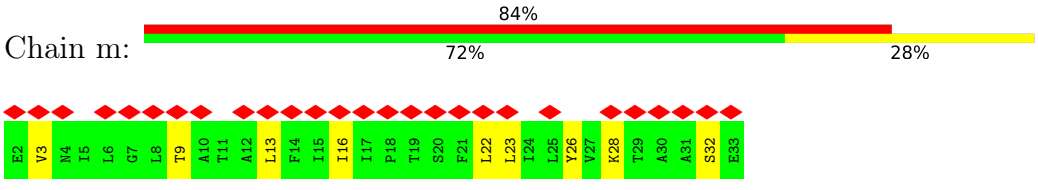
• Molecule 13: Photosystem II reaction center protein M

Chain M:



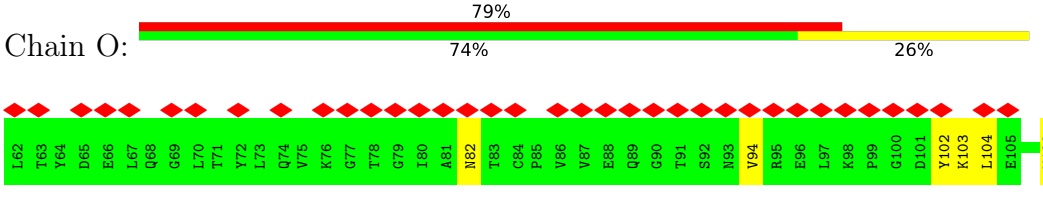
• Molecule 13: Photosystem II reaction center protein M

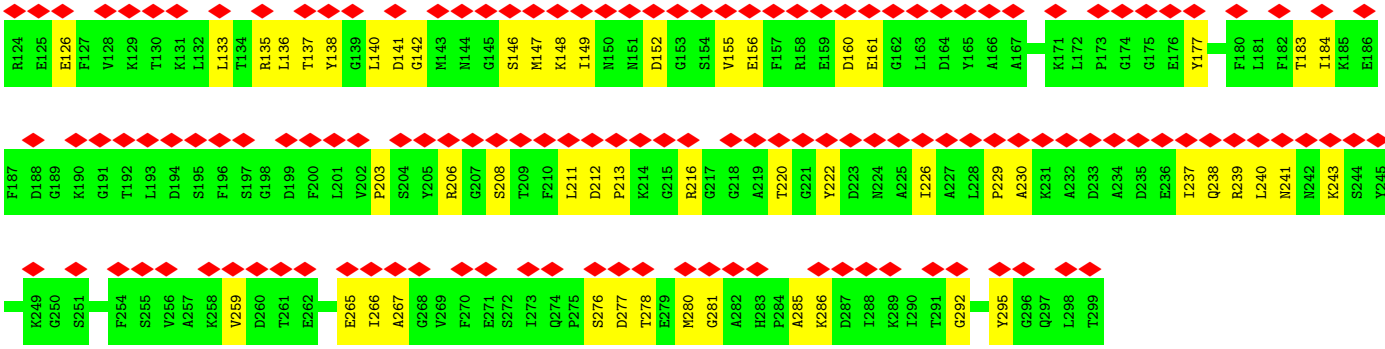
Chain m:



• Molecule 14: PsbO

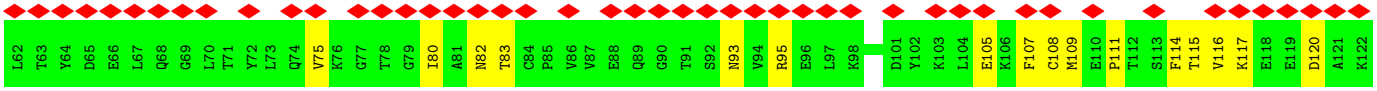
Chain O:





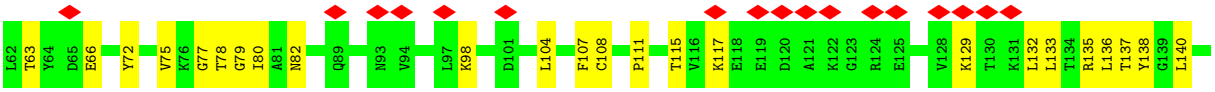
• Molecule 14: PsbO

Chain o:



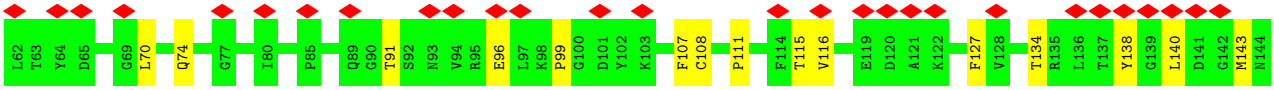
• Molecule 14: PsbO

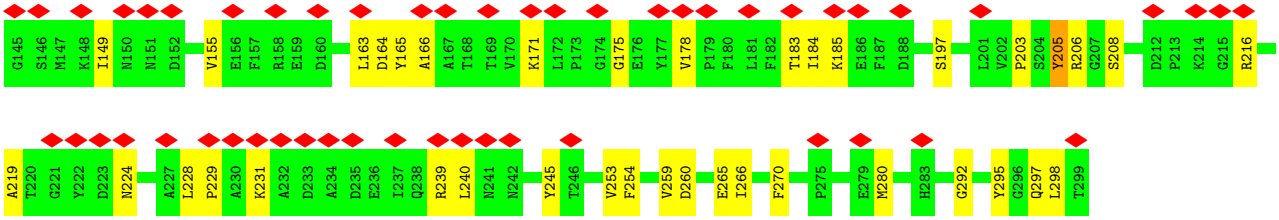
Chain O1:



• Molecule 14: PsbO

Chain o1:





• Molecule 15: PsbP

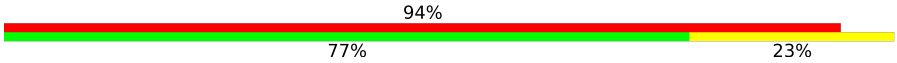
Chain P:

• Molecule 15: PsbP

Chain p:

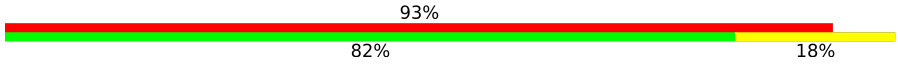
• Molecule 15: PsbP

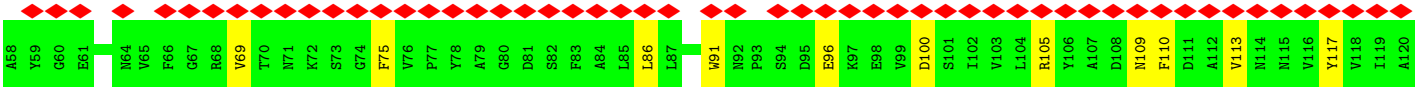
Chain P1:



• Molecule 15: PsbP

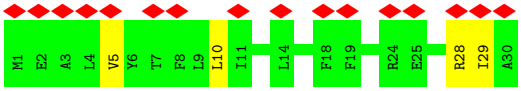
Chain p1:





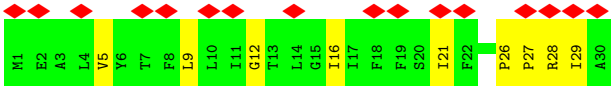
• Molecule 16: Photosystem II reaction center protein T

Chain T:



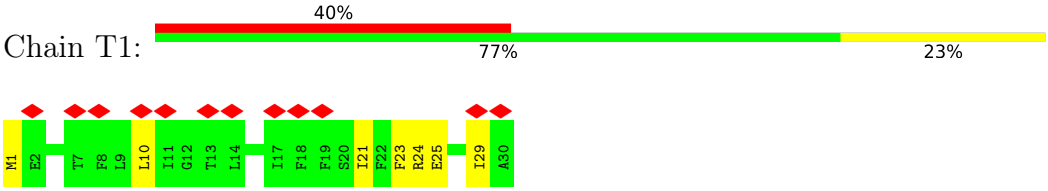
• Molecule 16: Photosystem II reaction center protein T

Chain t:



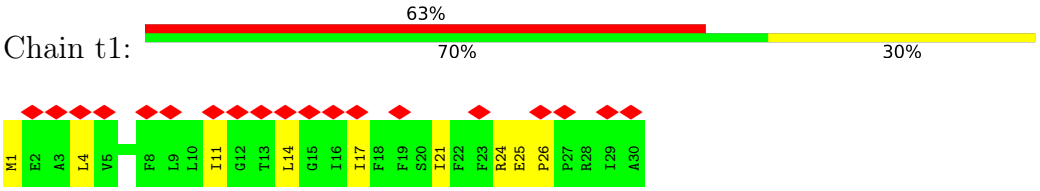
• Molecule 16: Photosystem II reaction center protein T

Chain T1:



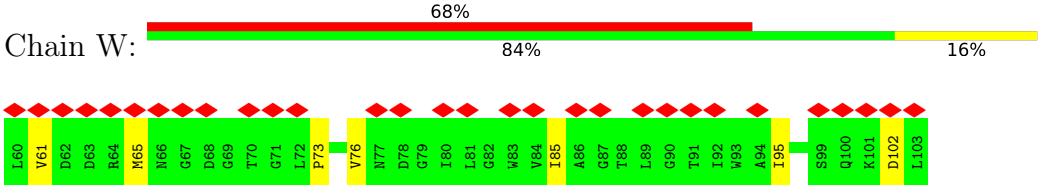
• Molecule 16: Photosystem II reaction center protein T

Chain t1:



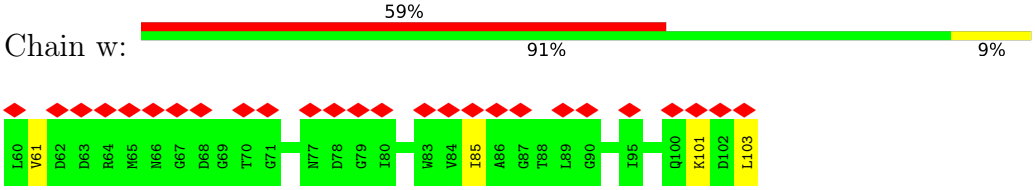
• Molecule 17: PsbW

Chain W:



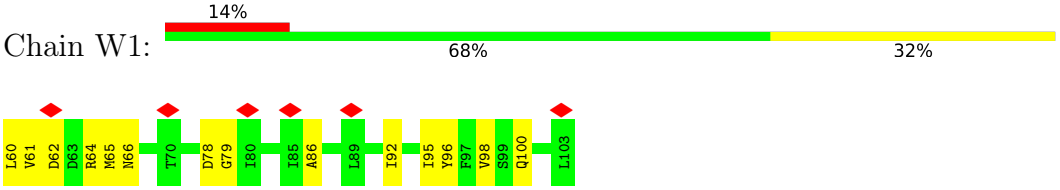
• Molecule 17: PsbW

Chain w:



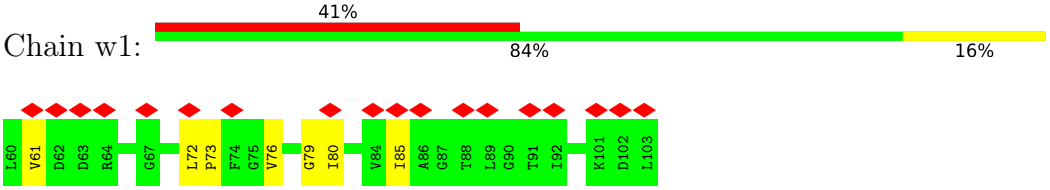
• Molecule 17: PsbW

Chain W1:



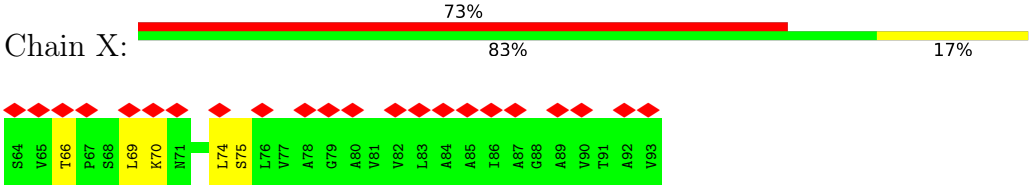
• Molecule 17: PsbW

Chain w1:



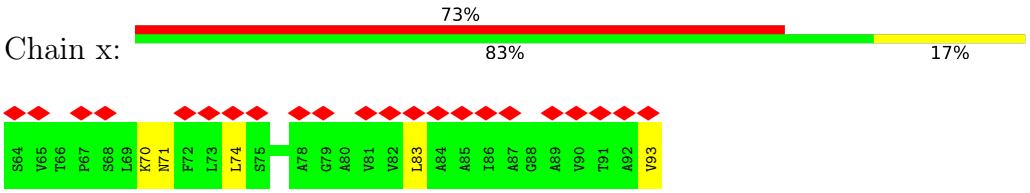
• Molecule 18: PsbX

Chain X:



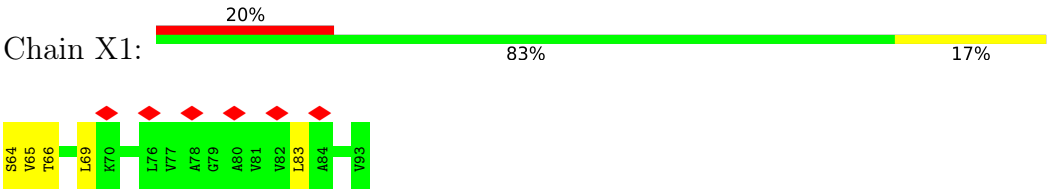
• Molecule 18: PsbX

Chain x:



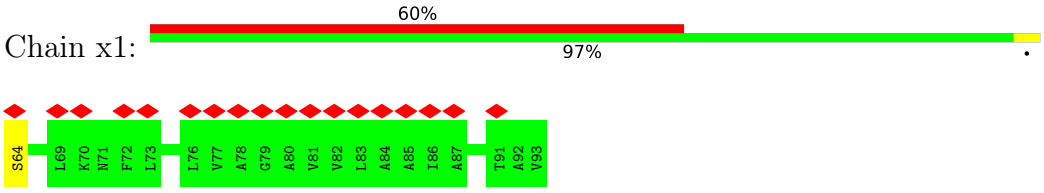
• Molecule 18: PsbX

Chain X1:



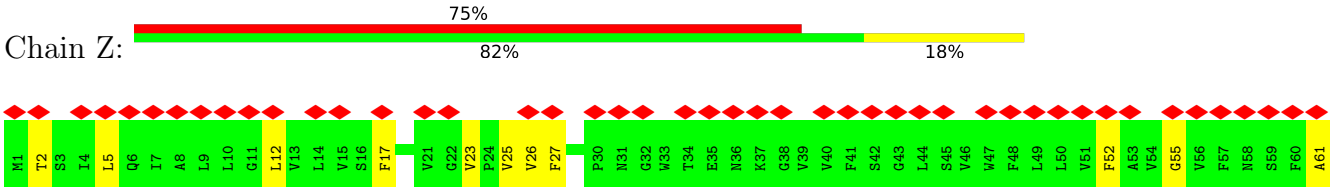
• Molecule 18: PsbX

Chain x1:



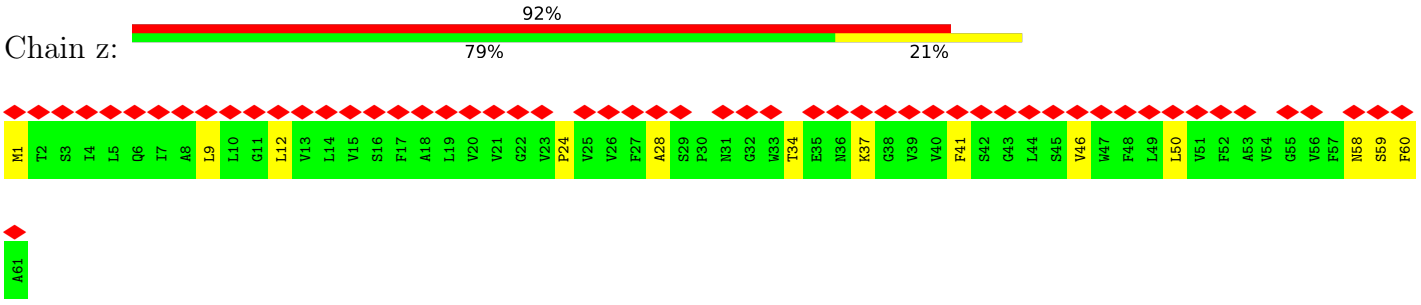
• Molecule 19: PsbZ

Chain Z:



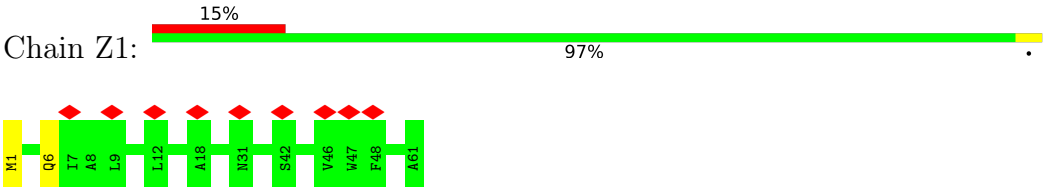
• Molecule 19: PsbZ

Chain z:



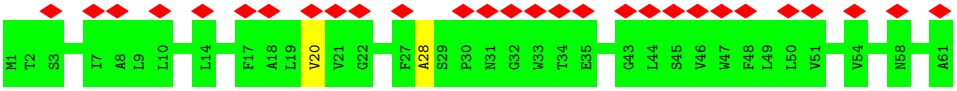
• Molecule 19: PsbZ

Chain Z1:



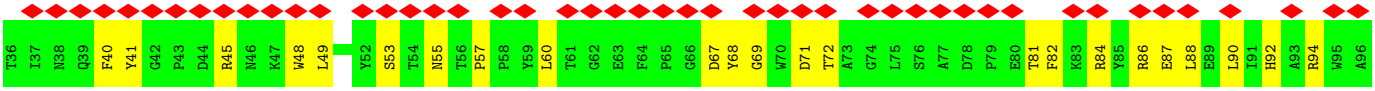
• Molecule 19: PsbZ

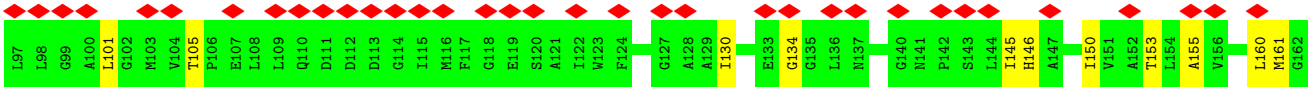
Chain z1:

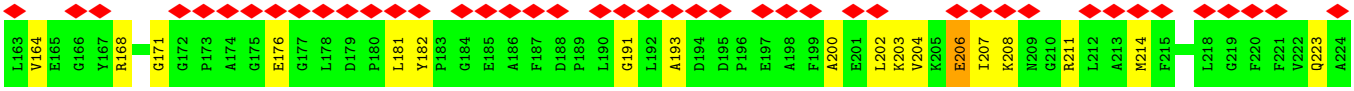


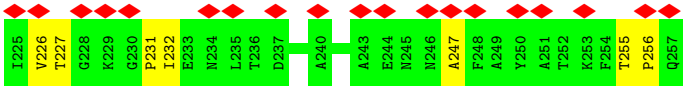
• Molecule 20: LHCII M3

Chain N:



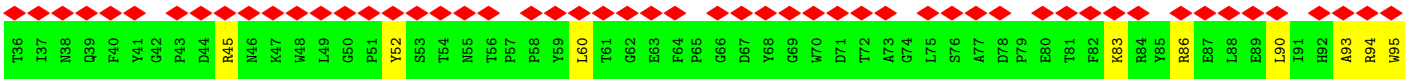


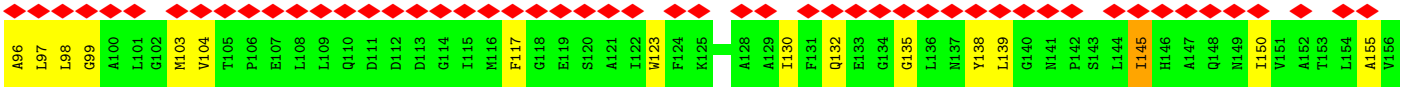


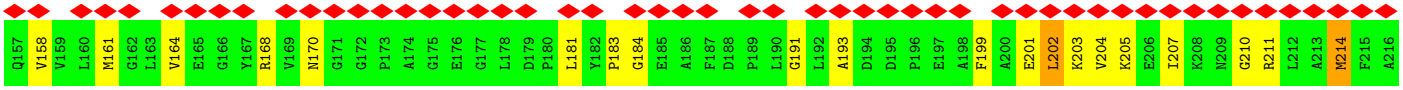


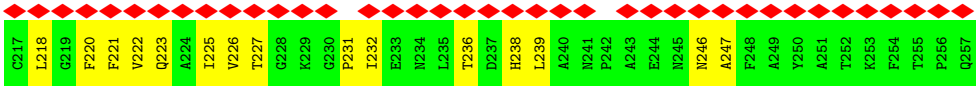
• Molecule 20: LHCII M3

Chain n:



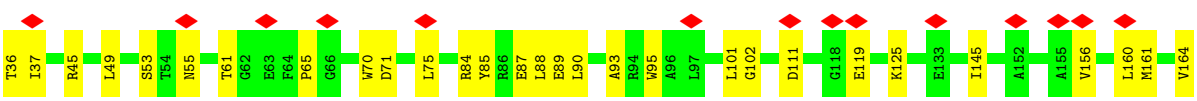






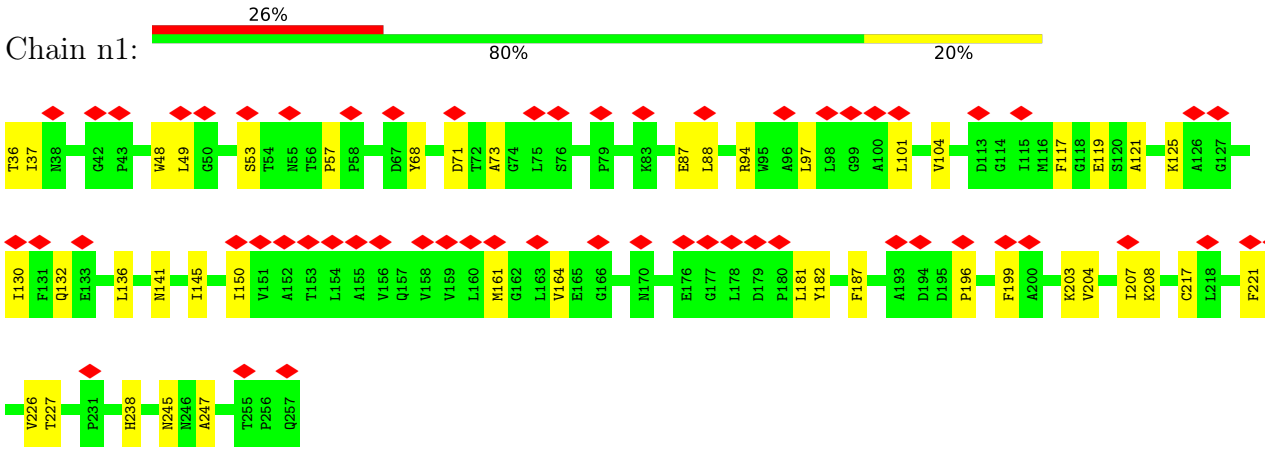
• Molecule 20: LHCII M3

Chain N1:



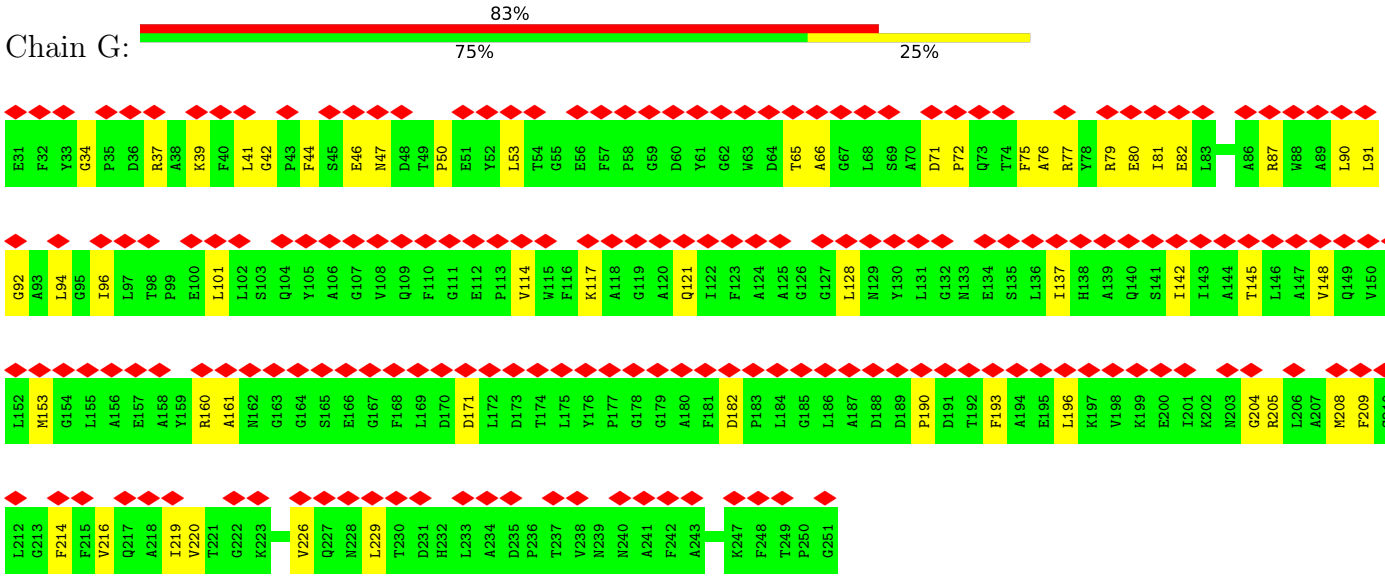
• Molecule 20: LHCII M3

Chain n1:



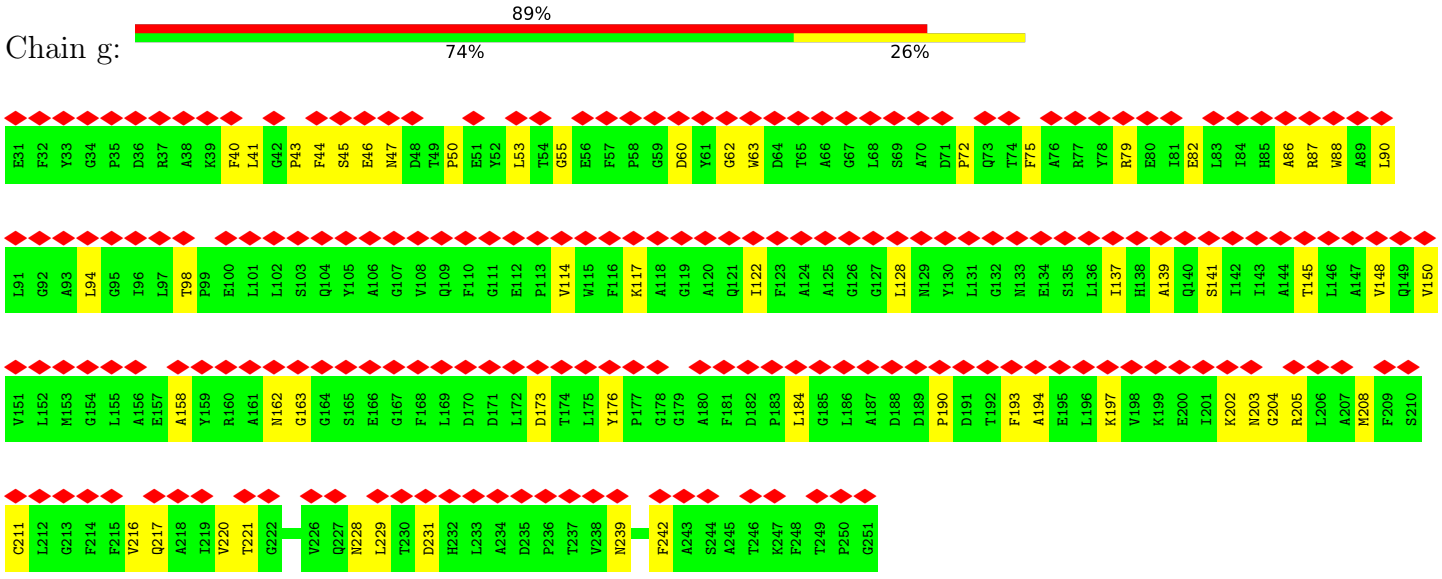
• Molecule 21: LHCII M2

Chain G:



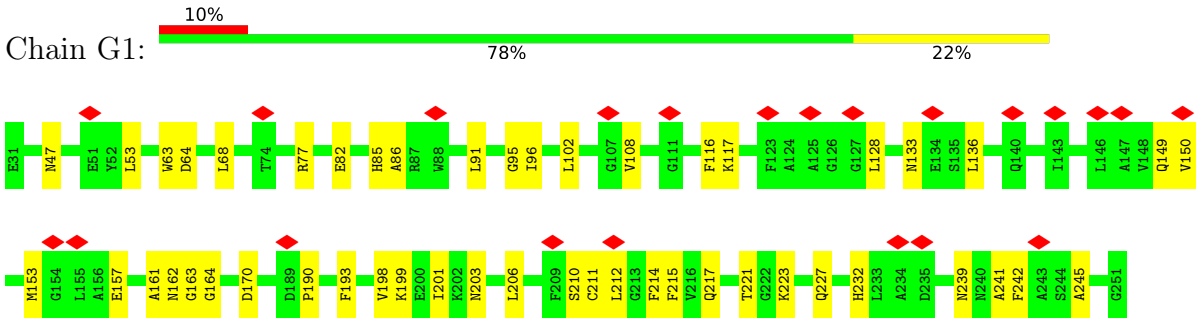
• Molecule 21: LHCII M2

Chain g:



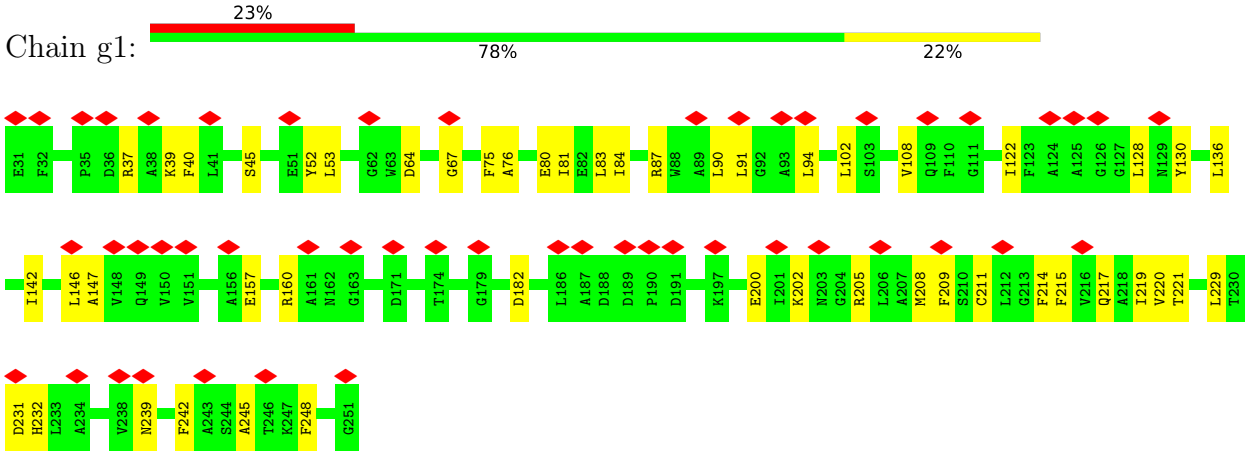
• Molecule 21: LHCII M2

Chain G1:



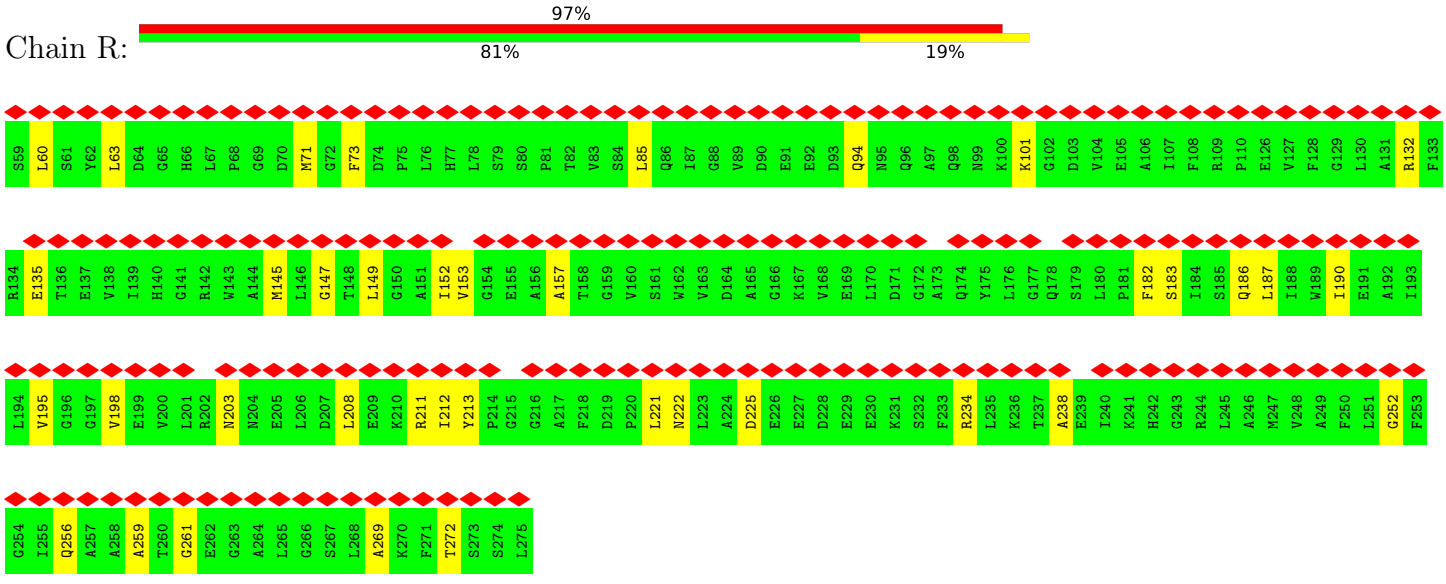
• Molecule 21: LHCII M2

Chain g1:



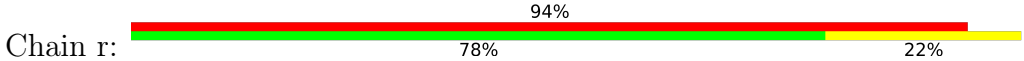
• Molecule 22: CP29

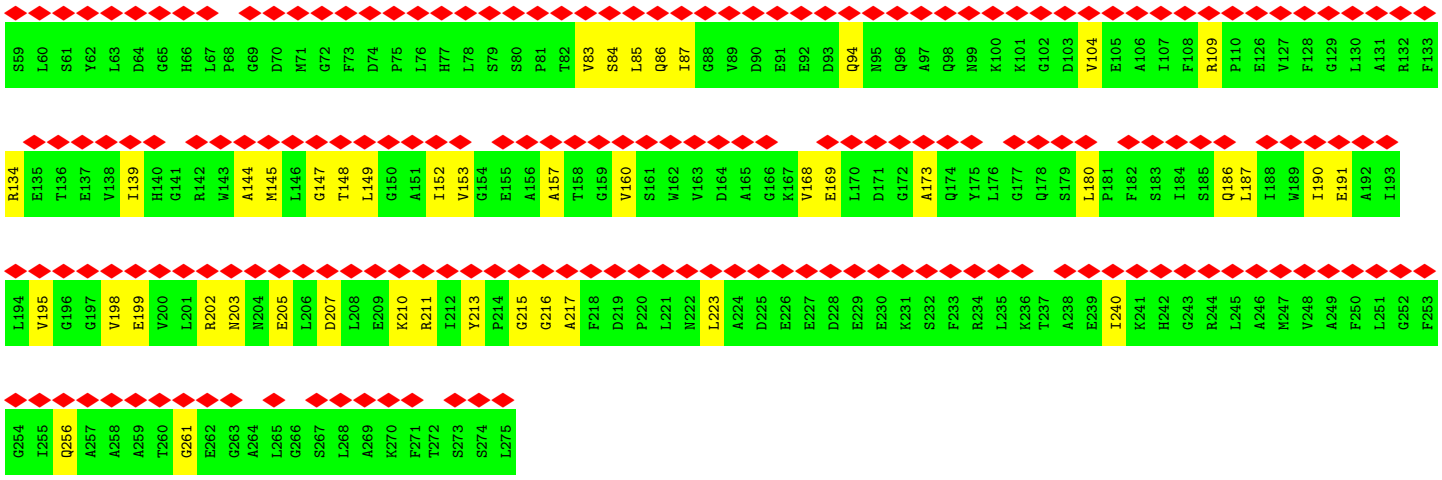
Chain R:



• Molecule 22: CP29

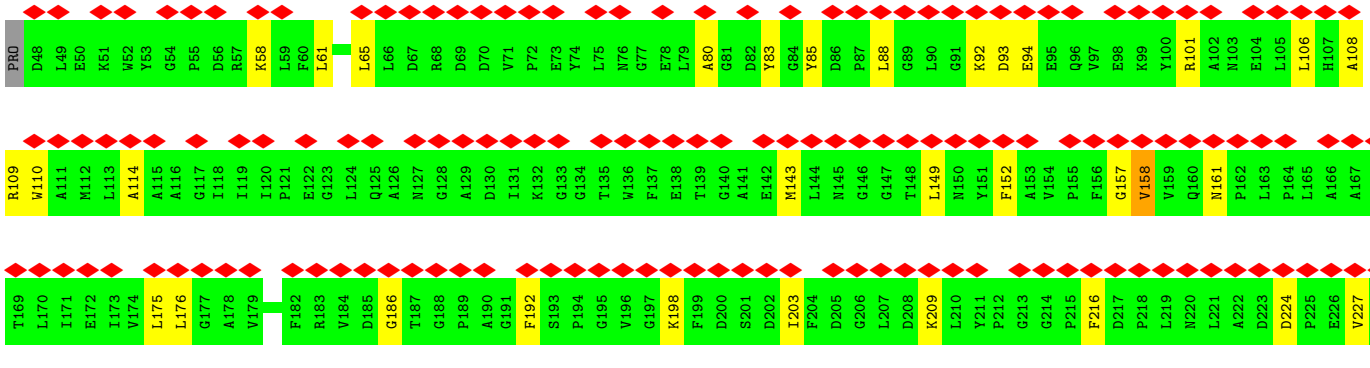
Chain r:





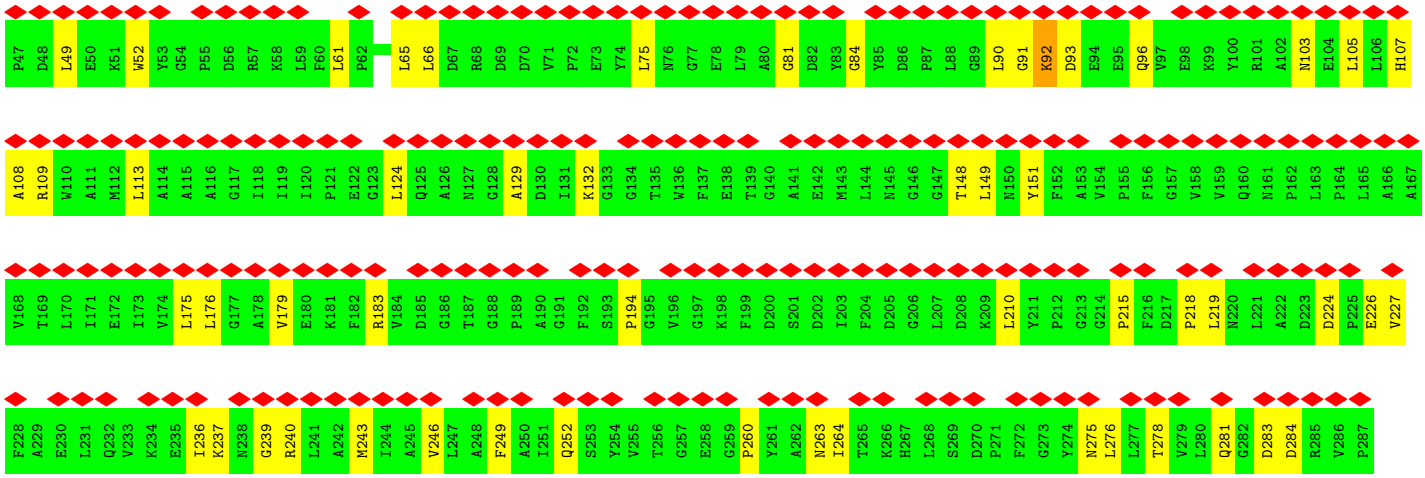
• Molecule 23: CP26

Chain S:



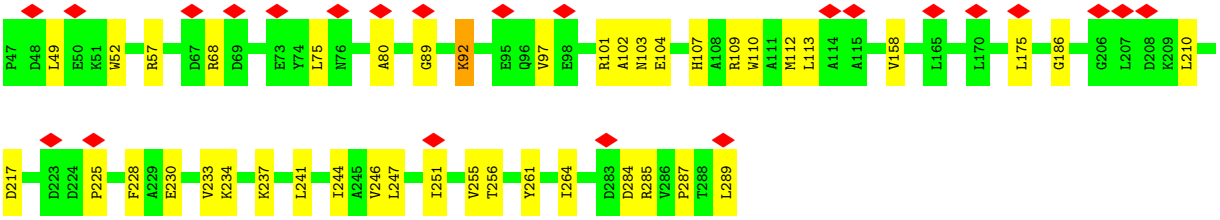
• Molecule 23: CP26

Chain s:



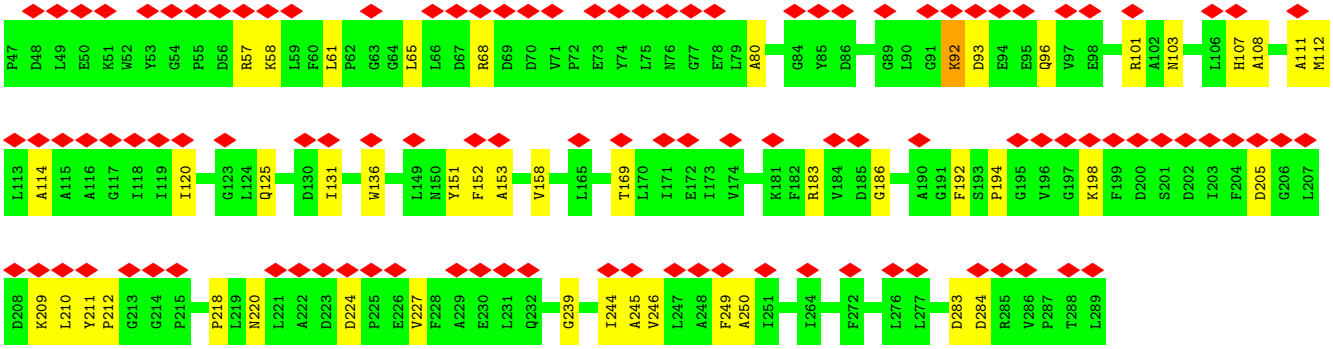
• Molecule 23: CP26

Chain S1:



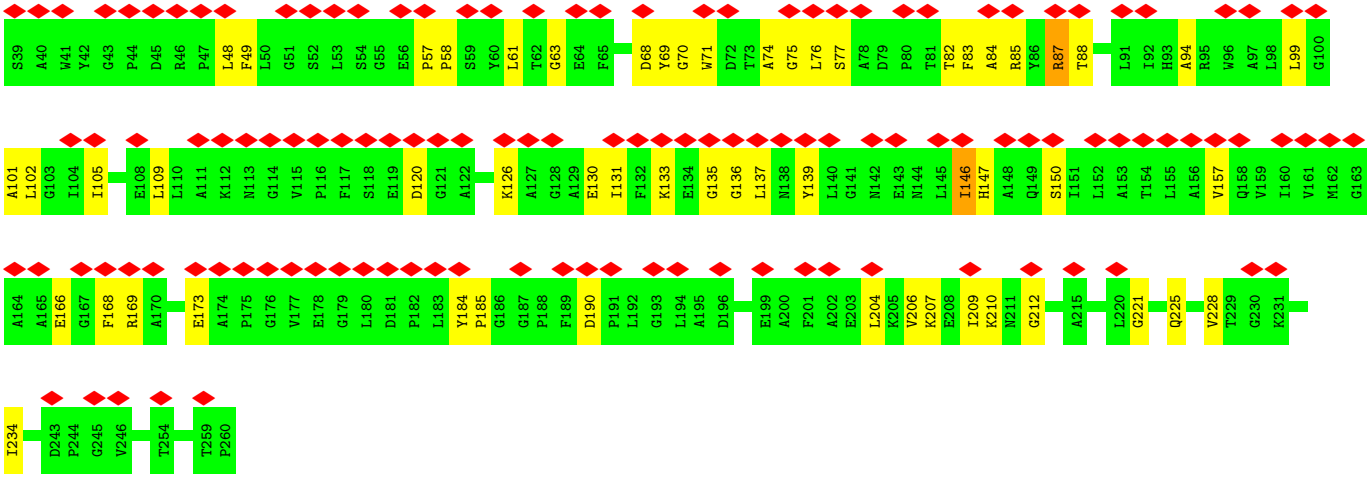
• Molecule 23: CP26

Chain s1:



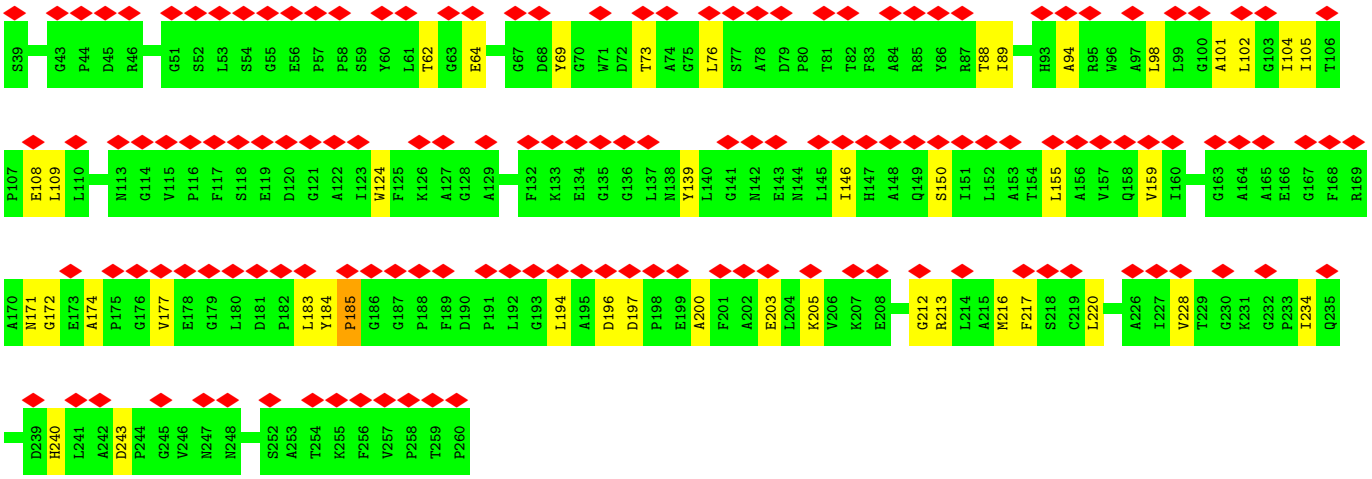
• Molecule 24: LHCII M1

Chain Y:



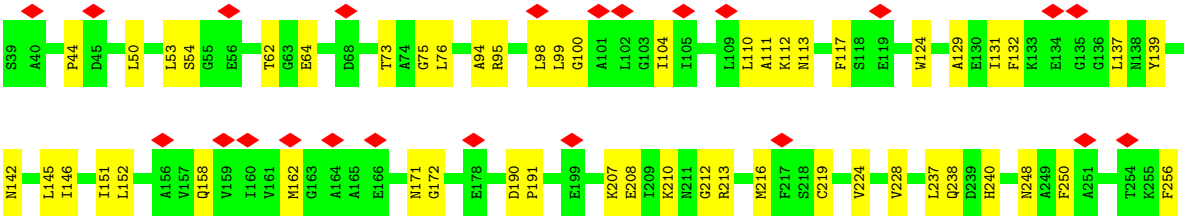
• Molecule 24: LHCII M1

Chain y:



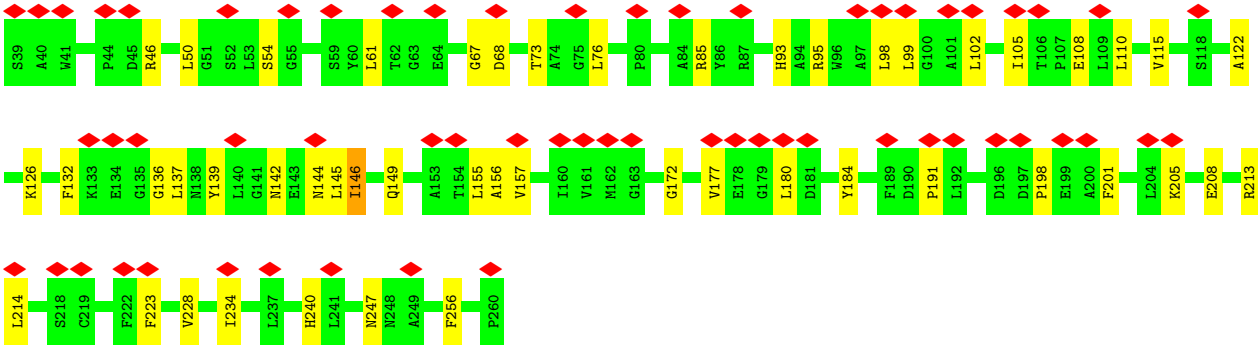
• Molecule 24: LHCII M1

Chain Y1:



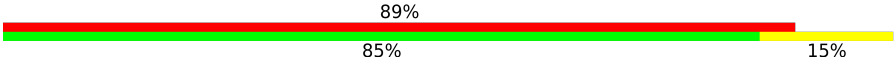
• Molecule 24: LHCII M1

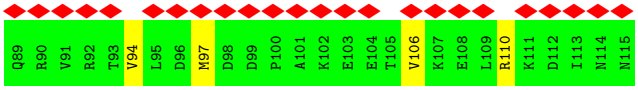
Chain y1:



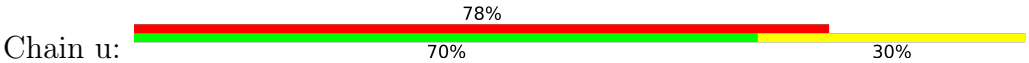
• Molecule 25: PsbU

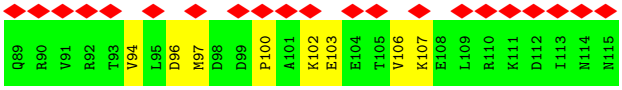
Chain U:



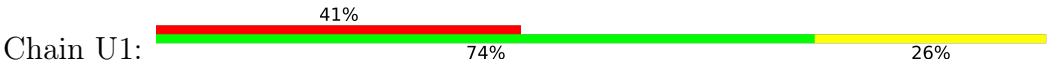


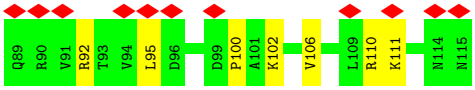
• Molecule 25: PsbU



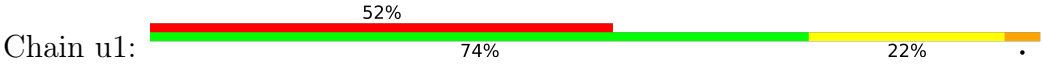


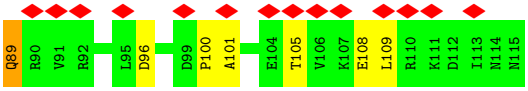
• Molecule 25: PsbU



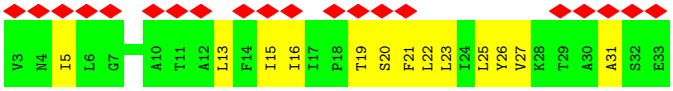


• Molecule 25: PsbU

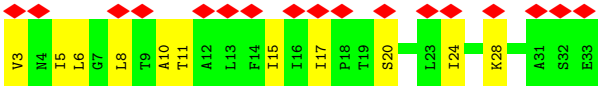




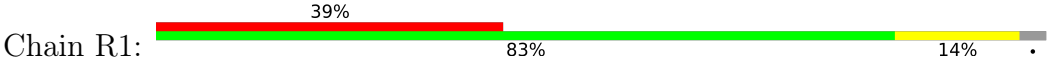
• Molecule 26: Photosystem II reaction center protein M

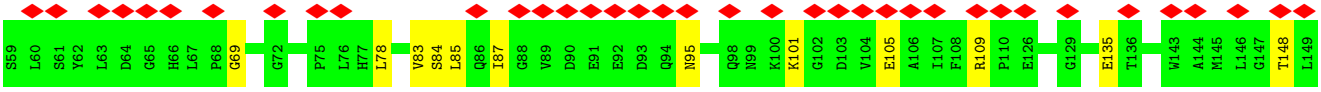


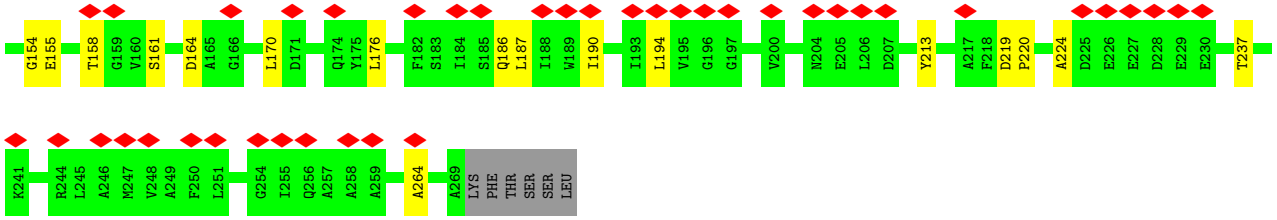
• Molecule 26: Photosystem II reaction center protein M



• Molecule 27: CP29

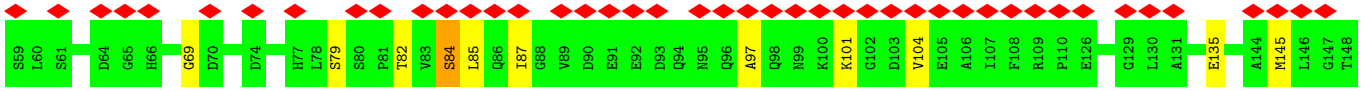


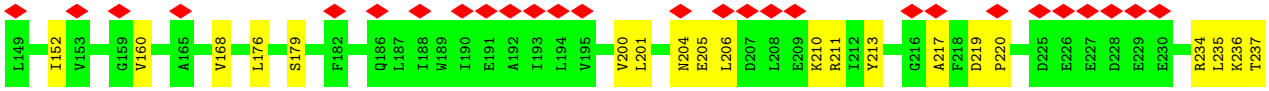


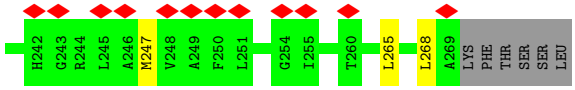


• Molecule 27: CP29

Chain r1:







4 Experimental information (i)

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	14307	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	NONE	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/Å^2$)	51.81	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K3 BIOQUANTUM (6k x 4k)	Depositor
Maximum map value	0.063	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.005	Depositor
Recommended contour level	0.0175	Depositor
Map size (Å)	460.8, 460.8, 460.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	0.96, 0.96, 0.96	Depositor

5 Model quality

5.1 Standard geometry

Bond lengths and bond angles in the following residue types are not validated in this section: GOL, SQD, 4RF, LHG, BCR, PHO, DGA, PL9, FE2, LMG, PTY, CHL, CLA, LUT, 3PH, C7Z, CL, LPX, SEP, NA, NEX, SPH, XAT, ERG, BCT, DGD, LMT, OEX, HEM, LMK, RRX

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#$\|Z\|$ >5	RMSZ	#$\|Z\|$ >5
1	A	0.26	0/2723	0.59	0/3715
1	A1	0.24	0/2723	0.57	0/3715
1	a	0.28	0/2723	0.63	0/3715
1	a1	0.23	0/2723	0.58	3/3715 (0.1%)
2	B	0.33	2/3912 (0.1%)	0.61	6/5327 (0.1%)
2	B1	0.18	0/3912	0.46	0/5327
2	b	0.22	0/3912	0.52	0/5327
2	b1	0.20	0/3912	0.48	0/5327
3	V	0.17	0/228	0.45	0/311
3	V1	0.21	0/228	0.50	0/311
3	v	0.20	0/228	0.52	0/311
3	v1	0.22	0/228	0.49	0/311
4	C	0.23	0/3602	0.54	2/4913 (0.0%)
4	C1	0.19	0/3602	0.48	0/4913
4	c	0.38	1/3602 (0.0%)	0.73	5/4913 (0.1%)
4	c1	0.21	0/3602	0.50	0/4913
5	D	0.24	0/2860	0.58	2/3899 (0.1%)
5	D1	0.21	0/2860	0.54	0/3899
5	d	0.25	0/2860	0.56	2/3899 (0.1%)
5	d1	0.20	0/2860	0.53	0/3899
6	E	0.20	0/639	0.52	0/870
6	E1	0.16	0/639	0.50	0/870
6	e	0.22	0/639	0.59	0/870
6	e1	0.17	0/639	0.44	0/870
7	F	0.23	0/259	0.53	0/351
7	F1	0.20	0/259	0.48	0/351
7	f	0.21	0/259	0.49	0/351
7	f1	0.16	0/259	0.42	0/351
8	H	3.98	6/513 (1.2%)	0.73	1/703 (0.1%)
8	H1	0.17	0/513	0.48	0/703
8	h	0.26	0/513	0.70	2/703 (0.3%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
8	h1	0.20	0/513	0.49	0/703
9	I	0.22	0/287	0.52	0/386
9	I1	0.25	0/287	0.57	0/386
9	i	0.24	0/287	0.57	0/386
9	i1	0.17	0/287	0.45	0/386
10	J	0.15	0/272	0.38	0/369
10	J1	0.14	0/272	0.39	0/369
10	j	0.18	0/272	0.39	0/369
10	j1	0.18	0/272	0.43	0/369
11	K	0.27	0/308	0.74	1/423 (0.2%)
11	K1	0.27	0/308	0.69	0/423
11	k	0.29	0/308	0.65	0/423
11	k1	0.29	0/308	0.62	1/423 (0.2%)
12	L	0.36	0/321	0.66	1/435 (0.2%)
12	L1	0.19	0/321	0.53	0/435
12	l	0.18	0/321	0.42	0/435
13	M	0.22	0/246	0.55	0/335
13	m	0.25	0/246	0.62	0/335
14	O	0.22	0/1855	0.55	0/2505
14	O1	0.20	0/1855	0.52	0/2505
14	o	0.21	0/1855	0.55	0/2505
14	o1	0.20	0/1855	0.54	0/2505
15	P	0.18	0/1473	0.50	0/1988
15	P1	0.19	0/1473	0.50	1/1988 (0.1%)
15	p	0.15	0/1473	0.41	0/1988
15	p1	0.16	0/1473	0.50	2/1988 (0.1%)
16	T	0.23	0/254	0.58	0/342
16	T1	0.22	0/254	0.51	0/342
16	t	0.22	0/254	0.61	0/342
16	t1	0.20	0/254	0.49	0/342
17	W	0.20	0/339	0.51	0/460
17	W1	0.19	0/339	0.52	0/460
17	w	0.19	0/339	0.44	0/460
17	w1	0.19	0/339	0.44	0/460
18	X	0.18	0/202	0.44	0/276
18	X1	0.19	0/202	0.49	0/276
18	x	0.20	0/202	0.49	0/276
18	x1	0.19	0/202	0.43	0/276
19	Z	0.21	0/469	0.53	0/641
19	Z1	0.13	0/469	0.39	0/641
19	z	0.18	0/469	0.40	0/641
19	z1	0.16	0/469	0.44	0/641
20	N	0.23	0/1751	0.56	1/2386 (0.0%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	#|Z| >5	RMSZ	#|Z| >5
20	N1	0.20	0/1751	0.51	0/2386
20	n	0.26	0/1751	0.69	4/2386 (0.2%)
20	n1	0.17	0/1750	0.46	0/2382
21	G	0.22	0/1725	0.61	0/2348
21	G1	0.18	0/1725	0.48	0/2348
21	g	0.22	0/1725	0.53	0/2348
21	g1	0.18	0/1725	0.49	0/2348
22	R	0.18	0/1561	0.46	0/2110
22	r	0.19	0/1561	0.49	0/2110
23	S	0.21	0/1895	0.53	1/2579 (0.0%)
23	S1	0.17	0/1903	0.49	0/2590
23	s	0.20	0/1902	0.53	0/2587
23	s1	0.18	0/1903	0.52	1/2590 (0.0%)
24	Y	0.31	0/1715	0.68	2/2338 (0.1%)
24	Y1	0.22	0/1715	0.49	1/2338 (0.0%)
24	y	0.39	2/1715 (0.1%)	0.73	4/2338 (0.2%)
24	y1	0.18	0/1715	0.47	0/2338
25	U	0.21	0/224	0.56	0/298
25	U1	0.22	0/224	0.54	0/298
25	u	0.23	0/224	0.70	0/298
25	u1	0.27	0/224	0.57	0/298
26	M1	0.23	0/237	0.58	0/323
26	m1	0.23	0/237	0.60	0/323
27	R1	0.16	0/1506	0.39	0/2035
27	r1	0.18	0/1506	0.52	0/2035
All	All	0.35	11/118105 (0.0%)	0.54	43/160649 (0.0%)

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
8	H	57	PHE	CD2-CE2	42.12	2.65	1.38
8	H	57	PHE	CD1-CE1	40.91	2.61	1.38
8	H	57	PHE	CE2-CZ	39.71	2.57	1.38
8	H	57	PHE	CE1-CZ	39.38	2.56	1.38
8	H	57	PHE	CG-CD2	27.71	1.97	1.38
8	H	57	PHE	CG-CD1	27.62	1.96	1.38
4	c	374	PRO	CG-CD	-14.17	1.02	1.50
2	B	88	PRO	CG-CD	-11.43	1.11	1.50
24	y	185	PRO	CG-CD	-10.74	1.14	1.50
2	B	50	PRO	CG-CD	-7.13	1.26	1.50
24	y	185	PRO	CB-CG	-7.06	1.14	1.49

All (43) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	y	185	PRO	N-CD-CG	-17.70	76.65	103.20
4	c	374	PRO	N-CD-CG	-16.63	78.26	103.20
2	B	88	PRO	N-CD-CG	-13.67	82.69	103.20
24	y	185	PRO	CB-CG-CD	12.76	146.92	106.10
24	y	185	PRO	CA-CB-CG	-11.76	82.17	104.50
2	B	50	PRO	CA-N-CD	-11.22	96.29	112.00
2	B	88	PRO	CA-N-CD	-10.52	97.28	112.00
4	c	374	PRO	CA-CB-CG	-9.50	86.45	104.50
2	B	50	PRO	N-CD-CG	-9.07	89.59	103.20
20	n	214	MET	CB-CG-SD	8.94	139.52	112.70
4	c	374	PRO	CA-N-CD	-8.73	99.78	112.00
24	Y	87	ARG	CG-CD-NE	-8.64	93.00	112.00
1	a1	39	PRO	N-CD-CG	-8.06	91.11	103.20
12	L	4	PRO	N-CD-CG	-7.78	91.53	103.20
2	B	88	PRO	CA-CB-CG	-7.67	89.93	104.50
1	a1	39	PRO	CA-N-CD	-7.60	101.36	112.00
24	y	185	PRO	CA-N-CD	-7.45	101.57	112.00
8	h	40	VAL	CA-C-N	7.41	131.01	120.49
8	h	40	VAL	C-N-CA	7.41	131.01	120.49
15	p1	91	TRP	CA-C-N	7.35	131.49	121.20
15	p1	91	TRP	C-N-CA	7.35	131.49	121.20
8	H	57	PHE	CD1-CG-CD2	7.31	129.56	118.60
20	n	184	GLY	CA-C-N	-7.28	111.63	122.56
20	n	184	GLY	C-N-CA	-7.28	111.63	122.56
5	D	59	TYR	CA-C-N	7.15	135.20	121.54
5	D	59	TYR	C-N-CA	7.15	135.20	121.54
11	K	43	VAL	N-CA-C	-6.53	106.37	112.83
5	d	59	TYR	CA-C-N	6.40	133.77	121.54
5	d	59	TYR	C-N-CA	6.40	133.77	121.54
1	a1	196	PRO	CA-N-CD	-6.22	103.29	112.00
4	C	256	GLY	CA-C-N	5.66	132.35	121.54
4	C	256	GLY	C-N-CA	5.66	132.35	121.54
4	c	374	PRO	N-CA-CB	-5.63	98.11	103.51
4	c	69	MET	CB-CG-SD	5.52	129.26	112.70
11	k1	25	LEU	N-CA-C	5.29	121.50	109.81
20	n	202	LEU	CA-CB-CG	5.27	134.73	116.30
2	B	50	PRO	CA-CB-CG	-5.26	94.50	104.50
24	Y1	44	PRO	CA-N-CD	-5.25	104.65	112.00
15	P1	161	ASP	CB-CA-C	-5.25	110.10	117.23
23	S	203	ILE	N-CA-C	-5.21	108.76	113.71
23	s1	220	ASN	CB-CA-C	-5.09	110.30	117.23
20	N	206	GLU	CA-CB-CG	5.07	124.24	114.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
24	Y	87	ARG	N-CA-CB	5.01	118.05	110.28

There are no chirality outliers.

There are no planarity outliers.

5.2 Too-close contacts (i)

In the following table, the Non-H and H(model) columns list the number of non-hydrogen atoms and hydrogen atoms in the chain respectively. The H(added) column lists the number of hydrogen atoms added and optimized by MolProbity. The Clashes column lists the number of clashes within the asymmetric unit, whereas Symm-Clashes lists symmetry-related clashes.

Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
1	A	2638	0	2541	81	0
1	A1	2638	0	2541	119	0
1	a	2638	0	2541	103	0
1	a1	2638	0	2541	108	0
2	B	3783	0	3663	90	0
2	B1	3783	0	3663	138	0
2	b	3783	0	3663	104	0
2	b1	3783	0	3663	126	0
3	V	227	0	261	3	0
3	V1	227	0	261	6	0
3	v	227	0	261	7	0
3	v1	227	0	261	5	0
4	C	3483	0	3376	102	0
4	C1	3483	0	3376	118	0
4	c	3483	0	3376	126	0
4	c1	3483	0	3376	124	0
5	D	2766	0	2654	87	0
5	D1	2766	0	2654	115	0
5	d	2766	0	2655	95	0
5	d1	2766	0	2655	108	0
6	E	621	0	605	8	0
6	E1	621	0	605	13	0
6	e	621	0	605	16	0
6	e1	621	0	605	11	0
7	F	252	0	265	5	0
7	F1	252	0	265	8	0
7	f	252	0	265	15	0
7	f1	252	0	265	7	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
8	H	503	0	532	38	0
8	H1	503	0	532	20	0
8	h	503	0	532	15	0
8	h1	503	0	532	29	0
9	I	279	0	288	9	0
9	I1	279	0	288	14	0
9	i	279	0	288	15	0
9	i1	279	0	288	9	0
10	J	266	0	286	4	0
10	J1	266	0	286	6	0
10	j	266	0	286	10	0
10	j1	266	0	286	3	0
11	K	297	0	312	9	0
11	K1	297	0	312	17	0
11	k	297	0	312	14	0
11	k1	297	0	312	15	0
12	L	313	0	325	13	0
12	L1	313	0	325	11	0
12	l	313	0	325	10	0
13	M	243	0	264	6	0
13	m	243	0	264	7	0
14	O	1820	0	1776	52	0
14	O1	1820	0	1776	57	0
14	o	1820	0	1776	56	0
14	o1	1820	0	1776	46	0
15	P	1444	0	1403	23	0
15	P1	1444	0	1403	32	0
15	p	1444	0	1403	16	0
15	p1	1444	0	1403	26	0
16	T	247	0	260	3	0
16	T1	247	0	260	7	0
16	t	247	0	260	6	0
16	t1	247	0	260	8	0
17	W	332	0	323	7	0
17	W1	332	0	323	14	0
17	w	332	0	323	4	0
17	w1	332	0	323	10	0
18	X	201	0	224	3	0
18	X1	201	0	224	5	0
18	x	201	0	224	4	0
18	x1	201	0	224	1	0
19	Z	457	0	478	10	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
19	Z1	457	0	478	2	0
19	z	457	0	478	11	0
19	z1	457	0	478	2	0
20	N	1703	0	1641	44	0
20	N1	1703	0	1641	40	0
20	n	1703	0	1641	44	0
20	n1	1703	0	1641	30	0
21	G	1680	0	1614	51	0
21	G1	1680	0	1614	37	0
21	g	1680	0	1614	45	0
21	g1	1680	0	1614	42	0
22	R	1533	0	1506	29	0
22	r	1533	0	1506	33	0
23	S	1849	0	1808	41	0
23	S1	1856	0	1816	32	0
23	s	1856	0	1815	41	0
23	s1	1856	0	1816	32	0
24	Y	1667	0	1624	43	0
24	Y1	1667	0	1624	51	0
24	y	1667	0	1624	45	0
24	y1	1667	0	1624	52	0
25	U	224	0	226	5	0
25	U1	224	0	226	5	0
25	u	224	0	226	7	0
25	u1	224	0	226	8	0
26	M1	234	0	258	11	0
26	m1	234	0	258	9	0
27	R1	1490	0	1454	25	0
27	r1	1490	0	1454	27	0
28	A	10	0	0	0	0
28	A1	10	0	0	1	0
28	a	10	0	0	1	0
28	a1	10	0	0	0	0
29	A	1	0	0	0	0
29	A1	1	0	0	0	0
29	a	1	0	0	0	0
29	a1	1	0	0	0	0
30	A	2	0	0	1	0
30	A1	2	0	0	0	0
30	a	2	0	0	1	0
30	a1	2	0	0	0	0
31	A	239	0	240	23	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
31	A1	240	0	239	16	0
31	B	1040	0	1143	69	0
31	B1	1040	0	1148	77	0
31	C	845	0	934	57	0
31	C1	845	0	929	66	0
31	D	130	0	144	7	0
31	D1	130	0	144	11	0
31	G	446	0	426	22	0
31	G1	466	0	467	24	0
31	N	468	0	467	22	0
31	N1	468	0	468	24	0
31	R	501	0	455	19	0
31	R1	409	0	391	17	0
31	S	625	0	587	24	0
31	S1	625	0	585	27	0
31	Y	570	0	611	33	0
31	Y1	570	0	611	37	0
31	a	239	0	239	14	0
31	a1	239	0	240	18	0
31	b	1040	0	1144	67	0
31	b1	1040	0	1146	88	0
31	c	845	0	930	57	0
31	c1	845	0	930	75	0
31	d	130	0	143	8	0
31	d1	130	0	143	8	0
31	g	446	0	427	22	0
31	g1	466	0	466	24	0
31	n	468	0	467	27	0
31	n1	468	0	468	21	0
31	r	501	0	453	15	0
31	r1	409	0	392	29	0
31	s	625	0	585	25	0
31	s1	625	0	585	28	0
31	y	570	0	612	50	0
31	y1	570	0	613	52	0
32	A	128	0	148	8	0
32	A1	128	0	148	9	0
32	a	128	0	148	9	0
32	a1	128	0	148	10	0
33	A	40	0	53	2	0
33	A1	40	0	53	4	0
33	B	80	0	106	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
33	B1	80	0	106	9	0
33	C	160	0	211	20	0
33	C1	160	0	211	25	0
33	D	40	0	54	1	0
33	D1	40	0	53	1	0
33	a	40	0	53	4	0
33	a1	40	0	53	4	0
33	b	80	0	106	5	0
33	b1	80	0	106	5	0
33	c	160	0	211	20	0
33	c1	160	0	212	31	0
33	d	40	0	53	5	0
33	d1	40	0	53	5	0
34	A	51	0	68	4	0
34	A1	51	0	68	2	0
34	B	54	0	77	3	0
34	B1	96	0	124	6	0
34	C	54	0	77	2	0
34	C1	54	0	77	2	0
34	M1	42	0	47	6	0
34	a	51	0	68	4	0
34	a1	51	0	68	7	0
34	b	54	0	77	2	0
34	b1	96	0	124	14	0
34	c	54	0	77	2	0
34	c1	54	0	77	5	0
34	m1	42	0	47	3	0
35	A	48	0	66	12	0
35	A1	48	0	66	7	0
35	B	44	0	58	3	0
35	B1	44	0	58	9	0
35	C	51	0	72	7	0
35	C1	106	0	158	14	0
35	D	46	0	62	3	0
35	D1	46	0	62	3	0
35	H	48	0	66	4	0
35	H1	48	0	66	5	0
35	J	45	0	60	2	0
35	W1	39	0	48	4	0
35	a	48	0	66	6	0
35	a1	48	0	66	7	0
35	b	44	0	58	5	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
35	b1	44	0	58	6	0
35	c	51	0	72	3	0
35	c1	106	0	158	17	0
35	d	46	0	62	4	0
35	d1	46	0	62	2	0
35	h	48	0	66	6	0
35	h1	48	0	66	3	0
35	j	45	0	60	5	0
35	w1	39	0	48	3	0
36	A	1	0	0	0	0
36	A1	1	0	0	0	0
36	a	1	0	0	0	0
36	a1	1	0	0	0	0
37	B	42	0	0	0	0
37	B1	42	0	0	0	0
37	b	42	0	0	0	0
37	b1	42	0	0	0	0
38	B	44	0	76	4	0
38	B1	44	0	76	5	0
38	C	44	0	76	2	0
38	C1	44	0	76	4	0
38	J1	29	0	40	2	0
38	b	44	0	76	3	0
38	b1	44	0	76	5	0
38	c	44	0	76	0	0
38	c1	44	0	76	3	0
38	j1	29	0	40	3	0
39	B	6	0	8	0	0
39	I1	6	0	8	0	0
39	b	12	0	16	2	0
39	y	6	0	8	0	0
40	B1	43	0	44	5	0
40	C	242	0	322	24	0
40	C1	176	0	226	24	0
40	b1	43	0	44	1	0
40	c	242	0	322	25	0
40	c1	176	0	226	24	0
41	C	47	0	67	1	0
41	C1	47	0	67	9	0
41	D	132	0	183	10	0
41	D1	132	0	183	11	0
41	G	49	0	74	6	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
41	G1	49	0	74	3	0
41	L	49	0	74	3	0
41	L1	49	0	74	9	0
41	N	49	0	74	0	0
41	N1	49	0	74	4	0
41	S	45	0	63	8	0
41	S1	45	0	63	6	0
41	Y	49	0	74	4	0
41	Y1	49	0	74	7	0
41	c	47	0	67	4	0
41	c1	47	0	67	9	0
41	d	132	0	183	10	0
41	d1	132	0	183	11	0
41	g	49	0	74	7	0
41	g1	49	0	74	5	0
41	l	49	0	74	9	0
41	n	49	0	74	7	0
41	n1	49	0	74	4	0
41	s	45	0	63	7	0
41	s1	45	0	63	3	0
41	y	49	0	74	7	0
41	y1	49	0	74	7	0
42	C	40	0	0	0	0
42	C1	40	0	0	1	0
42	c	40	0	0	0	0
42	c1	40	0	0	0	0
43	D	4	0	1	0	0
43	D1	4	0	1	0	0
43	d	4	0	1	0	0
43	d1	4	0	1	0	0
44	D	55	0	80	6	0
44	D1	55	0	80	8	0
44	d	55	0	80	4	0
44	d1	55	0	80	6	0
45	F	43	0	30	2	0
45	F1	43	0	30	1	0
45	f	43	0	30	5	0
45	f1	43	0	30	0	0
46	H	41	0	56	26	0
46	H1	41	0	56	5	0
46	h	41	0	56	3	0
46	h1	41	0	56	9	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
47	G	324	0	274	16	0
47	G1	340	0	305	16	0
47	N	380	0	383	21	0
47	N1	380	0	383	17	0
47	R	94	0	66	4	0
47	R1	94	0	67	4	0
47	S	194	0	144	14	0
47	S1	194	0	145	10	0
47	Y	310	0	307	17	0
47	Y1	310	0	307	14	0
47	g	324	0	274	16	0
47	g1	340	0	305	20	0
47	n	380	0	382	28	0
47	n1	380	0	381	19	0
47	r	94	0	66	3	0
47	r1	94	0	66	3	0
47	s	194	0	144	10	0
47	s1	194	0	144	10	0
47	y	310	0	306	14	0
47	y1	310	0	307	18	0
48	G	84	0	110	16	0
48	G1	84	0	110	7	0
48	N	84	0	110	6	0
48	N1	84	0	110	11	0
48	R	42	0	55	5	0
48	R1	42	0	55	6	0
48	S	84	0	110	9	0
48	S1	84	0	110	11	0
48	Y	84	0	110	10	0
48	Y1	84	0	110	15	0
48	g	84	0	110	14	0
48	g1	84	0	110	10	0
48	n	84	0	110	11	0
48	n1	84	0	110	12	0
48	r	42	0	55	3	0
48	r1	42	0	55	6	0
48	s	84	0	110	14	0
48	s1	84	0	110	9	0
48	y	84	0	110	11	0
48	y1	84	0	110	11	0
49	G	44	0	56	7	0
49	G1	44	0	56	8	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
49	N	44	0	56	5	0
49	N1	44	0	56	8	0
49	R	44	0	56	3	0
49	R1	44	0	56	3	0
49	Y	44	0	56	3	0
49	Y1	44	0	56	9	0
49	g	44	0	56	6	0
49	g1	44	0	56	8	0
49	n	44	0	56	5	0
49	n1	44	0	56	8	0
49	r	44	0	56	6	0
49	r1	44	0	56	4	0
49	y	44	0	56	5	0
49	y1	44	0	56	9	0
50	G	44	0	54	3	0
50	G1	44	0	54	0	0
50	N	44	0	54	2	0
50	N1	44	0	54	4	0
50	R	44	0	54	3	0
50	R1	44	0	54	4	0
50	S	44	0	54	2	0
50	S1	44	0	54	4	0
50	Y	44	0	54	0	0
50	Y1	44	0	54	2	0
50	g	44	0	54	0	0
50	g1	44	0	54	1	0
50	n	44	0	54	3	0
50	n1	44	0	54	0	0
50	r	44	0	54	0	0
50	r1	44	0	54	1	0
50	s	44	0	54	2	0
50	s1	44	0	54	1	0
50	y	44	0	54	0	0
50	y1	44	0	54	1	0
51	S	30	0	43	2	0
51	S1	30	0	43	0	0
51	s	30	0	43	1	0
51	s1	30	0	43	2	0
52	B1	48	0	75	10	0
52	S	48	0	75	3	0
52	S1	48	0	75	2	0
52	T1	48	0	75	1	0

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Mol	Chain	Non-H	H(model)	H(added)	Clashes	Symm-Clashes
52	b1	48	0	75	6	0
52	i	48	0	75	1	0
52	s	48	0	75	1	0
52	s1	48	0	75	3	0
52	t1	48	0	75	4	0
53	A1	21	0	37	5	0
53	Y	21	0	37	3	0
53	Y1	21	0	37	3	0
53	a1	21	0	37	5	0
53	y	21	0	37	4	0
53	y1	21	0	37	7	0
54	I1	57	0	98	3	0
54	K1	57	0	98	6	0
54	i1	57	0	98	5	0
54	k1	57	0	98	3	0
55	R1	35	0	45	0	0
55	r1	35	0	46	3	0
56	R1	29	0	38	8	0
56	r1	29	0	38	5	0
57	Y1	69	0	90	7	0
57	y1	69	0	90	5	0
All	All	151508	0	153084	4168	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 14.

All (4168) 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)
8:H:57:PHE:CD2	8:H:57:PHE:CG	1.97	1.52
8:H:57:PHE:CG	8:H:57:PHE:CD1	1.96	1.49
56:r1:626:ERG:O1	56:r1:626:ERG:C3	1.70	1.37
56:R1:626:ERG:O1	56:R1:626:ERG:C3	1.70	1.36
24:y:76:LEU:CD1	31:y:602:CLA:H42	1.68	1.22
14:O1:140:LEU:HD22	14:O1:163:LEU:O	1.43	1.17
46:H:101:RRX:C21	46:H:101:RRX:C22	2.24	1.15
24:y1:76:LEU:HD13	31:y1:602:CLA:H42	1.28	1.11
24:y1:76:LEU:CD1	31:y1:602:CLA:H11	1.85	1.05
24:y1:76:LEU:CD1	31:y1:602:CLA:H42	1.88	1.04
24:y:76:LEU:HD12	31:y:602:CLA:H11	1.36	1.03
24:y1:76:LEU:HD12	31:y1:602:CLA:H11	1.33	1.03

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:O1:138:TYR:OH	17:W1:60:LEU:HA	1.57	1.03
24:y:76:LEU:HD13	31:y:602:CLA:H42	1.45	0.98
25:u1:89:GLN:N	25:u1:89:GLN:HE21	1.60	0.98
24:y1:76:LEU:HD12	31:y1:602:CLA:C1	1.95	0.97
14:O:109:MET:HE3	14:O:140:LEU:CD1	1.98	0.94
8:H:57:PHE:CE1	8:H:57:PHE:CZ	2.56	0.94
8:H:57:PHE:CZ	8:H:57:PHE:CE2	2.57	0.92
8:H:57:PHE:CD2	46:H:101:RRX:H25	2.04	0.92
1:a1:38:ILE:HG22	33:a1:411:BCR:H10C	1.51	0.92
4:C1:153:LEU:HD21	31:C1:506:CLA:HAB	1.52	0.91
2:B:278:GLY:O	2:B:282:GLN:HB2	1.71	0.90
31:b:609:CLA:HAB	5:d:123:ILE:HG23	1.52	0.90
22:r:195:VAL:HG23	31:r:609:CLA:HAB	1.52	0.90
8:H:57:PHE:CD1	8:H:57:PHE:CE1	2.61	0.89
31:b1:616:CLA:HAB	31:r1:609:CLA:H51	1.54	0.89
8:H:57:PHE:CE2	46:H:101:RRX:C21	2.56	0.88
8:H:57:PHE:CE2	46:H:101:RRX:H25	2.08	0.87
1:A1:333:GLU:O	1:A1:337:HIS:NE2	2.08	0.86
8:H:57:PHE:CD2	8:H:57:PHE:CE2	2.65	0.85
8:H:57:PHE:CD2	46:H:101:RRX:C21	2.60	0.85
8:H:57:PHE:CZ	46:H:101:RRX:C21	2.59	0.85
14:O:109:MET:HE3	14:O:140:LEU:HD12	1.57	0.83
8:H:57:PHE:CE1	46:H:101:RRX:C21	2.62	0.83
24:y1:76:LEU:HD13	31:y1:602:CLA:C4	2.06	0.82
4:c:153:LEU:HD21	31:c:506:CLA:HAB	1.60	0.82
14:o1:140:LEU:HD23	14:o1:163:LEU:CD2	2.09	0.82
24:y:76:LEU:HD13	31:y:602:CLA:C4	2.10	0.82
8:H:57:PHE:CD1	46:H:101:RRX:C21	2.63	0.81
8:H:57:PHE:CZ	46:H:101:RRX:C22	2.65	0.80
24:Y1:158:GLN:HE22	47:Y1:607:CHL:HMC	1.45	0.80
31:B:609:CLA:HAB	5:D:123:ILE:HG12	1.63	0.80
24:y:76:LEU:CD1	31:y:602:CLA:C4	2.57	0.80
21:G1:91:LEU:HB3	31:G1:604:CLA:HAB	1.62	0.80
2:B1:26:HIS:HD1	31:B1:613:CLA:HHB	1.48	0.79
8:H:57:PHE:CE2	46:H:101:RRX:C22	2.67	0.78
31:C1:513:CLA:H101	33:C1:514:BCR:H21C	1.66	0.78
2:B:247:TRP:HB2	31:B:609:CLA:HBC1	1.66	0.78
4:C1:304:THR:HG22	4:C1:308:ARG:HH21	1.48	0.78
1:A:30:ILE:O	1:A:34:GLY:HA3	1.84	0.78
8:H:57:PHE:CG	46:H:101:RRX:C21	2.67	0.78
1:a1:196:PRO:HA	1:a1:199:MET:HB2	1.66	0.78

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:c1:503:CLA:H172	31:c1:510:CLA:HBB2	1.65	0.78
8:H:57:PHE:CD1	46:H:101:RRX:C22	2.67	0.77
8:H:57:PHE:CE1	46:H:101:RRX:C22	2.67	0.77
14:o1:140:LEU:CD2	14:o1:163:LEU:HD23	2.15	0.77
26:M1:27:VAL:HG11	26:m1:24:ILE:HG23	1.67	0.76
24:y:76:LEU:HD12	31:y:602:CLA:H42	1.67	0.76
31:c1:505:CLA:H43	33:c1:515:BCR:HC7	1.68	0.76
1:a:47:VAL:HG21	1:a:114:LEU:HD22	1.66	0.76
2:b:247:TRP:HB2	31:b:609:CLA:HBC1	1.67	0.76
4:C:153:LEU:HD21	31:C:506:CLA:HAB	1.65	0.76
40:C1:519:DGD:HB72	35:C1:521:LMG:H401	1.68	0.76
14:O:109:MET:HE3	14:O:140:LEU:HD13	1.68	0.75
4:C:101:VAL:HG23	33:C:514:BCR:H313	1.68	0.75
8:H:57:PHE:CD2	46:H:101:RRX:C22	2.70	0.75
31:b:603:CLA:HBD	31:b:603:CLA:H2	1.68	0.75
21:G1:212:LEU:HD11	31:G1:603:CLA:HAB	1.69	0.75
24:Y1:76:LEU:CD1	31:Y1:602:CLA:H42	2.17	0.75
1:A1:141:PRO:HG3	4:C1:434:GLY:HA3	1.68	0.74
4:c:454:VAL:HG13	5:d:251:ARG:HE	1.49	0.74
31:c1:506:CLA:H43	33:c1:515:BCR:HC8	1.70	0.74
20:N1:119:GLU:HB3	20:N1:125:LYS:HE2	1.70	0.74
2:b1:160:GLY:HA3	2:b1:180:PRO:HB3	1.69	0.74
5:D:152:VAL:HG21	5:D:279:LEU:HD12	1.70	0.73
40:c:523:DGD:HBW1	31:y:614:CLA:HBC1	1.69	0.73
4:c1:167:ALA:HA	4:c1:172:GLY:HA2	1.70	0.73
20:N:203:LYS:HA	20:N:206:GLU:HG2	1.68	0.73
2:b1:9:HIS:HB3	31:b1:613:CLA:HAB	1.69	0.73
4:c1:58:PHE:HE1	11:k1:23:ASP:HA	1.53	0.73
8:H:57:PHE:CG	46:H:101:RRX:C22	2.72	0.73
31:g:602:CLA:H72	48:g:621:LUT:H28	1.69	0.73
31:A1:405:CLA:H122	32:A1:408:PHO:H3A	1.69	0.73
24:y1:172:GLY:HA2	31:y1:608:CLA:HAC1	1.71	0.72
4:c:166:LYS:HD2	31:c:502:CLA:H171	1.72	0.72
23:S1:102:ALA:HA	23:S1:210:LEU:HD11	1.69	0.72
24:Y:133:LYS:HD2	24:Y:135:GLY:H	1.55	0.72
2:B1:64:PRO:HB3	2:B1:267:LEU:HB3	1.70	0.72
14:O1:140:LEU:CD2	14:O1:163:LEU:O	2.33	0.72
31:n1:602:CLA:H52	48:n1:621:LUT:H28	1.71	0.72
2:b:271:THR:HA	2:b:448:ARG:HH22	1.52	0.72
21:G:41:LEU:O	21:G:44:PHE:HB2	1.89	0.71
23:S1:186:GLY:HA2	47:S1:608:CHL:HAC1	1.70	0.71

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:80:ILE:HD11	31:C:503:CLA:HED3	1.73	0.71
2:b1:247:TRP:HB2	31:b1:609:CLA:HBC1	1.73	0.71
41:n1:624:LHG:H202	49:g1:622:XAT:H12	1.72	0.71
1:A1:334:ARG:NH2	14:O1:212:ASP:O	2.23	0.71
31:C1:507:CLA:H142	33:C1:515:BCR:H16C	1.70	0.71
8:h1:50:MET:HE1	46:h1:101:RRX:H16	1.73	0.71
24:y1:76:LEU:HD13	31:y1:602:CLA:H11	1.71	0.71
27:r1:145:MET:SD	31:r1:610:CLA:HAB	2.31	0.71
31:C1:504:CLA:H72	40:C1:519:DGD:HBE2	1.71	0.71
1:a1:85:THR:HA	1:a1:109:GLY:HA3	1.72	0.71
31:b1:603:CLA:H12	31:b1:603:CLA:HBD	1.71	0.71
14:O:117:LYS:HZ3	14:O:126:GLU:H	1.36	0.71
5:D:325:ILE:O	5:D:329:MET:HB3	1.91	0.71
14:o:120:ASP:OD2	14:o:124:ARG:NH2	2.24	0.71
2:b:347:LYS:O	2:b:397:VAL:HA	1.91	0.70
31:C:513:CLA:H101	33:C:514:BCR:H21C	1.73	0.70
1:a:27:ARG:NH2	16:t:21:ILE:O	2.24	0.70
14:O:141:ASP:OD1	14:O:142:GLY:N	2.25	0.70
22:R:71:MET:HG3	22:R:73:PHE:HD2	1.57	0.70
23:S1:109:ARG:NH1	47:S1:608:CHL:OBD	2.25	0.70
23:s1:246:VAL:HG11	48:s1:621:LUT:H12	1.72	0.70
5:d:294:ARG:HG3	5:d:296:TYR:HB2	1.74	0.70
5:d1:103:ARG:HH21	6:e1:77:LYS:HA	1.56	0.70
2:B:160:GLY:HA3	2:B:180:PRO:HB3	1.73	0.70
4:c:320:GLN:NE2	4:c:321:GLY:O	2.25	0.70
33:c1:516:BCR:H10C	19:z1:20:VAL:HG11	1.73	0.70
14:o:120:ASP:OD2	14:o:124:ARG:CZ	2.39	0.70
41:c1:525:LHG:H251	31:s1:611:CLA:HAB	1.73	0.70
27:R1:194:LEU:HD22	50:R1:622:NEX:H15	1.74	0.69
4:c1:153:LEU:HD21	31:c1:506:CLA:HAB	1.74	0.69
8:H1:47:THR:HA	8:H1:50:MET:HG2	1.74	0.69
24:Y:82:THR:HA	24:Y:85:ARG:HG2	1.74	0.69
4:C1:234:LEU:HB3	53:Y1:625:SPH:H151	1.74	0.69
1:a1:64:ARG:HH21	14:o1:134:THR:HG22	1.58	0.69
1:a1:234:ASN:OD1	5:d1:263:ASN:ND2	2.26	0.69
5:d:37:LEU:HD13	5:d:125:PHE:HB2	1.75	0.69
1:A1:331:MET:HE2	5:D1:324:GLY:HA3	1.75	0.69
38:C1:524:DGA:HBT1	35:W1:201:LMG:H372	1.74	0.69
23:s1:93:ASP:OD1	23:s1:96:GLN:NE2	2.25	0.69
20:N1:49:LEU:HB2	20:N1:53:SER:HB3	1.74	0.69
24:y:172:GLY:HA2	31:y:608:CLA:HAC1	1.75	0.69

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:G:34:GLY:O	21:G:37:ARG:HB2	1.93	0.68
31:y1:602:CLA:H72	48:y1:621:LUT:H30	1.75	0.68
25:u1:89:GLN:N	25:u1:89:GLN:NE2	2.39	0.68
31:B:606:CLA:HBB1	31:B:607:CLA:H51	1.74	0.68
22:r:147:GLY:HA3	49:r:622:XAT:H193	1.74	0.68
2:B1:11:VAL:HG13	2:B1:12:VAL:HG13	1.74	0.68
14:O:216:ARG:H	14:O:222:TYR:HB2	1.58	0.68
30:a:404:CL:CL	4:c:342:GLU:N	2.64	0.68
4:C1:145:MET:HE1	31:C1:507:CLA:HAC1	1.75	0.68
31:c1:513:CLA:H101	33:c1:514:BCR:H21C	1.74	0.68
5:d:122:LEU:HD22	5:d:150:ILE:HG22	1.75	0.68
21:g:41:LEU:HB3	21:g:44:PHE:HB2	1.76	0.68
4:C1:74:LEU:HD13	4:C1:77:LEU:HD12	1.76	0.68
4:c1:423:PHE:HE1	40:c1:518:DGD:HBH2	1.57	0.68
47:N:605:CHL:H101	31:S:612:CLA:HBB1	1.76	0.68
23:S:175:LEU:HD22	50:S:622:NEX:H35	1.76	0.68
31:S:613:CLA:HAB	41:S:624:LHG:H301	1.73	0.68
5:D1:148:ALA:HB1	5:D1:279:LEU:HB2	1.74	0.68
2:B:382:PRO:HA	5:D:345:VAL:HG12	1.76	0.67
8:H:60:PHE:HB2	46:H:101:RRX:H33	1.75	0.67
2:B1:364:GLU:OE2	5:D1:294:ARG:NH1	2.27	0.67
23:S:237:LYS:HE2	41:S:624:LHG:HC62	1.75	0.67
4:C:282:ASN:H	40:C:518:DGD:HE61	1.58	0.67
24:Y:102:LEU:HB2	48:Y:620:LUT:H35	1.76	0.67
23:s:107:HIS:CE1	48:s:621:LUT:H15	2.30	0.67
31:G1:602:CLA:H52	48:G1:621:LUT:H28	1.74	0.67
1:a1:37:MET:HE3	1:a1:125:CYS:HB2	1.77	0.67
31:b1:604:CLA:HAB	31:b1:606:CLA:H152	1.76	0.67
21:G:76:ALA:HA	21:G:79:ARG:HE	1.59	0.67
31:y1:603:CLA:HMA1	31:y1:603:CLA:H2	1.76	0.67
2:b:296:LEU:HD12	2:b:300:GLU:HG3	1.76	0.67
8:h:66:GLU:HG2	8:h:72:LEU:HB2	1.76	0.67
1:a:84:PRO:HD3	1:a:173:PRO:HB3	1.75	0.67
1:a:258:LEU:O	5:d:128:ARG:NH2	2.28	0.67
14:O1:138:TYR:HH	17:W1:60:LEU:HA	1.58	0.67
27:r1:69:GLY:H	27:r1:237:THR:HG22	1.59	0.67
20:n:222:VAL:HG21	31:n:613:CLA:HAC2	1.75	0.67
23:s:219:LEU:HD13	48:s:620:LUT:H24	1.76	0.67
1:a1:36:ILE:O	1:a1:40:THR:OG1	2.13	0.67
1:a1:82:VAL:HB	1:a1:174:LEU:HB2	1.77	0.67
2:b1:4:PRO:HD2	2:b1:7:ARG:HB2	1.77	0.67

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:213:VAL:HG11	4:c:280:PHE:HB2	1.75	0.67
31:Y1:602:CLA:H52	48:Y1:621:LUT:H28	1.76	0.67
31:r1:608:CLA:HBB1	31:r1:608:CLA:H8	1.76	0.67
31:b:616:CLA:H2	31:b:617:CLA:HBB2	1.75	0.67
24:y:76:LEU:CD1	31:y:602:CLA:H11	2.18	0.67
23:S:149:LEU:HD22	31:S:604:CLA:HED1	1.77	0.66
31:B1:608:CLA:H2	35:B1:622:LMG:H151	1.77	0.66
2:b1:330:MET:HG2	2:b1:444:ARG:HB2	1.77	0.66
4:C:203:LYS:HD3	4:C:209:ASP:HB3	1.76	0.66
4:c:244:PRO:O	4:c:249:ARG:NH2	2.29	0.66
1:A1:237:TYR:HB2	5:D1:265:ARG:HD3	1.77	0.66
1:A1:245:THR:OG1	5:D1:265:ARG:NH1	2.27	0.66
1:A1:274:PHE:HA	1:A1:277:VAL:HG12	1.77	0.66
15:p:174:ALA:HB3	15:p:186:LYS:HB2	1.76	0.66
31:Y1:613:CLA:H72	31:Y1:614:CLA:HMD3	1.76	0.66
1:a1:136:ARG:NH2	9:i1:27:ASP:OD1	2.28	0.66
21:g:75:PHE:HB3	21:g:79:ARG:HH21	1.60	0.66
5:d1:350:ASN:ND2	15:p1:195:ASP:OD1	2.28	0.66
31:C:505:CLA:HBB1	31:C:505:CLA:H71	1.76	0.66
24:Y:58:PRO:HD2	24:Y:61:LEU:HD12	1.77	0.66
8:h:41:LEU:HD12	8:h:42:PRO:HD2	1.78	0.66
31:Y1:603:CLA:HMA1	31:Y1:603:CLA:H2	1.78	0.66
15:P:187:PHE:HB2	15:P:205:VAL:HB	1.78	0.66
21:g:122:ILE:HG21	47:g:606:CHL:HBC1	1.77	0.66
24:Y1:76:LEU:HD12	31:Y1:602:CLA:H42	1.76	0.66
4:c1:166:LYS:HA	4:c1:170:PHE:HB2	1.78	0.66
5:d:68:ILE:HG23	5:d:69:GLU:HG3	1.76	0.65
33:A1:411:BCR:H19C	34:b1:626:SQD:H191	1.76	0.65
2:B1:160:GLY:HA3	2:B1:180:PRO:HB3	1.79	0.65
31:B:616:CLA:H2	31:B:617:CLA:HBB2	1.78	0.65
14:O:239:ARG:O	14:O:243:LYS:NZ	2.29	0.65
15:p:189:ILE:HB	15:p:203:GLN:HB2	1.78	0.65
20:n:52:TYR:HB3	21:g:162:ASN:HD21	1.61	0.65
15:P1:112:ALA:O	15:P1:115:ASN:ND2	2.30	0.65
24:y1:93:HIS:HD2	48:y1:621:LUT:H15	1.62	0.65
4:c:152:HIS:HA	4:c:155:ILE:HD12	1.79	0.65
53:A1:414:SPH:H4	9:I1:4:LEU:HD11	1.77	0.65
17:W1:86:ALA:HB1	35:W1:201:LMG:H361	1.78	0.65
2:b1:156:PHE:HB3	2:b1:162:PHE:HB2	1.78	0.65
5:d1:188:PHE:O	5:d1:294:ARG:NH1	2.30	0.65
31:n1:603:CLA:HAC1	47:n1:607:CHL:HBB2	1.79	0.65

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:298:ASN:HB2	4:C1:391:SER:HA	1.78	0.65
21:G:216:VAL:HG21	31:G:613:CLA:HAC2	1.77	0.65
31:A1:410:CLA:H2	9:I1:12:VAL:HG11	1.79	0.65
14:o1:171:LYS:HE3	14:o1:175:GLY:HA2	1.79	0.65
20:N:153:THR:HG22	47:N:605:CHL:HAC1	1.79	0.65
7:f:30:ILE:HG13	45:f:101:HEM:HAC	1.78	0.65
35:A1:413:LMG:H191	31:C1:505:CLA:H8	1.78	0.65
1:a1:126:TYR:HA	1:a1:129:ARG:HG2	1.77	0.65
31:A:406:CLA:HED2	5:D:198:MET:HE2	1.79	0.65
21:G:79:ARG:HA	21:G:82:GLU:HG2	1.79	0.65
20:n:161:MET:HA	20:n:164:VAL:HG12	1.78	0.65
20:n:226:VAL:HG23	20:n:227:THR:HG23	1.79	0.65
22:r:134:ARG:HH21	31:r:602:CLA:HED1	1.62	0.65
4:C1:253:VAL:HG21	4:C1:437:ARG:HG2	1.77	0.65
5:d:93:TRP:HB2	18:x:71:ASN:HB3	1.79	0.65
1:A1:230:ASN:ND2	27:R1:95:ASN:OD1	2.29	0.65
4:C:264:LEU:HD21	31:C:508:CLA:HAB	1.77	0.65
22:R:252:GLY:O	22:R:256:GLN:NE2	2.29	0.65
24:Y:109:LEU:HD21	24:Y:234:ILE:HG13	1.77	0.65
24:Y:185:PRO:HB3	31:Y:608:CLA:HBC2	1.78	0.65
24:Y1:172:GLY:HA2	31:Y1:608:CLA:HAC1	1.78	0.65
41:G1:624:LHG:H301	41:G1:624:LHG:H112	1.79	0.64
31:A:405:CLA:H112	31:A:406:CLA:HBB1	1.78	0.64
35:C:521:LMG:H151	35:J:101:LMG:H172	1.79	0.64
1:a:143:ILE:HG12	5:d:220:ASN:HD22	1.61	0.64
20:n:168:ARG:HH12	47:n:609:CHL:HED3	1.62	0.64
1:A1:137:LEU:HD12	5:D1:252:PHE:HE1	1.62	0.64
2:b1:320:ALA:HB1	5:d1:292:ASN:HB2	1.79	0.64
3:v1:8:GLN:HE22	11:k1:23:ASP:HB2	1.61	0.64
14:o:109:MET:SD	14:o:140:LEU:HD12	2.37	0.64
4:C1:295:PRO:HB2	4:C1:349:PHE:HB2	1.79	0.64
1:A:140:ARG:HH22	41:D:410:LHG:HC41	1.62	0.64
2:b:358:ARG:HD3	25:u:102:LYS:HE3	1.78	0.64
2:b1:296:LEU:HD12	2:b1:300:GLU:HG3	1.78	0.64
2:b1:371:ILE:HB	25:u1:100:PRO:HB3	1.80	0.64
31:n1:611:CLA:HAB	49:g1:622:XAT:H221	1.79	0.64
40:C:519:DGD:HB51	35:C:521:LMG:H381	1.79	0.64
22:R:149:LEU:HD11	48:R:620:LUT:H35	1.77	0.64
1:a1:333:GLU:HB3	1:a1:336:ALA:HB3	1.79	0.64
1:A:89:ILE:HD13	14:O:135:ARG:HH12	1.63	0.64
2:B:74:SER:HB3	2:B:93:TYR:HD2	1.62	0.64

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:S1:602:CLA:H72	48:S1:621:LUT:H28	1.78	0.64
33:c1:516:BCR:H21C	11:k1:34:LEU:HB3	1.78	0.64
5:d1:29:PHE:O	5:d1:128:ARG:NH1	2.31	0.64
14:o1:107:PHE:HB3	14:o1:143:MET:HB2	1.80	0.64
56:r1:626:ERG:O1	56:r1:626:ERG:C2	2.40	0.64
5:d:188:PHE:O	5:d:294:ARG:NH1	2.31	0.64
2:B1:384:ARG:HH12	5:D1:348:ARG:HD3	1.61	0.64
41:S1:624:LHG:H121	41:S1:624:LHG:H281	1.78	0.64
30:A:404:CL:CL	4:C:342:GLU:N	2.58	0.64
13:M:28:LYS:HE2	13:m:28:LYS:HE3	1.80	0.64
1:a:290:ILE:HG13	31:a:405:CLA:HED3	1.80	0.64
14:o:216:ARG:HA	14:o:222:TYR:H	1.62	0.64
14:o:238:GLN:NE2	14:o:281:GLY:O	2.31	0.64
31:B1:609:CLA:H151	31:B1:610:CLA:H172	1.78	0.64
31:N1:604:CLA:H121	50:N1:623:NEX:H402	1.79	0.64
27:R1:176:LEU:O	24:y1:142:ASN:ND2	2.31	0.64
6:e1:66:ILE:O	6:e1:75:GLN:NE2	2.30	0.64
31:R:609:CLA:H12	31:R:609:CLA:H3A	1.80	0.64
4:c:395:VAL:HG12	4:c:396:GLY:H	1.61	0.64
47:n:601:CHL:H111	41:n:624:LHG:H212	1.79	0.64
47:n:605:CHL:H152	31:s:605:CLA:HBA2	1.79	0.64
2:B1:30:VAL:HG12	31:B1:606:CLA:HHD	1.80	0.64
1:a:64:ARG:HH12	14:o:134:THR:HG23	1.63	0.64
2:b:160:GLY:HA3	2:b:180:PRO:HB3	1.79	0.64
4:c:414:LEU:O	4:c:418:HIS:ND1	2.31	0.64
2:B1:103:LEU:HB2	31:B1:607:CLA:H71	1.79	0.64
4:C1:200:TYR:HB3	4:C1:212:ILE:HG22	1.80	0.63
27:R1:213:TYR:HB3	31:R1:610:CLA:HED3	1.81	0.63
31:r1:603:CLA:HBB1	49:r1:621:XAT:H203	1.80	0.63
4:C:395:VAL:HG12	4:C:396:GLY:H	1.62	0.63
20:n:247:ALA:HB3	49:g:622:XAT:H193	1.79	0.63
31:b1:613:CLA:H171	31:b1:614:CLA:HBB2	1.79	0.63
9:I:13:THR:HG21	17:W:85:ILE:HG12	1.79	0.63
28:a:401:OEX:O2	4:c:345:ARG:NH2	2.31	0.63
1:A1:316:THR:HG22	5:D1:64:ALA:HB3	1.81	0.63
4:C1:435:ARG:NH2	31:C1:508:CLA:O1D	2.31	0.63
14:o1:164:ASP:HB2	14:o1:185:LYS:HB3	1.78	0.63
21:g1:130:TYR:HB3	21:g1:136:LEU:HD13	1.80	0.63
1:A:40:THR:HG23	31:A:410:CLA:HBB1	1.80	0.63
4:C1:221:ILE:O	4:C1:225:HIS:ND1	2.32	0.63
32:a1:409:PHO:H3A	31:d1:402:CLA:H121	1.80	0.63

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:p:179:LYS:HG3	15:p:180:LYS:HG3	1.80	0.63
33:C1:516:BCR:HC7	33:C1:517:BCR:H353	1.81	0.63
1:a1:181:ASN:HB2	5:d1:314:PHE:HB3	1.80	0.63
31:G1:611:CLA:HAB	49:Y1:622:XAT:H221	1.81	0.63
33:c1:514:BCR:H281	41:c1:525:LHG:H101	1.81	0.63
2:B1:338:VAL:HB	2:B1:431:GLU:HG3	1.81	0.63
3:V1:3:LEU:HA	3:V1:6:ILE:HD12	1.81	0.63
2:b1:75:TRP:NE1	2:b1:89:GLY:O	2.31	0.63
24:y1:98:LEU:HD13	31:y1:610:CLA:HAB	1.81	0.63
24:Y:61:LEU:HD13	24:Y:70:GLY:HA2	1.80	0.63
14:o:265:GLU:HG2	14:o:297:GLN:HG3	1.81	0.63
40:C1:520:DGD:HA82	40:C1:520:DGD:HBW2	1.79	0.63
14:O1:107:PHE:HB3	14:O1:143:MET:HB2	1.80	0.63
4:c1:14:ARG:O	4:c1:29:ARG:NH1	2.32	0.63
2:b:25:MET:HE3	33:b:618:BCR:H23C	1.79	0.62
31:B1:613:CLA:H171	31:B1:614:CLA:HBB2	1.80	0.62
31:a1:405:CLA:H112	31:a1:406:CLA:HBB1	1.81	0.62
4:c1:461:ASP:OD2	16:t1:24:ARG:NH2	2.32	0.62
41:c1:525:LHG:H142	34:c1:526:SQD:H322	1.81	0.62
21:G:91:LEU:HB3	31:G:604:CLA:HAB	1.81	0.62
31:n:603:CLA:H91	47:n:609:CHL:H142	1.81	0.62
1:A:82:VAL:HB	1:A:174:LEU:HB2	1.81	0.62
23:S:186:GLY:HA2	47:S:608:CHL:HAC1	1.81	0.62
20:n:94:ARG:HA	20:n:97:LEU:HD12	1.81	0.62
21:g:229:LEU:HD22	48:g:620:LUT:H172	1.79	0.62
31:C1:506:CLA:HBA2	31:C1:507:CLA:H202	1.81	0.62
5:d:47:GLY:HA2	33:d:404:BCR:H332	1.81	0.62
4:C1:390:GLY:HA3	4:C1:408:VAL:HG22	1.81	0.62
33:C1:516:BCR:H15C	11:K1:35:LEU:HD21	1.81	0.62
15:P1:174:ALA:HB3	15:P1:186:LYS:HB3	1.80	0.62
2:b1:37:MET:O	2:b1:41:GLU:N	2.26	0.62
5:d1:126:MET:HE2	5:d1:143:ALA:HB1	1.80	0.62
54:i1:101:4RF:H38	54:i1:101:4RF:H54	1.81	0.62
31:g1:611:CLA:HAB	49:y1:622:XAT:H221	1.81	0.62
4:C:437:ARG:NH2	9:I:27:ASP:OD2	2.32	0.62
1:a:51:ALA:O	1:a:55:ALA:HB2	1.99	0.62
1:A1:170:ASP:OD2	4:C1:345:ARG:NH1	2.33	0.62
2:B1:30:VAL:HG13	31:B1:614:CLA:HMC2	1.82	0.62
20:N1:75:LEU:HD11	31:N1:602:CLA:H42	1.81	0.62
31:c1:513:CLA:H142	41:c1:525:LHG:H132	1.81	0.62
2:B:70:GLY:HA2	2:B:178:VAL:HG11	1.79	0.62

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:305:ALA:O	14:O:216:ARG:NH2	2.32	0.62
31:R:602:CLA:HAB	49:R:621:XAT:H30	1.81	0.62
24:y:105:ILE:HG23	24:y:234:ILE:HD11	1.81	0.62
2:b1:142:HIS:ND1	31:b1:611:CLA:OBD	2.33	0.62
5:d1:47:GLY:HA2	33:d1:404:BCR:H332	1.82	0.62
5:d1:72:ASN:HB3	35:d1:411:LMG:HC3	1.80	0.62
23:S:93:ASP:OD1	23:S:94:GLU:N	2.32	0.62
23:S:234:LYS:HD3	31:S:612:CLA:HBD	1.81	0.62
15:P1:189:ILE:HB	15:P1:203:GLN:HB2	1.81	0.62
8:h1:28:THR:HA	8:h1:31:ARG:HG2	1.80	0.62
38:B:625:DGA:HA52	5:D:127:LEU:HD22	1.81	0.62
56:R1:626:ERG:O1	56:R1:626:ERG:C2	2.41	0.62
4:c1:227:TRP:HH2	31:y1:614:CLA:HAB	1.63	0.62
2:B:9:HIS:ND1	31:B:612:CLA:O1A	2.32	0.62
31:B:603:CLA:HAC1	8:H:57:PHE:HE1	1.63	0.62
41:c:625:LHG:H241	31:s:611:CLA:HAB	1.81	0.62
31:s1:604:CLA:H62	50:s1:623:NEX:H373	1.82	0.62
20:N:49:LEU:HB2	20:N:53:SER:HB3	1.80	0.62
31:Y:602:CLA:H72	48:Y:621:LUT:H30	1.81	0.62
31:B1:603:CLA:H152	35:H1:102:LMG:H341	1.82	0.62
21:G1:223:LYS:HD3	21:G1:227:GLN:HE22	1.65	0.62
1:a1:194:MET:HG3	1:a1:300:PHE:HB2	1.79	0.62
31:a1:405:CLA:H102	32:a1:408:PHO:HAA1	1.82	0.62
27:r1:152:ILE:HG23	27:r1:265:LEU:HD21	1.82	0.62
5:d:125:PHE:HE1	5:d:128:ARG:HH21	1.47	0.61
14:o:263:THR:HG23	14:o:265:GLU:HG3	1.82	0.61
1:A1:129:ARG:NH2	5:D1:255:GLN:O	2.33	0.61
1:a1:274:PHE:HA	1:a1:277:VAL:HG12	1.82	0.61
31:C:501:CLA:H193	31:C:507:CLA:HBB1	1.83	0.61
4:c:281:ASN:O	4:c:411:ARG:NH1	2.32	0.61
15:p:87:LEU:HD11	15:p:104:LEU:HD21	1.82	0.61
31:B1:615:CLA:H2	34:B1:621:SQD:H262	1.82	0.61
1:a:43:THR:HG23	33:a:411:BCR:H16C	1.82	0.61
1:a:303:ASN:O	4:c:403:ASN:ND2	2.33	0.61
31:a:406:CLA:HBA1	41:l:101:LHG:H221	1.80	0.61
2:b:242:ILE:HG23	2:b:462:PHE:HD2	1.65	0.61
14:O1:133:LEU:HD22	14:O1:169:THR:HB	1.83	0.61
15:P1:171:LEU:HB3	15:P1:188:GLU:HB3	1.82	0.61
2:B:73:GLN:NE2	2:B:85:SER:OG	2.34	0.61
2:b:27:THR:HG23	31:b:606:CLA:HAC1	1.82	0.61
31:g:603:CLA:H122	47:g:609:CHL:H102	1.82	0.61

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:416:THR:HA	2:B1:419:LYS:HE2	1.83	0.61
1:a1:328:MET:HE1	5:d1:183:LEU:HD22	1.82	0.61
53:a1:414:SPH:H91	54:i1:101:4RF:H40	1.81	0.61
31:b1:609:CLA:H2	38:b1:625:DGA:HB81	1.82	0.61
23:s1:108:ALA:HB1	23:s1:239:GLY:HA3	1.82	0.61
2:B:25:MET:HE3	33:B:618:BCR:H23C	1.82	0.61
31:c:504:CLA:H2	40:c:519:DGD:HB32	1.81	0.61
23:S1:264:ILE:HD13	48:S1:620:LUT:H163	1.81	0.61
31:Y1:602:CLA:H72	48:Y1:621:LUT:H30	1.82	0.61
5:D:323:GLU:HA	5:D:326:ARG:HD3	1.82	0.61
4:C1:413:TRP:HZ3	31:C1:504:CLA:H2	1.65	0.61
1:a1:211:PHE:HA	1:a1:214:MET:HG3	1.82	0.61
35:c1:521:LMG:H352	11:k1:30:VAL:HG21	1.82	0.61
21:g1:91:LEU:HB3	31:g1:604:CLA:HAB	1.83	0.61
3:v:4:THR:HG23	11:k:20:PRO:HG3	1.83	0.61
2:b1:220:ARG:HB2	8:h1:41:LEU:HG	1.80	0.61
2:B:364:GLU:N	5:D:326:ARG:HH22	1.98	0.61
2:B1:311:PHE:O	2:B1:317:ASN:ND2	2.34	0.61
31:C1:505:CLA:H172	40:C1:518:DGD:HA71	1.83	0.61
31:b1:609:CLA:HAB	5:d1:123:ILE:HD12	1.82	0.61
4:C:74:LEU:HD13	4:C:77:LEU:HD12	1.80	0.61
14:O:211:LEU:HD21	14:O:220:THR:HG23	1.82	0.61
20:N:247:ALA:HB1	49:G:622:XAT:H161	1.83	0.61
23:s:194:PRO:HB2	23:s:218:PRO:HB3	1.82	0.61
56:R1:626:ERG:O1	56:R1:626:ERG:C4	2.43	0.61
1:a1:234:ASN:ND2	41:d1:409:LHG:O2	2.34	0.61
2:b1:458:PHE:HE2	31:b1:608:CLA:HBB2	1.66	0.61
14:o1:140:LEU:HD21	14:o1:166:ALA:HB2	1.83	0.61
31:g1:613:CLA:H112	49:y1:622:XAT:H34	1.82	0.60
15:P:171:LEU:HB2	15:P:188:GLU:HG2	1.83	0.60
1:a:196:PRO:HB3	40:c:520:DGD:HA81	1.83	0.60
23:s:49:LEU:HD11	23:s:226:GLU:HA	1.84	0.60
24:y:108:GLU:HG3	24:y:234:ILE:HD12	1.82	0.60
14:O1:79:GLY:HA3	17:W1:66:ASN:HD21	1.65	0.60
4:c1:27:ASN:HB2	31:c1:508:CLA:H3A	1.82	0.60
31:A:410:CLA:HAB	9:I:15:PHE:CD2	2.36	0.60
47:G:601:CHL:HED3	41:G:630:LHG:H142	1.81	0.60
4:C1:101:VAL:HG13	33:C1:514:BCR:H313	1.83	0.60
31:Y1:610:CLA:H52	48:Y1:620:LUT:H30	1.81	0.60
2:b1:28:ALA:HB2	2:b1:107:LEU:HB2	1.83	0.60
31:b1:602:CLA:H162	46:h1:101:RRX:H42	1.83	0.60

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c1:390:GLY:HA3	4:c1:408:VAL:HG22	1.82	0.60
5:D:192:THR:HG23	31:D:402:CLA:HBC2	1.83	0.60
31:G:602:CLA:H52	48:G:621:LUT:H28	1.82	0.60
2:B1:223:ILE:HD12	27:R1:85:LEU:HD11	1.83	0.60
2:B1:321:LYS:NZ	2:B1:363:PHE:O	2.35	0.60
4:C1:147:ASN:O	4:C1:151:TYR:N	2.31	0.60
23:S1:247:LEU:HD11	31:S1:603:CLA:HBC1	1.84	0.60
4:C:152:HIS:ND1	31:C:507:CLA:OBD	2.33	0.60
7:F:42:ILE:HG12	15:P:65:VAL:HG22	1.84	0.60
21:g:41:LEU:HB2	21:g:45:SER:HB2	1.82	0.60
7:F1:33:LEU:HD13	7:F1:36:ILE:HD11	1.82	0.60
8:H1:69:ASN:ND2	35:H1:102:LMG:O10	2.35	0.60
1:A:107:TYR:HB2	14:O:133:LEU:HD12	1.82	0.60
31:B:617:CLA:H2	50:R:622:NEX:H42	1.83	0.60
14:O:183:THR:HG21	14:O:203:PRO:HD2	1.82	0.60
5:d:85:LEU:O	6:e:69:ARG:NH1	2.35	0.60
2:B1:157:HIS:HA	2:B1:163:GLY:HA3	1.83	0.60
2:B1:357:ARG:NH1	2:B1:358:ARG:O	2.35	0.60
31:C1:504:CLA:H172	31:C1:508:CLA:H13	1.83	0.60
2:b1:119:ASP:OD1	2:b1:124:ARG:NH2	2.35	0.60
23:s1:194:PRO:HB2	23:s1:218:PRO:HB3	1.82	0.60
20:N:247:ALA:HB3	49:G:622:XAT:H193	1.82	0.60
23:S:264:ILE:HD12	48:S:620:LUT:H163	1.84	0.60
2:B1:319:PRO:HG3	2:B1:448:ARG:HD2	1.83	0.60
31:R1:610:CLA:H52	48:R1:620:LUT:H30	1.84	0.60
4:C:27:ASN:HB3	31:C:509:CLA:HAB	1.83	0.60
31:b:609:CLA:HBA1	38:b:623:DGA:HB52	1.83	0.60
14:o:108:CYS:HB2	14:o:295:TYR:HB3	1.84	0.60
31:r1:602:CLA:H52	49:r1:621:XAT:H28	1.84	0.60
1:A:36:ILE:O	1:A:40:THR:OG1	2.13	0.60
1:A1:82:VAL:HB	1:A1:174:LEU:HB2	1.84	0.60
5:D1:79:SER:HA	5:D1:172:SER:HB3	1.83	0.60
2:b1:37:MET:HB3	2:b1:41:GLU:HG3	1.83	0.60
2:b1:394:GLN:HB3	15:p1:147:ARG:HH21	1.67	0.60
14:o1:140:LEU:HD22	14:o1:163:LEU:HD23	1.81	0.60
31:n1:610:CLA:HBB2	48:n1:620:LUT:H34	1.84	0.60
14:O1:171:LYS:HE3	14:O1:175:GLY:HA2	1.82	0.60
2:B:137:LYS:NZ	2:B:217:LEU:O	2.35	0.59
4:c:101:VAL:HG23	33:c:514:BCR:H313	1.83	0.59
31:y:604:CLA:H43	47:y:606:CHL:HAA2	1.83	0.59
1:A1:303:ASN:O	4:C1:403:ASN:ND2	2.35	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:312:ARG:NH1	15:P1:91:TRP:O	2.34	0.59
31:c1:508:CLA:H151	31:c1:510:CLA:H152	1.83	0.59
15:p1:105:ARG:HG3	15:p1:117:TYR:HB3	1.84	0.59
20:n1:222:VAL:HG11	31:n1:613:CLA:HAC2	1.84	0.59
2:B:371:ILE:HG22	2:B:377:VAL:HA	1.84	0.59
5:D:307:GLU:O	14:O:239:ARG:NH1	2.35	0.59
45:F:101:HEM:HBC2	45:F:101:HEM:HHD	1.85	0.59
4:c:244:PRO:HA	31:c:506:CLA:HED1	1.85	0.59
2:b1:36:ALA:HB1	52:b1:624:3PH:H2C1	1.84	0.59
31:g1:603:CLA:HAC1	47:g1:607:CHL:HBB2	1.83	0.59
14:o:109:MET:HB3	14:o:140:LEU:HB2	1.84	0.59
4:C1:323:THR:OG1	14:O1:206:ARG:NH1	2.35	0.59
27:R1:69:GLY:H	27:R1:237:THR:HG22	1.66	0.59
14:O:208:SER:HB3	15:P:154:THR:HG21	1.85	0.59
21:G:114:VAL:HB	21:G:117:LYS:HB2	1.84	0.59
1:a:220:THR:O	5:d:139:ARG:NH2	2.33	0.59
4:c:460:LEU:HD21	5:d:255:GLN:HG2	1.84	0.59
21:g:98:THR:HG21	31:g:604:CLA:HAC2	1.84	0.59
21:g:211:CYS:HB3	48:g:621:LUT:H12	1.83	0.59
24:y:98:LEU:HD13	31:y:610:CLA:HAB	1.84	0.59
24:y:184:TYR:HB3	31:y:610:CLA:HED3	1.85	0.59
33:B1:619:BCR:HC42	35:B1:622:LMG:H341	1.84	0.59
1:a1:315:ASN:OD1	15:p1:109:ASN:ND2	2.32	0.59
4:c1:120:HIS:HA	4:c1:124:GLY:HA3	1.85	0.59
4:c1:274:ALA:HB2	31:c1:501:CLA:H42	1.83	0.59
52:t1:101:3PH:H382	52:t1:101:3PH:H2D2	1.84	0.59
56:r1:626:ERG:O1	56:r1:626:ERG:C4	2.41	0.59
41:D:408:LHG:H382	41:D:408:LHG:HC91	1.84	0.59
2:b:341:LEU:HD21	2:b:431:GLU:HG3	1.84	0.59
4:c:200:TYR:HA	4:c:203:LYS:HE2	1.83	0.59
20:n:130:ILE:HG12	20:n:150:ILE:HB	1.84	0.59
2:B1:146:ALA:HB2	31:B1:611:CLA:H92	1.85	0.59
2:B1:258:TYR:HE2	35:H1:102:LMG:HC91	1.68	0.59
35:C1:521:LMG:H341	35:C1:521:LMG:H242	1.83	0.59
54:K1:101:4RF:H24	54:K1:101:4RF:H92	1.84	0.59
31:g1:602:CLA:H72	48:g1:621:LUT:H28	1.84	0.59
41:D:409:LHG:O9	12:L:20:TRP:NE1	2.35	0.59
21:G:65:THR:OG1	48:G:621:LUT:O23	2.20	0.59
22:R:222:ASN:ND2	22:R:225:ASP:OD2	2.36	0.59
31:a:406:CLA:H141	44:d:405:PL9:H471	1.84	0.59
33:c:515:BCR:H312	9:i:23:PHE:HB3	1.85	0.59

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:o:157:PHE:HB3	14:o:189:GLY:HA3	1.84	0.59
20:n:247:ALA:HB1	49:g:622:XAT:H161	1.84	0.59
33:c1:516:BCR:H17C	11:k1:35:LEU:HB2	1.84	0.59
40:c1:520:DGD:O1A	5:d1:72:ASN:ND2	2.35	0.59
20:n1:119:GLU:OE2	20:n1:132:GLN:NE2	2.36	0.59
47:n1:609:CHL:HAA2	24:y1:73:THR:HG21	1.84	0.59
31:r1:603:CLA:H111	55:r1:625:LMT:H32	1.83	0.59
4:C:13:GLY:O	11:K:46:ARG:NH2	2.36	0.59
12:L:5:ASN:HB3	12:L:8:LYS:HG3	1.83	0.59
14:o:133:LEU:HD11	14:o:171:LYS:HE2	1.83	0.59
2:B1:247:TRP:HB2	31:B1:609:CLA:HBC1	1.84	0.59
35:B1:622:LMG:HC5	52:B1:624:3PH:H11	1.84	0.59
2:b1:22:VAL:O	2:b1:26:HIS:ND1	2.34	0.59
4:c1:166:LYS:HG2	31:c1:502:CLA:H192	1.85	0.59
20:n1:94:ARG:HA	20:n1:97:LEU:HD12	1.82	0.59
2:B:277:GLN:HB3	25:U:106:VAL:HG23	1.83	0.59
2:B:327:THR:HB	35:B:622:LMG:HC8	1.84	0.59
1:a:59:ASP:OD2	1:a:65:GLU:N	2.34	0.59
4:C1:33:LEU:HD11	4:C1:126:GLU:HB3	1.85	0.59
23:S1:237:LYS:NZ	41:S1:624:LHG:O5	2.36	0.59
1:a1:54:ALA:HB2	1:a1:72:LEU:HD12	1.85	0.59
2:b1:338:VAL:HB	2:b1:431:GLU:HG3	1.83	0.59
31:y1:613:CLA:H193	31:y1:614:CLA:HAA1	1.84	0.59
14:O:267:ALA:HB2	14:O:295:TYR:HD1	1.67	0.59
35:a:413:LMG:H411	31:c:505:CLA:H143	1.85	0.59
31:n:603:CLA:H101	31:y:603:CLA:H92	1.82	0.59
31:C1:501:CLA:H171	31:C1:507:CLA:H111	1.85	0.59
5:D1:252:PHE:O	5:D1:256:ILE:N	2.29	0.59
26:M1:31:ALA:HB2	26:m1:28:LYS:HG3	1.85	0.59
24:Y1:145:LEU:HD22	31:Y1:604:CLA:H91	1.85	0.59
2:b1:275:TRP:NE1	2:b1:359:MET:O	2.28	0.59
31:b1:608:CLA:H112	35:b1:622:LMG:H332	1.84	0.59
47:n1:605:CHL:H202	31:s1:604:CLA:HBC3	1.85	0.59
15:P:94:SER:OG	15:P:105:ARG:NH1	2.35	0.59
23:S:216:PHE:HE1	47:S:608:CHL:HBA2	1.68	0.59
4:c:338:ILE:HG21	4:c:347:TRP:HB2	1.85	0.59
4:c:406:ASN:HD21	40:c:519:DGD:HD4	1.68	0.59
1:a1:186:PHE:HE2	1:a1:192:ILE:HB	1.68	0.59
20:n:96:ALA:HB2	48:n:621:LUT:H202	1.85	0.58
21:g:220:VAL:HG23	21:g:221:THR:HG23	1.84	0.58
31:A1:410:CLA:HAB	9:I1:15:PHE:CD2	2.39	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b1:251:VAL:HG13	31:b1:603:CLA:H2	1.85	0.58
5:D:193:LEU:O	12:L:35:TYR:OH	2.19	0.58
4:c:225:HIS:HA	4:c:228:ILE:HG22	1.85	0.58
5:d:264:LYS:O	5:d:268:HIS:ND1	2.34	0.58
31:r:608:CLA:H8	31:r:608:CLA:HBB1	1.83	0.58
4:C1:393:ASN:ND2	40:C1:520:DGD:O1B	2.37	0.58
20:N:72:THR:HA	21:G:77:ARG:HH21	1.68	0.58
4:c:155:ILE:HG21	31:c:512:CLA:HBA2	1.84	0.58
31:y:603:CLA:HAC1	47:y:607:CHL:HBB2	1.85	0.58
6:E1:57:THR:O	6:E1:61:GLN:NE2	2.35	0.58
2:b1:296:LEU:HG	2:b1:301:ALA:HB2	1.84	0.58
31:c1:504:CLA:H61	40:c1:519:DGD:HB92	1.84	0.58
20:n1:221:PHE:HB3	47:n1:607:CHL:H62	1.85	0.58
2:b:462:PHE:HE2	31:b:612:CLA:HAB	1.69	0.58
33:c:516:BCR:H372	10:j:21:LEU:HD12	1.85	0.58
2:B1:144:PHE:HE2	31:R1:603:CLA:H61	1.68	0.58
4:C1:225:HIS:HA	4:C1:228:ILE:HG12	1.84	0.58
35:C1:523:LMG:H352	35:C1:523:LMG:H152	1.85	0.58
35:c1:523:LMG:H162	31:y1:611:CLA:HBC3	1.83	0.58
33:C:516:BCR:HC41	11:K:25:LEU:HD21	1.86	0.58
15:p:211:ASN:OD1	15:p:212:GLY:N	2.36	0.58
14:O1:111:PRO:HD2	14:O1:138:TYR:HD1	1.68	0.58
34:a1:412:SQD:H101	54:k1:101:4RF:H65	1.84	0.58
5:d1:189:HIS:HE1	5:d1:292:ASN:HD22	1.51	0.58
49:n1:622:XAT:H10	41:y1:624:LHG:H211	1.84	0.58
1:a:57:PRO:O	14:o:177:TYR:OH	2.22	0.58
1:a:116:VAL:HG13	1:a:158:PHE:HB3	1.84	0.58
2:b:145:LEU:HD21	31:b:616:CLA:HMB1	1.86	0.58
31:b:617:CLA:HMD3	8:h:24:THR:HG21	1.85	0.58
5:d:20:ASP:OD1	5:d:23:ARG:NH2	2.37	0.58
5:d:268:HIS:HA	5:d:271:MET:HG2	1.86	0.58
8:h:54:ILE:HG12	46:h:101:RRX:H9	1.85	0.58
1:a1:261:GLN:NE2	5:d1:27:PHE:O	2.30	0.58
31:b1:610:CLA:H2	31:b1:611:CLA:HBB2	1.84	0.58
4:c1:426:PHE:HE2	31:c1:505:CLA:HAB	1.69	0.58
14:o1:245:TYR:HE1	14:o1:280:MET:HA	1.69	0.58
31:g1:613:CLA:H12	31:g1:614:CLA:HED2	1.86	0.58
4:C:257:GLU:OE2	4:C:435:ARG:NH1	2.36	0.58
35:a:413:LMG:H392	40:c:518:DGD:HB61	1.85	0.58
21:g:40:PHE:CG	21:g:63:TRP:HB2	2.39	0.58
31:A1:405:CLA:H141	31:A1:406:CLA:H122	1.86	0.58

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y1:210:LYS:NZ	41:Y1:624:LHG:O4	2.37	0.58
1:a1:267:ASN:ND2	5:d1:232:PHE:O	2.36	0.58
34:a1:412:SQD:H383	40:c1:519:DGD:HAW2	1.86	0.58
2:b1:473:THR:O	27:r1:101:LYS:NZ	2.36	0.58
4:c1:200:TYR:HA	4:c1:203:LYS:HE3	1.85	0.58
23:s1:211:TYR:HB3	31:s1:610:CLA:HED3	1.86	0.58
24:y1:157:VAL:HG11	47:y1:605:CHL:HBC1	1.85	0.58
2:B:145:LEU:HD22	31:B:605:CLA:H162	1.85	0.58
22:R:153:VAL:O	22:R:157:ALA:CB	2.51	0.58
2:b:321:LYS:NZ	2:b:363:PHE:O	2.37	0.58
3:v:20:PRO:HA	3:v:23:VAL:HG12	1.85	0.58
4:c:425:PHE:HA	31:c:508:CLA:HMC2	1.85	0.58
21:g:43:PRO:HA	21:g:46:GLU:HG3	1.85	0.58
31:y:613:CLA:H143	41:y:624:LHG:H371	1.85	0.58
4:C1:364:ASP:HB3	4:C1:367:LYS:HB2	1.85	0.58
20:n1:49:LEU:HB2	20:n1:53:SER:HB3	1.86	0.58
2:B1:383:PHE:H	5:D1:345:VAL:HA	1.69	0.58
2:B1:470:GLY:HA2	31:B1:609:CLA:HED1	1.85	0.58
2:B1:476:ARG:HH12	27:R1:101:LYS:HG2	1.67	0.58
23:S1:234:LYS:HE3	31:S1:611:CLA:HED2	1.85	0.58
35:c1:521:LMG:H361	35:c1:521:LMG:H242	1.86	0.58
5:d1:21:TRP:O	5:d1:26:ARG:NH2	2.37	0.58
21:g1:229:LEU:HD11	48:g1:620:LUT:H172	1.86	0.58
23:s1:112:MET:SD	31:s1:610:CLA:HAB	2.43	0.58
33:C:516:BCR:H363	11:K:31:LEU:HG	1.86	0.58
20:N:171:GLY:HA3	20:N:176:GLU:HA	1.86	0.58
2:b:313:ASP:OD2	2:b:358:ARG:NH2	2.32	0.58
31:b:617:CLA:H2A	31:b:617:CLA:H12	1.86	0.58
2:B1:231:MET:HB2	31:B1:611:CLA:HAC2	1.86	0.58
31:C1:505:CLA:H43	33:C1:515:BCR:H331	1.86	0.58
20:N1:55:ASN:ND2	21:G1:161:ALA:O	2.36	0.58
31:b1:609:CLA:HAB	5:d1:123:ILE:HG23	1.85	0.58
4:C:95:ASP:HB3	23:S:287:PRO:HB3	1.84	0.57
4:C:203:LYS:HG3	4:C:211:TRP:HA	1.84	0.57
4:C:221:ILE:HG21	31:C:501:CLA:HED1	1.86	0.57
24:Y:48:LEU:HD21	24:Y:57:PRO:HG3	1.85	0.57
45:f:101:HEM:HBC2	45:f:101:HEM:HHD	1.86	0.57
4:C1:95:ASP:OD2	23:S1:285:ARG:NH2	2.35	0.57
38:C1:524:DGA:HBE2	35:W1:201:LMG:H392	1.86	0.57
4:c1:285:TYR:O	4:c1:411:ARG:NH2	2.32	0.57
2:B:462:PHE:HE1	31:B:612:CLA:HAB	1.67	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:608:CLA:H2	35:b:622:LMG:H151	1.86	0.57
1:A1:340:PRO:HD2	4:C1:305:PHE:HE2	1.69	0.57
14:O1:75:VAL:HG13	14:O1:80:ILE:HB	1.85	0.57
4:C:18:THR:HG23	4:C:19:THR:HG23	1.85	0.57
40:C:520:DGD:O1A	5:D:72:ASN:ND2	2.37	0.57
8:H:30:LEU:HB2	8:H:33:LEU:HD12	1.86	0.57
31:b:610:CLA:H2	31:b:611:CLA:HBB2	1.87	0.57
21:g:114:VAL:HB	21:g:117:LYS:HB2	1.86	0.57
2:B1:23:HIS:ND1	31:B1:616:CLA:OBD	2.35	0.57
40:B1:623:DGD:HD61	27:R1:170:LEU:HD11	1.85	0.57
4:C1:305:PHE:HD1	4:C1:308:ARG:HH22	1.51	0.57
35:C1:523:LMG:H382	31:Y1:614:CLA:H92	1.86	0.57
5:D1:172:SER:HB2	5:D1:177:SER:HB2	1.85	0.57
20:N1:45:ARG:NH1	20:N1:61:THR:O	2.37	0.57
2:b1:272:ARG:HH21	2:b1:361:THR:HB	1.70	0.57
31:y:610:CLA:H61	48:y:620:LUT:H30	1.86	0.57
4:C1:148:ILE:HA	4:C1:151:TYR:HB2	1.85	0.57
33:C1:514:BCR:H281	41:C1:525:LHG:H102	1.86	0.57
24:Y1:131:ILE:HG21	24:Y1:151:ILE:HD13	1.86	0.57
14:O:103:LYS:HA	14:O:146:SER:HA	1.85	0.57
18:X:66:THR:HG23	18:X:69:LEU:H	1.70	0.57
22:R:145:MET:HG3	48:R:620:LUT:H402	1.85	0.57
1:a:225:ARG:NH1	2:b:478:VAL:O	2.37	0.57
22:r:187:LEU:O	22:r:191:GLU:HB3	2.04	0.57
4:C1:136:GLY:O	4:C1:144:LYS:NZ	2.37	0.57
31:S1:604:CLA:H43	47:S1:606:CHL:HAA2	1.86	0.57
8:h1:50:MET:HE3	8:h1:54:ILE:HD11	1.86	0.57
24:y1:99:LEU:HG	31:y1:610:CLA:HMC3	1.87	0.57
5:D:216:ALA:O	5:D:220:ASN:ND2	2.36	0.57
1:a:298:ASN:HB2	4:c:391:SER:HA	1.86	0.57
2:b:231:MET:HG3	31:b:611:CLA:HAC1	1.87	0.57
2:b:272:ARG:NH2	5:d:165:SER:OG	2.37	0.57
14:o:111:PRO:HD2	14:o:138:TYR:HD1	1.69	0.57
19:z:59:SER:O	23:s:281:GLN:NE2	2.38	0.57
1:A:199:MET:HE1	5:D:74:LEU:HD13	1.86	0.57
22:R:213:TYR:HB3	31:R:610:CLA:HED3	1.87	0.57
23:S:234:LYS:O	23:S:238:ASN:ND2	2.37	0.57
5:d:59:TYR:HE1	6:e:66:ILE:HG23	1.70	0.57
15:p:105:ARG:HG3	15:p:117:TYR:HB3	1.86	0.57
31:C1:511:CLA:H101	33:C1:517:BCR:H402	1.85	0.57
47:N1:609:CHL:HMB2	47:Y1:601:CHL:HHB	1.86	0.57

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b1:612:CLA:H203	31:b1:614:CLA:H8	1.85	0.57
4:c1:33:LEU:HB3	4:c1:36:LYS:HB3	1.86	0.57
2:B:365:THR:H	5:D:326:ARG:NH2	2.02	0.57
4:c:193:ASN:HD21	4:c:196:ILE:HD12	1.70	0.57
8:h:42:PRO:HD3	22:r:84:SER:HA	1.86	0.57
14:o:276:SER:OG	14:o:277:ASP:N	2.37	0.57
2:B1:9:HIS:CG	31:B1:613:CLA:HAB	2.40	0.57
31:C1:513:CLA:H62	41:C1:525:LHG:H292	1.85	0.57
5:D1:53:THR:HG21	7:F1:32:PHE:HZ	1.69	0.57
34:A:412:SQD:H372	40:C:519:DGD:HAF1	1.85	0.57
35:A:413:LMG:H402	40:C:518:DGD:HBT2	1.86	0.57
40:C:519:DGD:HB42	35:C:521:LMG:H322	1.85	0.57
20:N:161:MET:HA	20:N:164:VAL:HG22	1.87	0.57
2:b:434:ARG:NH2	2:b:440:ASP:O	2.37	0.57
16:T1:1:MET:H1	52:b1:624:3PH:H352	1.69	0.57
20:N1:87:GLU:HA	20:N1:181:LEU:HD21	1.85	0.57
38:c1:524:DGA:HAW2	35:w1:201:LMG:H381	1.87	0.57
7:f1:44:ARG:HB3	15:p1:69:VAL:HG23	1.87	0.57
14:o1:138:TYR:CE2	17:w1:61:VAL:HG13	2.40	0.57
20:n1:203:LYS:HD2	31:n1:610:CLA:HMA3	1.85	0.57
4:C:14:ARG:O	4:C:29:ARG:NH1	2.38	0.57
1:A1:334:ARG:HH22	14:O1:215:GLY:H	1.52	0.57
3:V1:33:LEU:O	11:K1:39:TRP:NE1	2.28	0.57
4:C1:334:THR:HG21	14:O1:77:GLY:HA2	1.86	0.57
31:n1:602:CLA:H72	48:n1:621:LUT:H30	1.86	0.57
31:g1:610:CLA:H52	48:g1:620:LUT:H30	1.87	0.57
35:A:413:LMG:O5	4:C:209:ASP:OD2	2.23	0.56
31:C:504:CLA:H52	40:C:520:DGD:HB41	1.86	0.56
22:R:221:LEU:HD13	48:R:620:LUT:H222	1.87	0.56
23:s:105:LEU:HB3	23:s:210:LEU:HD11	1.87	0.56
20:N1:182:TYR:HB3	31:N1:610:CLA:HED3	1.87	0.56
20:N1:188:ASP:OD1	48:N1:620:LUT:O23	2.22	0.56
53:a1:414:SPH:HN22	54:i1:101:4RF:H41	1.69	0.56
4:c1:244:PRO:HA	31:c1:506:CLA:HED3	1.86	0.56
4:c1:414:LEU:O	4:c1:418:HIS:ND1	2.30	0.56
24:Y:184:TYR:HB3	31:Y:610:CLA:HED3	1.87	0.56
1:a:269:ARG:HD3	5:d:222:LEU:HD13	1.87	0.56
31:b:606:CLA:HMA3	31:b:607:CLA:H3A	1.86	0.56
31:y:603:CLA:HMA3	31:y:603:CLA:H2	1.87	0.56
2:B1:277:GLN:HB2	25:U1:106:VAL:HB	1.87	0.56
3:v1:7:LEU:HD22	11:k1:20:PRO:HB2	1.85	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c1:68:PRO:O	4:c1:72:GLN:NE2	2.34	0.56
4:c1:319:ALA:HA	15:p1:158:GLY:HA3	1.86	0.56
4:c1:437:ARG:NH2	9:i1:27:ASP:OD2	2.37	0.56
2:B:385:LYS:HG3	15:P:150:TRP:HB2	1.87	0.56
45:F:101:HEM:HBB2	45:F:101:HEM:HHC	1.87	0.56
14:O:278:THR:HG22	14:O:285:ALA:HB2	1.87	0.56
22:R:147:GLY:HA3	49:R:621:XAT:H193	1.86	0.56
2:b:223:ILE:HG12	8:h:42:PRO:HA	1.87	0.56
2:b:277:GLN:HB3	25:u:106:VAL:HG23	1.87	0.56
41:c:625:LHG:H132	34:c:626:SQD:H301	1.88	0.56
2:B1:104:SER:HA	2:B1:107:LEU:HD12	1.87	0.56
4:C1:435:ARG:HH12	31:C1:508:CLA:HED2	1.71	0.56
56:R1:626:ERG:H213	9:i1:6:ILE:HD13	1.87	0.56
1:a1:63:ILE:HG22	14:o1:206:ARG:HH22	1.71	0.56
4:c1:163:LEU:HD12	4:c1:166:LYS:HD3	1.85	0.56
5:d1:122:LEU:HB3	5:d1:150:ILE:HG12	1.86	0.56
20:n1:88:LEU:HD21	31:n1:603:CLA:HAA2	1.87	0.56
31:D:402:CLA:H201	35:D:411:LMG:H332	1.85	0.56
4:c:27:ASN:ND2	31:c:510:CLA:O1A	2.38	0.56
15:P1:182:LYS:NZ	15:P1:209:VAL:O	2.36	0.56
20:N1:70:TRP:HZ3	31:N1:602:CLA:HBC2	1.71	0.56
31:S1:602:CLA:H2	48:S1:621:LUT:H24	1.86	0.56
2:B:389:LYS:NZ	15:P:143:TYR:O	2.39	0.56
40:C:520:DGD:HBN2	40:C:520:DGD:HBT1	1.86	0.56
19:Z:2:THR:HA	19:Z:5:LEU:HD12	1.86	0.56
21:g:190:PRO:HA	21:g:193:PHE:HB3	1.88	0.56
15:P1:116:VAL:HG23	15:P1:219:VAL:HG22	1.88	0.56
23:S1:244:ILE:HD11	31:S1:602:CLA:HAC1	1.86	0.56
31:c1:511:CLA:HBA1	33:c1:517:BCR:H282	1.86	0.56
41:d1:409:LHG:H142	41:d1:409:LHG:H281	1.87	0.56
31:A:405:CLA:H143	32:A:408:PHO:H72	1.86	0.56
47:n:605:CHL:H143	48:s:620:LUT:H403	1.87	0.56
1:A1:85:THR:HA	1:A1:109:GLY:HA3	1.87	0.56
24:Y1:237:LEU:HB2	48:Y1:620:LUT:H22	1.87	0.56
2:b1:106:LEU:HD11	31:b1:607:CLA:H122	1.86	0.56
2:b1:148:LEU:HD13	31:r1:603:CLA:H112	1.87	0.56
20:n1:226:VAL:HG23	20:n1:227:THR:HG23	1.87	0.56
1:A:225:ARG:NE	2:B:480:ALA:O	2.37	0.56
14:O:118:GLU:OE2	14:O:120:ASP:OD2	2.23	0.56
2:b:382:PRO:HG2	2:b:385:LYS:HG2	1.88	0.56
15:p:94:SER:OG	15:p:105:ARG:NH1	2.38	0.56

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:n:104:VAL:HB	20:n:232:ILE:HD11	1.86	0.56
4:c1:334:THR:OG1	4:c1:336:GLU:OE1	2.23	0.56
17:w1:73:PRO:HB2	35:w1:201:LMG:H112	1.88	0.56
27:r1:79:SER:OG	31:r1:602:CLA:O1A	2.23	0.56
33:C:517:BCR:H391	11:K:36:ALA:HB2	1.88	0.56
31:y:602:CLA:H52	48:y:621:LUT:H28	1.88	0.56
2:B1:127:ARG:NH1	27:R1:105:GLU:OE1	2.38	0.56
31:S1:613:CLA:HAB	41:S1:624:LHG:H331	1.88	0.56
4:c1:320:GLN:HA	4:c1:326:GLY:HA2	1.87	0.56
14:o1:140:LEU:HA	14:o1:163:LEU:HD22	1.88	0.56
15:p1:206:LYS:HD3	15:p1:241:PHE:HB3	1.86	0.56
4:C:201:ILE:O	4:C:211:TRP:NE1	2.32	0.56
2:b:63:LEU:HD13	2:b:66:LEU:HD12	1.88	0.56
2:B1:6:TYR:OH	41:L1:101:LHG:O5	2.23	0.56
1:a1:26:ASN:O	5:d1:255:GLN:NE2	2.38	0.56
2:b1:214:LEU:HD23	2:b1:217:LEU:HD13	1.88	0.56
4:c1:238:TRP:HD1	53:y1:625:SPH:H102	1.70	0.56
14:o1:138:TYR:OH	17:w1:61:VAL:HG22	2.05	0.56
2:B:330:MET:HA	2:B:444:ARG:HB2	1.88	0.56
41:C:525:LHG:H262	31:S:611:CLA:HAB	1.88	0.56
5:D:79:SER:HA	5:D:172:SER:HB3	1.87	0.56
47:G:605:CHL:HHC	47:G:605:CHL:HBB1	1.87	0.56
31:R:602:CLA:H122	49:R:621:XAT:H361	1.87	0.56
2:b:222:SER:OG	8:h:43:GLY:O	2.24	0.56
6:e:76:VAL:O	6:e:80:SER:HB2	2.05	0.56
20:n:132:GLN:NE2	20:n:135:GLY:O	2.39	0.56
31:n:603:CLA:H152	47:n:609:CHL:H143	1.88	0.56
1:A1:44:ALA:HB1	1:A1:115:VAL:HG23	1.88	0.56
2:B1:30:VAL:HG11	31:B1:613:CLA:H112	1.89	0.56
2:b1:193:TYR:HB2	8:h1:83:SER:HB2	1.88	0.56
2:b1:249:ALA:HA	2:b1:252:VAL:HG12	1.87	0.56
4:c1:164:VAL:HA	4:c1:222:ILE:HD11	1.88	0.56
21:g1:205:ARG:HA	21:g1:208:MET:HG2	1.88	0.56
23:s1:192:PHE:H	23:s1:198:LYS:HA	1.70	0.56
2:B:359:MET:HG2	2:B:366:PHE:HB2	1.89	0.55
4:C:27:ASN:ND2	31:C:510:CLA:O1A	2.39	0.55
6:E:57:THR:O	6:E:61:GLN:NE2	2.39	0.55
20:N:204:VAL:HA	20:N:207:ILE:HG22	1.87	0.55
41:n:624:LHG:H131	49:g:622:XAT:H403	1.86	0.55
31:C1:504:CLA:H43	40:C1:520:DGD:HB32	1.88	0.55
41:D1:410:LHG:O3	41:D1:410:LHG:O1	2.23	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:N1:603:CLA:HED1	31:Y1:602:CLA:H121	1.89	0.55
20:N:84:ARG:CZ	24:Y:75:GLY:HA3	2.36	0.55
47:n:606:CHL:HBB2	47:n:607:CHL:HAB	1.88	0.55
21:g:158:ALA:O	21:g:162:ASN:ND2	2.35	0.55
1:a1:318:ALA:HA	1:a1:321:ILE:HD12	1.88	0.55
32:a1:408:PHO:HED1	44:d1:405:PL9:H152	1.88	0.55
31:g1:602:CLA:H72	48:g1:621:LUT:H30	1.87	0.55
1:A:67:VAL:HG13	5:D:313:THR:HA	1.87	0.55
1:A:228:THR:HG23	1:A:230:ASN:H	1.71	0.55
21:G:47:ASN:ND2	24:Y:173:GLU:OE2	2.39	0.55
2:b:371:ILE:HG22	2:b:377:VAL:HA	1.89	0.55
4:c:384:MET:O	15:p:228:LYS:NZ	2.38	0.55
49:n:622:XAT:H10	41:y:624:LHG:H211	1.89	0.55
24:y:150:SER:OG	47:y:605:CHL:OMC	2.21	0.55
1:A1:64:ARG:NH1	14:O1:167:ALA:O	2.37	0.55
1:A1:140:ARG:HH22	5:D1:222:LEU:H	1.54	0.55
1:A1:322:ASN:O	1:A1:326:LEU:N	2.39	0.55
4:C1:155:ILE:HG23	31:C1:512:CLA:H72	1.88	0.55
5:D1:250:ASN:ND2	5:D1:261:PHE:O	2.37	0.55
18:X1:66:THR:HG23	18:X1:69:LEU:H	1.72	0.55
20:N1:247:ALA:HB3	49:G1:622:XAT:H193	1.87	0.55
31:G1:613:CLA:H112	49:Y1:622:XAT:H34	1.88	0.55
31:b1:603:CLA:H161	35:h1:102:LMG:H412	1.89	0.55
4:c1:118:VAL:HG22	33:c1:517:BCR:H383	1.88	0.55
6:e1:57:THR:OG1	6:e1:59:ASP:OD1	2.23	0.55
33:C:516:BCR:H313	19:Z:17:PHE:HA	1.87	0.55
15:P:174:ALA:HB3	15:P:186:LYS:HB2	1.87	0.55
20:n:83:LYS:HD2	20:n:86:ARG:HH22	1.72	0.55
31:r:609:CLA:H111	31:r:609:CLA:HBB1	1.89	0.55
24:y:76:LEU:HD11	31:y:602:CLA:H42	1.79	0.55
2:B1:68:ARG:NH1	31:B1:604:CLA:OBD	2.38	0.55
31:B1:615:CLA:H51	34:M1:101:SQD:H141	1.88	0.55
4:C1:264:LEU:HD21	31:C1:508:CLA:HAB	1.88	0.55
5:D1:24:GLN:OE1	5:D1:26:ARG:NH2	2.37	0.55
11:K1:18:PHE:HE2	19:Z1:6:GLN:HG2	1.71	0.55
20:N1:220:PHE:HZ	48:N1:620:LUT:H173	1.72	0.55
24:Y1:248:ASN:HD21	24:Y1:250:PHE:HB2	1.71	0.55
35:c1:523:LMG:H402	53:y1:625:SPH:H142	1.89	0.55
40:C:519:DGD:HB71	35:C:521:LMG:H401	1.87	0.55
6:E:71:ASN:OD1	25:U:110:ARG:NH1	2.40	0.55
22:R:153:VAL:O	22:R:157:ALA:HB3	2.06	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a:192:ILE:HA	1:a:293:MET:HE1	1.88	0.55
15:p:120:ALA:HB1	15:p:213:LYS:HD2	1.87	0.55
21:g:229:LEU:HB2	48:g:620:LUT:H22	1.87	0.55
27:R1:135:GLU:HG2	31:R1:609:CLA:HED3	1.89	0.55
20:n1:150:ILE:HG22	57:y1:626:PTY:HC22	1.89	0.55
1:A:9:GLU:HG3	1:A:11:THR:HG23	1.89	0.55
1:A:298:ASN:HB2	4:C:391:SER:HA	1.89	0.55
31:R:603:CLA:HBB2	47:R:607:CHL:HAB	1.87	0.55
31:c:504:CLA:H51	40:c:519:DGD:HB52	1.88	0.55
7:F1:22:ILE:HG23	7:F1:23:HIS:HD1	1.71	0.55
15:P1:88:PRO:HB2	15:P1:91:TRP:CD1	2.41	0.55
20:N1:173:PRO:HG2	47:N1:608:CHL:HBB2	1.88	0.55
2:b1:24:LEU:HD21	31:b1:617:CLA:CAB	2.35	0.55
20:n1:97:LEU:HD22	31:n1:610:CLA:HAB	1.89	0.55
27:r1:213:TYR:HB3	31:r1:610:CLA:HED3	1.89	0.55
2:B:247:TRP:HE1	31:B:603:CLA:H101	1.72	0.55
1:a:228:THR:HG23	1:a:230:ASN:H	1.71	0.55
20:N1:251:ALA:HA	49:G1:622:XAT:H22	1.88	0.55
21:G1:211:CYS:O	21:G1:215:PHE:N	2.35	0.55
25:U1:110:ARG:HH21	25:U1:111:LYS:HD3	1.71	0.55
2:b1:348:ASP:OD2	2:b1:352:ARG:NH1	2.40	0.55
31:b1:616:CLA:H171	31:r1:609:CLA:H72	1.87	0.55
4:c1:109:SER:HA	33:c1:514:BCR:H16C	1.89	0.55
8:H:61:LEU:HD23	8:H:64:ILE:HD11	1.88	0.55
21:G:208:MET:HE2	31:G:602:CLA:HAB	1.87	0.55
35:b:622:LMG:H291	12:l:36:ILE:HD12	1.89	0.55
4:c:142:LYS:HB3	4:c:244:PRO:HG2	1.89	0.55
1:A1:310:ASN:O	15:P1:89:SER:OG	2.25	0.55
1:A1:337:HIS:CE1	5:D1:352:LEU:HD22	2.42	0.55
2:B1:3:LEU:HD13	2:B1:8:VAL:HA	1.88	0.55
5:D1:164:GLN:NE2	5:D1:290:ALA:O	2.39	0.55
21:G1:82:GLU:O	21:G1:86:ALA:N	2.39	0.55
23:S1:89:GLY:O	23:S1:92:LYS:NZ	2.39	0.55
2:b1:103:LEU:HD22	31:b1:607:CLA:H51	1.88	0.55
2:b1:355:PHE:HB2	25:u1:100:PRO:HB2	1.89	0.55
14:o1:138:TYR:HE2	17:w1:61:VAL:HG13	1.71	0.55
21:g1:84:ILE:HD13	21:g1:87:ARG:HD2	1.88	0.55
47:g1:608:CHL:HBB1	47:g1:608:CHL:HHC	1.88	0.55
24:y1:184:TYR:HB3	31:y1:610:CLA:HED3	1.89	0.55
14:O:212:ASP:OD2	14:O:216:ARG:NE	2.40	0.55
47:G:601:CHL:H12	47:Y:609:CHL:H43	1.89	0.55

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:385:LYS:HB3	15:p:149:ALA:HB3	1.88	0.55
23:s:108:ALA:HB1	23:s:239:GLY:HA3	1.87	0.55
5:D1:222:LEU:HA	5:D1:244:TYR:HA	1.87	0.55
47:N1:601:CHL:H202	47:G1:607:CHL:H13	1.89	0.55
47:Y1:601:CHL:HHD	41:Y1:624:LHG:HC41	1.89	0.55
1:A:9:GLU:N	17:W:102:ASP:O	2.40	0.55
32:a:409:PHO:HBC3	5:d:279:LEU:HD22	1.88	0.55
14:o:159:GLU:OE2	14:o:186:GLU:N	2.33	0.55
20:n:199:PHE:O	20:n:203:LYS:HB2	2.06	0.55
47:n:601:CHL:HED3	31:n:602:CLA:HBC1	1.89	0.55
1:A1:331:MET:HE1	5:D1:321:LEU:HA	1.88	0.55
2:B1:357:ARG:NH2	5:D1:337:GLU:OE1	2.40	0.55
5:D1:192:THR:HG23	31:D1:402:CLA:HBC2	1.89	0.55
15:P1:225:ARG:HH21	15:P1:228:LYS:HE2	1.72	0.55
21:G1:47:ASN:HB2	24:Y1:171:ASN:HB2	1.88	0.55
2:b1:288:VAL:O	2:b1:292:THR:OG1	2.23	0.55
4:c1:452:GLU:OE2	5:d1:248:THR:OG1	2.25	0.55
14:O:109:MET:HE1	14:O:184:ILE:HG13	1.89	0.54
22:R:234:ARG:NH1	31:R:612:CLA:O1A	2.40	0.54
31:c:511:CLA:H13	33:c:517:BCR:H21C	1.89	0.54
2:b1:90:ILE:HG22	34:b1:626:SQD:H101	1.89	0.54
2:b1:223:ILE:HG21	27:r1:85:LEU:HD13	1.88	0.54
5:d1:152:VAL:HG22	31:d1:402:CLA:HED1	1.89	0.54
1:A:340:PRO:HB2	15:P:224:LYS:HG3	1.89	0.54
22:R:238:ALA:HB2	31:R:611:CLA:HED2	1.89	0.54
22:R:256:GLN:O	22:R:261:GLY:N	2.41	0.54
24:Y:150:SER:OG	47:Y:605:CHL:OMC	2.23	0.54
6:e:38:VAL:HG11	7:f:39:MET:HE3	1.88	0.54
47:g:601:CHL:HED3	41:g:624:LHG:H142	1.89	0.54
1:a1:187:GLN:HE22	1:a1:192:ILE:HG22	1.72	0.54
35:c1:523:LMG:H171	31:y1:612:CLA:HBC1	1.88	0.54
9:i1:20:ILE:HG23	9:i1:21:PHE:HD1	1.72	0.54
8:H:66:GLU:HG3	8:H:72:LEU:HB2	1.88	0.54
14:O:148:LYS:HB2	14:O:156:GLU:HB3	1.90	0.54
48:G:621:LUT:H372	31:Y:603:CLA:HED3	1.90	0.54
2:b:272:ARG:NH2	2:b:276:ASP:OD2	2.41	0.54
31:b:605:CLA:H41	31:b:605:CLA:H92	1.89	0.54
40:C1:519:DGD:HB91	35:C1:521:LMG:H421	1.89	0.54
5:D1:106:GLN:NE2	6:E1:48:GLY:O	2.38	0.54
27:R1:224:ALA:HB3	31:R1:610:CLA:HAA2	1.88	0.54
27:r1:205:GLU:HG3	27:r1:210:LYS:HG2	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:225:ARG:NH1	1:A:227:THR:O	2.40	0.54
32:A:408:PHO:HAB	5:D:205:LEU:HD13	1.90	0.54
31:A:410:CLA:H3A	35:A:413:LMG:H122	1.89	0.54
15:P:68:ARG:HH22	15:P:72:LYS:HZ3	1.54	0.54
21:G:39:LYS:NZ	21:G:46:GLU:OE1	2.41	0.54
47:G:601:CHL:HMA3	41:G:630:LHG:H121	1.88	0.54
23:S:85:TYR:HE2	47:S:601:CHL:HAA2	1.71	0.54
5:d:51:GLY:HA2	5:d:55:VAL:HB	1.88	0.54
8:h:44:TRP:O	8:h:47:THR:OG1	2.26	0.54
14:o:158:ARG:NH1	14:o:188:ASP:OD1	2.41	0.54
21:g:86:ALA:HB1	21:g:204:GLY:HA3	1.88	0.54
49:n1:622:XAT:H8	41:y1:624:LHG:H221	1.89	0.54
21:g1:37:ARG:NH2	21:g1:53:LEU:O	2.41	0.54
35:A:413:LMG:H402	40:C:518:DGD:HB92	1.88	0.54
31:N:603:CLA:H101	31:Y:603:CLA:H92	1.90	0.54
24:Y:207:LYS:NZ	31:Y:611:CLA:O2D	2.41	0.54
2:b:333:GLY:O	2:b:441:GLY:N	2.41	0.54
4:c:174:TYR:HA	4:c:184:VAL:HA	1.89	0.54
4:c:177:TRP:HZ2	4:c:283:THR:HG22	1.72	0.54
1:A1:42:LEU:HD11	34:b1:626:SQD:H361	1.90	0.54
4:C1:135:PHE:HD1	31:C1:512:CLA:HBC2	1.71	0.54
31:C1:501:CLA:H203	31:C1:507:CLA:H13	1.89	0.54
35:a1:413:LMG:H402	40:c1:518:DGD:HBT2	1.89	0.54
2:b1:149:LEU:HD22	31:b1:604:CLA:HAC2	1.88	0.54
4:c1:221:ILE:O	4:c1:225:HIS:ND1	2.40	0.54
14:o1:111:PRO:HA	14:o1:292:GLY:HA3	1.90	0.54
21:g1:87:ARG:NH2	21:g1:200:GLU:OE2	2.41	0.54
31:B:603:CLA:H2	31:B:603:CLA:HBD	1.90	0.54
41:G:630:LHG:H221	49:Y:622:XAT:H10	1.89	0.54
2:b:415:SER:HA	2:b:418:LYS:HE2	1.90	0.54
31:n:610:CLA:H51	48:n:620:LUT:H373	1.89	0.54
21:g:208:MET:SD	31:g:602:CLA:HAB	2.47	0.54
35:A1:413:LMG:H422	40:C1:518:DGD:HBW2	1.89	0.54
2:B1:64:PRO:O	2:B1:67:THR:OG1	2.23	0.54
2:B1:75:TRP:NE1	2:B1:89:GLY:O	2.30	0.54
4:C1:252:PHE:HE1	33:C1:515:BCR:HC21	1.72	0.54
5:D1:246:MET:O	5:D1:250:ASN:N	2.32	0.54
5:D1:350:ASN:ND2	15:P1:195:ASP:OD1	2.41	0.54
15:P1:205:VAL:HG22	15:P1:218:LYS:HG3	1.90	0.54
24:Y1:99:LEU:HB3	31:Y1:604:CLA:HAB	1.90	0.54
31:a1:410:CLA:HAC2	33:a1:411:BCR:H363	1.89	0.54

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
23:s1:58:LYS:HE3	41:s1:624:LHG:HC11	1.90	0.54
31:B:613:CLA:H171	31:B:614:CLA:HBB2	1.89	0.54
31:c:513:CLA:H101	33:c:514:BCR:H23C	1.90	0.54
14:o:107:PHE:HB2	14:o:143:MET:HB2	1.89	0.54
24:Y1:190:ASP:OD1	48:Y1:620:LUT:O23	2.26	0.54
2:b1:357:ARG:NH1	25:u1:101:ALA:O	2.40	0.54
21:g1:122:ILE:HG21	21:g1:142:ILE:HD13	1.88	0.54
1:A:312:ARG:NE	15:P:92:ASN:OD1	2.41	0.54
31:n:604:CLA:H121	50:n:623:NEX:H402	1.89	0.54
4:C1:42:VAL:HG23	4:C1:117:GLY:HA2	1.90	0.54
14:O1:172:LEU:HB3	14:O1:176:GLU:HB2	1.90	0.54
2:b1:268:PHE:HB3	2:b1:448:ARG:HB2	1.89	0.54
31:b1:610:CLA:OBD	8:h1:46:THR:OG1	2.25	0.54
31:C:503:CLA:H172	31:C:510:CLA:HBB2	1.88	0.54
4:c:228:ILE:HD11	31:c:507:CLA:H72	1.90	0.54
41:n:624:LHG:H221	49:g:622:XAT:H8	1.90	0.54
33:B1:618:BCR:H322	26:M1:13:LEU:HD11	1.90	0.54
47:G1:605:CHL:HHC	47:G1:605:CHL:HBB1	1.90	0.54
31:S1:611:CLA:H203	31:S1:612:CLA:HAB	1.90	0.54
5:d1:55:VAL:HG21	5:d1:110:LEU:HD23	1.90	0.54
5:d1:98:GLN:HB3	6:e1:73:LEU:HD22	1.90	0.54
21:g1:202:LYS:NZ	41:g1:624:LHG:O4	2.36	0.54
20:N:87:GLU:HG3	20:N:181:LEU:HD13	1.90	0.54
31:n:613:CLA:HBB1	48:n:620:LUT:H192	1.90	0.54
1:A1:63:ILE:HA	4:C1:325:LEU:HD11	1.89	0.54
1:A1:317:TRP:O	1:A1:321:ILE:N	2.35	0.54
5:D1:58:TRP:HA	5:D1:63:LEU:H	1.72	0.54
1:a1:257:ARG:O	5:d1:128:ARG:NH2	2.39	0.54
4:c1:101:VAL:HG13	33:c1:514:BCR:H313	1.89	0.54
31:r1:608:CLA:HMB3	50:r1:622:NEX:H35	1.89	0.54
14:O:109:MET:CE	14:O:140:LEU:HD13	2.35	0.53
22:r:86:GLN:NE2	22:r:87:ILE:O	2.41	0.53
34:A1:412:SQD:H112	34:A1:412:SQD:H242	1.90	0.53
8:H1:67:ILE:O	8:H1:79:ASN:ND2	2.41	0.53
1:a1:84:PRO:HA	1:a1:112:TYR:CG	2.42	0.53
4:c1:338:ILE:HG21	4:c1:347:TRP:HB2	1.88	0.53
14:o1:140:LEU:CD2	14:o1:163:LEU:CD2	2.76	0.53
31:R:608:CLA:HMB2	50:R:622:NEX:H14	1.90	0.53
31:R:612:CLA:HHC	31:R:612:CLA:HBB1	1.90	0.53
33:c:516:BCR:H361	10:j:21:LEU:HD11	1.89	0.53
10:j:28:ALA:HA	35:j:101:LMG:H341	1.90	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:o:115:THR:HG22	14:o:129:LYS:HA	1.89	0.53
21:g:228:ASN:ND2	31:g:613:CLA:O1D	2.37	0.53
1:A1:234:ASN:HD22	5:D1:265:ARG:HB3	1.73	0.53
2:B1:385:LYS:NZ	14:O1:221:GLY:O	2.41	0.53
14:O1:108:CYS:N	14:O1:295:TYR:O	2.35	0.53
21:G1:210:SER:O	21:G1:214:PHE:N	2.39	0.53
1:a1:190:HIS:O	1:a1:299:GLY:N	2.41	0.53
4:c1:153:LEU:HD11	31:c1:506:CLA:HAB	1.90	0.53
20:n1:36:THR:OG1	20:n1:37:ILE:N	2.37	0.53
21:g1:214:PHE:HZ	48:g1:620:LUT:H8	1.73	0.53
31:s1:602:CLA:CAB	48:s1:621:LUT:H32	2.38	0.53
47:s1:608:CHL:HHC	47:s1:608:CHL:HBB1	1.90	0.53
2:B:381:VAL:HG22	2:B:418:LYS:HG2	1.89	0.53
4:C:315:ASN:HD21	14:O:161:GLU:HB2	1.73	0.53
35:A1:413:LMG:H372	40:C1:518:DGD:HA62	1.89	0.53
18:X1:65:VAL:HG13	18:X1:69:LEU:HD22	1.91	0.53
31:G1:602:CLA:CAB	48:G1:621:LUT:H32	2.38	0.53
24:Y1:162:MET:HE1	50:Y1:623:NEX:H30	1.90	0.53
1:a1:241:GLN:NE2	1:a1:243:GLU:O	2.36	0.53
31:a1:410:CLA:HAA2	35:a1:413:LMG:H111	1.91	0.53
31:b1:615:CLA:H51	34:m1:101:SQD:H131	1.90	0.53
2:B:245:VAL:HG23	31:B:613:CLA:H202	1.90	0.53
33:C:515:BCR:H332	9:I:20:ILE:HD13	1.89	0.53
23:S:237:LYS:NZ	41:S:624:LHG:O4	2.42	0.53
4:c:171:GLY:HA2	4:c:186:ILE:HB	1.89	0.53
6:e:14:LEU:HB3	10:j:15:VAL:HG11	1.91	0.53
31:g:602:CLA:H2	48:g:621:LUT:H382	1.90	0.53
1:A1:100:ALA:N	1:A1:104:GLU:OE2	2.40	0.53
31:A1:410:CLA:H142	35:A1:413:LMG:H141	1.89	0.53
40:B1:623:DGD:O5D	40:B1:623:DGD:O4D	2.23	0.53
3:V1:7:LEU:HA	3:V1:10:VAL:HG12	1.89	0.53
23:S1:57:ARG:O	23:S1:68:ARG:NH2	2.37	0.53
23:S1:246:VAL:HG21	48:S1:621:LUT:H12	1.90	0.53
31:a1:407:CLA:HED2	31:a1:407:CLA:H2A	1.91	0.53
4:c1:71:GLU:O	40:c1:519:DGD:O4E	2.27	0.53
5:d1:90:LEU:O	5:d1:104:TRP:NE1	2.40	0.53
5:d1:148:ALA:HB1	5:d1:279:LEU:HB2	1.91	0.53
8:h1:69:ASN:HD22	35:h1:102:LMG:HC92	1.73	0.53
21:g1:102:LEU:HB3	21:g1:108:VAL:HB	1.89	0.53
1:A:156:ALA:HA	1:A:160:ILE:HB	1.91	0.53
1:A:162:PRO:HB3	1:A:168:PHE:HA	1.91	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:91:TRP:CD2	31:B:607:CLA:HBA2	2.44	0.53
40:C:519:DGD:HB92	35:C:521:LMG:H421	1.91	0.53
4:c:296:GLU:HB3	4:c:349:PHE:CZ	2.43	0.53
14:o:209:THR:OG1	15:p:195:ASP:OD1	2.25	0.53
31:n:604:CLA:H161	31:s:610:CLA:H171	1.89	0.53
31:A1:406:CLA:HED2	5:D1:198:MET:HE2	1.90	0.53
4:C1:320:GLN:HA	4:C1:326:GLY:HA2	1.90	0.53
4:C1:414:LEU:O	4:C1:418:HIS:ND1	2.41	0.53
31:C1:512:CLA:H121	34:C1:526:SQD:H351	1.91	0.53
56:R1:626:ERG:C3	56:R1:626:ERG:HO1	2.13	0.53
24:Y1:94:ALA:HB1	24:Y1:212:GLY:HA3	1.91	0.53
33:b1:619:BCR:H14C	52:b1:624:3PH:H2E1	1.90	0.53
4:c1:48:ILE:HG22	31:c1:503:CLA:HHD	1.91	0.53
5:d1:222:LEU:HD23	5:d1:244:TYR:HB3	1.90	0.53
47:n1:605:CHL:HHC	47:n1:605:CHL:HBB1	1.90	0.53
1:A:42:LEU:HA	1:A:45:ILE:HG22	1.91	0.53
31:A:405:CLA:H191	41:D:409:LHG:H181	1.90	0.53
2:B:41:GLU:O	2:B:45:PHE:HB2	2.08	0.53
4:C:205:PRO:HA	4:C:211:TRP:HB2	1.90	0.53
31:G:603:CLA:H92	31:G:603:CLA:HMA2	1.91	0.53
1:a:283:ILE:HA	1:a:286:THR:HG22	1.89	0.53
14:o:140:LEU:HD22	14:o:163:LEU:O	2.09	0.53
24:y:94:ALA:HB1	24:y:212:GLY:HA3	1.90	0.53
2:B1:40:PHE:HB2	52:B1:624:3PH:H2A1	1.90	0.53
14:O1:149:ILE:HA	14:O1:155:VAL:HG12	1.90	0.53
20:N1:238:HIS:ND1	20:N1:245:ASN:O	2.35	0.53
24:Y1:76:LEU:HD12	31:Y1:602:CLA:H11	1.89	0.53
4:c1:230:THR:HB	57:y1:626:PTY:H171	1.91	0.53
4:c1:445:LYS:NZ	5:d1:224:GLU:O	2.42	0.53
21:g1:87:ARG:NH1	47:g1:608:CHL:OBD	2.41	0.53
1:A:64:ARG:HD3	4:C:325:LEU:HD11	1.91	0.53
31:B:613:CLA:H162	31:B:613:CLA:H8	1.89	0.53
4:C:281:ASN:O	4:C:411:ARG:NH1	2.41	0.53
5:D:188:PHE:HZ	5:D:330:ALA:HB2	1.74	0.53
31:N:602:CLA:CAB	48:N:621:LUT:H32	2.39	0.53
1:a:106:LEU:HD11	33:a:411:BCR:H402	1.90	0.53
2:b:357:ARG:NH2	25:u:103:GLU:OE2	2.42	0.53
15:p:179:LYS:HE3	15:p:244:VAL:HG13	1.90	0.53
1:A1:147:TYR:OH	32:A1:408:PHO:O1A	2.23	0.53
4:C1:246:PRO:HD2	35:C1:523:LMG:HC2	1.89	0.53
31:a1:410:CLA:H142	35:a1:413:LMG:H141	1.89	0.53

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b1:441:GLY:HA3	14:o1:228:LEU:HD12	1.90	0.53
2:B:247:TRP:HZ3	31:B:604:CLA:H121	1.74	0.53
31:D:402:CLA:H201	35:D:411:LMG:H362	1.90	0.53
4:c:150:GLY:HA2	4:c:236:GLY:HA2	1.91	0.53
4:c:201:ILE:O	4:c:211:TRP:NE1	2.32	0.53
1:A1:142:TRP:HZ2	4:C1:435:ARG:HE	1.56	0.53
1:A1:340:PRO:HA	5:D1:352:LEU:H	1.74	0.53
24:Y1:162:MET:HE2	47:Y1:606:CHL:HMA1	1.91	0.53
34:a1:412:SQD:H312	31:c1:508:CLA:H71	1.89	0.53
3:v1:33:LEU:OXT	11:k1:39:TRP:NE1	2.40	0.53
34:A:412:SQD:O7	5:D:233:ARG:NH1	2.42	0.53
2:B:73:GLN:NE2	2:B:86:SER:O	2.39	0.53
4:C:323:THR:HG23	4:C:325:LEU:HD13	1.91	0.53
31:C:504:CLA:H71	40:C:519:DGD:HB72	1.90	0.53
22:R:182:PHE:HB3	22:R:187:LEU:HG	1.91	0.53
24:Y:84:ALA:HA	24:Y:87:ARG:CZ	2.39	0.53
24:Y:210:LYS:NZ	41:Y:624:LHG:O4	2.42	0.53
4:c:198:PHE:HA	4:c:201:ILE:HG22	1.91	0.53
2:B1:275:TRP:O	25:U1:102:LYS:NZ	2.42	0.53
2:B1:434:ARG:NH1	14:O1:230:ALA:O	2.41	0.53
1:a1:74:GLY:O	5:d1:301:GLN:NE2	2.42	0.53
2:b1:379:ALA:HB2	2:b1:395:VAL:HG11	1.90	0.53
4:c1:355:GLU:OE2	4:c1:358:ARG:NH1	2.41	0.53
26:m1:5:ILE:HD12	26:m1:8:LEU:HD12	1.91	0.53
24:y1:137:LEU:HD21	31:y1:604:CLA:HAA2	1.89	0.53
1:A:176:ILE:HD11	44:D:405:PL9:H452	1.90	0.53
31:B:605:CLA:HMB1	31:B:608:CLA:HAB	1.91	0.53
31:G:603:CLA:HBC3	48:G:621:LUT:H203	1.91	0.53
23:S:234:LYS:HE3	31:S:611:CLA:HED2	1.91	0.53
1:a:84:PRO:HA	1:a:112:TYR:CG	2.44	0.53
1:a:332:HIS:CD2	1:a:333:GLU:HG2	2.44	0.53
4:c:267:VAL:HA	4:c:270:MET:HE3	1.90	0.53
24:y:220:LEU:HD12	31:y:603:CLA:HAB	1.90	0.53
14:O1:115:THR:HG22	14:O1:129:LYS:HA	1.91	0.53
14:O1:239:ARG:O	14:O1:243:LYS:NZ	2.42	0.53
21:G1:96:ILE:HD11	21:G1:214:PHE:CD2	2.44	0.53
25:u1:105:THR:HB	25:u1:108:GLU:HG3	1.92	0.53
23:S:276:LEU:HD11	31:S:613:CLA:H2	1.90	0.52
1:a:188:ALA:HB2	1:a:328:MET:HB3	1.91	0.52
2:b:212:ALA:O	2:b:216:HIS:ND1	2.40	0.52
1:A1:24:THR:O	5:D1:255:GLN:NE2	2.41	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:57:PRO:O	14:O1:177:TYR:OH	2.27	0.52
2:B1:117:TYR:HD1	8:H1:22:ILE:HD13	1.73	0.52
31:B1:615:CLA:H43	34:M1:101:SQD:H241	1.91	0.52
4:C1:120:HIS:HA	4:C1:124:GLY:HA3	1.90	0.52
31:C1:504:CLA:HBB1	40:C1:519:DGD:HB82	1.91	0.52
20:N1:36:THR:OG1	20:N1:37:ILE:N	2.39	0.52
47:N1:605:CHL:HHC	47:N1:605:CHL:HBB1	1.90	0.52
47:G1:601:CHL:H202	47:Y1:607:CHL:H13	1.91	0.52
31:G1:603:CLA:HMA1	31:G1:603:CLA:H12	1.91	0.52
1:a1:304:GLN:HG2	1:a1:313:VAL:HG11	1.91	0.52
31:c1:506:CLA:HBB2	31:c1:507:CLA:H52	1.90	0.52
5:d1:273:PHE:HZ	41:d1:408:LHG:H131	1.74	0.52
31:A:410:CLA:H2	9:I:12:VAL:HG11	1.91	0.52
2:B:16:PRO:HG2	2:B:123:PHE:HB3	1.91	0.52
40:C:523:DGD:HBW1	31:Y:614:CLA:HBC1	1.92	0.52
5:D:292:ASN:OD1	5:D:294:ARG:NH1	2.42	0.52
1:a:161:TYR:HH	1:a:190:HIS:HE2	1.56	0.52
34:a:412:SQD:O8	4:c:24:TRP:NE1	2.38	0.52
2:b:23:HIS:ND1	31:b:616:CLA:OBD	2.42	0.52
2:b:51:VAL:HG13	2:b:308:LYS:HD3	1.90	0.52
2:b:470:GLY:HA2	31:b:609:CLA:HED1	1.91	0.52
4:c:207:GLY:HA2	40:c:518:DGD:HD2	1.91	0.52
10:j:32:TYR:HB2	35:j:101:LMG:H312	1.91	0.52
12:l:27:VAL:HG11	41:l:101:LHG:H201	1.90	0.52
2:B1:15:ASP:OD2	12:L1:5:ASN:ND2	2.37	0.52
5:D1:25:ASP:N	5:D1:25:ASP:OD1	2.42	0.52
31:Y1:614:CLA:H2	57:Y1:626:PTY:H372	1.91	0.52
1:A:283:ILE:HA	1:A:286:THR:HG22	1.90	0.52
15:P:121:GLN:O	15:P:214:LEU:N	2.36	0.52
21:G:66:ALA:HB2	48:G:621:LUT:H221	1.91	0.52
21:G:229:LEU:HD12	48:G:620:LUT:H163	1.91	0.52
1:a:224:ILE:HD11	2:b:484:GLU:HA	1.91	0.52
4:c:185:ARG:NH2	4:c:219:GLU:OE2	2.43	0.52
21:g:88:TRP:NE1	47:g:608:CHL:O1D	2.31	0.52
1:A1:187:GLN:NE2	1:A1:191:ASN:OD1	2.35	0.52
24:Y1:129:ALA:HB2	47:Y1:607:CHL:HED2	1.91	0.52
24:Y1:207:LYS:HG3	31:Y1:611:CLA:HED2	1.92	0.52
31:b1:611:CLA:H71	31:b1:616:CLA:HBA2	1.90	0.52
33:b1:618:BCR:H313	26:m1:10:ALA:HA	1.90	0.52
31:r1:603:CLA:HAB	55:r1:625:LMT:H22	1.89	0.52
2:B:384:ARG:HH11	5:D:348:ARG:HH22	1.56	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:C:507:CLA:H2	31:C:507:CLA:HMA3	1.92	0.52
22:R:195:VAL:HA	22:R:198:VAL:HG12	1.92	0.52
2:b:158:VAL:HB	2:b:166:ILE:HD11	1.91	0.52
2:b:443:PHE:HE1	14:o:229:PRO:HG2	1.73	0.52
31:b:609:CLA:HAB	5:d:123:ILE:HD12	1.91	0.52
16:t:12:GLY:O	16:t:16:ILE:HG12	2.10	0.52
2:B1:224:ARG:NH1	5:D1:10:GLU:OE1	2.43	0.52
5:D1:161:PRO:HB3	5:D1:170:ALA:HB2	1.91	0.52
6:E1:54:GLU:HG3	6:E1:81:ALA:HB2	1.91	0.52
15:P1:178:ASP:HB2	15:P1:184:TYR:HE2	1.74	0.52
31:n1:603:CLA:HED2	31:n1:603:CLA:H12	1.91	0.52
49:n1:622:XAT:H35	47:y1:601:CHL:H72	1.92	0.52
21:g1:128:LEU:HD22	47:g1:606:CHL:HMD2	1.92	0.52
47:n:609:CHL:HAA1	24:y:73:THR:HG21	1.92	0.52
23:s:151:TYR:OH	47:s:606:CHL:OBD	2.26	0.52
23:s:276:LEU:HD22	31:s:613:CLA:H43	1.90	0.52
31:y:603:CLA:HHC	31:y:603:CLA:HBB1	1.91	0.52
2:B1:348:ASP:OD1	2:B1:352:ARG:N	2.42	0.52
4:C1:67:LYS:O	4:C1:72:GLN:NE2	2.43	0.52
5:D1:253:TRP:O	5:D1:258:GLY:N	2.42	0.52
6:E1:8:ARG:HB3	6:E1:13:ILE:HD11	1.91	0.52
14:O1:265:GLU:OE1	14:O1:295:TYR:OH	2.22	0.52
31:N1:613:CLA:H142	49:G1:622:XAT:H15	1.91	0.52
47:G1:609:CHL:HBB1	47:G1:609:CHL:HHC	1.90	0.52
35:c1:523:LMG:H441	53:y1:625:SPH:H81	1.90	0.52
5:d1:111:TRP:HZ3	5:d1:167:TRP:HB3	1.75	0.52
41:n1:624:LHG:H191	49:g1:622:XAT:H14	1.92	0.52
24:y1:155:LEU:HD13	47:y1:607:CHL:HAC2	1.91	0.52
49:N:622:XAT:H34	31:Y:613:CLA:H112	1.91	0.52
5:d:51:GLY:HA3	5:d:78:VAL:HG22	1.92	0.52
5:d:195:PRO:HD3	12:l:35:TYR:CZ	2.45	0.52
1:A1:331:MET:HA	5:D1:349:GLY:H	1.74	0.52
2:B1:96:ALA:O	2:B1:100:HIS:ND1	2.34	0.52
4:C1:166:LYS:HA	4:C1:170:PHE:HB2	1.90	0.52
21:G1:133:ASN:HB3	21:G1:136:LEU:HG	1.92	0.52
27:R1:220:PRO:HD2	48:R1:620:LUT:H23	1.92	0.52
1:a1:340:PRO:HA	5:d1:352:LEU:HA	1.91	0.52
4:c1:330:MET:HE3	4:c1:331:ARG:H	1.75	0.52
23:s1:186:GLY:HA2	47:s1:608:CHL:HMC	1.90	0.52
4:C:337:ILE:HB	4:C:363:LEU:H	1.74	0.52
23:S:152:PHE:HA	23:S:158:VAL:H	1.74	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:c:520:DGD:HA22	35:d:411:LMG:H111	1.91	0.52
12:l:23:LEU:HG	41:l:101:LHG:H181	1.92	0.52
14:o:260:ASP:HB3	14:o:265:GLU:H	1.74	0.52
22:r:153:VAL:O	22:r:157:ALA:CB	2.58	0.52
31:B1:605:CLA:H2	31:B1:613:CLA:H152	1.92	0.52
8:H1:74:LEU:HB2	8:H1:77:VAL:HG22	1.92	0.52
47:N1:601:CHL:HHC	47:N1:601:CHL:HBB1	1.91	0.52
4:c1:218:LEU:HA	4:c1:221:ILE:HB	1.91	0.52
1:A:269:ARG:NH1	5:D:231:THR:O	2.42	0.52
14:O:276:SER:HB3	14:O:286:LYS:H	1.74	0.52
20:N:81:THR:HG23	20:N:84:ARG:HH22	1.75	0.52
31:N:604:CLA:H121	50:N:623:NEX:H402	1.91	0.52
23:S:186:GLY:HA2	47:S:608:CHL:HMC	1.92	0.52
1:a:54:ALA:HB2	1:a:72:LEU:HD12	1.91	0.52
16:t:26:PRO:HB2	16:t:28:ARG:HH12	1.74	0.52
20:n:138:TYR:HH	50:n:623:NEX:H1	1.47	0.52
21:g:217:GLN:O	21:g:221:THR:OG1	2.23	0.52
47:s:601:CHL:HED2	41:s:624:LHG:H152	1.91	0.52
31:A1:410:CLA:H62	35:A1:413:LMG:H132	1.91	0.52
35:A1:413:LMG:H371	40:C1:518:DGD:HB41	1.92	0.52
52:S1:626:3PH:H342	52:S1:626:3PH:H2	1.92	0.52
33:c1:516:BCR:H361	10:j1:21:LEU:HD21	1.92	0.52
8:h1:66:GLU:O	8:h1:71:SER:N	2.42	0.52
21:g1:182:ASP:OD1	48:g1:620:LUT:O23	2.27	0.52
23:s1:103:ASN:O	23:s1:107:HIS:ND1	2.35	0.52
24:y1:76:LEU:CD1	31:y1:602:CLA:C4	2.75	0.52
1:A:325:ASN:HA	1:A:328:MET:HE2	1.92	0.52
23:S:109:ARG:NH1	47:S:608:CHL:OBD	2.43	0.52
22:r:256:GLN:O	22:r:261:GLY:N	2.37	0.52
2:B1:319:PRO:HB3	2:B1:446:SER:HB3	1.91	0.52
31:B1:603:CLA:H43	8:H1:65:LEU:HA	1.91	0.52
2:b1:354:LEU:HB3	2:b1:370:LEU:HB3	1.92	0.52
4:c1:203:LYS:HB3	4:c1:211:TRP:HA	1.92	0.52
4:c1:359:GLY:N	4:c1:362:GLY:O	2.42	0.52
1:A:340:PRO:HA	5:D:351:ALA:HB1	1.91	0.52
33:B:619:BCR:HC21	35:B:622:LMG:H142	1.90	0.52
1:a:131:TRP:HE1	4:c:434:GLY:HA2	1.74	0.52
12:l:27:VAL:HG21	41:l:101:LHG:H192	1.92	0.52
22:r:223:LEU:HD22	31:r:610:CLA:H2	1.92	0.52
1:A1:216:GLY:HA2	5:D1:268:HIS:HB3	1.90	0.52
5:D1:276:VAL:HG12	41:D1:408:LHG:H261	1.91	0.52

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
8:H1:75:ASP:OD2	18:X1:64:SER:N	2.43	0.52
20:N1:156:VAL:HG11	47:N1:605:CHL:HBC1	1.92	0.52
31:S1:611:CLA:H91	31:S1:611:CLA:H142	1.91	0.52
31:a1:407:CLA:HED1	5:d1:175:VAL:HG22	1.92	0.52
31:c1:505:CLA:H93	31:c1:505:CLA:HBB1	1.91	0.52
23:s1:183:ARG:O	23:s1:209:LYS:NZ	2.42	0.52
1:A:229:GLU:HG3	22:R:94:GLN:HB2	1.92	0.51
4:C:36:LYS:NZ	4:C:121:SER:O	2.38	0.51
31:N:613:CLA:H162	49:G:622:XAT:H32	1.92	0.51
5:d:165:SER:HB2	5:d:169:PHE:HE2	1.75	0.51
10:j:32:TYR:HD1	35:j:101:LMG:H292	1.75	0.51
47:g:605:CHL:HBB1	47:g:605:CHL:HHC	1.91	0.51
1:A1:84:PRO:HA	1:A1:112:TYR:CG	2.44	0.51
2:B1:16:PRO:HG2	2:B1:123:PHE:HB3	1.90	0.51
47:y1:609:CHL:HHC	47:y1:609:CHL:HBB1	1.92	0.51
1:A:85:THR:HA	1:A:109:GLY:HA3	1.92	0.51
1:A:163:ILE:HD11	40:C:518:DGD:HA31	1.92	0.51
4:C:59:GLU:HG3	4:C:74:LEU:HD22	1.92	0.51
1:a:328:MET:HE1	5:d:183:LEU:HD22	1.92	0.51
2:b:167:TRP:HE3	2:b:178:VAL:HG23	1.75	0.51
31:c:507:CLA:H2	31:c:507:CLA:HMA3	1.91	0.51
14:o:114:PHE:O	14:o:130:THR:OG1	2.27	0.51
20:n:191:GLY:O	20:n:193:ALA:N	2.43	0.51
22:r:207:ASP:OD1	22:r:207:ASP:N	2.41	0.51
1:A1:29:TYR:O	1:A1:129:ARG:NE	2.36	0.51
5:D1:179:PHE:HA	5:D1:182:ILE:HG22	1.92	0.51
31:c1:511:CLA:HBA2	31:c1:511:CLA:HBD	1.92	0.51
27:r1:234:ARG:HH12	31:r1:612:CLA:H43	1.75	0.51
1:A:27:ARG:O	1:A:27:ARG:NH1	2.39	0.51
5:D:48:TRP:HA	5:D:78:VAL:HG21	1.92	0.51
5:d:186:GLN:NE2	5:d:322:ASN:OD1	2.42	0.51
23:s:124:LEU:HB3	23:s:129:ALA:HB3	1.92	0.51
26:M1:20:SER:HB2	34:M1:101:SQD:H302	1.92	0.51
16:T1:24:ARG:HE	16:T1:25:GLU:H	1.58	0.51
14:O:104:LEU:HD22	14:O:147:MET:HE2	1.93	0.51
47:N:605:CHL:H161	31:S:610:CLA:H112	1.93	0.51
31:R:610:CLA:H11	48:R:620:LUT:H28	1.92	0.51
47:S:608:CHL:HHC	47:S:608:CHL:HBB1	1.91	0.51
2:b:41:GLU:O	2:b:45:PHE:HB2	2.09	0.51
2:b:237:VAL:HB	31:b:611:CLA:HBC2	1.92	0.51
40:c:523:DGD:HG31	31:y:611:CLA:HBA1	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:n:605:CHL:HHC	47:n:605:CHL:HBB1	1.92	0.51
20:N1:205:LYS:O	20:N1:209:ASN:ND2	2.37	0.51
23:S1:101:ARG:HA	23:S1:104:GLU:HB3	1.92	0.51
1:A:290:ILE:HG13	31:A:405:CLA:HED3	1.92	0.51
4:C:285:TYR:O	4:C:411:ARG:NH2	2.31	0.51
14:O:237:ILE:HG23	14:O:241:ASN:HB3	1.93	0.51
47:Y:605:CHL:HHC	47:Y:605:CHL:HBB1	1.93	0.51
5:d:192:THR:HG23	31:d:402:CLA:HBC2	1.93	0.51
6:e:22:ILE:HG13	6:e:23:HIS:HD1	1.75	0.51
14:o:130:THR:HG22	14:o:172:LEU:HA	1.92	0.51
14:o:183:THR:HG21	14:o:203:PRO:HD2	1.91	0.51
31:s:602:CLA:H112	48:s:621:LUT:H371	1.93	0.51
47:s:608:CHL:H143	50:s:623:NEX:H35	1.92	0.51
47:y:606:CHL:HHC	47:y:606:CHL:HBB1	1.93	0.51
4:C1:245:TRP:NE1	31:C1:506:CLA:OBD	2.36	0.51
4:C1:437:ARG:HH22	9:I1:27:ASP:HB2	1.73	0.51
14:O1:189:GLY:HA2	14:O1:198:GLY:HA3	1.93	0.51
31:b1:604:CLA:HBC1	31:b1:605:CLA:H72	1.93	0.51
4:c1:155:ILE:HG23	31:c1:512:CLA:H72	1.93	0.51
5:d1:149:PRO:HB3	31:d1:402:CLA:H41	1.91	0.51
31:B:603:CLA:HAC1	8:H:57:PHE:CE1	2.45	0.51
5:D:72:ASN:OD1	5:D:73:PHE:N	2.39	0.51
8:H:78:THR:OG1	8:H:83:SER:OG	2.27	0.51
19:Z:5:LEU:HD11	19:Z:61:ALA:HB3	1.93	0.51
20:N:155:ALA:HA	31:Y:613:CLA:H201	1.91	0.51
1:A1:318:ALA:HA	1:A1:321:ILE:HD12	1.92	0.51
2:B1:141:ILE:HG22	2:B1:145:LEU:HD23	1.93	0.51
47:S1:606:CHL:HHC	47:S1:606:CHL:HBB1	1.93	0.51
47:Y1:606:CHL:H71	31:r1:610:CLA:H121	1.92	0.51
5:d1:105:PHE:HZ	33:d1:404:BCR:HC42	1.75	0.51
17:w1:79:GLY:HA2	35:w1:201:LMG:HC72	1.93	0.51
47:N:605:CHL:HHC	47:N:605:CHL:HBB1	1.93	0.51
23:S:108:ALA:HB1	23:S:239:GLY:HA3	1.93	0.51
2:b:23:HIS:HB3	31:b:616:CLA:HED2	1.93	0.51
2:b:157:HIS:HA	2:b:163:GLY:HA3	1.91	0.51
11:k:40:GLN:HE21	11:k:45:PHE:HA	1.74	0.51
9:I1:31:ASN:ND2	9:I1:35:GLY:O	2.38	0.51
20:N1:93:ALA:HB1	20:N1:210:GLY:HA3	1.92	0.51
24:Y1:145:LEU:HD11	27:r1:176:LEU:HD21	1.92	0.51
1:a1:156:ALA:HA	1:a1:160:ILE:HB	1.92	0.51
1:a1:304:GLN:HB2	4:c1:402:ILE:HG23	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b1:37:MET:HA	2:b1:40:PHE:HB3	1.93	0.51
31:b1:602:CLA:H13	46:h1:101:RRX:H42	1.93	0.51
15:p1:96:GLU:OE2	15:p1:105:ARG:NH1	2.44	0.51
47:g1:601:CHL:H12	47:y1:609:CHL:H43	1.93	0.51
24:y1:46:ARG:NH2	24:y1:61:LEU:O	2.44	0.51
15:P:206:LYS:HB2	15:P:217:LEU:HB3	1.93	0.51
21:G:219:ILE:HG23	21:G:220:VAL:HG13	1.92	0.51
31:G:602:CLA:H91	31:Y:603:CLA:H72	1.91	0.51
14:o:117:LYS:HD3	14:o:287:ASP:HB2	1.92	0.51
2:B1:282:GLN:HE22	2:B1:286:LYS:HD3	1.76	0.51
31:B1:617:CLA:H61	50:R1:622:NEX:H172	1.91	0.51
4:C1:454:VAL:HG21	5:D1:248:THR:HA	1.92	0.51
5:D1:62:GLY:HA3	6:E1:63:ALA:HB1	1.93	0.51
31:S1:602:CLA:CAB	48:S1:621:LUT:H32	2.41	0.51
2:b1:64:PRO:HB3	2:b1:267:LEU:HB3	1.93	0.51
2:b1:252:VAL:HG22	2:b1:256:MET:HE1	1.93	0.51
38:c1:524:DGA:HBF2	31:y1:612:CLA:H13	1.93	0.51
5:d1:188:PHE:HA	5:d1:326:ARG:HD3	1.93	0.51
52:t1:101:3PH:H2A2	52:t1:101:3PH:H2F2	1.92	0.51
21:g1:220:VAL:HG11	49:y1:622:XAT:H163	1.93	0.51
47:g1:609:CHL:HHC	47:g1:609:CHL:HBB1	1.93	0.51
23:s1:112:MET:HG3	23:s1:239:GLY:HA2	1.93	0.51
4:C:125:PRO:HD3	31:C:513:CLA:HED3	1.93	0.51
8:H:29:LEU:HD22	22:R:203:ASN:HD22	1.76	0.51
21:G:153:MET:HE1	47:G:609:CHL:CMC	2.40	0.51
24:Y:157:VAL:HG21	47:Y:605:CHL:HBC1	1.92	0.51
24:Y:190:ASP:OD1	48:Y:620:LUT:O23	2.25	0.51
2:b:468:TRP:NE1	31:b:612:CLA:O1D	2.36	0.51
4:c:212:ILE:HG21	4:c:273:THR:HG23	1.93	0.51
21:g:184:LEU:HD13	48:g:620:LUT:H222	1.93	0.51
1:A1:281:VAL:HA	1:A1:284:TRP:CE3	2.46	0.51
5:D1:30:VAL:HG12	5:D1:38:LEU:HD11	1.92	0.51
8:H1:66:GLU:HB2	8:H1:71:SER:HB2	1.93	0.51
15:P1:204:LEU:HB2	15:P1:219:VAL:HB	1.92	0.51
47:Y1:601:CHL:H162	41:Y1:624:LHG:H221	1.91	0.51
2:b1:74:SER:HA	2:b1:92:SER:HB2	1.92	0.51
2:b1:440:ASP:HB3	5:d1:299:VAL:HG21	1.93	0.51
4:c1:60:VAL:HA	4:c1:63:PHE:HB2	1.93	0.51
5:d1:106:GLN:NE2	6:e1:48:GLY:O	2.44	0.51
14:o1:115:THR:HB	14:o1:127:PHE:HB3	1.93	0.51
49:n1:622:XAT:H14	47:y1:601:CHL:H71	1.92	0.51

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:84:PRO:HA	1:A:112:TYR:CG	2.45	0.51
4:c:298:SER:OG	4:c:343:THR:OG1	2.20	0.51
4:c:397:GLY:H	4:c:401:GLU:HG2	1.76	0.51
1:A1:42:LEU:HA	1:A1:45:ILE:HG22	1.93	0.51
4:C1:78:PRO:HB3	4:C1:289:PHE:HB3	1.92	0.51
4:C1:350:ARG:HH21	14:O1:72:TYR:HD2	1.57	0.51
23:S1:57:ARG:H	23:S1:68:ARG:HH22	1.59	0.51
1:a1:228:THR:OG1	1:a1:230:ASN:OD1	2.20	0.51
2:b1:274:GLN:HE22	8:h1:81:TRP:NE1	2.08	0.51
7:f1:33:LEU:HD23	7:f1:36:ILE:HD11	1.93	0.51
31:r1:609:CLA:H41	31:r1:609:CLA:H93	1.93	0.51
1:A:196:PRO:HG3	40:C:520:DGD:HB62	1.93	0.50
5:D:82:ALA:HB3	5:D:85:LEU:HD23	1.91	0.50
14:O:82:ASN:HD22	14:O:136:LEU:HD22	1.76	0.50
47:G:609:CHL:HBB1	47:G:609:CHL:HHC	1.92	0.50
2:b:454:GLY:HA2	35:b:622:LMG:H191	1.91	0.50
20:n:223:GLN:O	20:n:227:THR:OG1	2.29	0.50
23:s:109:ARG:NH1	47:s:608:CHL:OBD	2.40	0.50
31:S1:605:CLA:H11	31:S1:610:CLA:H193	1.93	0.50
24:Y1:95:ARG:HA	24:Y1:98:LEU:HD12	1.93	0.50
1:a1:322:ASN:HD21	15:p1:110:PHE:HD1	1.58	0.50
1:a1:332:HIS:NE2	1:a1:342:ASP:OD2	2.43	0.50
35:a1:413:LMG:O5	4:c1:209:ASP:OD2	2.26	0.50
40:c1:520:DGD:HAW2	35:d1:411:LMG:H191	1.92	0.50
5:d1:122:LEU:HD21	31:d1:402:CLA:H8	1.92	0.50
47:y1:605:CHL:HHC	47:y1:605:CHL:HBB1	1.93	0.50
2:B:364:GLU:H	5:D:326:ARG:HH22	1.58	0.50
40:C:523:DGD:O2D	38:C:524:DGA:OB1	2.29	0.50
31:G:604:CLA:H42	50:G:623:NEX:H23	1.93	0.50
47:S:606:CHL:HHC	47:S:606:CHL:HBB1	1.92	0.50
47:Y:609:CHL:HHC	47:Y:609:CHL:HBB1	1.94	0.50
1:a:184:ILE:HD11	5:d:186:GLN:HG2	1.93	0.50
4:c:167:ALA:HB1	4:c:187:ILE:HD12	1.93	0.50
8:h:29:LEU:HD13	22:r:203:ASN:HD21	1.76	0.50
2:B1:66:LEU:HB3	2:B1:71:VAL:HB	1.93	0.50
2:B1:274:GLN:HE22	8:H1:81:TRP:CD1	2.28	0.50
4:C1:213:VAL:HG12	40:C1:518:DGD:HD61	1.92	0.50
21:G1:68:LEU:HD11	31:Y1:603:CLA:H11	1.92	0.50
23:S1:110:TRP:HD1	31:S1:609:CLA:HMD3	1.77	0.50
1:a1:27:ARG:NH2	16:t1:21:ILE:O	2.43	0.50
32:a1:408:PHO:HHC	5:d1:205:LEU:HD12	1.91	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c1:257:GLU:HG2	4:c1:436:ALA:HB2	1.92	0.50
41:d1:408:LHG:H331	41:d1:408:LHG:H102	1.93	0.50
47:g1:605:CHL:HHC	47:g1:605:CHL:HBB1	1.92	0.50
27:r1:87:ILE:HA	27:r1:104:VAL:HA	1.93	0.50
1:A:78:ILE:HG13	12:L:35:TYR:HE1	1.76	0.50
2:B:256:MET:O	2:B:448:ARG:NH1	2.45	0.50
2:B:442:VAL:HA	14:O:229:PRO:HD2	1.94	0.50
4:C:87:VAL:HG21	4:C:289:PHE:HZ	1.76	0.50
14:O:216:ARG:HB3	14:O:243:LYS:HE2	1.92	0.50
31:G:603:CLA:H152	47:G:609:CHL:H102	1.93	0.50
1:a:163:ILE:HD11	40:c:518:DGD:HA31	1.94	0.50
4:c:59:GLU:HG2	4:c:74:LEU:HD22	1.93	0.50
31:g:602:CLA:H101	48:g:621:LUT:H371	1.92	0.50
47:s:607:CHL:HHC	47:s:607:CHL:HBB1	1.92	0.50
34:B1:621:SQD:H151	34:M1:101:SQD:H122	1.93	0.50
4:C1:167:ALA:HA	4:C1:172:GLY:HA2	1.94	0.50
1:a1:28:LEU:HD21	5:d1:258:GLY:HA2	1.94	0.50
2:b1:30:VAL:HG12	31:b1:606:CLA:HHD	1.93	0.50
4:c1:104:VAL:HG21	33:c1:514:BCR:HC32	1.94	0.50
4:c1:287:SER:OG	4:c1:296:GLU:OE1	2.30	0.50
15:p1:178:ASP:OD1	15:p1:182:LYS:N	2.38	0.50
2:B:458:PHE:HB3	31:B:605:CLA:HBC2	1.92	0.50
24:Y:49:PHE:HB3	24:Y:69:TYR:HB3	1.93	0.50
1:a:97:TRP:CD1	9:i:5:LYS:HD2	2.46	0.50
5:d:12:ARG:NH2	5:d:20:ASP:OD2	2.44	0.50
1:A1:221:SER:HA	5:D1:139:ARG:HB3	1.91	0.50
2:B1:361:THR:HG22	5:D1:292:ASN:HD22	1.75	0.50
31:B1:604:CLA:H152	8:H1:57:PHE:HE2	1.77	0.50
4:C1:48:ILE:HG22	31:C1:503:CLA:HHD	1.93	0.50
4:C1:272:PHE:HB3	40:C1:518:DGD:HB51	1.93	0.50
14:O1:192:THR:HG23	14:O1:195:SER:H	1.77	0.50
15:P1:99:VAL:HG12	15:P1:101:SER:H	1.76	0.50
31:N1:602:CLA:H52	48:N1:621:LUT:H28	1.92	0.50
47:G1:608:CHL:HBB1	47:G1:608:CHL:HHC	1.93	0.50
35:a1:413:LMG:H291	4:c1:205:PRO:HD3	1.92	0.50
31:b1:611:CLA:H43	31:b1:613:CLA:H51	1.93	0.50
4:c1:439:ALA:HA	4:c1:444:GLU:HB3	1.94	0.50
21:g1:146:LEU:HD21	49:g1:622:XAT:H202	1.92	0.50
27:r1:206:LEU:O	27:r1:211:ARG:NH1	2.44	0.50
24:y1:102:LEU:HD13	31:y1:612:CLA:HBB2	1.94	0.50
24:y1:198:PRO:HA	24:y1:201:PHE:HB3	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:95:PRO:HD2	1:A:98:GLU:HB2	1.92	0.50
1:A:191:ASN:HB2	4:C:399:ALA:HB1	1.94	0.50
1:A:286:THR:OG1	31:A:405:CLA:O1D	2.29	0.50
31:C:503:CLA:H101	31:C:507:CLA:H42	1.92	0.50
23:S:61:LEU:HD22	23:S:65:LEU:HD23	1.93	0.50
31:b:610:CLA:OBD	8:h:46:THR:OG1	2.28	0.50
5:d:274:VAL:HG23	5:d:275:PRO:HD3	1.93	0.50
20:n:204:VAL:HA	20:n:207:ILE:HG22	1.94	0.50
31:n:603:CLA:H71	31:g:603:CLA:H71	1.94	0.50
21:g:47:ASN:ND2	24:y:171:ASN:O	2.45	0.50
23:s:246:VAL:HA	23:s:249:PHE:HD2	1.76	0.50
47:s:608:CHL:HHC	47:s:608:CHL:HBB1	1.94	0.50
1:A1:180:PHE:HA	1:A1:183:MET:HB3	1.93	0.50
1:A1:181:ASN:HD22	5:D1:314:PHE:HD1	1.59	0.50
4:C1:187:ILE:HG13	4:C1:222:ILE:HG13	1.94	0.50
5:D1:53:THR:HG22	5:D1:67:TYR:CD2	2.46	0.50
5:D1:80:THR:HG22	5:D1:111:TRP:CE2	2.47	0.50
6:E1:51:ARG:NH1	6:E1:53:ASN:OD1	2.45	0.50
31:Y1:613:CLA:H12	31:Y1:614:CLA:HED2	1.94	0.50
1:a1:228:THR:HA	27:r1:97:ALA:HA	1.93	0.50
4:c1:112:VAL:HB	33:c1:514:BCR:H362	1.94	0.50
4:c1:227:TRP:CH2	31:y1:614:CLA:HAB	2.46	0.50
5:d1:189:HIS:HA	5:d1:294:ARG:HG2	1.93	0.50
5:d1:236:ASN:ND2	5:d1:238:THR:O	2.45	0.50
47:r1:607:CHL:HBB1	47:r1:607:CHL:HHC	1.94	0.50
1:A:296:ASN:HB3	4:C:389:LEU:HD13	1.92	0.50
47:S:608:CHL:H12	48:S:620:LUT:H373	1.93	0.50
2:b:170:ASP:HB2	2:b:175:THR:H	1.77	0.50
31:b:602:CLA:HAB	46:h:101:RRX:H32	1.93	0.50
4:c:67:LYS:HE2	4:c:71:GLU:HG3	1.93	0.50
4:c:319:ALA:O	14:o:165:TYR:OH	2.21	0.50
13:m:13:LEU:HA	13:m:16:ILE:HG12	1.93	0.50
47:n:607:CHL:HBB2	47:n:609:CHL:HBC1	1.92	0.50
47:y:609:CHL:HHC	47:y:609:CHL:HBB1	1.93	0.50
1:A1:337:HIS:HE1	5:D1:352:LEU:HD22	1.75	0.50
47:N1:601:CHL:H171	47:G1:607:CHL:H161	1.94	0.50
47:Y1:605:CHL:HBB1	47:Y1:605:CHL:HHC	1.92	0.50
31:Y1:614:CLA:HMB2	57:Y1:626:PTY:H161	1.94	0.50
2:b1:369:VAL:HG23	2:b1:380:ASP:HB3	1.93	0.50
4:c1:246:PRO:HA	4:c1:249:ARG:HG2	1.94	0.50
4:c1:257:GLU:OE2	4:c1:432:HIS:ND1	2.44	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
14:o1:297:GLN:NE2	14:o1:298:LEU:O	2.44	0.50
20:n1:247:ALA:HB1	49:g1:622:XAT:H161	1.94	0.50
21:g1:39:LYS:NZ	21:g1:45:SER:O	2.37	0.50
2:B:326:ARG:HB3	2:B:444:ARG:HD3	1.93	0.50
2:B:384:ARG:HH21	15:P:193:THR:HG21	1.76	0.50
49:N:622:XAT:H163	24:Y:228:VAL:HG21	1.93	0.50
2:b:170:ASP:HB3	2:b:174:LEU:H	1.76	0.50
47:s:606:CHL:HHC	47:s:606:CHL:HBB1	1.92	0.50
31:y:610:CLA:H142	31:y:612:CLA:H172	1.93	0.50
4:C1:102:SER:O	4:C1:106:HIS:ND1	2.35	0.50
4:C1:338:ILE:HG21	4:C1:347:TRP:HB2	1.93	0.50
26:M1:16:ILE:HD13	26:m1:17:ILE:HD11	1.93	0.50
21:G1:162:ASN:ND2	21:G1:164:GLY:O	2.44	0.50
2:b1:26:HIS:CE1	31:b1:613:CLA:HMB2	2.46	0.50
14:o1:140:LEU:HD21	14:o1:165:TYR:C	2.37	0.50
23:s1:152:PHE:HD1	23:s1:158:VAL:H	1.58	0.50
2:B:372:ASP:HB2	2:B:378:ARG:HG3	1.92	0.50
4:C:69:MET:HG2	4:C:74:LEU:HD12	1.93	0.50
24:Y:76:LEU:HD12	31:Y:602:CLA:C4	2.42	0.50
24:Y:99:LEU:HB3	31:Y:604:CLA:HAB	1.94	0.50
23:s:240:ARG:HA	23:s:243:MET:HG3	1.93	0.50
31:s:611:CLA:H203	31:s:612:CLA:HBB1	1.94	0.50
14:O1:104:LEU:HD22	14:O1:147:MET:HB2	1.94	0.50
47:N1:606:CHL:HHC	47:N1:606:CHL:HBB1	1.93	0.50
1:a1:114:LEU:O	1:a1:118:HIS:ND1	2.44	0.50
4:c1:41:HIS:O	4:c1:45:ALA:N	2.43	0.50
21:g1:87:ARG:HA	21:g1:90:LEU:HD12	1.93	0.50
21:g1:91:LEU:HD13	31:g1:604:CLA:HBB2	1.94	0.50
1:A:93:PHE:HB2	4:C:206:PHE:CG	2.46	0.50
1:A:343:LEU:HD11	4:C:387:ALA:HB1	1.94	0.50
31:B:608:CLA:H201	13:M:11:THR:HA	1.94	0.50
40:C:523:DGD:HAH1	53:Y:625:SPH:H102	1.94	0.50
11:K:18:PHE:HD2	11:K:21:ILE:HD11	1.76	0.50
47:N:601:CHL:H102	49:G:622:XAT:H12	1.94	0.50
47:Y:606:CHL:HHC	47:Y:606:CHL:HBB1	1.94	0.50
9:i:9:TYR:HD2	17:w:85:ILE:HD11	1.77	0.50
31:B1:608:CLA:H122	35:B1:622:LMG:H332	1.93	0.50
5:D1:259:VAL:HG13	16:T1:21:ILE:HG22	1.94	0.50
23:S1:217:ASP:OD1	48:S1:620:LUT:O23	2.30	0.50
23:S1:241:LEU:HG	41:S1:624:LHG:H242	1.94	0.50
1:a1:124[B]:CYS:HB3	31:c1:505:CLA:HBB2	1.93	0.50

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:a1:257:ARG:HA	1:a1:261:GLN:HE22	1.76	0.50
1:a1:281:VAL:HA	1:a1:284:TRP:HB2	1.94	0.50
49:n1:622:XAT:H34	31:y1:613:CLA:H111	1.93	0.50
1:A:309:SER:HA	7:F:44:ARG:HB2	1.94	0.49
35:A:413:LMG:H191	31:C:505:CLA:H8	1.94	0.49
35:A:413:LMG:H381	31:C:505:CLA:H143	1.94	0.49
44:D:405:PL9:H513	16:T:10:LEU:HD22	1.93	0.49
31:N:602:CLA:H151	31:G:603:CLA:H143	1.93	0.49
1:a:315:ASN:ND2	5:d:332:GLN:OE1	2.37	0.49
31:b:612:CLA:H172	31:b:614:CLA:H8	1.94	0.49
31:c:509:CLA:H143	31:c:509:CLA:HAA1	1.94	0.49
41:g:624:LHG:O1	49:y:622:XAT:O23	2.29	0.49
31:y:610:CLA:H93	31:y:612:CLA:H8	1.94	0.49
2:B1:41:GLU:HB3	2:B1:60:MET:HE1	1.94	0.49
2:B1:74:SER:HB2	2:B1:93:TYR:HD2	1.77	0.49
2:B1:340:TRP:NE1	2:B1:428:GLU:OE2	2.45	0.49
31:B1:605:CLA:HBB1	31:B1:608:CLA:CAB	2.42	0.49
4:C1:287:SER:HA	4:C1:411:ARG:HH21	1.77	0.49
12:L1:22:LEU:HA	12:L1:25:ILE:HG12	1.94	0.49
24:Y1:104:ILE:HD13	48:Y1:621:LUT:H41	1.94	0.49
47:Y1:609:CHL:HHC	47:Y1:609:CHL:HBB1	1.92	0.49
4:c1:264:LEU:HD21	31:c1:508:CLA:HAB	1.94	0.49
20:n1:238:HIS:ND1	20:n1:245:ASN:O	2.40	0.49
57:y1:626:PTY:H401	57:y1:626:PTY:H212	1.94	0.49
4:C:43:ALA:HB2	4:C:117:GLY:HA3	1.94	0.49
20:N:231:PRO:HG2	20:N:232:ILE:HD12	1.94	0.49
1:a:291:SER:HB3	4:c:419:PHE:HE2	1.77	0.49
31:a:410:CLA:HAB	9:i:15:PHE:CD2	2.47	0.49
31:b:605:CLA:HAB	31:b:612:CLA:H191	1.94	0.49
4:c:267:VAL:HG22	31:c:502:CLA:HAC1	1.94	0.49
6:e:23:HIS:NE2	45:f:101:HEM:ND	2.59	0.49
31:n:602:CLA:H62	48:n:621:LUT:H28	1.93	0.49
4:C1:246:PRO:HA	4:C1:249:ARG:HG2	1.93	0.49
38:C1:524:DGA:HAF1	35:W1:201:LMG:H352	1.93	0.49
31:R1:604:CLA:HAC2	31:y1:604:CLA:H151	1.93	0.49
1:a1:124[A]:CYS:HB3	31:c1:505:CLA:HBB2	1.93	0.49
2:b1:477:ASP:OD2	5:d1:134:ARG:NH2	2.45	0.49
31:b1:608:CLA:H52	35:b1:622:LMG:H151	1.93	0.49
4:c1:74:LEU:HD13	4:c1:77:LEU:HD12	1.92	0.49
5:d1:187:GLY:O	5:d1:326:ARG:NH1	2.40	0.49
14:o1:197:SER:HB3	14:o1:253:VAL:HG22	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:139:MET:HE1	5:D:252:PHE:HB2	1.93	0.49
4:C:191:THR:HG23	4:C:219:GLU:HB3	1.93	0.49
4:C:287:SER:OG	4:C:296:GLU:OE2	2.30	0.49
4:C:307:VAL:HA	4:C:310:GLN:HG2	1.95	0.49
47:N:601:CHL:HBB1	47:N:601:CHL:HHC	1.92	0.49
31:G:613:CLA:H12	31:G:614:CLA:HED2	1.94	0.49
31:Y:612:CLA:HAB	48:Y:620:LUT:C14	2.42	0.49
1:a:24:THR:HG23	4:c:457:MET:HE3	1.94	0.49
4:c:157:GLY:HA3	4:c:233:ILE:HG13	1.94	0.49
4:c:315:ASN:HD22	14:o:161:GLU:HG3	1.77	0.49
33:d:404:BCR:H14C	7:f:32:PHE:CD2	2.47	0.49
20:n:98:LEU:HB3	31:n:604:CLA:HAB	1.93	0.49
1:A1:143:ILE:HG21	5:D1:253:TRP:HH2	1.77	0.49
14:O1:132:LEU:HD13	17:W1:61:VAL:HG21	1.94	0.49
20:n1:161:MET:HA	20:n1:164:VAL:HB	1.93	0.49
47:y1:606:CHL:HHC	47:y1:606:CHL:HBB1	1.94	0.49
4:C:63:PHE:HE2	4:C:93:VAL:HG11	1.77	0.49
4:C:166:LYS:HA	4:C:170:PHE:HB2	1.95	0.49
4:C:267:VAL:HG22	31:C:502:CLA:HAC1	1.94	0.49
1:a:85:THR:HG21	1:a:113:GLN:HG3	1.93	0.49
1:a:225:ARG:HG3	2:b:481:GLY:HA2	1.94	0.49
32:a:409:PHO:H2A	32:a:409:PHO:HED2	1.94	0.49
2:B1:5:TRP:NE1	41:L1:101:LHG:O10	2.43	0.49
2:B1:256:MET:O	2:B1:448:ARG:NH1	2.44	0.49
34:B1:626:SQD:H361	1:a1:42:LEU:HD11	1.93	0.49
9:I1:27:ASP:HA	9:I1:30:ARG:HG3	1.94	0.49
23:S1:285:ARG:HH12	23:S1:287:PRO:HA	1.76	0.49
24:Y1:111:ALA:HB2	24:Y1:117:PHE:HD2	1.77	0.49
21:g1:211:CYS:HA	21:g1:214:PHE:HD2	1.77	0.49
21:g1:231:ASP:HB3	21:g1:239:ASN:HD21	1.77	0.49
23:s1:245:ALA:O	23:s1:249:PHE:N	2.45	0.49
31:s1:602:CLA:H2	48:s1:621:LUT:H24	1.95	0.49
24:y1:126:LYS:HA	47:y1:607:CHL:HED3	1.94	0.49
1:A:13:LEU:HD13	22:r:217:ALA:HA	1.95	0.49
2:B:384:ARG:HD3	5:D:348:ARG:HH22	1.77	0.49
47:g:609:CHL:HHC	47:g:609:CHL:HBB1	1.93	0.49
3:V1:25:LEU:HA	3:V1:28:VAL:HG22	1.94	0.49
31:N1:610:CLA:H61	31:N1:612:CLA:HMA3	1.94	0.49
1:a1:193:LEU:HD21	1:a1:202:VAL:HG21	1.93	0.49
4:c1:36:LYS:NZ	31:c1:511:CLA:H2A	2.27	0.49
16:t1:14:LEU:HD23	16:t1:17:ILE:HD11	1.95	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:357:ARG:NH1	2:B:358:ARG:O	2.46	0.49
38:B:625:DGA:HA82	5:D:127:LEU:HD13	1.93	0.49
4:C:454:VAL:HG21	5:D:248:THR:HA	1.95	0.49
5:D:19:ASP:OD1	5:D:32:TRP:NE1	2.41	0.49
20:N:202:LEU:HB3	31:N:610:CLA:HMA3	1.94	0.49
47:N:606:CHL:H192	52:S:626:3PH:H2A1	1.94	0.49
1:a:269:ARG:NH1	5:d:231:THR:OG1	2.46	0.49
31:b:602:CLA:CAB	46:h:101:RRX:H32	2.43	0.49
31:c:501:CLA:C1B	31:c:501:CLA:H2	2.42	0.49
40:c:520:DGD:HBH2	35:d:411:LMG:H192	1.94	0.49
14:o:116:VAL:HG22	14:o:288:ILE:HG12	1.93	0.49
21:g:173:ASP:OD2	21:g:176:TYR:N	2.46	0.49
46:H1:101:RRX:H46	18:X1:69:LEU:HD11	1.95	0.49
47:G1:601:CHL:HHC	47:G1:601:CHL:HBB1	1.92	0.49
4:C:30:LEU:HD21	31:C:511:CLA:HMA2	1.94	0.49
4:C:167:ALA:HB1	4:C:187:ILE:HD12	1.94	0.49
5:D:87:HIS:CD2	5:D:162:LEU:HA	2.48	0.49
25:U:94:VAL:HA	25:U:97:MET:HB2	1.93	0.49
1:a:269:ARG:NH2	5:d:225:ASP:OD2	2.45	0.49
2:b:70:GLY:HA2	2:b:178:VAL:HG11	1.94	0.49
2:b:403:GLY:O	2:b:407:ASN:ND2	2.46	0.49
2:b:463:PHE:HZ	5:d:150:ILE:HD11	1.78	0.49
23:s:61:LEU:HB2	23:s:66:LEU:HB2	1.94	0.49
1:A1:285:LEU:O	1:A1:289:GLY:N	2.41	0.49
31:B1:604:CLA:HHC	31:B1:606:CLA:H161	1.94	0.49
5:D1:285:GLY:O	5:D1:289:LEU:N	2.45	0.49
21:G1:198:VAL:HA	21:G1:201:ILE:HG22	1.94	0.49
47:Y1:606:CHL:HHC	47:Y1:606:CHL:HBB1	1.95	0.49
1:a1:40:THR:HG22	1:a1:118:HIS:HD2	1.77	0.49
1:a1:201:GLY:HA2	1:a1:282:CYS:HB3	1.95	0.49
1:a1:234:ASN:O	5:d1:263:ASN:ND2	2.32	0.49
1:a1:257:ARG:HG3	5:d1:132:ILE:HD13	1.95	0.49
2:b1:18:ARG:NE	2:b1:115:TRP:O	2.45	0.49
2:b1:141:ILE:HD13	31:b1:616:CLA:HBB1	1.94	0.49
4:c1:122:LEU:HD13	19:z1:28:ALA:HB2	1.94	0.49
4:c1:427:VAL:HA	4:c1:430:LEU:HB2	1.95	0.49
35:c1:521:LMG:H172	11:k1:27:ILE:HD13	1.95	0.49
20:n1:182:TYR:HB3	31:n1:610:CLA:HED3	1.95	0.49
47:g1:601:CHL:H171	47:y1:607:CHL:H152	1.95	0.49
47:r1:606:CHL:HHC	47:r1:606:CHL:HBB1	1.95	0.49
31:y1:610:CLA:H93	31:y1:612:CLA:H8	1.94	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:142:LYS:HE2	4:C:249:ARG:HG2	1.95	0.49
15:P:108:ASP:OD1	15:P:108:ASP:N	2.46	0.49
18:X:70:LYS:HE2	18:X:74:LEU:HD21	1.94	0.49
20:N:208:LYS:NZ	31:N:611:CLA:O2D	2.46	0.49
2:b:299:SER:HA	2:b:402:TYR:HB3	1.93	0.49
2:B1:221:PRO:HG2	8:H1:40:VAL:HG12	1.94	0.49
4:C1:444:GLU:HG2	4:C1:445:LYS:HG3	1.94	0.49
7:F1:44:ARG:NH1	10:J1:42:LEU:OXT	2.45	0.49
16:T1:1:MET:HE3	52:b1:624:3PH:H332	1.93	0.49
1:a1:343:LEU:HD22	4:c1:389:LEU:HD13	1.95	0.49
2:b1:326:ARG:HB3	2:b1:444:ARG:HD3	1.94	0.49
47:g1:606:CHL:HBB1	47:g1:606:CHL:HHC	1.95	0.49
1:A:93:PHE:HZ	31:A:410:CLA:HAA1	1.77	0.49
2:B:190:PHE:HZ	31:B:602:CLA:HBB1	1.77	0.49
4:C:198:PHE:HA	4:C:201:ILE:HG22	1.94	0.49
31:C:512:CLA:H193	34:C:526:SQD:H281	1.95	0.49
6:E:74:GLU:HA	6:E:77:LYS:HE3	1.95	0.49
20:N:71:ASP:O	21:G:77:ARG:NE	2.39	0.49
23:S:152:PHE:HD1	23:S:157:GLY:HA3	1.78	0.49
4:c:162:LEU:HD21	31:c:502:CLA:H203	1.94	0.49
4:c:209:ASP:O	4:c:214:SER:OG	2.31	0.49
5:d:186:GLN:HB2	31:d:402:CLA:HBC1	1.94	0.49
31:n:610:CLA:CAB	48:n:620:LUT:H32	2.43	0.49
21:g:231:ASP:OD2	21:g:239:ASN:ND2	2.46	0.49
1:A1:58:VAL:HB	1:A1:83:VAL:HB	1.95	0.49
1:A1:330:VAL:O	5:D1:349:GLY:N	2.41	0.49
4:C1:49:VAL:HG13	4:C1:106:HIS:HD2	1.78	0.49
20:N1:247:ALA:HB1	49:G1:622:XAT:H161	1.93	0.49
31:S1:604:CLA:H62	50:S1:623:NEX:H373	1.95	0.49
24:Y1:76:LEU:HD13	31:Y1:602:CLA:H42	1.95	0.49
31:a1:407:CLA:HAB	31:d1:402:CLA:H51	1.95	0.49
31:c1:512:CLA:HMB1	41:c1:525:LHG:H112	1.94	0.49
8:h1:29:LEU:HD12	27:r1:200:VAL:HA	1.94	0.49
47:g1:601:CHL:HHC	47:g1:601:CHL:HBB1	1.94	0.49
5:D:178:ILE:O	5:D:182:ILE:HG12	2.13	0.49
5:D:350:ASN:O	5:D:352:LEU:N	2.45	0.49
47:S:607:CHL:HHC	47:S:607:CHL:HBB1	1.93	0.49
21:G1:85:HIS:HD2	48:G1:621:LUT:H201	1.78	0.49
47:R1:607:CHL:HHC	47:R1:607:CHL:HBB1	1.95	0.49
31:b1:602:CLA:H162	46:h1:101:RRX:H39	1.95	0.49
4:c1:261:SER:HB2	4:c1:429:HIS:HD2	1.77	0.49

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:c1:504:CLA:HBB1	40:c1:519:DGD:HB82	1.95	0.49
8:h1:62:LEU:HA	8:h1:65:LEU:HB2	1.95	0.49
15:p1:182:LYS:NZ	15:p1:209:VAL:O	2.46	0.49
47:n1:601:CHL:HBB1	47:n1:601:CHL:HHC	1.94	0.49
23:s1:80:ALA:O	23:s1:101:ARG:NH2	2.45	0.49
23:s1:92:LYS:HB2	23:s1:96:GLN:HE21	1.78	0.49
24:y1:139:TYR:HB3	24:y1:145:LEU:HB3	1.95	0.49
31:B:610:CLA:O2A	46:H:101:RRX:O2	2.31	0.48
31:Y:603:CLA:H172	47:Y:607:CHL:H143	1.95	0.48
40:c:523:DGD:HAH1	53:y:625:SPH:H102	1.94	0.48
41:y:624:LHG:O1	53:y:625:SPH:N2	2.39	0.48
1:A1:209:SER:HB3	5:D1:204:VAL:HG13	1.94	0.48
4:C1:139:TRP:HH2	31:C1:509:CLA:H191	1.79	0.48
2:b1:60:MET:HB3	2:b1:63:LEU:HB3	1.94	0.48
2:b1:158:VAL:HA	2:b1:165:GLY:HA2	1.95	0.48
4:c1:241:TYR:HB2	53:y1:625:SPH:H92	1.94	0.48
14:o1:140:LEU:HD23	14:o1:163:LEU:HD22	1.94	0.48
14:o1:224:ASN:HA	14:o1:240:LEU:HD13	1.95	0.48
21:g1:94:LEU:HB3	31:g1:604:CLA:HMC2	1.94	0.48
24:y1:177:VAL:HB	24:y1:180:LEU:HD13	1.95	0.48
24:y1:240:HIS:ND1	24:y1:247:ASN:O	2.37	0.48
5:D:328:TRP:HZ2	5:D:348:ARG:HB2	1.78	0.48
2:b:330:MET:HA	2:b:444:ARG:HB2	1.94	0.48
5:d:119:ALA:O	5:d:123:ILE:HG12	2.13	0.48
21:g:194:ALA:HA	21:g:197:LYS:HE2	1.95	0.48
31:g:602:CLA:CBB	48:g:621:LUT:H32	2.43	0.48
24:y:174:ALA:HB3	24:y:177:VAL:HB	1.95	0.48
2:B1:371:ILE:HG23	25:U1:100:PRO:HB2	1.94	0.48
11:K1:22:VAL:HA	11:K1:25:LEU:HD12	1.93	0.48
21:G1:245:ALA:HA	49:Y1:622:XAT:H22	1.95	0.48
31:a1:410:CLA:H2	9:i1:12:VAL:HG21	1.95	0.48
2:b1:467:ILE:O	2:b1:471:SER:OG	2.26	0.48
31:b1:615:CLA:H2	34:b1:621:SQD:H262	1.95	0.48
41:c1:525:LHG:H162	31:s1:611:CLA:HBB2	1.94	0.48
5:d1:12:ARG:NH2	5:d1:20:ASP:OD2	2.46	0.48
21:g1:217:GLN:O	21:g1:221:THR:OG1	2.22	0.48
33:B:618:BCR:H402	34:B:621:SQD:H461	1.96	0.48
38:C:524:DGA:HB42	38:C:524:DGA:HA51	1.95	0.48
1:a:228:THR:OG1	1:a:229:GLU:N	2.46	0.48
2:b:236:SER:HB2	2:b:473:THR:HG21	1.94	0.48
2:b:392:ILE:HG23	2:b:397:VAL:HG22	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:b:615:CLA:H12	34:b:621:SQD:H262	1.95	0.48
4:c:102:SER:O	4:c:106:HIS:ND1	2.45	0.48
15:p:207:ALA:HB1	15:p:214:LEU:HD21	1.95	0.48
20:n:45:ARG:NH2	20:n:60:LEU:O	2.45	0.48
21:g:82:GLU:OE2	21:g:205:ARG:NH2	2.40	0.48
31:y:602:CLA:CAB	48:y:621:LUT:H32	2.43	0.48
25:u:94:VAL:HA	25:u:97:MET:HG3	1.94	0.48
31:A1:406:CLA:H72	32:A1:408:PHO:HMA1	1.96	0.48
31:C1:507:CLA:H112	33:C1:515:BCR:H362	1.95	0.48
1:a1:277:VAL:HG23	41:d1:410:LHG:H292	1.95	0.48
4:c1:36:LYS:HZ1	31:c1:511:CLA:H2A	1.77	0.48
35:c1:523:LMG:HC5	31:y1:611:CLA:HMA3	1.94	0.48
47:n1:606:CHL:HHC	47:n1:606:CHL:HBB1	1.95	0.48
24:y1:105:ILE:HG23	24:y1:234:ILE:HD11	1.95	0.48
24:y1:142:ASN:OD1	24:y1:144:ASN:ND2	2.46	0.48
5:D:161:PRO:HB3	5:D:170:ALA:HB2	1.95	0.48
15:P:68:ARG:NH1	15:P:69:VAL:O	2.46	0.48
20:N:82:PHE:O	20:N:86:ARG:HG3	2.13	0.48
23:S:88:LEU:HD13	48:S:621:LUT:H222	1.96	0.48
24:Y:101:ALA:O	24:Y:105:ILE:HG12	2.13	0.48
1:a:114:LEU:O	1:a:118:HIS:ND1	2.45	0.48
4:c:246:PRO:HD3	4:c:249:ARG:HH21	1.79	0.48
14:o:132:LEU:HD22	17:w:61:VAL:HG21	1.96	0.48
31:s:610:CLA:H152	31:s:610:CLA:H111	1.68	0.48
15:P1:119:ILE:HD12	15:P1:216:LEU:HD22	1.94	0.48
15:P1:225:ARG:HE	15:P1:228:LYS:HE2	1.79	0.48
21:G1:217:GLN:O	21:G1:221:THR:OG1	2.24	0.48
31:S1:610:CLA:H2	48:S1:620:LUT:H373	1.95	0.48
24:Y1:137:LEU:HD21	31:Y1:604:CLA:HAA2	1.96	0.48
31:c1:513:CLA:H122	33:c1:514:BCR:H23C	1.95	0.48
5:d1:225:ASP:HB2	5:d1:234:ALA:HB1	1.94	0.48
20:n1:217:CYS:HB3	48:n1:621:LUT:H12	1.94	0.48
35:A:413:LMG:H301	31:C:505:CLA:H192	1.94	0.48
2:B:236:SER:HA	2:B:473:THR:HG21	1.94	0.48
21:G:128:LEU:HD21	31:G:604:CLA:HAA2	1.95	0.48
9:i:21:PHE:O	9:i:25:SER:HB3	2.13	0.48
22:r:199:GLU:OE1	22:r:202:ARG:NH2	2.45	0.48
22:r:216:GLY:HA3	31:r:608:CLA:H142	1.95	0.48
2:B1:137:LYS:HZ1	2:B1:217:LEU:HD22	1.78	0.48
31:B1:602:CLA:H3A	31:B1:602:CLA:HBA2	1.61	0.48
5:D1:160:TYR:HD1	5:D1:290:ALA:HA	1.78	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b1:124:ARG:HH21	8:h1:21:GLY:HA2	1.79	0.48
2:b1:170:ASP:CG	2:b1:174:LEU:H	2.21	0.48
2:b1:175:THR:OG1	2:b1:176:GLY:N	2.46	0.48
4:c1:71:GLU:HA	4:c1:407:PHE:HE1	1.78	0.48
14:o1:99:PRO:HA	14:o1:149:ILE:HB	1.93	0.48
31:g1:602:CLA:H52	48:g1:621:LUT:H28	1.95	0.48
31:s1:611:CLA:H91	31:s1:611:CLA:H142	1.95	0.48
1:A:170:ASP:OD2	4:C:345:ARG:NH1	2.47	0.48
4:C:277:PHE:HB3	4:C:285:TYR:CE2	2.48	0.48
8:H:57:PHE:CE1	46:H:101:RRX:H22	2.49	0.48
47:R:607:CHL:HBB1	47:R:607:CHL:HHC	1.95	0.48
31:b:604:CLA:H192	31:b:610:CLA:H91	1.95	0.48
38:b:623:DGA:HAG2	18:x:83:LEU:HD21	1.96	0.48
31:c:508:CLA:HED2	41:d:410:LHG:HC2	1.95	0.48
5:d:43:PHE:HE1	33:d:404:BCR:H323	1.78	0.48
19:z:46:VAL:O	19:z:50:LEU:HG	2.13	0.48
47:g:608:CHL:HHC	47:g:608:CHL:HBB1	1.94	0.48
24:y:185:PRO:HB3	31:y:608:CLA:HBC2	1.95	0.48
1:A1:131:TRP:HZ2	4:C1:437:ARG:HD3	1.79	0.48
4:C1:425:PHE:O	4:C1:429:HIS:N	2.38	0.48
40:C1:519:DGD:HA61	35:C1:521:LMG:H362	1.94	0.48
5:D1:351:ALA:HA	15:P1:197:ASN:HA	1.94	0.48
14:O1:82:ASN:HD22	14:O1:136:LEU:HD22	1.79	0.48
27:R1:219:ASP:OD1	48:R1:620:LUT:O23	2.30	0.48
24:Y1:112:LYS:NZ	57:Y1:627:PTY:O4	2.44	0.48
1:a1:220:THR:O	5:d1:139:ARG:NH2	2.36	0.48
2:b1:117:TYR:HD1	8:h1:22:ILE:HD13	1.78	0.48
2:b1:230:SER:O	2:b1:236:SER:OG	2.30	0.48
4:c1:392:LEU:HD13	40:c1:520:DGD:HB51	1.94	0.48
27:r1:160:VAL:HG11	27:r1:168:VAL:HG21	1.95	0.48
5:D:122:LEU:HD22	5:D:150:ILE:HG22	1.96	0.48
47:G:601:CHL:HHC	47:G:601:CHL:HBB1	1.96	0.48
23:S:268:LEU:HD13	31:S:614:CLA:HAB	1.95	0.48
31:S:602:CLA:HBA2	31:S:602:CLA:H3A	1.57	0.48
24:Y:135:GLY:O	24:Y:147:HIS:ND1	2.44	0.48
1:a:36:ILE:HA	31:a:410:CLA:HBB2	1.95	0.48
4:c:88:GLY:N	4:c:92:GLU:O	2.37	0.48
47:s:608:CHL:HAB	31:s:617:CLA:HMD1	1.95	0.48
28:A1:401:OEX:O2	4:C1:345:ARG:NH2	2.45	0.48
2:B1:158:VAL:HA	2:B1:165:GLY:HA2	1.96	0.48
31:B1:612:CLA:H102	41:L1:101:LHG:H331	1.96	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
7:F1:22:ILE:HG12	45:F1:101:HEM:HMD3	1.96	0.48
57:Y1:626:PTY:H182	57:Y1:626:PTY:H362	1.96	0.48
34:a1:412:SQD:H62	5:d1:233:ARG:HD3	1.96	0.48
5:d1:223:PHE:HE2	5:d1:242:GLU:HG3	1.79	0.48
20:n1:130:ILE:HG22	20:n1:136:LEU:HB2	1.95	0.48
21:g1:91:LEU:HB3	31:g1:604:CLA:CAB	2.44	0.48
8:H:57:PHE:CD2	46:H:101:RRX:C23	2.97	0.48
24:Y:131:ILE:HA	24:Y:136:GLY:HA2	1.94	0.48
1:a:297:LEU:HD13	4:c:416:THR:HG21	1.96	0.48
35:h:102:LMG:H151	35:h:102:LMG:H182	1.61	0.48
21:g:150:VAL:HG23	47:g:609:CHL:HBB2	1.96	0.48
31:s:603:CLA:HAA1	31:s:609:CLA:H42	1.94	0.48
24:y:213:ARG:HA	24:y:216:MET:HG2	1.95	0.48
1:A1:95:PRO:HD2	1:A1:98:GLU:HB2	1.94	0.48
44:D1:405:PL9:H513	16:T1:10:LEU:HD22	1.94	0.48
12:L1:32:PHE:HA	12:L1:35:TYR:HD2	1.79	0.48
27:R1:154:GLY:O	27:R1:158:THR:OG1	2.31	0.48
1:a1:123:VAL:HB	1:a1:151:VAL:HG22	1.96	0.48
1:a1:157:VAL:HG23	1:a1:158:PHE:HD1	1.79	0.48
33:a1:411:BCR:H373	53:a1:414:SPH:H101	1.95	0.48
2:b1:74:SER:HB3	2:b1:93:TYR:HD2	1.78	0.48
2:b1:224:ARG:HH12	2:b1:228:GLY:HA3	1.79	0.48
15:p1:148:GLN:NE2	15:p1:150:TRP:O	2.46	0.48
21:g1:157:GLU:OE1	21:g1:160:ARG:NH2	2.39	0.48
2:B:245:VAL:HG22	31:B:605:CLA:HAC1	1.95	0.48
31:B:609:CLA:H101	38:B:625:DGA:HAV1	1.95	0.48
31:B:617:CLA:HMD3	8:H:24:THR:HG21	1.94	0.48
41:d:409:LHG:H141	41:d:409:LHG:H282	1.96	0.48
6:e:8:ARG:NH2	7:f:18:ARG:HE	2.12	0.48
4:C1:166:LYS:NZ	4:C1:172:GLY:O	2.37	0.48
4:C1:270:MET:HE1	31:C1:501:CLA:H112	1.95	0.48
31:C1:505:CLA:H203	40:C1:518:DGD:HA41	1.94	0.48
40:C1:519:DGD:HA31	35:C1:521:LMG:H342	1.94	0.48
31:D1:402:CLA:H62	31:D1:402:CLA:H41	1.59	0.48
20:N1:166:GLY:HA3	24:Y1:53:LEU:HD13	1.95	0.48
27:R1:78:LEU:HD22	49:R1:621:XAT:H23	1.96	0.48
1:a1:329:GLU:O	1:a1:332:HIS:ND1	2.27	0.48
4:c1:237:ILE:HD11	34:c1:526:SQD:H121	1.96	0.48
4:c1:291:GLY:O	4:c1:411:ARG:NE	2.27	0.48
27:r1:201:LEU:HA	27:r1:204:ASN:HB2	1.95	0.48
27:r1:236:LYS:HD3	31:r1:610:CLA:HMA3	1.95	0.48

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:B:615:CLA:H12	34:B:621:SQD:H241	1.95	0.48
21:G:214:PHE:HZ	48:G:620:LUT:H8	1.79	0.48
1:a:135:TYR:CE1	4:c:437:ARG:HG3	2.48	0.48
4:c:59:GLU:HB3	4:c:77:LEU:HG	1.96	0.48
4:c:433:ALA:HA	31:c:505:CLA:HED2	1.95	0.48
14:o:238:GLN:HE21	14:o:282:ALA:HA	1.79	0.48
31:g:603:CLA:HBC1	47:g:609:CHL:HAC1	1.95	0.48
31:g:613:CLA:H8	31:g:613:CLA:H122	1.65	0.48
31:r:610:CLA:H102	31:r:610:CLA:H13	1.61	0.48
24:y:62:THR:OG1	24:y:64:GLU:OE2	2.32	0.48
2:B1:479:PHE:O	5:D1:139:ARG:NH2	2.46	0.48
31:B1:609:CLA:H51	38:B1:625:DGA:HB92	1.96	0.48
7:F1:39:MET:HA	7:F1:42:ILE:HD12	1.94	0.48
14:O1:111:PRO:HD2	14:O1:138:TYR:CD1	2.48	0.48
1:a1:41:LEU:HD21	32:a1:408:PHO:H42	1.96	0.48
1:a1:104:GLU:O	1:a1:108:ASN:ND2	2.43	0.48
1:a1:172:MET:SD	1:a1:179:THR:OG1	2.60	0.48
2:b1:124:ARG:O	8:h1:31:ARG:NH2	2.47	0.48
31:b1:608:CLA:H112	31:b1:608:CLA:H152	1.62	0.48
4:c1:408:VAL:HB	4:c1:413:TRP:HE1	1.78	0.48
2:B:365:THR:HG21	14:O:226:ILE:HD12	1.96	0.47
4:C:454:VAL:HG13	5:D:251:ARG:HD2	1.96	0.47
21:G:148:VAL:HG11	47:G:605:CHL:HBC1	1.96	0.47
48:G:621:LUT:H362	47:Y:609:CHL:H11	1.96	0.47
31:b:610:CLA:C2	31:b:611:CLA:HBB2	2.44	0.47
40:c:520:DGD:HBN1	35:d:411:LMG:H192	1.96	0.47
7:f:23:HIS:NE2	45:f:101:HEM:NA	2.62	0.47
47:g:601:CHL:HHC	47:g:601:CHL:HBB1	1.96	0.47
48:r:620:LUT:H391	48:r:620:LUT:H31	1.71	0.47
1:A1:156:ALA:HA	1:A1:160:ILE:HB	1.96	0.47
1:A1:162:PRO:HB3	1:A1:168:PHE:HA	1.95	0.47
31:A1:406:CLA:HAA2	44:D1:405:PL9:H351	1.96	0.47
2:B1:458:PHE:HE1	35:B1:622:LMG:H211	1.79	0.47
14:O1:233:ASP:N	14:O1:233:ASP:OD1	2.46	0.47
31:N1:602:CLA:H52	48:N1:621:LUT:H30	1.95	0.47
21:G1:63:TRP:HZ3	31:G1:602:CLA:HBC2	1.79	0.47
27:R1:155:GLU:OE2	27:R1:264:ALA:N	2.44	0.47
31:S1:611:CLA:H92	31:S1:611:CLA:H61	1.73	0.47
1:a1:29:TYR:H	5:d1:255:GLN:HB3	1.79	0.47
2:b1:257:TRP:CD1	35:h1:102:LMG:H211	2.49	0.47
2:b1:272:ARG:HG3	2:b1:320:ALA:HB3	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c1:224:GLY:HA3	33:c1:515:BCR:H402	1.95	0.47
31:c1:508:CLA:HAC1	41:d1:410:LHG:H341	1.95	0.47
40:c1:519:DGD:HB72	35:c1:521:LMG:H401	1.95	0.47
2:B:3:LEU:HD23	31:B:615:CLA:HED1	1.96	0.47
4:C:207:GLY:HA2	40:C:518:DGD:HD2	1.96	0.47
5:D:87:HIS:HD2	5:D:162:LEU:HA	1.80	0.47
5:D:331:ALA:HA	5:D:339:LEU:HB2	1.96	0.47
15:P:206:LYS:HG2	15:P:238:LEU:HD22	1.96	0.47
49:G:622:XAT:H31	49:G:622:XAT:H391	1.76	0.47
1:a:65:GLU:HG3	14:o:210:PHE:HZ	1.79	0.47
1:a:201:GLY:HA3	1:a:286:THR:HB	1.96	0.47
4:c:77:LEU:HD22	4:c:99:TYR:CD2	2.49	0.47
47:n:607:CHL:H13	47:n:607:CHL:H102	1.72	0.47
23:s:107:HIS:HE1	48:s:621:LUT:H15	1.78	0.47
23:s:149:LEU:HD22	31:s:604:CLA:HED1	1.96	0.47
31:s:602:CLA:HBA2	31:s:602:CLA:H3A	1.63	0.47
47:y:605:CHL:HHC	47:y:605:CHL:HBB1	1.95	0.47
1:A1:334:ARG:HG3	1:A1:335:ASN:ND2	2.29	0.47
2:B1:382:PRO:HG2	2:B1:385:LYS:HG2	1.96	0.47
5:D1:122:LEU:HD23	5:D1:150:ILE:HG13	1.96	0.47
27:R1:220:PRO:HB3	24:y1:191:PRO:HB3	1.96	0.47
31:Y1:602:CLA:H141	31:Y1:602:CLA:H18	1.94	0.47
1:a1:140:ARG:NH2	41:d1:410:LHG:O5	2.41	0.47
2:b1:243:ALA:HB2	2:b1:466:HIS:CE1	2.49	0.47
40:c1:519:DGD:HA72	40:c1:520:DGD:HB91	1.95	0.47
20:n1:187:PHE:HB3	47:n1:608:CHL:H11	1.95	0.47
20:N:130:ILE:HG21	20:N:150:ILE:HD13	1.95	0.47
2:b:251:VAL:HG22	31:b:603:CLA:H72	1.96	0.47
4:c:384:MET:SD	4:c:385:THR:OG1	2.63	0.47
31:c:509:CLA:H161	31:c:509:CLA:H141	1.74	0.47
12:l:18:LEU:HD11	13:m:23:LEU:HD22	1.94	0.47
1:A1:45:ILE:HD11	31:A1:406:CLA:H203	1.96	0.47
1:A1:126:TYR:HB3	1:A1:147:TYR:HE2	1.78	0.47
2:B1:264:PRO:HD2	2:B1:268:PHE:HE2	1.78	0.47
31:B1:608:CLA:HBC1	33:B1:618:BCR:HC8	1.96	0.47
5:D1:56:THR:OG1	5:D1:69:GLU:OE2	2.30	0.47
6:E1:38:VAL:HG12	6:E1:43:ALA:HB2	1.96	0.47
2:b1:181:VAL:HG21	2:b1:195:PRO:HB2	1.95	0.47
52:b1:624:3PH:H3D2	52:b1:624:3PH:H3G2	1.69	0.47
14:o1:260:ASP:HB3	14:o1:265:GLU:HG2	1.96	0.47
20:n1:117:PHE:HB2	20:n1:121:ALA:HB2	1.96	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
27:r1:179:SER:HB2	56:r1:626:ERG:H121	1.96	0.47
4:C:33:LEU:HD22	4:C:126:GLU:HG3	1.95	0.47
24:Y:120:ASP:HB3	24:Y:126:LYS:HB3	1.97	0.47
35:c:521:LMG:HC71	35:j:101:LMG:HC92	1.97	0.47
5:d:167:TRP:O	5:d:170:ALA:HB3	2.14	0.47
11:k:15:TYR:OH	19:z:58:ASN:ND2	2.38	0.47
47:n:601:CHL:H62	47:n:601:CHL:H41	1.54	0.47
1:A1:194:MET:HB3	1:A1:300:PHE:HB2	1.96	0.47
2:B1:257:TRP:CE2	5:D1:291:LEU:HD22	2.49	0.47
2:B1:341:LEU:HG	2:B1:406:LEU:HD23	1.96	0.47
4:C1:78:PRO:HB2	4:C1:290:TYR:CE1	2.50	0.47
4:C1:152:HIS:HE1	31:C1:509:CLA:H162	1.79	0.47
5:D1:49:LEU:HD21	35:D1:411:LMG:H342	1.96	0.47
33:D1:404:BCR:H381	10:J1:23:ALA:HB1	1.95	0.47
38:b1:625:DGA:HBG1	31:d1:403:CLA:H92	1.95	0.47
52:t1:101:3PH:H2A2	52:t1:101:3PH:H2I3	1.96	0.47
47:n1:605:CHL:H143	31:s1:612:CLA:HBB1	1.97	0.47
34:A:412:SQD:H341	40:C:519:DGD:HAF1	1.96	0.47
31:B:612:CLA:H71	41:L:101:LHG:H321	1.97	0.47
8:H:69:ASN:ND2	35:H:102:LMG:O10	2.47	0.47
14:O:102:TYR:HB3	14:O:147:MET:HB3	1.95	0.47
31:n:604:CLA:HBA2	31:n:604:CLA:H3A	1.39	0.47
1:A1:42:LEU:HD23	33:A1:411:BCR:C11	2.45	0.47
1:A1:281:VAL:HG22	1:A1:284:TRP:HZ3	1.78	0.47
2:B1:60:MET:HE2	2:B1:63:LEU:HD22	1.95	0.47
38:B1:625:DGA:HAW1	5:D1:36:LEU:HD21	1.96	0.47
4:C1:232:CYS:O	4:C1:236:GLY:N	2.45	0.47
4:C1:410:PRO:HA	4:C1:413:TRP:HD1	1.79	0.47
21:G1:199:LYS:HG3	31:G1:611:CLA:HED2	1.97	0.47
31:G1:613:CLA:H12	31:G1:614:CLA:HED2	1.96	0.47
24:Y1:100:GLY:O	24:Y1:104:ILE:HG12	2.14	0.47
24:Y1:104:ILE:HG23	24:Y1:124:TRP:CD1	2.48	0.47
31:Y1:602:CLA:H142	48:Y1:621:LUT:H361	1.94	0.47
31:Y1:602:CLA:HBB1	31:Y1:602:CLA:H51	1.96	0.47
31:n1:602:CLA:HBA1	48:n1:621:LUT:H382	1.96	0.47
31:A:405:CLA:H102	32:A:408:PHO:HAA1	1.97	0.47
2:B:157:HIS:HA	2:B:163:GLY:HA3	1.97	0.47
31:B:605:CLA:CMB	31:B:608:CLA:HAB	2.45	0.47
5:D:152:VAL:HG22	31:D:402:CLA:HED1	1.96	0.47
14:O:216:ARG:HH11	14:O:240:LEU:HD23	1.79	0.47
20:N:88:LEU:O	20:N:92:HIS:ND1	2.47	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:N:607:CHL:H151	47:N:609:CHL:H71	1.96	0.47
21:G:182:ASP:OD1	48:G:620:LUT:O23	2.29	0.47
1:a:135:TYR:OH	9:i:31:ASN:ND2	2.48	0.47
20:n:90:LEU:HB2	20:n:181:LEU:HD11	1.95	0.47
21:g:75:PHE:O	21:g:79:ARG:HB2	2.15	0.47
23:s:224:ASP:HB2	23:s:227:VAL:HG22	1.96	0.47
1:A1:328:MET:HG3	5:D1:325:ILE:HD11	1.97	0.47
2:B1:330:MET:HA	2:B1:444:ARG:HB2	1.97	0.47
4:C1:441:ALA:HA	9:I1:31:ASN:HD22	1.78	0.47
5:D1:92:VAL:O	5:D1:99:GLY:N	2.36	0.47
5:D1:217:THR:O	5:D1:221:THR:OG1	2.32	0.47
31:N1:604:CLA:H62	31:N1:604:CLA:H41	1.68	0.47
21:G1:153:MET:HE3	21:G1:157:GLU:HG2	1.97	0.47
21:G1:232:HIS:CG	31:G1:613:CLA:HAA2	2.49	0.47
47:G1:606:CHL:HHC	47:G1:606:CHL:HBB1	1.95	0.47
31:b1:609:CLA:HBA1	38:b1:625:DGA:HB52	1.97	0.47
8:h1:47:THR:HA	8:h1:50:MET:HB3	1.96	0.47
47:s1:601:CHL:HBB1	47:s1:601:CHL:HHC	1.96	0.47
31:B:606:CLA:HBC2	31:B:613:CLA:H112	1.96	0.47
38:B:625:DGA:HAE1	38:B:625:DGA:HAF2	1.66	0.47
4:C:129:GLU:OE2	4:C:137:TYR:N	2.48	0.47
31:C:501:CLA:HMD2	31:C:502:CLA:H91	1.96	0.47
14:O:136:LEU:CD2	14:O:138:TYR:OH	2.63	0.47
14:O:160:ASP:OD1	14:O:160:ASP:N	2.46	0.47
20:N:168:ARG:NH2	47:N:609:CHL:O1D	2.44	0.47
21:G:205:ARG:NH2	31:G:602:CLA:O2D	2.48	0.47
47:G:608:CHL:HBB1	47:G:608:CHL:HHC	1.95	0.47
47:R:606:CHL:HHC	47:R:606:CHL:HBB1	1.95	0.47
23:S:85:TYR:OH	47:S:601:CHL:O1A	2.32	0.47
23:S:283:ASP:OD1	23:S:284:ASP:N	2.47	0.47
24:Y:130:GLU:HB2	24:Y:137:LEU:HD22	1.97	0.47
24:Y:131:ILE:HG23	24:Y:137:LEU:HD23	1.97	0.47
1:a:106:LEU:HD21	33:a:411:BCR:H383	1.95	0.47
1:a:195:HIS:HD2	1:a:299:GLY:HA2	1.79	0.47
34:a:412:SQD:H61	5:d:233:ARG:HD3	1.97	0.47
2:b:460:LEU:HG	5:d:280:TRP:HZ3	1.80	0.47
31:c:501:CLA:H41	31:c:501:CLA:H61	1.61	0.47
33:c:516:BCR:C21	11:k:34:LEU:HG	2.45	0.47
9:i:13:THR:HG21	17:w:85:ILE:HG12	1.96	0.47
49:y:622:XAT:H15	49:y:622:XAT:H201	1.69	0.47
1:A1:218:LEU:HB3	1:A1:251:ALA:HB1	1.95	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:312:ARG:HD2	6:E1:56:PHE:CZ	2.50	0.47
2:B1:376:VAL:HG21	15:P1:97:LYS:HE2	1.97	0.47
4:C1:96:THR:HA	4:C1:99:TYR:HD2	1.79	0.47
5:D1:53:THR:HA	5:D1:67:TYR:H	1.79	0.47
17:W1:96:TYR:O	17:W1:100:GLN:NE2	2.40	0.47
20:N1:161:MET:HA	20:N1:164:VAL:HB	1.96	0.47
20:N1:184:GLY:HA3	31:N1:610:CLA:HED2	1.96	0.47
31:N1:610:CLA:H51	48:N1:620:LUT:H30	1.95	0.47
21:G1:53:LEU:HD11	21:G1:64:ASP:HB2	1.97	0.47
1:a1:66:PRO:HG3	1:a1:107:TYR:HE1	1.80	0.47
1:a1:88:ALA:HB1	4:c1:333:PRO:HG3	1.97	0.47
1:a1:149:ALA:HB2	1:a1:280:VAL:HG13	1.97	0.47
2:b1:373:LYS:HG3	25:u1:96:ASP:HB3	1.97	0.47
34:b1:626:SQD:H121	34:b1:626:SQD:H91	1.64	0.47
4:c1:394:SER:O	4:c1:407:PHE:N	2.48	0.47
44:d1:405:PL9:H401	41:d1:409:LHG:H211	1.97	0.47
20:n1:247:ALA:HB3	49:g1:622:XAT:H193	1.97	0.47
47:n1:607:CHL:H193	47:y1:601:CHL:H122	1.97	0.47
24:y1:67:GLY:O	24:y1:213:ARG:NH1	2.42	0.47
1:A:330:VAL:HB	5:D:348:ARG:HG3	1.97	0.47
4:C:175:ASP:O	4:C:182:GLY:HA2	2.15	0.47
5:D:312:GLU:HB3	14:O:213:PRO:HG3	1.96	0.47
31:R:608:CLA:HBA2	31:R:608:CLA:H3A	1.63	0.47
2:b:422:ARG:HH12	14:o:229:PRO:HB3	1.80	0.47
5:d:302:GLU:HG2	14:o:227:ALA:HB1	1.97	0.47
21:g:55:GLY:HA2	21:g:60:ASP:HB3	1.97	0.47
31:g:611:CLA:HAC1	41:g:624:LHG:H282	1.97	0.47
48:y:620:LUT:H35	48:y:620:LUT:H401	1.75	0.47
1:A1:272:HIS:HA	1:A1:275:LEU:HD12	1.96	0.47
34:B1:626:SQD:H132	53:a1:414:SPH:H71	1.96	0.47
5:D1:317:LYS:O	5:D1:321:LEU:N	2.45	0.47
49:N1:622:XAT:H15	49:N1:622:XAT:H201	1.69	0.47
49:N1:622:XAT:H28	41:Y1:624:LHG:H352	1.97	0.47
31:R1:608:CLA:HMB3	50:R1:622:NEX:H35	1.96	0.47
23:S1:261:TYR:HA	23:S1:264:ILE:HG22	1.95	0.47
24:Y1:224:VAL:HG21	31:Y1:613:CLA:HAC2	1.97	0.47
49:Y1:622:XAT:H15	49:Y1:622:XAT:H201	1.70	0.47
2:b1:385:LYS:HB3	15:p1:149:ALA:HB3	1.97	0.47
31:b1:610:CLA:HBB1	46:h1:101:RRX:H6	1.95	0.47
31:c1:504:CLA:H142	31:c1:504:CLA:H111	1.77	0.47
54:k1:101:4RF:H85	54:k1:101:4RF:H78	1.74	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
15:p1:189:ILE:HB	15:p1:203:GLN:HB2	1.97	0.47
27:r1:235:LEU:HG	31:r1:610:CLA:HMA2	1.97	0.47
31:s1:604:CLA:H61	47:s1:606:CHL:HBA2	1.96	0.47
24:y1:76:LEU:HD12	31:y1:602:CLA:O2A	2.15	0.47
2:B:464:PHE:HD2	31:B:612:CLA:HAC2	1.80	0.47
4:C:234:LEU:HB3	53:Y:625:SPH:H151	1.96	0.47
4:C:394:SER:HB3	4:C:406:ASN:ND2	2.30	0.47
35:C:521:LMG:H312	11:K:27:ILE:HG22	1.97	0.47
12:L:17:SER:OG	41:L:101:LHG:O8	2.32	0.47
21:G:50:PRO:HB2	21:G:53:LEU:HD23	1.96	0.47
22:R:269:ALA:O	22:R:272:THR:OG1	2.30	0.47
23:S:106:LEU:HD12	23:S:110:TRP:CZ3	2.50	0.47
2:b:11:VAL:HG23	2:b:12:VAL:HG13	1.95	0.47
33:c:515:BCR:H351	33:c:515:BCR:H15C	1.74	0.47
6:e:68:ASP:OD1	6:e:69:ARG:N	2.48	0.47
21:g:50:PRO:HG2	21:g:53:LEU:HD12	1.96	0.47
21:g:216:VAL:HG21	31:g:613:CLA:HAC2	1.96	0.47
22:r:195:VAL:HA	22:r:198:VAL:HG22	1.97	0.47
2:B1:478:VAL:O	5:D1:139:ARG:NE	2.32	0.47
52:B1:624:3PH:H381	16:t1:4:LEU:HD21	1.97	0.47
4:C1:174:TYR:HA	4:C1:184:VAL:HA	1.97	0.47
4:C1:277:PHE:HB3	4:C1:285:TYR:HE2	1.79	0.47
4:C1:398:VAL:N	4:C1:401:GLU:OE1	2.48	0.47
40:C1:520:DGD:HA82	40:C1:520:DGD:HBT1	1.97	0.47
14:O1:133:LEU:HD12	14:O1:171:LYS:HB2	1.97	0.47
2:b1:365:THR:OG1	5:d1:326:ARG:NH2	2.36	0.47
4:c1:27:ASN:HB3	31:c1:509:CLA:HAB	1.97	0.47
40:c1:519:DGD:HB22	35:c1:521:LMG:H311	1.97	0.47
54:k1:101:4RF:H81	54:k1:101:4RF:H75	1.58	0.47
15:p1:113:VAL:O	15:p1:220:GLN:NE2	2.42	0.47
2:B:134:ASP:OD2	2:B:220:ARG:NH1	2.47	0.47
31:B:603:CLA:H91	31:B:603:CLA:H112	1.76	0.47
41:Y:624:LHG:H272	41:Y:624:LHG:H242	1.65	0.47
41:Y:624:LHG:H301	41:Y:624:LHG:H112	1.97	0.47
33:b:618:BCR:H341	39:b:624:GOL:H12	1.97	0.47
4:c:58:PHE:HE1	11:k:23:ASP:HA	1.79	0.47
4:c:330:MET:HE2	4:c:340:GLY:HA2	1.97	0.47
45:f:101:HEM:HBB2	45:f:101:HEM:HHC	1.96	0.47
11:k:28:ILE:HD13	11:k:31:LEU:HD12	1.97	0.47
20:n:214:MET:HE2	31:n:602:CLA:HAB	1.96	0.47
33:C1:517:BCR:H351	33:C1:517:BCR:H15C	1.56	0.47

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
6:E1:22:ILE:HG13	6:E1:23:HIS:HD1	1.79	0.47
11:K1:12:PRO:HB2	11:K1:15:TYR:HD1	1.79	0.47
1:a1:166:GLY:HA3	4:c1:346:PHE:HE1	1.80	0.47
1:a1:196:PRO:HG2	40:c1:520:DGD:HB81	1.96	0.47
1:a1:341:LEU:HD23	1:a1:343:LEU:HD21	1.97	0.47
2:b1:57:ARG:HD2	2:b1:330:MET:HE3	1.96	0.47
2:b1:363:PHE:HA	5:d1:326:ARG:HD2	1.95	0.47
4:c1:33:LEU:HD23	4:c1:36:LYS:HG2	1.97	0.47
5:d1:171:PRO:HG3	5:d1:181:PHE:CE2	2.50	0.47
49:y1:622:XAT:H31	49:y1:622:XAT:H391	1.70	0.47
31:A:410:CLA:H12	35:A:413:LMG:H111	1.96	0.46
2:B:471:SER:O	2:B:475:PHE:HB2	2.15	0.46
31:B:604:CLA:HAB	31:B:606:CLA:H152	1.97	0.46
4:C:306:LEU:HD13	4:C:328:TYR:HB3	1.97	0.46
31:C:508:CLA:HBC3	31:C:510:CLA:H92	1.96	0.46
20:N:208:LYS:HD2	31:N:611:CLA:C3D	2.45	0.46
1:a:258:LEU:HB3	1:a:259:ILE:HD12	1.97	0.46
40:c:523:DGD:HAE1	41:y:624:LHG:H362	1.96	0.46
14:o:171:LYS:HD2	14:o:175:GLY:HA2	1.97	0.46
15:p:179:LYS:NZ	15:p:243:VAL:O	2.42	0.46
1:A1:59:ASP:HA	1:A1:66:PRO:HA	1.97	0.46
31:B1:602:CLA:CAB	46:H1:101:RRX:H32	2.45	0.46
44:D1:405:PL9:H353	41:L1:101:LHG:H223	1.97	0.46
33:a1:411:BCR:H351	33:a1:411:BCR:H15C	1.69	0.46
34:a1:412:SQD:H362	31:c1:508:CLA:H142	1.96	0.46
2:b1:434:ARG:HH22	14:o1:231:LYS:HD3	1.80	0.46
34:b1:621:SQD:H161	34:m1:101:SQD:H151	1.96	0.46
4:c1:330:MET:HE3	4:c1:331:ARG:HB2	1.96	0.46
31:c1:504:CLA:H13	40:c1:519:DGD:HAT1	1.97	0.46
31:A:405:CLA:H141	31:A:406:CLA:H122	1.97	0.46
33:A:411:BCR:H351	33:A:411:BCR:H15C	1.79	0.46
3:V:7:LEU:HA	3:V:10:VAL:HG12	1.96	0.46
5:D:194:ASN:O	5:D:198:MET:HG3	2.16	0.46
1:a:308:ASP:OD1	1:a:312:ARG:N	2.48	0.46
2:b:324:LEU:HD22	5:d:293:LEU:HB3	1.97	0.46
31:d:403:CLA:H101	8:h:55:LEU:HD11	1.98	0.46
24:y:69:TYR:HB2	31:y:602:CLA:HMD3	1.96	0.46
1:A1:114:LEU:O	1:A1:118:HIS:ND1	2.34	0.46
31:C1:510:CLA:H112	31:C1:510:CLA:H152	1.65	0.46
5:D1:261:PHE:HE1	44:D1:405:PL9:H112	1.80	0.46
14:O1:183:THR:HG21	14:O1:202:VAL:HA	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:n1:204:VAL:HA	20:n1:207:ILE:HG22	1.97	0.46
31:s1:603:CLA:H143	31:s1:603:CLA:H161	1.84	0.46
33:C:514:BCR:HC7	19:Z:55:GLY:HA3	1.97	0.46
40:C:520:DGD:O1B	10:J:35:TYR:OH	2.34	0.46
19:Z:23:VAL:O	19:Z:27:PHE:HB2	2.15	0.46
1:a:156:ALA:HA	1:a:160:ILE:HB	1.97	0.46
4:c:215:VAL:HG11	33:c:515:BCR:H291	1.97	0.46
16:t:5:VAL:O	16:t:9:LEU:HG	2.16	0.46
21:g:88:TRP:CD1	47:g:608:CHL:HED2	2.49	0.46
2:B1:322:GLY:O	2:B1:326:ARG:NH1	2.49	0.46
31:C1:501:CLA:H203	31:C1:507:CLA:H162	1.97	0.46
5:D1:87:HIS:CD2	5:D1:162:LEU:HA	2.50	0.46
41:G1:624:LHG:C20	49:Y1:622:XAT:H12	2.46	0.46
5:d1:264:LYS:HZ3	44:d1:405:PL9:H532	1.80	0.46
5:d1:306:ALA:HA	14:o1:216:ARG:HH22	1.80	0.46
20:n1:196:PRO:HA	20:n1:199:PHE:HB3	1.95	0.46
2:B:149:LEU:HD11	31:B:605:CLA:H152	1.97	0.46
4:C:277:PHE:HB3	4:C:285:TYR:HE2	1.80	0.46
31:C:513:CLA:H62	31:C:513:CLA:H41	1.58	0.46
20:N:223:GLN:O	20:N:227:THR:OG1	2.29	0.46
21:G:75:PHE:O	21:G:79:ARG:HG2	2.15	0.46
41:G:630:LHG:H291	41:G:630:LHG:H112	1.97	0.46
53:Y:625:SPH:H131	53:Y:625:SPH:H162	1.72	0.46
14:o:140:LEU:HB3	14:o:143:MET:HE1	1.98	0.46
31:g:602:CLA:H201	41:g:624:LHG:H172	1.98	0.46
1:A1:50:ILE:HG12	34:b1:626:SQD:H281	1.96	0.46
52:B1:624:3PH:H361	16:t1:4:LEU:HD11	1.97	0.46
5:D1:88:SER:O	5:D1:167:TRP:NE1	2.47	0.46
7:F1:16:THR:HG23	7:F1:19:TRP:H	1.81	0.46
54:I1:102:4RF:H47	54:I1:102:4RF:H8	1.96	0.46
31:c1:506:CLA:H152	31:c1:506:CLA:H111	1.76	0.46
47:y1:607:CHL:HAA1	49:y1:622:XAT:H41	1.98	0.46
1:A:60:ILE:HD12	1:A:84:PRO:HD2	1.97	0.46
22:R:149:LEU:HA	22:R:152:ILE:HG22	1.97	0.46
22:R:195:VAL:HG23	31:R:609:CLA:CAB	2.45	0.46
31:Y:602:CLA:H143	31:Y:602:CLA:H161	1.79	0.46
2:b:224:ARG:NH2	5:d:16:ASP:OD1	2.39	0.46
21:g:87:ARG:NH1	47:g:608:CHL:OBD	2.48	0.46
49:r:622:XAT:H371	49:r:622:XAT:H28	1.98	0.46
35:C1:521:LMG:H182	38:J1:101:DGA:HA82	1.97	0.46
5:D1:323:GLU:HA	5:D1:326:ARG:HG3	1.98	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:N1:621:LUT:H35	48:N1:621:LUT:H401	1.81	0.46
21:G1:116:PHE:HD1	21:G1:117:LYS:HE3	1.80	0.46
23:S1:112:MET:SD	31:S1:610:CLA:HAB	2.55	0.46
24:Y1:100:GLY:O	24:Y1:104:ILE:N	2.46	0.46
1:a1:166:GLY:HA3	4:c1:346:PHE:CE1	2.51	0.46
4:c1:156:LEU:HD11	31:c1:509:CLA:H61	1.97	0.46
31:r1:612:CLA:H3A	31:r1:612:CLA:HBA1	1.57	0.46
23:s1:151:TYR:CZ	23:s1:153:ALA:HB2	2.51	0.46
2:B:247:TRP:CZ3	31:B:604:CLA:H121	2.49	0.46
13:M:20:SER:O	13:M:24:ILE:HG13	2.16	0.46
20:N:160:LEU:HD21	50:N:623:NEX:C34	2.46	0.46
21:G:41:LEU:HB3	21:G:44:PHE:HB2	1.97	0.46
24:Y:228:VAL:HG11	31:Y:613:CLA:HMD2	1.97	0.46
5:d:191:TRP:CE3	5:d:289:LEU:HD11	2.51	0.46
7:f:16:THR:HG22	7:f:17:VAL:H	1.81	0.46
9:i:8:VAL:HA	9:i:11:VAL:HG12	1.98	0.46
48:r:620:LUT:H201	48:r:620:LUT:H15	1.71	0.46
47:r:606:CHL:HBB1	47:r:606:CHL:HHC	1.96	0.46
47:r:607:CHL:HBB1	47:r:607:CHL:HHC	1.98	0.46
24:y:240:HIS:CG	31:y:613:CLA:HAA2	2.51	0.46
1:A1:97:TRP:NE1	35:A1:413:LMG:O3	2.47	0.46
1:A1:134:SER:O	1:A1:138:GLY:N	2.49	0.46
31:C1:506:CLA:H162	31:C1:506:CLA:H193	1.78	0.46
31:C1:513:CLA:HMC1	33:C1:514:BCR:H372	1.97	0.46
5:D1:152:VAL:HG22	31:D1:402:CLA:HED1	1.97	0.46
25:U1:92:ARG:HH21	25:U1:95:LEU:HD13	1.80	0.46
2:b1:153:PHE:CD1	31:b1:607:CLA:HAB	2.51	0.46
41:d1:410:LHG:H291	41:d1:410:LHG:H322	1.55	0.46
31:g1:602:CLA:H91	31:y1:603:CLA:H71	1.97	0.46
32:A:409:PHO:HBA1	32:A:409:PHO:H3A	1.45	0.46
31:B:606:CLA:H61	31:B:606:CLA:H41	1.70	0.46
3:V:26:LEU:HD21	19:Z:25:VAL:HA	1.98	0.46
4:C:421:LEU:HD22	31:C:502:CLA:HMC3	1.97	0.46
5:D:317:LYS:O	5:D:321:LEU:HG	2.15	0.46
1:a:51:ALA:O	1:a:55:ALA:CB	2.64	0.46
2:b:41:GLU:HB3	2:b:60:MET:SD	2.56	0.46
31:b:606:CLA:H61	31:b:606:CLA:H41	1.78	0.46
49:n:622:XAT:H15	49:n:622:XAT:H201	1.66	0.46
22:r:153:VAL:O	22:r:157:ALA:HB3	2.15	0.46
31:s:602:CLA:H62	31:s:602:CLA:H41	1.67	0.46
47:y:601:CHL:H102	41:y:624:LHG:H192	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:96:ILE:HD12	9:I1:4:LEU:HD13	1.98	0.46
31:B1:602:CLA:HAB	46:H1:101:RRX:H32	1.97	0.46
21:G1:241:ALA:HB3	49:Y1:622:XAT:H193	1.97	0.46
48:S1:620:LUT:H35	48:S1:620:LUT:H401	1.72	0.46
1:a1:142:TRP:HZ3	41:d1:410:LHG:HC41	1.80	0.46
2:b1:128:THR:HG23	2:b1:130:LYS:H	1.81	0.46
31:b1:610:CLA:C4A	46:h1:101:RRX:H15	2.46	0.46
31:b1:615:CLA:H8	34:m1:101:SQD:H282	1.98	0.46
31:c1:511:CLA:H51	11:k1:39:TRP:CG	2.51	0.46
15:p1:75:PHE:HZ	15:p1:233:GLU:HA	1.80	0.46
21:g1:219:ILE:HG22	21:g1:248:PHE:HZ	1.81	0.46
56:r1:626:ERG:C3	56:r1:626:ERG:HO1	2.13	0.46
24:y1:46:ARG:HD2	24:y1:68:ASP:HB3	1.97	0.46
24:y1:93:HIS:CD2	48:y1:621:LUT:H15	2.47	0.46
24:y1:145:LEU:HD23	47:y1:605:CHL:HED2	1.97	0.46
31:y1:614:CLA:H8	57:y1:626:PTY:H411	1.98	0.46
4:C:261:SER:O	4:C:429:HIS:ND1	2.48	0.46
4:C:395:VAL:HG22	4:C:403:ASN:HD21	1.81	0.46
20:N:57:PRO:HG3	20:N:71:ASP:HB2	1.96	0.46
1:a:334:ARG:HD3	5:d:320:LEU:HD21	1.98	0.46
34:a:412:SQD:H292	31:c:508:CLA:H93	1.96	0.46
2:b:96:ALA:O	2:b:100:HIS:ND1	2.47	0.46
5:d:19:ASP:OD2	5:d:23:ARG:NH1	2.49	0.46
6:e:44:TYR:HA	6:e:49:SER:HB3	1.98	0.46
48:n:620:LUT:H11	48:n:620:LUT:H191	1.82	0.46
31:g:602:CLA:H151	48:g:621:LUT:H393	1.97	0.46
23:s:132:LYS:NZ	23:s:148:THR:OG1	2.49	0.46
31:y:613:CLA:H2	31:y:614:CLA:HMD1	1.96	0.46
1:A1:41:LEU:O	1:A1:45:ILE:N	2.36	0.46
2:B1:389:LYS:HD3	15:P1:98:GLU:HG3	1.97	0.46
31:B1:609:CLA:H193	31:D1:403:CLA:HAA2	1.97	0.46
11:K1:28:ILE:HA	11:K1:31:LEU:HB3	1.97	0.46
20:N1:71:ASP:O	21:G1:77:ARG:NH1	2.48	0.46
41:N1:624:LHG:H131	49:G1:622:XAT:H403	1.97	0.46
21:G1:128:LEU:HD22	47:G1:606:CHL:HMD1	1.98	0.46
27:R1:148:THR:HG21	48:R1:620:LUT:H12	1.97	0.46
1:a1:207:GLY:HA2	1:a1:210:LEU:HD12	1.97	0.46
40:c1:518:DGD:HA72	40:c1:518:DGD:HA42	1.76	0.46
5:d1:89:LEU:HD22	5:d1:116:LEU:HD12	1.96	0.46
5:d1:305:ALA:O	14:o1:239:ARG:NH2	2.46	0.46
31:r1:608:CLA:H61	31:r1:608:CLA:H41	1.70	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:9:HIS:HB3	31:B:613:CLA:HAB	1.96	0.46
31:C:513:CLA:HBA2	31:C:513:CLA:H3A	1.69	0.46
21:G:171:ASP:OD1	21:G:171:ASP:N	2.49	0.46
47:G:606:CHL:HBB1	47:G:606:CHL:HHC	1.97	0.46
2:b:357:ARG:NH1	2:b:358:ARG:O	2.48	0.46
31:b:609:CLA:H141	31:d:403:CLA:H12	1.97	0.46
5:d:286:VAL:HA	5:d:289:LEU:HD12	1.96	0.46
20:n:238:HIS:NE2	31:n:613:CLA:O2D	2.34	0.46
1:A1:157:VAL:HG23	1:A1:158:PHE:HD1	1.80	0.46
1:A1:191:ASN:HB2	4:C1:399:ALA:HB1	1.98	0.46
31:B1:611:CLA:H102	31:B1:616:CLA:HBA2	1.97	0.46
4:C1:257:GLU:OE2	4:C1:432:HIS:ND1	2.49	0.46
17:W1:95:ILE:HA	17:W1:98:VAL:HG22	1.98	0.46
47:S1:601:CHL:HBB1	47:S1:601:CHL:HHC	1.98	0.46
31:b1:615:CLA:H41	31:b1:615:CLA:H61	1.53	0.46
4:c1:139:TRP:HH2	31:c1:509:CLA:H191	1.79	0.46
31:c1:512:CLA:O2D	31:c1:513:CLA:HBB2	2.15	0.46
31:A:405:CLA:H141	31:A:406:CLA:H162	1.97	0.46
4:C:250:ARG:HG2	9:I:26:ASN:ND2	2.31	0.46
5:D:51:GLY:HA2	5:D:55:VAL:HB	1.98	0.46
44:D:405:PL9:H101	44:D:405:PL9:H121	1.75	0.46
15:P:128:ILE:O	15:P:131:TYR:HB2	2.16	0.46
47:S:601:CHL:HBB1	47:S:601:CHL:HHC	1.97	0.46
47:Y:606:CHL:H62	47:Y:606:CHL:H41	1.76	0.46
1:a:230:ASN:OD1	1:a:231:GLU:N	2.43	0.46
1:a:269:ARG:NH2	5:d:222:LEU:O	2.49	0.46
4:c:283:THR:OG1	4:c:284:ALA:N	2.49	0.46
31:c:506:CLA:H143	31:c:506:CLA:H112	1.74	0.46
5:d:134:ARG:NH2	5:d:137:ASN:OD1	2.40	0.46
33:d:404:BCR:H17C	7:f:29:THR:HG22	1.98	0.46
41:l:101:LHG:H261	13:m:22:LEU:HD21	1.98	0.46
20:n:158:VAL:HG13	47:n:609:CHL:HBB2	1.98	0.46
24:y:76:LEU:HD12	31:y:602:CLA:C1	2.27	0.46
24:y:139:TYR:CE2	31:y:604:CLA:H2	2.50	0.46
31:y:603:CLA:CAD	47:y:609:CHL:H2	2.46	0.46
31:C1:505:CLA:C4B	31:C1:505:CLA:H52	2.46	0.46
5:D1:341:LEU:HD12	5:D1:342:PRO:HD2	1.97	0.46
8:H1:61:LEU:HD13	8:H1:64:ILE:HD11	1.98	0.46
2:b1:121:GLU:O	8:h1:31:ARG:NH1	2.49	0.46
38:b1:625:DGA:HA61	5:d1:32:TRP:HB2	1.98	0.46
47:s1:607:CHL:HHC	47:s1:607:CHL:HBB1	1.97	0.46

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:127:MET:SD	1:A:151:VAL:HG11	2.57	0.45
2:B:166:ILE:O	2:B:178:VAL:HA	2.16	0.45
3:V:16:VAL:HG13	33:C:516:BCR:H362	1.97	0.45
41:D:409:LHG:H162	12:L:23:LEU:HD21	1.97	0.45
31:N:603:CLA:HAC1	47:N:607:CHL:HBB2	1.99	0.45
21:G:101:LEU:HD21	21:G:226:VAL:HG11	1.98	0.45
4:c:282:ASN:ND2	40:c:518:DGD:O3E	2.46	0.45
31:c:513:CLA:NB	33:c:514:BCR:H383	2.31	0.45
5:d:48:TRP:HA	5:d:78:VAL:HG21	1.98	0.45
14:o:149:ILE:HD13	14:o:155:VAL:HG12	1.96	0.45
22:r:186:GLN:O	22:r:190:ILE:HG12	2.16	0.45
2:B1:221:PRO:O	8:H1:41:LEU:N	2.37	0.45
2:B1:349:GLN:HG2	2:B1:396:GLY:HA3	1.98	0.45
33:C1:514:BCR:H10C	42:C1:527:LMK:C35	2.46	0.45
31:N1:614:CLA:HBC1	48:N1:620:LUT:H162	1.98	0.45
31:R1:612:CLA:H52	31:R1:612:CLA:H11	1.77	0.45
1:a1:245:THR:HG1	5:d1:265:ARG:HE	1.62	0.45
31:b1:602:CLA:HBA2	31:b1:602:CLA:H151	1.98	0.45
31:c1:513:CLA:H91	31:c1:513:CLA:H112	1.81	0.45
52:t1:101:3PH:H3A2	52:t1:101:3PH:H2F1	1.98	0.45
31:n1:613:CLA:HBD	31:n1:613:CLA:HBA1	1.98	0.45
31:s1:610:CLA:HBA2	31:s1:610:CLA:H3A	1.52	0.45
48:y1:620:LUT:H15	48:y1:620:LUT:H201	1.83	0.45
35:A:413:LMG:H411	31:C:505:CLA:H143	1.98	0.45
2:B:308:LYS:HA	2:B:308:LYS:HD2	1.70	0.45
33:B:618:BCR:H15C	33:B:618:BCR:H351	1.73	0.45
4:C:63:PHE:HZ	4:C:93:VAL:HG21	1.80	0.45
4:C:319:ALA:HB1	4:C:327:LYS:H	1.80	0.45
7:F:35:ALA:O	7:F:39:MET:HG3	2.16	0.45
14:O:149:ILE:HG22	14:O:155:VAL:HA	1.98	0.45
15:P:204:LEU:HB3	15:P:238:LEU:HD21	1.98	0.45
1:a:323:ARG:HG3	5:d:332:GLN:NE2	2.31	0.45
34:a:412:SQD:H383	31:c:508:CLA:H142	1.97	0.45
2:b:424:ALA:HB2	2:b:429:ILE:HD11	1.98	0.45
23:s:103:ASN:ND2	31:s:609:CLA:OBD	2.44	0.45
31:s:611:CLA:HAC1	41:s:624:LHG:H291	1.97	0.45
24:y:102:LEU:HD23	48:y:620:LUT:H401	1.99	0.45
1:A1:106:LEU:HD11	33:A1:411:BCR:H292	1.97	0.45
1:A1:252:HIS:O	1:A1:256:GLY:N	2.49	0.45
1:A1:273:PHE:O	1:A1:277:VAL:N	2.42	0.45
2:B1:260:SER:N	2:B1:263:THR:OG1	2.49	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B1:368:VAL:HA	2:B1:425:GLN:HE21	1.81	0.45
20:N1:90:LEU:HD12	20:N1:181:LEU:HD13	1.97	0.45
47:S1:608:CHL:HHC	47:S1:608:CHL:HBB1	1.97	0.45
1:a1:129:ARG:HH22	5:d1:256:ILE:HA	1.81	0.45
35:a1:413:LMG:H371	40:c1:518:DGD:HB41	1.96	0.45
2:b1:220:ARG:NE	8:h1:39:LYS:O	2.48	0.45
5:d1:50:THR:HA	5:d1:53:THR:HG22	1.98	0.45
31:d1:402:CLA:H41	31:d1:402:CLA:H62	1.66	0.45
21:g1:209:PHE:CE2	31:g1:613:CLA:HAB	2.51	0.45
1:A:164:GLY:HA3	1:A:294:ALA:HB1	1.99	0.45
32:A:408:PHO:H61	32:A:408:PHO:H2	1.63	0.45
2:B:30:VAL:HG12	31:B:606:CLA:HHD	1.97	0.45
5:D:8:TYR:CZ	22:R:85:LEU:HD11	2.51	0.45
21:G:34:GLY:O	21:G:37:ARG:CB	2.62	0.45
32:a:409:PHO:H142	32:a:409:PHO:H112	1.82	0.45
2:b:220:ARG:NE	8:h:39:LYS:O	2.45	0.45
31:b:609:CLA:H72	5:d:36:LEU:HD11	1.99	0.45
20:n:93:ALA:HB1	20:n:210:GLY:HA3	1.97	0.45
47:n:601:CHL:HBB1	47:n:601:CHL:HHC	1.97	0.45
48:n:621:LUT:H31	48:n:621:LUT:H391	1.85	0.45
5:D1:279:LEU:HD22	31:D1:402:CLA:HBA2	1.99	0.45
14:O1:132:LEU:HD23	17:W1:64:ARG:HH21	1.82	0.45
23:S1:49:LEU:HD23	23:S1:230:GLU:HG3	1.98	0.45
23:S1:110:TRP:CZ3	47:S1:608:CHL:HED3	2.51	0.45
1:a1:197:PHE:CZ	40:c1:519:DGD:HBN1	2.51	0.45
35:a1:413:LMG:H291	35:a1:413:LMG:H322	1.82	0.45
31:b1:608:CLA:H91	31:b1:608:CLA:H111	1.78	0.45
14:o1:208:SER:HA	14:o1:245:TYR:CE2	2.52	0.45
21:g1:232:HIS:CG	31:g1:613:CLA:HAA2	2.52	0.45
31:A:405:CLA:H42	31:A:406:CLA:HMC1	1.99	0.45
2:B:392:ILE:HA	2:B:395:VAL:HG12	1.98	0.45
31:B:610:CLA:H62	31:B:610:CLA:H41	1.69	0.45
31:C:502:CLA:H61	31:C:512:CLA:H11	1.97	0.45
31:C:509:CLA:H161	31:C:509:CLA:H141	1.68	0.45
31:C:511:CLA:H101	33:C:517:BCR:H23C	1.97	0.45
20:N:40:PHE:HA	20:N:45:ARG:HB2	1.99	0.45
47:G:601:CHL:H203	47:Y:607:CHL:H142	1.99	0.45
2:b:468:TRP:HE3	5:d:144:ILE:HG12	1.81	0.45
4:c:40:ALA:HB2	31:c:511:CLA:HMA1	1.99	0.45
4:c:295:PRO:HB3	4:c:346:PHE:HB3	1.98	0.45
31:c:509:CLA:H11	31:c:509:CLA:H51	1.70	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:g:128:LEU:HB2	21:g:139:ALA:HB3	1.97	0.45
22:r:160:VAL:HG11	22:r:168:VAL:HG11	1.99	0.45
53:A1:414:SPH:H62	9:I1:4:LEU:HD11	1.99	0.45
2:B1:145:LEU:HD11	31:B1:611:CLA:H93	1.98	0.45
5:D1:348:ARG:HH22	15:P1:198:GLU:HG3	1.81	0.45
19:Z1:1:MET:SD	19:Z1:1:MET:N	2.86	0.45
21:G1:206:LEU:HD11	31:G1:611:CLA:HHD	1.98	0.45
27:R1:161:SER:OG	27:R1:164:ASP:OD1	2.26	0.45
31:a1:405:CLA:H2	32:a1:408:PHO:CHC	2.46	0.45
2:b1:136:PRO:HD3	2:b1:231:MET:HE1	1.99	0.45
35:c1:523:LMG:H411	53:y1:625:SPH:H101	1.98	0.45
10:j1:29:ILE:HA	10:j1:32:TYR:HD2	1.82	0.45
20:n1:87:GLU:HA	20:n1:181:LEU:HD21	1.99	0.45
31:B:603:CLA:H143	31:B:603:CLA:H162	1.79	0.45
4:C:155:ILE:HG21	31:C:512:CLA:HBA1	1.99	0.45
14:O:238:GLN:NE2	14:O:281:GLY:O	2.41	0.45
47:N:601:CHL:H62	47:N:601:CHL:H41	1.63	0.45
2:b:472:ARG:HH21	39:b:625:GOL:H12	1.81	0.45
22:r:149:LEU:HB2	48:r:620:LUT:H35	1.98	0.45
2:B1:135:LEU:HA	2:B1:138:ILE:HD12	1.99	0.45
4:C1:261:SER:O	4:C1:429:HIS:ND1	2.39	0.45
20:N1:102:GLY:HA3	48:N1:621:LUT:H182	1.98	0.45
20:N1:160:LEU:HD12	47:N1:606:CHL:HMA1	1.97	0.45
48:Y1:620:LUT:H15	48:Y1:620:LUT:H201	1.70	0.45
31:b1:615:CLA:H91	31:b1:615:CLA:H112	1.81	0.45
31:b1:615:CLA:H71	34:b1:621:SQD:H291	1.99	0.45
31:y1:613:CLA:H72	41:y1:624:LHG:H161	1.99	0.45
33:C:517:BCR:H342	19:Z:12:LEU:HG	1.99	0.45
47:N:606:CHL:HHC	47:N:606:CHL:HBB1	1.99	0.45
49:N:622:XAT:H31	49:N:622:XAT:H391	1.71	0.45
21:G:209:PHE:HE1	31:G:602:CLA:H203	1.81	0.45
31:Y:604:CLA:H8	31:Y:604:CLA:H52	1.71	0.45
31:Y:610:CLA:H142	31:Y:612:CLA:H172	1.99	0.45
1:a:97:TRP:NE1	35:a:413:LMG:O2	2.45	0.45
31:a:406:CLA:HED2	5:d:198:MET:SD	2.57	0.45
31:b:617:CLA:H112	31:b:617:CLA:H91	1.75	0.45
31:c:505:CLA:H43	9:i:19:PHE:HE1	1.81	0.45
5:d:325:ILE:O	5:d:329:MET:HB3	2.16	0.45
20:n:202:LEU:HA	20:n:205:LYS:HB2	1.97	0.45
22:r:202:ARG:HH11	22:r:211:ARG:HH12	1.65	0.45
23:s:252:GLN:HE22	48:s:620:LUT:H42	1.81	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:s:620:LUT:H193	41:s:624:LHG:H372	1.99	0.45
2:B1:331:ASN:HB2	2:B1:336:ILE:HG13	1.98	0.45
31:B1:603:CLA:H202	31:B1:603:CLA:H161	1.79	0.45
4:C1:282:ASN:OD1	40:C1:518:DGD:O5E	2.29	0.45
33:C1:516:BCR:H15C	33:C1:516:BCR:H351	1.75	0.45
47:N1:601:CHL:H111	41:N1:624:LHG:H202	1.98	0.45
31:N1:603:CLA:H51	31:G1:603:CLA:H41	1.98	0.45
49:N1:622:XAT:H31	49:N1:622:XAT:H391	1.62	0.45
47:S1:607:CHL:HHC	47:S1:607:CHL:HBB1	1.97	0.45
2:b1:65:PHE:HE1	31:b1:605:CLA:HED2	1.81	0.45
2:b1:385:LYS:HB2	15:p1:150:TRP:HE1	1.81	0.45
4:c1:458:ARG:O	5:d1:251:ARG:NH1	2.50	0.45
15:p1:187:PHE:HD2	15:p1:205:VAL:HB	1.82	0.45
27:r1:82:THR:OG1	27:r1:84:SEP:O2P	2.34	0.45
24:y1:99:LEU:HD21	31:y1:610:CLA:H171	1.99	0.45
31:C:509:CLA:H11	31:C:509:CLA:H51	1.64	0.45
8:H:50:MET:HE3	46:H:101:RRX:H16	1.99	0.45
14:O:276:SER:OG	14:O:277:ASP:N	2.48	0.45
24:Y:85:ARG:HA	24:Y:88:THR:HG22	1.98	0.45
1:a:97:TRP:HA	9:i:1:MET:HE2	1.98	0.45
1:a:301:ASN:HB3	4:c:395:VAL:HG21	1.98	0.45
2:b:257:TRP:HZ3	2:b:449:GLY:HA2	1.82	0.45
14:o:181:LEU:HB2	14:o:205:TYR:HD1	1.81	0.45
48:s:621:LUT:H11	48:s:621:LUT:H191	1.87	0.45
31:y:602:CLA:H143	31:y:602:CLA:H161	1.82	0.45
1:A1:34:GLY:HA2	1:A1:37:MET:SD	2.57	0.45
1:A1:312:ARG:HG3	15:P1:91:TRP:O	2.17	0.45
2:B1:154:GLY:HA3	2:B1:202:HIS:HB2	1.99	0.45
4:C1:83:LEU:HD11	4:C1:166:LYS:HG2	1.99	0.45
10:J1:32:TYR:HA	38:J1:101:DGA:HA31	1.98	0.45
31:Y1:610:CLA:H93	31:Y1:612:CLA:H8	1.99	0.45
48:Y1:620:LUT:H11	48:Y1:620:LUT:H191	1.87	0.45
2:b1:455:HIS:O	2:b1:459:ALA:N	2.44	0.45
31:b1:607:CLA:H141	31:b1:607:CLA:H161	1.77	0.45
4:c1:249:ARG:HA	4:c1:254:TRP:HE1	1.81	0.45
41:c1:525:LHG:O10	31:s1:611:CLA:HAB	2.17	0.45
5:d1:82:ALA:HB1	5:d1:336:HIS:CE1	2.52	0.45
31:n1:613:CLA:H203	21:g1:147:ALA:HB2	1.99	0.45
23:s1:169:THR:HB	47:s1:607:CHL:HBC1	1.98	0.45
31:B:602:CLA:H13	46:H:101:RRX:H39	1.99	0.45
31:B:607:CLA:H141	31:B:607:CLA:H162	1.73	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:B:613:CLA:H162	31:B:613:CLA:H122	1.76	0.45
20:N:60:LEU:HD23	20:N:69:GLY:HA2	1.98	0.45
31:Y:602:CLA:CAB	48:Y:621:LUT:H32	2.47	0.45
31:b:615:CLA:HBD	31:b:615:CLA:HBA1	1.98	0.45
5:d:81:PRO:HG2	5:d:167:TRP:HB2	1.99	0.45
5:d:188:PHE:HZ	5:d:330:ALA:HB2	1.82	0.45
31:n:603:CLA:HED2	47:n:609:CHL:H93	1.98	0.45
48:g:621:LUT:H372	31:y:603:CLA:HED3	1.99	0.45
1:A1:247:ASN:HB3	1:A1:250:ALA:HB3	1.99	0.45
2:B1:245:VAL:HG22	31:B1:605:CLA:HAC1	1.98	0.45
5:D1:97:ALA:HA	6:E1:73:LEU:HD21	1.99	0.45
5:D1:253:TRP:HB2	5:D1:260:ALA:HB2	1.99	0.45
31:G1:603:CLA:H91	47:G1:609:CHL:H121	1.98	0.45
32:a1:409:PHO:H11	5:d1:125:PHE:HB2	1.99	0.45
31:a1:410:CLA:H8	9:i1:16:VAL:HG11	1.98	0.45
2:b1:157:HIS:HA	2:b1:163:GLY:HA3	1.98	0.45
2:b1:231:MET:HG3	31:b1:611:CLA:HAC2	1.99	0.45
33:b1:619:BCR:HC42	35:b1:622:LMG:H341	1.98	0.45
31:c1:508:CLA:H62	31:c1:508:CLA:H41	1.73	0.45
31:c1:513:CLA:HAB	33:c1:514:BCR:H24C	1.98	0.45
47:n1:601:CHL:HHB	47:g1:609:CHL:HMB2	1.98	0.45
49:r1:621:XAT:H31	49:r1:621:XAT:H391	1.86	0.45
1:A:274:PHE:HA	1:A:277:VAL:HG12	1.99	0.45
1:A:289:GLY:O	1:A:293:MET:HG2	2.17	0.45
31:A:407:CLA:HMA2	35:D:411:LMG:H372	1.99	0.45
35:A:413:LMG:H331	31:C:506:CLA:H192	1.98	0.45
2:B:278:GLY:O	2:B:282:GLN:CB	2.54	0.45
2:B:441:GLY:HA2	14:O:230:ALA:HB3	1.99	0.45
31:B:612:CLA:H193	31:B:612:CLA:H162	1.70	0.45
40:C:523:DGD:HB92	40:C:523:DGD:HBH2	1.98	0.45
14:O:265:GLU:OE1	14:O:295:TYR:OH	2.27	0.45
16:T:28:ARG:HD3	16:T:28:ARG:HA	1.83	0.45
31:N:613:CLA:H13	49:G:622:XAT:H34	1.99	0.45
2:b:172:TYR:HB2	2:b:174:LEU:HD23	1.99	0.45
2:b:359:MET:HB2	2:b:425:GLN:NE2	2.31	0.45
31:b:608:CLA:H92	35:b:622:LMG:H201	1.98	0.45
3:v:12:LEU:HA	11:k:24:VAL:HG21	1.98	0.45
33:c:516:BCR:H15C	11:k:35:LEU:HD12	1.99	0.45
44:d:405:PL9:H252	41:l:101:LHG:H151	1.99	0.45
21:g:53:LEU:HD13	21:g:62:GLY:HA2	1.99	0.45
22:r:85:LEU:HD22	22:r:104:VAL:HG11	1.98	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A1:204:GLY:HA3	1:A1:282:CYS:SG	2.57	0.45
33:A1:411:BCR:H15C	33:A1:411:BCR:H351	1.71	0.45
2:B1:287:ARG:HD2	2:B1:305:ILE:HD13	1.99	0.45
2:B1:460:LEU:HB3	5:D1:280:TRP:HZ3	1.82	0.45
4:C1:271:GLY:HA3	4:C1:422:GLY:HA3	1.99	0.45
26:M1:5:ILE:HG21	26:m1:5:ILE:HG21	1.98	0.45
47:G1:601:CHL:H171	47:Y1:607:CHL:H152	1.99	0.45
31:G1:613:CLA:H61	49:Y1:622:XAT:H203	1.99	0.45
31:R1:604:CLA:H12	47:R1:606:CHL:C3D	2.47	0.45
24:Y1:112:LYS:NZ	24:Y1:238:GLN:OE1	2.35	0.45
33:b1:618:BCR:H24C	34:b1:621:SQD:H261	1.98	0.45
4:c1:438:ALA:O	4:c1:443:PHE:N	2.40	0.45
5:d1:84:SER:H	5:d1:336:HIS:CE1	2.35	0.45
31:g1:611:CLA:H72	31:g1:611:CLA:H112	1.75	0.45
31:g1:613:CLA:H72	41:g1:624:LHG:H152	1.99	0.45
2:B:55:MET:HE2	2:B:64:PRO:HG3	1.98	0.45
31:B:608:CLA:H41	31:B:608:CLA:H62	1.63	0.45
33:C:514:BCR:H341	19:Z:52:PHE:HD1	1.82	0.45
5:D:262:SER:N	41:D:409:LHG:O5	2.47	0.45
20:N:41:TYR:HE2	20:N:200:ALA:HB1	1.81	0.45
48:N:621:LUT:H15	48:N:621:LUT:H201	1.80	0.45
47:G:601:CHL:H62	47:G:601:CHL:H41	1.58	0.45
31:b:604:CLA:H193	31:b:604:CLA:H162	1.85	0.45
31:c:508:CLA:H202	31:c:508:CLA:H161	1.74	0.45
5:d:29:PHE:HB3	5:d:128:ARG:NH1	2.31	0.45
5:d:148:ALA:HB2	5:d:276:VAL:HG13	1.99	0.45
41:n:624:LHG:H221	49:g:622:XAT:H10	1.98	0.45
22:r:169:GLU:HA	22:r:173:ALA:HA	1.99	0.45
25:u:96:ASP:O	25:u:100:PRO:HD3	2.17	0.45
1:A1:283:ILE:HG13	32:A1:408:PHO:HBC3	1.99	0.45
2:B1:324:LEU:HD21	5:D1:196:PHE:HE2	1.82	0.45
38:C1:524:DGA:HAT2	38:C1:524:DGA:HAH1	1.69	0.45
54:K1:101:4RF:H68	54:K1:101:4RF:H78	1.99	0.45
20:N1:101:LEU:HB2	31:N1:604:CLA:HMC1	1.98	0.45
20:N1:208:LYS:HE3	41:N1:624:LHG:HC61	1.99	0.45
23:S1:225:PRO:HA	23:S1:228:PHE:HB3	1.99	0.45
24:Y1:142:ASN:HB3	24:Y1:145:LEU:HB2	1.98	0.45
24:Y1:191:PRO:HB3	27:r1:220:PRO:HB3	1.99	0.45
31:Y1:613:CLA:H143	41:Y1:624:LHG:H361	1.98	0.45
31:b1:608:CLA:H3A	31:b1:608:CLA:HBA2	1.56	0.45
4:c1:225:HIS:HA	4:c1:228:ILE:HG22	1.99	0.45

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:c1:512:CLA:HED2	31:c1:512:CLA:H2A	1.99	0.45
33:d1:404:BCR:H373	7:f1:33:LEU:HD21	1.97	0.45
31:n1:604:CLA:HBA2	31:n1:604:CLA:H3A	1.43	0.45
31:n1:613:CLA:H202	31:n1:614:CLA:HBA2	1.98	0.45
21:g1:40:PHE:CZ	47:g1:601:CHL:HAA1	2.52	0.45
47:g1:601:CHL:HHD	41:g1:624:LHG:HC41	1.99	0.45
31:s1:604:CLA:HBB1	48:s1:621:LUT:H181	1.98	0.45
1:A:89:ILE:HB	14:O:135:ARG:HH22	1.82	0.44
31:B:615:CLA:H192	33:B:618:BCR:H343	1.98	0.44
4:C:296:GLU:HB3	4:C:349:PHE:CZ	2.53	0.44
4:C:307:VAL:HG23	4:C:310:GLN:HE21	1.82	0.44
31:C:511:CLA:H193	19:Z:23:VAL:HG21	1.99	0.44
14:O:135:ARG:O	14:O:137:THR:N	2.50	0.44
1:a:41:LEU:HG	1:a:122:GLY:HA3	1.99	0.44
2:b:65:PHE:HE2	31:b:605:CLA:H2A	1.81	0.44
2:b:192:PRO:HG3	8:h:68:TYR:HD1	1.81	0.44
31:b:611:CLA:H8	31:b:611:CLA:H51	1.80	0.44
31:c:511:CLA:H122	19:z:24:PRO:HG3	2.00	0.44
41:d:410:LHG:H252	41:d:410:LHG:H282	1.78	0.44
6:e:53:ASN:ND2	6:e:54:GLU:OE2	2.50	0.44
20:n:223:GLN:HE22	20:n:231:PRO:HB3	1.82	0.44
21:g:141:SER:OG	47:g:605:CHL:OMC	2.27	0.44
31:g:613:CLA:H72	41:g:624:LHG:H152	1.99	0.44
49:r:622:XAT:H32	31:r:602:CLA:CBB	2.47	0.44
23:s:283:ASP:N	23:s:283:ASP:OD1	2.50	0.44
41:s:624:LHG:H271	41:s:624:LHG:HC91	1.98	0.44
24:y:104:ILE:HD11	24:y:124:TRP:CE2	2.52	0.44
48:y:621:LUT:H11	48:y:621:LUT:H191	1.84	0.44
1:A1:47:VAL:HG21	1:A1:114:LEU:HD22	1.99	0.44
4:C1:119:TYR:O	4:C1:124:GLY:N	2.50	0.44
4:C1:249:ARG:HA	4:C1:254:TRP:CZ2	2.53	0.44
5:D1:92:VAL:HA	5:D1:97:ALA:HB3	1.99	0.44
11:K1:45:PHE:HE2	54:K1:101:4RF:H5	1.82	0.44
14:O1:140:LEU:HD21	14:O1:165:TYR:C	2.42	0.44
31:N1:610:CLA:H91	31:N1:610:CLA:H112	1.80	0.44
27:R1:186:GLN:NE2	54:i1:101:4RF:O40	2.50	0.44
48:S1:621:LUT:H35	48:S1:621:LUT:H401	1.86	0.44
47:Y1:607:CHL:H143	47:Y1:609:CHL:H101	1.99	0.44
1:a1:338:ASN:HB3	4:c1:327:LYS:HG2	1.99	0.44
31:b1:609:CLA:H18	31:d1:403:CLA:HMA1	1.99	0.44
5:d1:84:SER:H	5:d1:336:HIS:HE1	1.65	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:s1:620:LUT:H15	48:s1:620:LUT:H201	1.82	0.44
49:y1:622:XAT:H11	49:y1:622:XAT:H191	1.89	0.44
31:B:610:CLA:C2	31:B:611:CLA:HBB2	2.47	0.44
31:B:617:CLA:H2A	31:B:617:CLA:H12	1.99	0.44
31:C:511:CLA:H102	33:C:517:BCR:H402	2.00	0.44
5:D:213:ILE:HG22	44:D:405:PL9:HC2	1.99	0.44
20:N:171:GLY:HA2	47:N:608:CHL:HMC	1.98	0.44
31:N:610:CLA:H161	31:N:610:CLA:H193	1.84	0.44
21:G:77:ARG:O	21:G:80:GLU:HG2	2.16	0.44
31:G:602:CLA:H3A	31:G:602:CLA:HBA2	1.47	0.44
2:b:30:VAL:HG13	31:b:606:CLA:HAC2	1.99	0.44
2:b:118:TRP:HH2	12:l:1:MET:H2	1.66	0.44
2:b:463:PHE:HE1	31:b:609:CLA:HBB1	1.81	0.44
4:c:14:ARG:O	4:c:29:ARG:NH1	2.50	0.44
5:d:210:LEU:HA	5:d:213:ILE:HG22	1.99	0.44
14:o:93:ASN:O	14:o:95:ARG:N	2.50	0.44
19:z:41:PHE:HE1	23:s:65:LEU:HD12	1.82	0.44
20:n:99:GLY:O	20:n:103:MET:HG2	2.16	0.44
47:n:606:CHL:HHC	47:n:606:CHL:HBB1	1.99	0.44
48:n:621:LUT:H11	48:n:621:LUT:H191	1.88	0.44
1:A1:67:VAL:HG13	5:D1:313:THR:HA	1.98	0.44
1:A1:139:MET:N	1:A1:139:MET:SD	2.90	0.44
1:A1:211:PHE:HA	1:A1:214:MET:HG3	1.99	0.44
4:C1:142:LYS:HE2	4:C1:254:TRP:CD2	2.52	0.44
31:C1:505:CLA:H91	31:C1:505:CLA:H111	1.73	0.44
11:K1:11:LEU:HD12	11:K1:19:SER:HB2	1.99	0.44
17:W1:78:ASP:OD1	17:W1:79:GLY:N	2.49	0.44
48:G1:620:LUT:H15	48:G1:620:LUT:H201	1.81	0.44
47:R1:606:CHL:HHC	47:R1:606:CHL:HBB1	1.98	0.44
31:S1:610:CLA:HBA2	31:S1:610:CLA:H3A	1.51	0.44
31:S1:613:CLA:H11	31:S1:613:CLA:H52	1.68	0.44
24:Y1:212:GLY:O	24:Y1:216:MET:HG3	2.17	0.44
31:b1:608:CLA:CAB	35:b1:622:LMG:H182	2.46	0.44
4:c1:78:PRO:O	4:c1:82:THR:OG1	2.28	0.44
31:c1:505:CLA:HBA2	31:c1:505:CLA:H3A	1.66	0.44
35:c1:523:LMG:H401	41:y1:624:LHG:H381	1.99	0.44
49:g1:622:XAT:H31	49:g1:622:XAT:H391	1.77	0.44
51:s1:625:LPX:H8	52:s1:626:3PH:H291	1.99	0.44
2:B:260:SER:H	2:B:263:THR:HB	1.82	0.44
4:C:265:ALA:HB2	4:C:429:HIS:CG	2.52	0.44
4:C:456:SER:OG	4:C:457:MET:SD	2.75	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
40:C:523:DGD:HB71	40:C:523:DGD:HA82	1.99	0.44
5:D:219:GLU:HA	5:D:222:LEU:HD23	2.00	0.44
8:H:29:LEU:HD12	22:R:132:ARG:HH12	1.82	0.44
31:G:602:CLA:H72	48:G:621:LUT:H28	1.99	0.44
2:b:357:ARG:NH2	5:d:337:GLU:OE1	2.49	0.44
5:d:202:ALA:HB2	44:d:405:PL9:H353	1.98	0.44
41:l:101:LHG:H111	41:l:101:LHG:HC81	1.76	0.44
53:y:625:SPH:H131	53:y:625:SPH:H162	1.67	0.44
2:B1:57:ARG:HH22	2:B1:432:PHE:HE1	1.66	0.44
4:C1:47:LEU:HD12	33:C1:517:BCR:H372	1.99	0.44
4:C1:438:ALA:O	4:C1:442:GLY:N	2.50	0.44
35:C1:521:LMG:H111	35:C1:521:LMG:H141	1.85	0.44
9:I1:21:PHE:O	9:I1:25:SER:OG	2.26	0.44
49:N1:622:XAT:C34	31:Y1:613:CLA:H111	2.47	0.44
1:a1:153:ALA:HB3	31:a1:405:CLA:H11	1.99	0.44
32:a1:408:PHO:HAB	5:d1:205:LEU:HD12	2.00	0.44
34:a1:412:SQD:H261	34:a1:412:SQD:H292	1.78	0.44
2:b1:383:PHE:H	5:d1:345:VAL:HA	1.82	0.44
38:b1:625:DGA:HBG3	8:h1:55:LEU:HA	1.99	0.44
4:c1:58:PHE:CZ	11:k1:26:PRO:HD3	2.52	0.44
15:p1:121:GLN:O	15:p1:214:LEU:N	2.46	0.44
31:n1:603:CLA:HMA3	31:n1:603:CLA:H2	1.99	0.44
31:g1:603:CLA:HMD3	47:g1:609:CHL:HBA2	1.99	0.44
27:r1:101:LYS:HD3	27:r1:101:LYS:HA	1.86	0.44
35:H:102:LMG:H151	35:H:102:LMG:H182	1.52	0.44
11:K:40:GLN:HA	11:K:43:VAL:HG12	2.00	0.44
14:O:135:ARG:HB3	14:O:136:LEU:H	1.68	0.44
31:S:611:CLA:H62	51:S:625:LPX:H21	1.99	0.44
31:Y:610:CLA:CBB	48:Y:620:LUT:H32	2.47	0.44
31:Y:612:CLA:HED2	31:Y:612:CLA:H2A	1.99	0.44
1:a:234:ASN:HB3	1:a:238:LYS:HD3	2.00	0.44
2:b:359:MET:HB2	2:b:425:GLN:HE22	1.83	0.44
31:b:613:CLA:H193	31:b:613:CLA:H162	1.76	0.44
4:c:192:THR:HG22	4:c:223:GLY:HA2	1.98	0.44
4:c:232:CYS:HA	31:c:506:CLA:HMC2	1.99	0.44
31:c:509:CLA:H71	31:c:509:CLA:H112	1.72	0.44
5:d:73:PHE:HB2	35:d:411:LMG:H291	1.99	0.44
10:j:31:PHE:O	10:j:34:SER:OG	2.35	0.44
11:k:29:PRO:HA	11:k:32:PHE:HD2	1.83	0.44
18:x:70:LYS:HE3	18:x:74:LEU:HG	1.99	0.44
21:g:242:PHE:HZ	24:y:155:LEU:HD13	1.81	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:y:602:CLA:H101	31:y:602:CLA:H13	1.68	0.44
2:B1:68:ARG:HH11	31:B1:604:CLA:HED2	1.82	0.44
2:B1:170:ASP:CG	2:B1:174:LEU:H	2.24	0.44
31:B1:611:CLA:H141	31:B1:613:CLA:HAA1	1.99	0.44
31:B1:616:CLA:H13	31:R1:609:CLA:H8	2.00	0.44
4:C1:282:ASN:N	40:C1:518:DGD:O5E	2.40	0.44
4:C1:393:ASN:HB3	40:C1:520:DGD:HD62	1.99	0.44
5:D1:191:TRP:CE2	5:D1:197:HIS:HB2	2.52	0.44
15:P1:125:LYS:HG3	15:P1:131:TYR:HE1	1.83	0.44
15:P1:204:LEU:HB3	15:P1:238:LEU:HD21	1.98	0.44
31:a1:406:CLA:H41	44:d1:405:PL9:H162	1.99	0.44
5:d1:267:LEU:O	5:d1:271:MET:HG2	2.17	0.44
21:g1:231:ASP:HB3	21:g1:239:ASN:ND2	2.32	0.44
49:g1:622:XAT:H15	49:g1:622:XAT:H201	1.72	0.44
31:r1:603:CLA:HBA2	31:r1:603:CLA:H3A	1.56	0.44
23:s1:93:ASP:OD1	23:s1:93:ASP:N	2.50	0.44
31:s1:610:CLA:H91	31:s1:610:CLA:H111	1.83	0.44
1:A:325:ASN:HB3	4:C:400:THR:HG22	2.00	0.44
2:B:242:ILE:HA	2:B:245:VAL:HG12	1.99	0.44
4:C:227:TRP:O	4:C:231:LEU:HG	2.17	0.44
5:D:29:PHE:O	5:D:128:ARG:NH1	2.38	0.44
41:D:408:LHG:HC81	41:L:101:LHG:HC82	1.99	0.44
14:O:109:MET:CE	14:O:140:LEU:CD1	2.82	0.44
21:G:39:LYS:HE3	21:G:42:GLY:O	2.17	0.44
33:b:618:BCR:H351	33:b:618:BCR:H15C	1.78	0.44
31:c:501:CLA:H193	31:c:507:CLA:HBB1	1.99	0.44
40:c:519:DGD:O2D	35:j:101:LMG:O10	2.30	0.44
35:h:102:LMG:H291	35:h:102:LMG:H111	1.99	0.44
47:n:601:CHL:HED1	41:n:624:LHG:H282	1.99	0.44
49:n:622:XAT:H31	49:n:622:XAT:H391	1.67	0.44
49:n:622:XAT:H172	24:y:228:VAL:HG21	2.00	0.44
2:B1:58:GLN:HB2	2:B1:60:MET:HG2	1.98	0.44
2:B1:368:VAL:HB	2:B1:381:VAL:HG12	1.98	0.44
31:B1:603:CLA:H101	31:B1:603:CLA:H13	1.85	0.44
41:C1:525:LHG:H112	31:S1:611:CLA:HBB2	1.99	0.44
5:D1:274:VAL:HA	44:D1:405:PL9:H253	2.00	0.44
48:N1:621:LUT:H15	48:N1:621:LUT:H201	1.83	0.44
21:G1:199:LYS:O	21:G1:203:ASN:ND2	2.43	0.44
31:R1:608:CLA:H92	31:R1:608:CLA:H62	1.84	0.44
24:Y1:191:PRO:HD2	48:Y1:620:LUT:H23	2.00	0.44
1:a1:76:ASN:O	1:a1:80:GLY:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b1:258:TYR:OH	5:d1:162:LEU:O	2.35	0.44
2:b1:413:ASP:HB3	2:b1:416:THR:HG22	1.99	0.44
31:b1:615:CLA:H193	31:b1:615:CLA:H161	1.86	0.44
31:b1:616:CLA:H8	31:b1:616:CLA:H52	1.81	0.44
5:d1:221:THR:HG21	5:d1:249:ALA:HB2	1.99	0.44
1:A:344:ALA:OXT	4:C:345:ARG:NH1	2.50	0.44
4:C:57:LEU:HD13	33:C:517:BCR:HC21	1.99	0.44
5:D:314:PHE:HA	5:D:317:LYS:HD3	1.99	0.44
20:N:226:VAL:HG13	20:N:227:THR:HG23	1.99	0.44
31:R:612:CLA:HED2	31:R:612:CLA:H12	2.00	0.44
31:Y:602:CLA:HAB	48:Y:621:LUT:H32	1.99	0.44
4:c:120:HIS:HA	4:c:124:GLY:HA3	1.99	0.44
44:d:405:PL9:H162	41:d:409:LHG:H131	2.00	0.44
13:m:32:SER:O	13:m:32:SER:OG	2.35	0.44
14:o:143:MET:HG3	14:o:162:GLY:HA3	2.00	0.44
47:n:606:CHL:H192	52:s:626:3PH:H2A1	1.99	0.44
48:s:620:LUT:H35	48:s:620:LUT:H401	1.81	0.44
2:B1:26:HIS:ND1	31:B1:613:CLA:HHB	2.24	0.44
2:B1:187:ALA:HB1	8:H1:74:LEU:HD13	1.99	0.44
34:B1:621:SQD:H102	34:B1:621:SQD:H131	1.80	0.44
4:C1:317:ALA:HB1	14:O1:163:LEU:HD22	2.00	0.44
31:C1:512:CLA:H41	31:C1:512:CLA:H62	1.70	0.44
41:C1:525:LHG:O8	41:S1:624:LHG:O1	2.35	0.44
14:O1:135:ARG:HA	17:W1:64:ARG:HH22	1.82	0.44
47:N1:606:CHL:HBB2	47:N1:607:CHL:HAB	1.99	0.44
21:G1:212:LEU:HD11	31:G1:603:CLA:CAB	2.45	0.44
2:b1:162:PHE:O	40:b1:623:DGD:O2E	2.32	0.44
31:b1:609:CLA:H3A	31:b1:609:CLA:HBA2	1.72	0.44
4:c1:237:ILE:HG12	34:c1:526:SQD:H101	1.99	0.44
31:c1:505:CLA:H111	31:c1:505:CLA:H91	1.81	0.44
26:m1:20:SER:O	26:m1:24:ILE:HD12	2.17	0.44
55:r1:625:LMT:H91	55:r1:625:LMT:H61	1.81	0.44
4:C:191:THR:OG1	4:C:220:ASP:OD1	2.30	0.44
4:C:447:ILE:H	5:D:223:PHE:HA	1.82	0.44
44:D:405:PL9:H322	44:D:405:PL9:H28	1.79	0.44
20:N:72:THR:HA	21:G:77:ARG:NH2	2.32	0.44
22:R:186:GLN:O	22:R:190:ILE:HG12	2.18	0.44
1:a:162:PRO:HB3	1:a:168:PHE:HA	1.98	0.44
31:b:608:CLA:H62	31:b:608:CLA:H41	1.59	0.44
4:c:160:ALA:O	4:c:164:VAL:HG23	2.18	0.44
6:e:12:ASP:OD1	6:e:12:ASP:N	2.50	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:n:117:PHE:HZ	20:n:139:LEU:HD23	1.82	0.44
31:r:612:CLA:H52	31:r:612:CLA:H8	1.69	0.44
23:s:237:LYS:HG3	23:s:240:ARG:HH21	1.83	0.44
41:s:624:LHG:H302	41:s:624:LHG:H332	1.72	0.44
24:y:101:ALA:HB1	48:y:620:LUT:H12	2.00	0.44
31:B1:610:CLA:HBA1	31:B1:610:CLA:H3A	1.87	0.44
35:B1:622:LMG:H142	35:B1:622:LMG:H171	1.72	0.44
4:C1:199:GLY:O	4:C1:203:LYS:HG3	2.17	0.44
44:D1:405:PL9:H311	41:L1:101:LHG:H182	2.00	0.44
41:D1:409:LHG:HC91	41:D1:409:LHG:H122	1.69	0.44
14:O1:235:ASP:N	14:O1:235:ASP:OD1	2.51	0.44
31:N1:602:CLA:CBB	48:N1:621:LUT:H32	2.47	0.44
49:G1:622:XAT:H391	49:G1:622:XAT:H31	1.74	0.44
23:S1:255:VAL:HG23	23:S1:256:THR:HG23	1.99	0.44
49:Y1:622:XAT:H31	49:Y1:622:XAT:H391	1.74	0.44
50:Y1:623:NEX:H171	50:Y1:623:NEX:H193	1.99	0.44
1:a1:59:ASP:OD2	1:a1:64:ARG:NH1	2.49	0.44
1:a1:123:VAL:O	1:a1:127:MET:HG2	2.18	0.44
4:c1:393:ASN:HB3	40:c1:520:DGD:HD62	1.99	0.44
31:c1:503:CLA:H61	31:c1:503:CLA:H41	1.59	0.44
33:c1:516:BCR:H352	11:k1:28:ILE:HG23	2.00	0.44
5:d1:13:THR:HG23	5:d1:15:PHE:H	1.83	0.44
14:o1:254:PHE:CD1	14:o1:270:PHE:HB2	2.53	0.44
27:r1:217:ALA:HB1	31:r1:608:CLA:H93	2.00	0.44
31:s1:603:CLA:H92	31:s1:603:CLA:H61	1.90	0.44
24:y1:146:ILE:N	47:y1:605:CHL:O1D	2.51	0.44
24:y1:201:PHE:CE2	24:y1:205:LYS:HE3	2.53	0.44
31:B:608:CLA:HBA2	31:B:608:CLA:H3A	1.59	0.44
33:C:517:BCR:H351	33:C:517:BCR:H15C	1.67	0.44
5:D:29:PHE:HB3	5:D:128:ARG:NH2	2.33	0.44
20:N:211:ARG:HA	20:N:214:MET:HE3	1.99	0.44
47:N:605:CHL:H13	31:S:605:CLA:HBA2	2.00	0.44
1:a:105:TRP:NE1	1:a:110:GLY:HA3	2.33	0.44
2:b:334:ASP:OD1	2:b:334:ASP:N	2.51	0.44
4:c:78:PRO:O	4:c:82:THR:OG1	2.30	0.44
4:c:122:LEU:HD13	19:z:28:ALA:HB2	2.00	0.44
4:c:177:TRP:CZ2	4:c:283:THR:HG22	2.53	0.44
5:d:87:HIS:CD2	5:d:166:GLY:HA2	2.53	0.44
12:l:24:LEU:HD12	41:l:101:LHG:H122	2.00	0.44
31:r:603:CLA:HBB2	47:r:607:CHL:HAB	2.00	0.44
23:s:81:GLY:HA3	23:s:240:ARG:HH12	1.82	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:y:601:CHL:H51	41:y:624:LHG:H162	1.99	0.44
32:A1:409:PHO:HBA1	32:A1:409:PHO:H3A	1.42	0.44
2:B1:270:PRO:HB3	2:B1:280:PHE:HE2	1.82	0.44
5:D1:90:LEU:HB3	5:D1:109:GLY:HA2	2.00	0.44
20:N1:205:LYS:HG3	31:N1:611:CLA:HED2	2.00	0.44
31:N1:604:CLA:HBA2	31:N1:604:CLA:H3A	1.35	0.44
31:N1:610:CLA:H61	31:N1:610:CLA:H41	1.54	0.44
31:Y1:602:CLA:CAB	48:Y1:621:LUT:H32	2.48	0.44
1:a1:319:ASP:HA	1:a1:322:ASN:HB3	2.00	0.44
4:c1:265:ALA:HB2	4:c1:429:HIS:CE1	2.52	0.44
8:h1:67:ILE:HG13	8:h1:72:LEU:HB3	2.00	0.44
14:o1:108:CYS:O	14:o1:295:TYR:N	2.42	0.44
31:n1:603:CLA:CAD	47:n1:609:CHL:H2	2.48	0.44
49:n1:622:XAT:H201	49:n1:622:XAT:H15	1.72	0.44
2:B:317:ASN:HA	2:B:330:MET:HE1	2.00	0.44
31:C:501:CLA:H61	31:C:501:CLA:H41	1.55	0.44
31:C:504:CLA:H62	31:C:504:CLA:H41	1.67	0.44
31:R:612:CLA:H52	31:R:612:CLA:H8	1.66	0.44
23:S:83:TYR:OH	41:S:624:LHG:O5	2.29	0.44
24:Y:204:LEU:HD23	24:Y:207:LYS:HG3	2.00	0.44
31:c:505:CLA:H42	33:c:515:BCR:HC7	2.00	0.44
31:c:511:CLA:H62	33:c:517:BCR:H402	1.99	0.44
16:t:27:PRO:O	16:t:28:ARG:NH1	2.43	0.44
20:n:139:LEU:HD23	20:n:139:LEU:HA	1.86	0.44
31:g:602:CLA:CAB	48:g:621:LUT:H32	2.48	0.44
31:y:602:CLA:HBB1	31:y:602:CLA:H51	1.99	0.44
48:y:621:LUT:H35	48:y:621:LUT:H401	1.86	0.44
2:B1:24:LEU:HG	31:B1:616:CLA:HED3	2.00	0.44
2:B1:183:PRO:HA	2:B1:199:PRO:HG2	2.00	0.44
2:B1:423:LYS:HB3	2:B1:429:ILE:HG12	1.99	0.44
4:C1:37:LEU:O	4:C1:41:HIS:ND1	2.51	0.44
24:Y1:139:TYR:HB3	24:Y1:145:LEU:HB3	1.99	0.44
1:a1:226:GLU:OE1	5:d1:265:ARG:NH2	2.51	0.44
1:a1:331:MET:SD	5:d1:347:PRO:HB2	2.57	0.44
31:a1:407:CLA:HBB2	5:d1:153:PHE:CD1	2.53	0.44
31:b1:603:CLA:H43	8:h1:64:ILE:HG13	2.00	0.44
33:c1:515:BCR:H332	9:i1:20:ILE:HD12	1.99	0.44
14:o1:149:ILE:HA	14:o1:155:VAL:HG12	1.99	0.44
24:y1:98:LEU:HD22	31:y1:610:CLA:HAB	2.00	0.44
24:y1:105:ILE:HD12	24:y1:234:ILE:HD11	1.99	0.44
31:y1:612:CLA:HED2	31:y1:612:CLA:H12	2.00	0.44

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
1:A:175:GLY:O	1:A:179:THR:OG1	2.31	0.43
1:A:190:HIS:HB3	1:A:293:MET:SD	2.59	0.43
2:B:333:GLY:O	2:B:441:GLY:N	2.38	0.43
4:C:15:ASP:HB3	11:K:46:ARG:HD2	1.98	0.43
31:C:511:CLA:H13	33:C:517:BCR:H21C	1.99	0.43
6:E:62:ASP:OD1	6:E:63:ALA:N	2.47	0.43
21:G:92:GLY:O	21:G:96:ILE:HG12	2.17	0.43
2:b:365:THR:O	5:d:326:ARG:NH1	2.51	0.43
31:b:607:CLA:H143	31:b:607:CLA:H8	1.99	0.43
31:b:612:CLA:H161	31:b:612:CLA:H121	1.67	0.43
4:c:203:LYS:HD2	4:c:209:ASP:HB3	2.00	0.43
4:c:205:PRO:HA	4:c:211:TRP:H	1.83	0.43
4:c:300:ALA:HB1	4:c:383:TYR:HB2	2.00	0.43
6:e:8:ARG:HH21	7:f:18:ARG:HE	1.64	0.43
14:o:277:ASP:CG	14:o:279:GLU:H	2.25	0.43
20:n:218:LEU:CD2	31:n:603:CLA:HAB	2.48	0.43
21:g:90:LEU:HD21	21:g:203:ASN:HB3	2.00	0.43
23:s:75:LEU:HD22	23:s:84:GLY:HA2	1.99	0.43
1:A1:36:ILE:HA	31:A1:410:CLA:CBB	2.48	0.43
1:A1:50:ILE:HD11	34:b1:626:SQD:H302	1.99	0.43
2:B1:39:LEU:HG	2:B1:97:ALA:HB1	1.99	0.43
41:C1:525:LHG:H311	41:S1:624:LHG:H101	1.99	0.43
5:D1:92:VAL:HG21	5:D1:101:LEU:HD23	2.00	0.43
26:M1:15:ILE:O	26:M1:19:THR:OG1	2.23	0.43
20:N1:65:PRO:HG3	20:N1:203:LYS:HB3	1.99	0.43
20:N1:111:ASP:OD1	20:N1:111:ASP:N	2.48	0.43
49:G1:622:XAT:H15	49:G1:622:XAT:H201	1.75	0.43
56:R1:626:ERG:H212	17:w1:80:ILE:HG12	1.98	0.43
1:a1:89:ILE:HD11	1:a1:108:ASN:HB3	1.99	0.43
32:a1:409:PHO:H3A	32:a1:409:PHO:HBA1	1.69	0.43
2:b1:139:PHE:O	2:b1:143:LEU:N	2.44	0.43
31:b1:613:CLA:H171	31:b1:613:CLA:H13	1.78	0.43
4:c1:71:GLU:HA	4:c1:407:PHE:CE1	2.52	0.43
40:c1:519:DGD:O3D	40:c1:520:DGD:O5E	2.29	0.43
6:e1:69:ARG:NH2	8:h1:69:ASN:O	2.30	0.43
48:n1:620:LUT:H15	48:n1:620:LUT:H201	1.87	0.43
21:g1:67:GLY:HA2	24:y1:85:ARG:CZ	2.48	0.43
21:g1:215:PHE:HB3	47:g1:607:CHL:H93	2.00	0.43
4:C:162:LEU:HD21	31:C:502:CLA:H18	1.99	0.43
31:C:511:CLA:H93	31:C:511:CLA:H61	1.84	0.43
47:N:607:CHL:H2	47:N:607:CHL:HMA3	1.99	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:N:610:CLA:H91	31:N:610:CLA:H111	1.78	0.43
49:N:622:XAT:H30	41:Y:624:LHG:H383	2.00	0.43
21:G:160:ARG:HE	47:G:608:CHL:C4D	2.31	0.43
22:R:256:GLN:HA	22:R:259:ALA:HB3	2.01	0.43
23:S:114:ALA:HA	48:S:621:LUT:H182	2.00	0.43
2:b:264:PRO:HD2	2:b:268:PHE:HE2	1.83	0.43
31:b:610:CLA:HBA2	31:b:610:CLA:H3A	1.69	0.43
31:b:613:CLA:H61	31:b:613:CLA:H102	1.66	0.43
4:c:157:GLY:HA2	4:c:229:GLY:HA2	1.99	0.43
4:c:264:LEU:HD21	31:c:508:CLA:HAB	1.99	0.43
40:c:523:DGD:HB21	40:c:523:DGD:HA21	2.01	0.43
22:r:213:TYR:HB3	31:r:610:CLA:HED3	2.00	0.43
24:y:217:PHE:CE1	31:y:602:CLA:HAC1	2.53	0.43
1:A1:57:PRO:HB2	1:A1:66:PRO:HB2	1.99	0.43
31:C1:513:CLA:NB	33:C1:514:BCR:H383	2.33	0.43
40:C1:519:DGD:HA22	10:J1:31:PHE:CE2	2.54	0.43
12:L1:15:ARG:NH1	16:T1:23:PHE:O	2.43	0.43
17:W1:92:ILE:HA	17:W1:95:ILE:HG22	1.99	0.43
23:S1:113:LEU:HB3	31:S1:604:CLA:HAB	2.00	0.43
3:v1:4:THR:HG23	11:k1:20:PRO:HG3	2.00	0.43
5:d1:5:ILE:HG22	5:d1:10:GLU:HG2	2.00	0.43
47:n1:605:CHL:HAA1	52:s1:626:3PH:H3C2	2.00	0.43
47:n1:609:CHL:H43	47:y1:601:CHL:H12	2.00	0.43
49:n1:622:XAT:H201	31:y1:613:CLA:H203	1.99	0.43
31:B:612:CLA:H142	31:B:612:CLA:H111	1.79	0.43
20:N:134:GLY:O	20:N:146:HIS:NE2	2.50	0.43
47:Y:607:CHL:H151	47:Y:609:CHL:H101	2.00	0.43
4:c:58:PHE:CE1	11:k:23:ASP:HA	2.54	0.43
4:c:98:PRO:HA	4:c:101:VAL:HG12	2.00	0.43
40:c:523:DGD:HAE2	53:y:625:SPH:H142	2.00	0.43
21:g:72:PRO:HA	21:g:75:PHE:HB2	2.00	0.43
23:s:113:LEU:HB3	31:s:604:CLA:HAB	2.00	0.43
31:y:613:CLA:H93	31:y:613:CLA:H111	1.79	0.43
53:A1:414:SPH:H132	54:I1:102:4RF:H4	2.00	0.43
2:B1:321:LYS:HE2	2:B1:359:MET:HE1	2.01	0.43
31:C1:512:CLA:NB	33:C1:514:BCR:H401	2.33	0.43
5:D1:159:ILE:HG21	5:D1:287:VAL:HG22	2.01	0.43
27:R1:83:VAL:HG23	27:R1:109:ARG:HA	2.00	0.43
31:R1:603:CLA:H92	31:R1:603:CLA:H62	1.83	0.43
1:a1:162:PRO:O	1:a1:166:GLY:N	2.50	0.43
1:a1:163:ILE:HD11	40:c1:518:DGD:HA31	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b1:54:PRO:O	2:b1:58:GLN:HG3	2.18	0.43
33:b1:618:BCR:H15C	33:b1:618:BCR:H351	1.68	0.43
4:c1:394:SER:HA	4:c1:408:VAL:HG23	2.01	0.43
14:o1:116:VAL:HG11	14:o1:178:VAL:HG11	1.99	0.43
31:s1:603:CLA:HMA2	31:s1:609:CLA:HBD	2.00	0.43
31:y1:614:CLA:H91	31:y1:614:CLA:H112	1.88	0.43
1:A:94:TYR:OH	1:A:104:GLU:HG2	2.18	0.43
2:B:341:LEU:HD11	2:B:431:GLU:HG2	1.99	0.43
47:N:606:CHL:HBB2	47:N:607:CHL:HAB	2.00	0.43
21:G:77:ARG:O	21:G:81:ILE:HG12	2.18	0.43
22:R:135:GLU:OE2	22:R:211:ARG:NH1	2.51	0.43
31:R:610:CLA:H102	31:R:610:CLA:H13	1.75	0.43
24:Y:206:VAL:HA	24:Y:209:ILE:HG22	2.00	0.43
31:b:603:CLA:H91	31:b:603:CLA:H112	1.72	0.43
31:b:612:CLA:H193	31:b:612:CLA:H162	1.77	0.43
4:c:95:ASP:OD1	4:c:96:THR:N	2.51	0.43
4:c:125:PRO:HD3	31:c:513:CLA:HED3	2.01	0.43
4:c:249:ARG:HA	4:c:254:TRP:HE1	1.84	0.43
4:c:391:SER:HB3	4:c:394:SER:O	2.18	0.43
5:d:201:VAL:HG13	31:d:402:CLA:HMB1	2.00	0.43
13:m:9:THR:O	13:m:13:LEU:HG	2.18	0.43
20:n:201:GLU:O	20:n:205:LYS:HG2	2.18	0.43
47:n:607:CHL:C2C	47:y:601:CHL:H143	2.48	0.43
31:g:603:CLA:H2A	31:g:603:CLA:H12	2.00	0.43
31:y:612:CLA:H101	31:y:612:CLA:H62	1.74	0.43
1:A1:304:GLN:HE22	4:C1:402:ILE:HA	1.83	0.43
31:A1:405:CLA:NB	31:D1:402:CLA:HBB1	2.33	0.43
31:B1:615:CLA:HHD	26:M1:21:PHE:CE1	2.53	0.43
31:C1:508:CLA:H2	31:C1:510:CLA:H12	2.01	0.43
5:D1:189:HIS:HB3	5:D1:289:LEU:HD13	2.00	0.43
20:N1:95:TRP:NE1	47:N1:608:CHL:HED2	2.33	0.43
27:R1:187:LEU:HD12	27:R1:190:ILE:HD11	2.01	0.43
31:S1:603:CLA:H11	31:S1:603:CLA:H51	1.83	0.43
24:Y1:228:VAL:HG22	24:Y1:256:PHE:HE2	1.83	0.43
1:a1:29:TYR:CG	1:a1:133:LEU:HD13	2.53	0.43
1:a1:118:HIS:O	1:a1:122:GLY:N	2.52	0.43
1:a1:260:PHE:O	1:a1:264:SER:OG	2.34	0.43
2:b1:57:ARG:NH2	2:b1:335:GLY:O	2.51	0.43
4:c1:393:ASN:ND2	40:c1:520:DGD:O1B	2.51	0.43
31:c1:501:CLA:HMB2	33:c1:515:BCR:H23C	2.01	0.43
31:c1:505:CLA:H92	31:c1:505:CLA:H61	1.77	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:c1:507:CLA:HBA2	31:c1:509:CLA:H72	2.00	0.43
44:d1:405:PL9:H351	44:d1:405:PL9:H371	1.58	0.43
26:m1:3:VAL:HG13	26:m1:6:LEU:HB2	2.00	0.43
20:n1:48:TRP:N	20:n1:68:TYR:O	2.49	0.43
23:s1:136:TRP:CZ2	23:s1:250:ALA:HA	2.53	0.43
31:A:407:CLA:HMC1	31:D:402:CLA:H2	2.01	0.43
4:C:76:LEU:HD12	31:C:503:CLA:CGD	2.49	0.43
31:C:504:CLA:HAA1	40:C:519:DGD:HD61	2.00	0.43
5:D:80:THR:HG22	5:D:111:TRP:CE2	2.54	0.43
5:D:89:LEU:HD21	35:H:102:LMG:H301	2.00	0.43
31:R:612:CLA:H52	31:R:612:CLA:H11	1.79	0.43
23:S:224:ASP:HB3	23:S:227:VAL:HG12	1.99	0.43
1:a:331:MET:HE1	5:d:347:PRO:HB2	2.00	0.43
33:b:619:BCR:HC21	35:b:622:LMG:H142	2.00	0.43
5:d:85:LEU:HD23	5:d:90:LEU:HD21	1.99	0.43
41:d:408:LHG:H352	41:d:408:LHG:H111	2.00	0.43
8:h:75:ASP:OD1	8:h:76:GLY:N	2.52	0.43
14:o:105:GLU:OE1	14:o:299:THR:OG1	2.26	0.43
20:n:123:TRP:CD1	48:n:621:LUT:H41	2.53	0.43
24:y:102:LEU:HD23	48:y:620:LUT:H35	2.01	0.43
1:A1:142:TRP:HZ3	41:D1:410:LHG:HC41	1.82	0.43
1:A1:145:VAL:O	1:A1:148:SER:OG	2.33	0.43
32:A1:409:PHO:HBA1	31:D1:402:CLA:H142	2.00	0.43
2:B1:254:GLY:HA2	35:H1:102:LMG:H202	1.99	0.43
4:C1:33:LEU:HD12	4:C1:33:LEU:HA	1.89	0.43
31:R1:603:CLA:HBB1	49:R1:621:XAT:H203	2.01	0.43
56:R1:626:ERG:H212	56:R1:626:ERG:H162	1.80	0.43
1:a1:335:ASN:ND2	5:d1:350:ASN:OD1	2.32	0.43
31:b1:608:CLA:C2B	35:b1:622:LMG:H162	2.48	0.43
15:p1:177:LYS:HE2	15:p1:177:LYS:HB2	1.87	0.43
16:t1:11:ILE:HA	16:t1:14:LEU:HB2	1.99	0.43
31:s1:613:CLA:H11	31:s1:613:CLA:H52	1.65	0.43
24:y1:228:VAL:HG22	24:y1:256:PHE:HE2	1.84	0.43
32:A:409:PHO:H142	32:A:409:PHO:H112	1.84	0.43
4:C:390:GLY:HA2	4:C:396:GLY:O	2.19	0.43
31:C:512:CLA:HBA1	31:C:512:CLA:H3A	1.75	0.43
8:H:67:ILE:HG13	8:H:72:LEU:HD23	2.01	0.43
1:a:108:ASN:HD22	1:a:108:ASN:C	2.25	0.43
2:b:359:MET:HG2	2:b:366:PHE:HB2	2.01	0.43
24:y:89:ILE:HG21	31:y:603:CLA:HAA2	2.01	0.43
24:y:196:ASP:OD1	24:y:197:ASP:N	2.51	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
53:A1:414:SPH:H151	34:b1:626:SQD:H202	2.01	0.43
4:C1:238:TRP:HA	53:Y1:625:SPH:H102	2.00	0.43
31:C1:504:CLA:H61	31:C1:504:CLA:H93	1.82	0.43
33:C1:514:BCR:H351	33:C1:514:BCR:H15C	1.64	0.43
41:C1:525:LHG:O10	31:S1:611:CLA:HAB	2.18	0.43
5:D1:53:THR:HG22	5:D1:67:TYR:HD2	1.83	0.43
31:R1:603:CLA:H3A	31:R1:603:CLA:HBA2	1.77	0.43
23:S1:103:ASN:O	23:S1:107:HIS:ND1	2.27	0.43
48:Y1:620:LUT:H35	48:Y1:620:LUT:H401	1.83	0.43
2:b1:192:PRO:HB2	2:b1:193:TYR:CD2	2.53	0.43
2:b1:193:TYR:HB3	8:h1:84:LEU:HD12	2.01	0.43
2:b1:321:LYS:HA	2:b1:321:LYS:HD2	1.81	0.43
33:c1:514:BCR:H15C	33:c1:514:BCR:H351	1.66	0.43
33:c1:517:BCR:H15C	33:c1:517:BCR:H351	1.61	0.43
35:c1:523:LMG:HC72	31:y1:611:CLA:HBA1	2.00	0.43
38:c1:524:DGA:HAS2	17:w1:85:ILE:HG22	1.99	0.43
23:s1:283:ASP:N	23:s1:283:ASP:OD1	2.51	0.43
24:y1:108:GLU:HG3	24:y1:122:ALA:HB1	2.01	0.43
31:y1:613:CLA:H143	41:y1:624:LHG:H361	2.01	0.43
1:A:76:ASN:ND2	12:L:34:SER:HB3	2.33	0.43
2:B:148:LEU:HD23	2:B:148:LEU:HA	1.81	0.43
2:B:463:PHE:HD2	5:D:280:TRP:HH2	1.66	0.43
35:C:521:LMG:H111	35:C:521:LMG:H141	1.61	0.43
31:N:603:CLA:HED2	31:N:603:CLA:H12	2.00	0.43
31:S:613:CLA:H52	31:S:613:CLA:H11	1.71	0.43
1:a:17:PHE:HE2	9:i:18:LEU:HD22	1.83	0.43
2:b:273:TYR:O	2:b:277:GLN:HB2	2.18	0.43
4:c:285:TYR:O	4:c:411:ARG:NH2	2.36	0.43
14:o:267:ALA:HB2	14:o:295:TYR:HD1	1.84	0.43
20:n:225:ILE:HD11	47:n:607:CHL:H41	2.00	0.43
31:n:610:CLA:H41	31:n:610:CLA:H61	1.83	0.43
31:r:604:CLA:H3A	31:r:604:CLA:HBA2	1.61	0.43
23:s:236:ILE:HG12	23:s:240:ARG:CZ	2.49	0.43
24:y:200:ALA:HA	24:y:203:GLU:HG2	2.01	0.43
31:A1:406:CLA:H93	31:A1:406:CLA:HBA2	2.01	0.43
34:A1:412:SQD:H45	34:A1:412:SQD:H1	1.76	0.43
35:C1:521:LMG:H202	11:K1:27:ILE:HD12	2.00	0.43
5:D1:149:PRO:HB3	31:D1:402:CLA:H41	2.01	0.43
8:H1:53:ALA:O	46:H1:101:RRX:H21	2.19	0.43
54:I1:102:4RF:H23	54:I1:102:4RF:H73	2.01	0.43
15:P1:198:GLU:HG2	15:P1:224:LYS:HD3	2.00	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
21:G1:164:GLY:HA3	21:G1:170:ASP:HA	2.01	0.43
4:c1:423:PHE:CE1	40:c1:518:DGD:HBH2	2.45	0.43
35:c1:521:LMG:H302	38:j1:101:DGA:HA61	2.01	0.43
5:d1:189:HIS:ND1	5:d1:289:LEU:HD22	2.34	0.43
10:j1:32:TYR:CE1	38:j1:101:DGA:HA41	2.54	0.43
47:n1:601:CHL:H61	47:n1:601:CHL:H41	1.82	0.43
31:y1:614:CLA:H152	31:y1:614:CLA:H18	1.82	0.43
2:B:208:LEU:HD23	31:B:603:CLA:HAC2	1.99	0.43
31:C:512:CLA:H201	31:C:512:CLA:HBB1	2.01	0.43
31:N:602:CLA:H102	31:N:603:CLA:HMB1	2.01	0.43
31:N:604:CLA:H193	47:N:608:CHL:H2	2.00	0.43
21:G:193:PHE:HA	21:G:196:LEU:HD23	2.01	0.43
1:a:148:SER:OG	1:a:284:TRP:NE1	2.39	0.43
5:d:319:ILE:O	5:d:323:GLU:HG3	2.19	0.43
14:o:209:THR:HA	14:o:220:THR:HG22	2.00	0.43
31:y:602:CLA:H92	31:y:603:CLA:HMA1	2.01	0.43
1:A1:321:ILE:HG12	5:D1:179:PHE:CD1	2.53	0.43
2:B1:458:PHE:CE1	35:B1:622:LMG:H211	2.53	0.43
31:B1:605:CLA:H41	31:B1:605:CLA:H61	1.79	0.43
35:C1:523:LMG:H202	31:Y1:612:CLA:HBC1	2.00	0.43
12:L1:1:MET:HE3	12:L1:6:PRO:HG3	2.01	0.43
14:O1:169:THR:HA	14:O1:179:PRO:HA	2.01	0.43
14:O1:216:ARG:HG2	14:O1:217:GLY:H	1.83	0.43
15:P1:81:ASP:OD1	15:P1:81:ASP:N	2.51	0.43
49:N1:622:XAT:H30	41:Y1:624:LHG:H342	1.99	0.43
49:R1:621:XAT:H391	49:R1:621:XAT:H31	1.71	0.43
1:a1:104:GLU:OE2	1:a1:108:ASN:ND2	2.52	0.43
31:b1:611:CLA:H102	31:b1:616:CLA:HAA1	1.99	0.43
4:c1:414:LEU:HD21	31:c1:502:CLA:HED3	2.01	0.43
4:c1:445:LYS:HE2	5:d1:231:THR:HA	2.00	0.43
54:i1:101:4RF:H38	54:i1:101:4RF:H60	2.01	0.43
17:w1:72:LEU:HD12	17:w1:73:PRO:HD2	2.00	0.43
48:r1:620:LUT:H11	48:r1:620:LUT:H191	1.77	0.43
2:B:231:MET:HG2	31:B:611:CLA:HMC3	2.01	0.43
2:B:315:ILE:O	2:B:318:ASN:CB	2.67	0.43
4:C:395:VAL:HG22	4:C:403:ASN:ND2	2.33	0.43
20:N:182:TYR:HB3	31:N:610:CLA:HED3	2.00	0.43
21:G:94:LEU:HD22	31:G:604:CLA:HMC2	2.01	0.43
1:a:26:ASN:O	5:d:255:GLN:NE2	2.52	0.43
1:a:78:ILE:HD11	5:d:298:PHE:CZ	2.54	0.43
1:a:289:GLY:O	1:a:293:MET:HG3	2.18	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:460:LEU:HD11	5:d:151:ALA:HB1	2.00	0.43
38:b:623:DGA:HBG1	31:d:403:CLA:H71	2.00	0.43
4:c:21:PHE:HE2	31:c:508:CLA:HED1	1.83	0.43
7:f:19:TRP:HE3	7:f:20:LEU:HD23	1.83	0.43
21:g:94:LEU:O	21:g:98:THR:OG1	2.28	0.43
21:g:145:THR:HA	21:g:148:VAL:HG12	2.01	0.43
47:y:601:CHL:H62	47:y:601:CHL:H41	1.70	0.43
1:A1:210:LEU:HD13	31:A1:407:CLA:H43	2.00	0.43
1:A1:281:VAL:HA	1:A1:284:TRP:HE3	1.83	0.43
31:A1:407:CLA:HMB3	31:D1:402:CLA:H102	2.00	0.43
32:A1:409:PHO:H161	32:A1:409:PHO:H122	1.89	0.43
31:B1:609:CLA:H61	31:B1:610:CLA:H101	2.01	0.43
4:C1:64:VAL:N	4:C1:72:GLN:OE1	2.39	0.43
4:C1:357:LEU:HD11	4:C1:368:LEU:HA	2.00	0.43
4:C1:426:PHE:CE1	31:C1:505:CLA:HAB	2.54	0.43
5:D1:148:ALA:HB2	5:D1:276:VAL:HG13	2.00	0.43
41:G1:624:LHG:H201	49:Y1:622:XAT:H12	2.00	0.43
2:b1:41:GLU:HB3	2:b1:60:MET:SD	2.59	0.43
2:b1:68:ARG:O	2:b1:167:TRP:N	2.52	0.43
2:b1:399:VAL:HG11	2:b1:420:TYR:HD2	1.84	0.43
31:b1:616:CLA:H13	31:r1:609:CLA:H8	2.00	0.43
4:c1:252:PHE:HE2	31:c1:507:CLA:HAB	1.83	0.43
31:c1:504:CLA:H61	40:c1:519:DGD:HBE2	2.01	0.43
31:c1:508:CLA:H8	31:c1:510:CLA:H52	2.00	0.43
21:g1:83:LEU:HD12	21:g1:83:LEU:HA	1.92	0.43
1:A:30:ILE:O	1:A:34:GLY:CA	2.61	0.43
31:A:406:CLA:H92	31:A:406:CLA:H62	1.80	0.43
2:B:7:ARG:HE	31:B:612:CLA:HED1	1.84	0.43
2:B:476:ARG:HG3	22:R:101:LYS:HE2	2.01	0.43
31:C:513:CLA:NB	33:C:514:BCR:H383	2.33	0.43
33:D:404:BCR:H17C	7:F:29:THR:HG22	2.01	0.43
20:N:168:ARG:HA	47:N:608:CHL:C4C	2.49	0.43
22:R:183:SER:O	22:R:187:LEU:HB2	2.19	0.43
23:S:176:LEU:HD21	31:S:609:CLA:HHC	2.00	0.43
1:a:97:TRP:CG	9:i:5:LYS:HD2	2.54	0.43
2:b:464:PHE:HB2	5:d:280:TRP:CH2	2.54	0.43
31:b:608:CLA:H93	31:b:608:CLA:H61	1.86	0.43
34:b:621:SQD:H211	34:b:621:SQD:H181	1.92	0.43
4:c:307:VAL:HA	4:c:310:GLN:HG2	2.00	0.43
31:c:509:CLA:H142	31:c:509:CLA:H111	1.80	0.43
31:n:603:CLA:HMC2	47:n:607:CHL:H112	2.01	0.43

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
47:g:601:CHL:H8	47:y:607:CHL:H201	2.00	0.43
23:s:175:LEU:HD11	50:s:623:NEX:C15	2.48	0.43
24:y:88:THR:HG22	24:y:183:LEU:HD13	2.01	0.43
1:A1:284:TRP:CZ2	4:C1:427:VAL:HG21	2.53	0.43
31:B1:607:CLA:H151	31:B1:607:CLA:H111	1.77	0.43
31:B1:608:CLA:H52	35:B1:622:LMG:H132	2.00	0.43
31:B1:615:CLA:H141	31:B1:615:CLA:H161	1.81	0.43
33:B1:618:BCR:HC42	35:B1:622:LMG:H291	1.99	0.43
3:V1:16:VAL:O	33:C1:516:BCR:H16C	2.19	0.43
5:D1:269:PHE:O	5:D1:273:PHE:N	2.52	0.43
1:a1:207:GLY:HA2	1:a1:210:LEU:HB2	2.01	0.43
31:b1:608:CLA:H62	31:b1:608:CLA:H41	1.83	0.43
31:b1:609:CLA:CAB	5:d1:123:ILE:HG23	2.47	0.43
35:c1:523:LMG:H422	53:y1:625:SPH:H122	2.00	0.43
14:o1:205:TYR:HD2	14:o1:206:ARG:HD3	1.84	0.43
21:g1:75:PHE:HE1	31:g1:602:CLA:HAA2	1.83	0.43
23:s1:120:ILE:HD12	31:s1:605:CLA:HED2	2.01	0.43
31:y1:610:CLA:CBB	48:y1:620:LUT:H32	2.49	0.43
31:y1:614:CLA:H3A	57:y1:626:PTY:H331	2.01	0.43
4:C:141:ASP:OD1	4:C:141:ASP:N	2.50	0.42
4:C:373:GLN:HG2	4:C:375:TRP:HD1	1.84	0.42
8:H:57:PHE:CE1	46:H:101:RRX:C37	3.02	0.42
12:L:27:VAL:HA	12:L:30:VAL:HG22	2.01	0.42
1:a:221:SER:OG	5:d:139:ARG:O	2.35	0.42
1:a:277:VAL:HG23	41:d:410:LHG:H292	2.00	0.42
32:a:409:PHO:H3A	32:a:409:PHO:HBA1	1.51	0.42
31:b:609:CLA:H171	31:b:610:CLA:H172	2.02	0.42
31:b:614:CLA:H92	31:b:614:CLA:H61	1.84	0.42
5:d:189:HIS:HB3	5:d:289:LEU:HD22	2.01	0.42
7:f:44:ARG:NE	10:j:42:LEU:O	2.47	0.42
19:z:1:MET:HE2	19:z:60:PHE:HB2	2.01	0.42
23:s:91:GLY:O	23:s:93:ASP:N	2.52	0.42
24:y:220:LEU:HD13	31:y:602:CLA:H193	2.01	0.42
47:y:601:CHL:HMA2	47:y:601:CHL:H2	2.01	0.42
1:A1:312:ARG:HD2	6:E1:56:PHE:CE2	2.54	0.42
2:B1:233:SER:HG	2:B1:236:SER:HG	1.67	0.42
31:B1:602:CLA:H143	31:B1:602:CLA:H111	1.89	0.42
4:C1:44:HIS:HD2	31:C1:509:CLA:HMB3	1.84	0.42
4:C1:221:ILE:HD13	33:C1:515:BCR:H282	2.01	0.42
31:C1:501:CLA:H172	31:C1:506:CLA:HBB1	2.01	0.42
31:C1:513:CLA:H112	41:C1:525:LHG:H132	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:C1:525:LHG:H361	41:C1:525:LHG:H331	1.69	0.42
34:C1:526:SQD:H201	34:C1:526:SQD:H172	1.84	0.42
5:D1:203:GLY:HA2	44:D1:405:PL9:H23	2.01	0.42
44:D1:405:PL9:H28	44:D1:405:PL9:H321	1.72	0.42
52:T1:101:3PH:H382	34:b1:626:SQD:H362	2.01	0.42
20:N1:85:TYR:O	20:N1:89:GLU:N	2.48	0.42
21:G1:102:LEU:HB3	21:G1:108:VAL:HB	2.00	0.42
27:R1:190:ILE:HD12	47:R1:606:CHL:HED1	2.00	0.42
1:a1:37:MET:HG3	1:a1:129:ARG:HD2	2.01	0.42
2:b1:75:TRP:HZ2	2:b1:90:ILE:HA	1.84	0.42
2:b1:378:ARG:NH2	15:p1:100:ASP:OD1	2.52	0.42
2:b1:384:ARG:NH1	2:b1:387:GLU:OE2	2.52	0.42
5:d1:286:VAL:O	5:d1:290:ALA:N	2.51	0.42
31:g1:613:CLA:H152	49:y1:622:XAT:H34	2.01	0.42
31:r1:603:CLA:HMA3	31:r1:609:CLA:HBA2	2.00	0.42
24:y1:214:LEU:HD21	31:y1:611:CLA:HAC2	1.99	0.42
1:A:24:THR:O	5:D:255:GLN:NE2	2.51	0.42
2:B:158:VAL:HG23	2:B:199:PRO:HB3	2.01	0.42
4:C:45:ALA:O	4:C:49:VAL:HG22	2.18	0.42
4:C:161:TRP:HB3	34:C:526:SQD:H212	2.01	0.42
31:C:504:CLA:H112	31:C:504:CLA:H91	1.79	0.42
11:K:11:LEU:HD12	11:K:12:PRO:HD2	2.01	0.42
20:N:255:THR:HA	20:N:256:PRO:HD3	1.90	0.42
49:N:622:XAT:H15	49:N:622:XAT:H201	1.72	0.42
31:G:602:CLA:CBB	48:G:621:LUT:H32	2.50	0.42
1:a:224:ILE:HD12	1:a:224:ILE:HA	1.93	0.42
31:a:410:CLA:H12	35:a:413:LMG:H112	2.00	0.42
35:a:413:LMG:HC72	4:c:204:SER:HB3	2.01	0.42
2:b:422:ARG:HH21	14:o:226:ILE:HD13	1.84	0.42
31:b:611:CLA:HHC	31:b:611:CLA:HBB1	2.00	0.42
31:c:511:CLA:H93	31:c:511:CLA:H61	1.76	0.42
19:z:12:LEU:HD13	19:z:50:LEU:HB2	2.01	0.42
23:s:215:PRO:HB2	31:s:617:CLA:HBC2	2.01	0.42
23:s:264:ILE:HD12	48:s:620:LUT:H172	2.01	0.42
23:s:275:ASN:H	23:s:278:THR:HB	1.83	0.42
48:s:620:LUT:H11	48:s:620:LUT:H191	1.74	0.42
31:y:602:CLA:H152	31:y:602:CLA:H18	1.85	0.42
31:A1:406:CLA:H92	41:L1:101:LHG:H221	2.00	0.42
32:A1:409:PHO:HHB	31:D1:402:CLA:H121	2.01	0.42
31:B1:613:CLA:H192	31:B1:613:CLA:H162	1.89	0.42
31:B1:615:CLA:HMD3	26:M1:25:LEU:HD21	2.01	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
35:C1:523:LMG:H452	49:N1:622:XAT:H382	2.01	0.42
5:D1:189:HIS:HA	5:D1:294:ARG:HE	1.84	0.42
9:I1:5:LYS:HE2	9:I1:9:TYR:CZ	2.54	0.42
12:L1:36:ILE:HD12	12:L1:36:ILE:HA	1.88	0.42
31:G1:602:CLA:H3A	31:G1:602:CLA:HBA2	1.53	0.42
23:S1:287:PRO:HB2	23:S1:289:LEU:HD22	2.01	0.42
24:Y1:248:ASN:HD22	31:Y1:614:CLA:HED3	1.84	0.42
31:b1:614:CLA:H141	31:b1:614:CLA:H162	1.88	0.42
4:c1:290:TYR:O	4:c1:411:ARG:HG3	2.18	0.42
4:c1:454:VAL:HG21	5:d1:248:THR:HA	2.00	0.42
31:c1:513:CLA:H41	31:c1:513:CLA:H62	1.76	0.42
31:c1:513:CLA:HBA1	31:c1:513:CLA:HBD	2.01	0.42
35:c1:521:LMG:H192	38:j1:101:DGA:HA82	2.01	0.42
14:o1:140:LEU:CD2	14:o1:166:ALA:HB2	2.48	0.42
21:g1:52:TYR:OH	24:y1:85:ARG:NH1	2.52	0.42
23:s1:183:ARG:HA	47:s1:608:CHL:C3C	2.50	0.42
23:s1:212:PRO:HB3	47:s1:608:CHL:HBC2	2.00	0.42
24:y1:110:LEU:HB3	24:y1:115:VAL:HB	2.00	0.42
24:y1:214:LEU:HD23	41:y1:624:LHG:H272	2.01	0.42
31:y1:602:CLA:CBB	48:y1:621:LUT:H32	2.49	0.42
1:A:269:ARG:NH1	5:D:234:ALA:HB3	2.34	0.42
2:B:243:ALA:HA	2:B:246:PHE:CE2	2.54	0.42
48:R:620:LUT:H11	48:R:620:LUT:H191	1.74	0.42
23:S:176:LEU:HG	31:S:609:CLA:HAB	2.01	0.42
31:Y:602:CLA:H71	31:Y:603:CLA:HHB	2.01	0.42
1:a:303:ASN:HD22	1:a:322:ASN:ND2	2.17	0.42
1:a:338:ASN:HB3	4:c:327:LYS:HG3	2.01	0.42
31:a:405:CLA:H102	32:a:408:PHO:HAA1	2.01	0.42
31:b:610:CLA:C3D	8:h:50:MET:HB3	2.49	0.42
5:d:83:ASN:HD22	5:d:336:HIS:CD2	2.37	0.42
15:p:111:ASP:HB2	15:p:225:ARG:HH21	1.84	0.42
31:n:603:CLA:H12	31:n:603:CLA:HBA2	1.59	0.42
21:g:163:GLY:HA2	47:g:608:CHL:HAC1	2.00	0.42
1:A1:317:TRP:O	1:A1:321:ILE:HG13	2.19	0.42
2:B1:250:PHE:CE1	2:B1:459:ALA:HB1	2.55	0.42
2:B1:419:LYS:HA	2:B1:422:ARG:HD3	2.01	0.42
31:B1:615:CLA:H112	31:B1:615:CLA:H91	1.82	0.42
4:C1:209:ASP:O	4:C1:214:SER:OG	2.29	0.42
41:D1:409:LHG:H171	12:L1:23:LEU:HD21	2.02	0.42
15:P1:102:ILE:HD11	15:P1:117:TYR:HB2	2.01	0.42
49:G1:622:XAT:H11	49:G1:622:XAT:H191	1.87	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:S1:605:CLA:H12	31:S1:605:CLA:NA	2.34	0.42
31:b1:604:CLA:H91	31:b1:604:CLA:H112	1.77	0.42
31:b1:610:CLA:H141	31:b1:610:CLA:H161	1.72	0.42
4:c1:33:LEU:O	4:c1:37:LEU:N	2.52	0.42
4:c1:152:HIS:ND1	31:c1:509:CLA:H91	2.34	0.42
4:c1:449:ARG:HG3	5:d1:223:PHE:CD1	2.54	0.42
4:c1:452:GLU:OE2	5:d1:245:SER:OG	2.36	0.42
41:c1:525:LHG:H311	41:s1:624:LHG:H101	2.01	0.42
6:e1:75:GLN:HG2	6:e1:79:LEU:HD13	2.02	0.42
31:g1:602:CLA:H3A	31:g1:602:CLA:HBA2	1.38	0.42
47:g1:605:CHL:HMA2	47:g1:605:CHL:HAA1	1.88	0.42
41:g1:624:LHG:H202	49:y1:622:XAT:H12	2.01	0.42
24:y1:50:LEU:HB2	24:y1:54:SER:HA	2.00	0.42
31:y1:602:CLA:H92	31:y1:603:CLA:HMA3	2.01	0.42
1:A:57:PRO:HD2	14:O:177:TYR:HE2	1.84	0.42
2:B:226:TYR:CD1	2:B:231:MET:HB2	2.55	0.42
31:C:506:CLA:H143	31:C:506:CLA:H112	1.80	0.42
5:D:105:PHE:HE1	5:D:110:LEU:HD13	1.84	0.42
6:E:74:GLU:O	6:E:78:LYS:HG2	2.20	0.42
47:N:605:CHL:H141	31:S:604:CLA:HBC1	2.01	0.42
21:G:190:PRO:HA	21:G:193:PHE:HB3	1.99	0.42
21:G:204:GLY:O	21:G:208:MET:HG2	2.19	0.42
21:G:211:CYS:SG	48:G:621:LUT:H12	2.59	0.42
23:S:161:ASN:N	23:S:161:ASN:OD1	2.52	0.42
24:Y:74:ALA:HB2	48:Y:621:LUT:H221	2.02	0.42
25:U:110:ARG:HA	25:U:110:ARG:HD2	1.82	0.42
1:a:30:ILE:HG13	1:a:31:GLY:H	1.84	0.42
1:a:175:GLY:O	1:a:179:THR:OG1	2.32	0.42
1:a:229:GLU:HB2	22:r:94:GLN:NE2	2.34	0.42
2:b:471:SER:O	2:b:475:PHE:HB2	2.19	0.42
4:c:363:LEU:HB3	4:c:368:LEU:HD11	2.02	0.42
31:c:501:CLA:HBB1	31:c:501:CLA:H71	2.01	0.42
5:d:265:ARG:HH11	41:d:408:LHG:HC11	1.84	0.42
31:s:609:CLA:H41	31:s:609:CLA:H61	1.76	0.42
31:y:612:CLA:H93	31:y:612:CLA:H111	1.88	0.42
31:y:613:CLA:H51	31:y:613:CLA:H8	1.75	0.42
5:D1:196:PHE:CD1	5:D1:281:MET:HE3	2.55	0.42
41:D1:409:LHG:H252	12:L1:19:TYR:HB3	2.01	0.42
35:D1:411:LMG:H181	35:D1:411:LMG:H152	1.75	0.42
11:K1:24:VAL:O	11:K1:27:ILE:HG12	2.19	0.42
48:N1:621:LUT:H11	48:N1:621:LUT:H191	1.88	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
41:N1:624:LHG:H172	41:N1:624:LHG:H201	1.72	0.42
47:S1:606:CHL:HBB2	47:S1:607:CHL:CBB	2.49	0.42
24:Y1:110:LEU:HA	24:Y1:113:ASN:HB2	2.02	0.42
1:a1:135:TYR:CE1	4:c1:437:ARG:HB3	2.54	0.42
2:b1:272:ARG:HG2	2:b1:318:ASN:HD21	1.83	0.42
4:c1:419:PHE:O	4:c1:423:PHE:N	2.41	0.42
7:f1:30:ILE:HD13	7:f1:33:LEU:HD12	2.01	0.42
20:n1:204:VAL:HG12	20:n1:208:LYS:HD3	2.01	0.42
31:r1:612:CLA:HMC1	48:r1:620:LUT:H203	2.00	0.42
35:A:413:LMG:H181	31:C:505:CLA:H8	2.02	0.42
5:D:82:ALA:O	5:D:85:LEU:HB2	2.19	0.42
5:D:90:LEU:HA	5:D:90:LEU:HD12	1.77	0.42
5:D:213:ILE:HD13	5:D:213:ILE:HA	1.94	0.42
5:D:259:VAL:HG21	41:D:409:LHG:H271	2.00	0.42
19:Z:23:VAL:HA	19:Z:26:VAL:HG22	2.00	0.42
49:Y:622:XAT:H31	49:Y:622:XAT:H391	1.71	0.42
1:a:274:PHE:HA	1:a:277:VAL:HG12	2.01	0.42
32:a:409:PHO:H8	32:a:409:PHO:H121	1.84	0.42
2:b:270:PRO:O	2:b:448:ARG:NH1	2.37	0.42
4:c:129:GLU:HB3	4:c:136:GLY:HA3	2.01	0.42
31:c:506:CLA:H91	31:c:506:CLA:H151	2.01	0.42
41:c:625:LHG:H281	41:c:625:LHG:H251	1.82	0.42
31:n:613:CLA:H152	31:n:613:CLA:H18	1.95	0.42
49:g:622:XAT:H31	49:g:622:XAT:H391	1.74	0.42
1:A1:204:GLY:O	1:A1:208:GLY:N	2.44	0.42
2:B1:233:SER:OG	2:B1:236:SER:OG	2.33	0.42
5:D1:136:VAL:HG23	5:D1:138:LEU:HB2	2.01	0.42
8:H1:42:PRO:HG3	27:R1:83:VAL:HG13	2.00	0.42
14:O1:135:ARG:HE	14:O1:135:ARG:HB3	1.71	0.42
31:a1:405:CLA:HAA1	31:a1:406:CLA:HAC2	2.01	0.42
2:b1:126:PRO:HD3	8:h1:31:ARG:HH21	1.85	0.42
2:b1:352:ARG:HD3	2:b1:372:ASP:CG	2.45	0.42
2:b1:389:LYS:HA	2:b1:394:GLN:NE2	2.35	0.42
31:b1:602:CLA:HAC1	46:h1:101:RRX:H56	2.02	0.42
31:b1:612:CLA:H92	31:b1:612:CLA:H62	1.84	0.42
31:c1:501:CLA:H61	31:c1:501:CLA:H41	1.58	0.42
31:c1:502:CLA:H42	31:c1:503:CLA:H112	2.02	0.42
5:d1:80:THR:HG22	5:d1:111:TRP:CE2	2.54	0.42
33:d1:404:BCR:H16C	7:f1:32:PHE:HD2	1.85	0.42
14:o1:259:VAL:HG12	14:o1:266:ILE:HG22	2.01	0.42
31:r1:610:CLA:H92	31:r1:610:CLA:H61	1.77	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:r1:620:LUT:H35	48:r1:620:LUT:H401	1.88	0.42
1:A:43:THR:HG23	33:A:411:BCR:H362	2.00	0.42
1:A:183:MET:HB3	31:A:405:CLA:HBC2	2.01	0.42
1:A:316:THR:HA	5:D:63:LEU:HB2	2.02	0.42
10:J:28:ALA:HA	35:J:101:LMG:H341	2.00	0.42
20:N:101:LEU:O	20:N:105:THR:OG1	2.33	0.42
47:S:608:CHL:CMB	50:S:622:NEX:H15	2.49	0.42
1:a:126:TYR:CZ	32:a:408:PHO:HBA1	2.54	0.42
2:b:7:ARG:O	2:b:10:THR:OG1	2.29	0.42
2:b:254:GLY:HA3	35:h:102:LMG:H151	2.02	0.42
31:b:608:CLA:H91	31:b:608:CLA:H112	1.88	0.42
31:b:612:CLA:H92	31:b:612:CLA:H61	1.88	0.42
14:o:80:ILE:O	14:o:83:THR:OG1	2.31	0.42
31:s:609:CLA:H61	31:s:609:CLA:H93	1.84	0.42
48:s:620:LUT:H362	48:s:620:LUT:H23	1.87	0.42
2:B1:247:TRP:CD1	31:B1:604:CLA:H122	2.54	0.42
4:C1:166:LYS:NZ	4:C1:170:PHE:O	2.41	0.42
14:O1:187:PHE:HD1	14:O1:200:PHE:HB3	1.84	0.42
20:N1:168:ARG:HH12	47:N1:609:CHL:HED2	1.84	0.42
49:N1:622:XAT:H34	31:Y1:613:CLA:H111	2.01	0.42
21:G1:242:PHE:HB3	24:Y1:132:PHE:CZ	2.54	0.42
23:S1:52:TRP:CD2	23:S1:233:VAL:HG11	2.54	0.42
1:a1:308:ASP:OD1	1:a1:312:ARG:N	2.53	0.42
2:b1:170:ASP:OD1	2:b1:174:LEU:N	2.48	0.42
4:c1:28:ALA:HA	4:c1:31:ILE:HD11	2.02	0.42
4:c1:176:THR:HB	4:c1:286:PRO:HB3	2.00	0.42
4:c1:367:LYS:HE3	4:c1:367:LYS:HB2	1.84	0.42
31:c1:506:CLA:H41	9:i1:20:ILE:HD11	2.00	0.42
8:h1:75:ASP:OD2	18:x1:64:SER:OG	2.33	0.42
49:n1:622:XAT:H363	41:y1:624:LHG:HC41	2.01	0.42
31:y1:611:CLA:H202	31:y1:611:CLA:H162	1.90	0.42
1:A:167:SER:O	1:A:170:ASP:HB2	2.20	0.42
5:D:56:THR:OG1	5:D:69:GLU:OE2	2.24	0.42
5:D:184:PHE:HD1	5:D:329:MET:HE1	1.85	0.42
5:D:188:PHE:HE1	5:D:326:ARG:HA	1.84	0.42
5:D:343:GLU:OE2	15:P:112:ALA:HB3	2.19	0.42
10:J:26:LEU:HA	10:J:26:LEU:HD12	1.81	0.42
17:W:73:PRO:O	17:W:76:VAL:HG22	2.19	0.42
23:S:143:MET:HE1	47:S:606:CHL:HMD3	2.01	0.42
52:S:626:3PH:H3C1	52:S:626:3PH:H392	1.88	0.42
24:Y:63:GLY:HA2	24:Y:68:ASP:HB3	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b:264:PRO:HD2	2:b:268:PHE:CE2	2.55	0.42
4:c:76:LEU:HA	4:c:79:HIS:ND1	2.34	0.42
33:c:517:BCR:H351	33:c:517:BCR:H15C	1.63	0.42
34:c:626:SQD:H111	51:s:625:LPX:H19A	2.01	0.42
33:d:404:BCR:H14C	7:f:32:PHE:CE2	2.55	0.42
7:f:44:ARG:NH2	10:j:42:LEU:OXT	2.41	0.42
14:o:82:ASN:HD22	14:o:136:LEU:HD22	1.85	0.42
21:g:62:GLY:N	31:g:602:CLA:OBD	2.53	0.42
1:A1:321:ILE:HA	5:D1:179:PHE:CE1	2.55	0.42
31:B1:613:CLA:H61	31:B1:613:CLA:H102	1.73	0.42
4:C1:142:LYS:HE2	4:C1:254:TRP:CG	2.55	0.42
5:D1:201:VAL:HG13	31:D1:402:CLA:HAB	2.02	0.42
41:D1:410:LHG:H291	41:D1:410:LHG:H322	1.77	0.42
47:N1:606:CHL:H62	47:N1:606:CHL:H41	1.59	0.42
50:N1:623:NEX:H11	50:N1:623:NEX:H191	1.85	0.42
21:G1:149:GLN:NE2	47:G1:607:CHL:OMC	2.53	0.42
50:S1:623:NEX:H15	50:S1:623:NEX:H201	1.89	0.42
31:b1:606:CLA:H62	31:b1:606:CLA:H41	1.77	0.42
5:d1:155:SER:HA	5:d1:159:ILE:HB	2.01	0.42
26:m1:11:THR:O	26:m1:15:ILE:HG12	2.19	0.42
20:n1:73:ALA:HA	21:g1:81:ILE:HD11	2.02	0.42
1:A:157:VAL:HG21	1:A:172:MET:HE2	2.01	0.42
31:B:610:CLA:C4B	46:H:101:RRX:H20	2.50	0.42
4:C:308:ARG:HD3	4:C:311:ARG:HH21	1.83	0.42
5:D:134:ARG:NH2	5:D:137:ASN:OD1	2.53	0.42
48:N:620:LUT:H15	48:N:620:LUT:H201	1.76	0.42
48:N:621:LUT:H11	48:N:621:LUT:H191	1.81	0.42
21:G:87:ARG:HA	21:G:90:LEU:HD12	2.00	0.42
48:G:620:LUT:H35	48:G:620:LUT:H401	1.81	0.42
22:R:60:LEU:HB2	22:R:63:LEU:HD23	2.00	0.42
48:S:620:LUT:H35	48:S:620:LUT:H401	1.81	0.42
1:a:140:ARG:HH22	41:d:410:LHG:HC42	1.85	0.42
1:a:183:MET:HG2	31:a:405:CLA:HBC2	2.01	0.42
31:b:611:CLA:H202	31:b:616:CLA:HMD3	2.02	0.42
3:v:7:LEU:HA	3:v:10:VAL:HG12	2.02	0.42
31:c:503:CLA:H193	31:c:503:CLA:H161	1.80	0.42
5:d:88:SER:HB2	6:e:69:ARG:NH2	2.34	0.42
14:o:212:ASP:OD1	14:o:216:ARG:N	2.53	0.42
49:y:622:XAT:H31	49:y:622:XAT:H391	1.86	0.42
1:A1:332:HIS:ND1	1:A1:333:GLU:OE1	2.26	0.42
2:B1:39:LEU:HD12	52:B1:624:3PH:H3D2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
33:B1:619:BCR:H351	33:B1:619:BCR:H15C	1.83	0.42
5:D1:171:PRO:HG3	5:D1:181:PHE:CD1	2.54	0.42
17:W1:62:ASP:N	17:W1:62:ASP:OD1	2.53	0.42
31:a1:405:CLA:H141	31:a1:405:CLA:H162	1.84	0.42
53:a1:414:SPH:H183	53:a1:414:SPH:H152	1.86	0.42
4:c1:163:LEU:HD13	31:c1:501:CLA:HMD2	2.01	0.42
5:d1:156:VAL:HG22	5:d1:286:VAL:HG11	2.02	0.42
31:n1:613:CLA:H2	31:n1:613:CLA:H61	1.62	0.42
48:r1:620:LUT:H31	48:r1:620:LUT:H391	1.94	0.42
2:B:91:TRP:HB3	31:B:607:CLA:HAA1	2.02	0.42
2:B:135:LEU:HA	2:B:138:ILE:HD12	2.01	0.42
2:B:201:HIS:HB2	31:B:603:CLA:C1B	2.50	0.42
9:I:3:THR:HG21	22:r:180:LEU:HG	2.01	0.42
15:P:119:ILE:HB	15:P:216:LEU:HB3	2.01	0.42
21:G:160:ARG:HH21	47:G:608:CHL:C1A	2.32	0.42
31:G:604:CLA:C1C	50:G:623:NEX:H222	2.50	0.42
23:S:268:LEU:HD12	51:S:625:LPX:H4	2.02	0.42
1:a:140:ARG:NH2	41:d:410:LHG:HC42	2.34	0.42
1:a:176:ILE:HD13	31:a:406:CLA:HED3	2.01	0.42
31:b:610:CLA:H141	31:b:610:CLA:H161	1.87	0.42
4:c:120:HIS:HE1	31:c:513:CLA:O1D	2.03	0.42
5:d:89:LEU:HD11	35:h:102:LMG:H301	2.01	0.42
5:d:265:ARG:HG3	5:d:266:TRP:N	2.34	0.42
52:i:101:3PH:H281	52:i:101:3PH:H2B2	1.83	0.42
19:z:34:THR:HA	19:z:37:LYS:HE2	2.01	0.42
49:n:622:XAT:H11	49:n:622:XAT:H191	1.93	0.42
31:r:602:CLA:HED2	31:r:602:CLA:H2A	2.01	0.42
2:B1:4:PRO:HD2	2:B1:7:ARG:HB2	2.02	0.42
2:B1:468:TRP:NE1	31:B1:612:CLA:O1D	2.49	0.42
31:B1:604:CLA:H41	31:B1:604:CLA:H61	1.54	0.42
31:B1:604:CLA:H193	31:B1:604:CLA:H162	1.79	0.42
31:B1:605:CLA:H192	40:B1:623:DGD:HA42	2.02	0.42
52:B1:624:3PH:H341	16:t1:1:MET:HB3	2.02	0.42
4:C1:101:VAL:HG12	4:C1:105:LEU:HD23	2.02	0.42
5:D1:157:PHE:CE1	5:D1:171:PRO:HB2	2.55	0.42
8:H1:59:VAL:O	8:H1:63:ILE:N	2.48	0.42
9:I1:5:LYS:NZ	17:W1:65:MET:HE1	2.35	0.42
31:N1:610:CLA:H52	31:N1:610:CLA:H8	1.85	0.42
57:Y1:626:PTY:H112	57:Y1:626:PTY:H332	2.01	0.42
1:a1:157:VAL:HG23	1:a1:158:PHE:CD1	2.55	0.42
2:b1:462:PHE:HA	31:b1:612:CLA:HMC2	2.02	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c1:96:THR:HA	4:c1:99:TYR:CD2	2.54	0.42
31:c1:502:CLA:H43	31:c1:503:CLA:H52	2.02	0.42
14:o1:219:ALA:O	15:p1:150:TRP:NE1	2.53	0.42
21:g1:90:LEU:HD13	31:g1:610:CLA:HAB	2.02	0.42
47:g1:601:CHL:H202	47:y1:607:CHL:H13	2.02	0.42
31:s1:603:CLA:H51	31:s1:603:CLA:H11	1.78	0.42
51:s1:625:LPX:H15A	51:s1:625:LPX:H18A	1.92	0.42
31:B:616:CLA:H92	31:B:616:CLA:H61	1.81	0.42
4:C:95:ASP:OD1	4:C:95:ASP:N	2.51	0.42
6:E:25:ILE:O	6:E:29:SER:HB2	2.20	0.42
20:N:45:ARG:NE	20:N:67:ASP:OD2	2.52	0.42
20:N:211:ARG:NH2	31:N:602:CLA:O2D	2.53	0.42
31:N:610:CLA:H61	48:N:620:LUT:H30	2.02	0.42
23:S:237:LYS:HE2	41:S:624:LHG:HC41	2.02	0.42
1:a:131:TRP:CZ3	31:c:505:CLA:HAA2	2.55	0.42
31:a:410:CLA:HMA3	35:a:413:LMG:H131	2.02	0.42
3:v:12:LEU:O	3:v:16:VAL:HG12	2.20	0.42
4:c:119:TYR:OH	31:c:513:CLA:O1D	2.33	0.42
4:c:360:PRO:O	14:o:75:VAL:HG11	2.20	0.42
5:d:264:LYS:HB2	5:d:268:HIS:CE1	2.55	0.42
20:n:220:PHE:HE1	20:n:231:PRO:HG3	1.85	0.42
47:n:608:CHL:H2	31:s:610:CLA:H203	2.02	0.42
22:r:205:GLU:HG2	31:r:608:CLA:HBC1	2.01	0.42
31:s:613:CLA:H52	31:s:613:CLA:H11	1.68	0.42
4:C1:26:GLY:HA3	31:C1:511:CLA:HMD2	2.02	0.42
4:C1:155:ILE:HD11	31:C1:512:CLA:HMB1	2.01	0.42
14:O1:78:THR:O	17:W1:66:ASN:ND2	2.52	0.42
14:O1:202:VAL:O	14:O1:248:GLY:N	2.47	0.42
15:P1:192:ARG:HG2	15:P1:200:GLY:HA3	2.02	0.42
31:R1:608:CLA:CMB	50:R1:622:NEX:H35	2.49	0.42
52:S1:626:3PH:H321	52:S1:626:3PH:H351	1.53	0.42
31:Y1:602:CLA:CBB	48:Y1:621:LUT:H32	2.50	0.42
1:a1:204:GLY:O	1:a1:208:GLY:N	2.46	0.42
1:a1:321:ILE:HD13	5:d1:179:PHE:HD2	1.85	0.42
31:b1:610:CLA:HBA2	31:b1:610:CLA:H3A	1.57	0.42
4:c1:252:PHE:CE2	31:c1:507:CLA:HAB	2.55	0.42
48:n1:621:LUT:H15	48:n1:621:LUT:H201	1.89	0.42
21:g1:245:ALA:HB1	49:y1:622:XAT:H183	2.02	0.42
31:r1:608:CLA:H93	31:r1:608:CLA:H111	1.83	0.42
31:r1:609:CLA:H102	31:r1:609:CLA:H13	1.81	0.42
23:s1:205:ASP:OD1	23:s1:205:ASP:N	2.44	0.42

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:s1:609:CLA:H93	31:s1:609:CLA:H111	1.89	0.42
24:y1:223:PHE:HB3	47:y1:607:CHL:H71	2.01	0.42
31:y1:608:CLA:H43	31:y1:610:CLA:H192	2.02	0.42
1:A:27:ARG:NH2	5:D:258:GLY:O	2.53	0.41
31:B:612:CLA:H151	33:B:619:BCR:H342	2.02	0.41
14:O:136:LEU:HD23	14:O:138:TYR:OH	2.20	0.41
14:O:243:LYS:HE3	14:O:280:MET:HE3	2.02	0.41
14:O:259:VAL:HG12	14:O:266:ILE:HG22	2.02	0.41
31:R:609:CLA:H121	31:R:609:CLA:H8	1.86	0.41
31:S:609:CLA:H41	31:S:609:CLA:H62	1.85	0.41
31:Y:602:CLA:H91	31:Y:602:CLA:H111	1.85	0.41
48:Y:621:LUT:H15	48:Y:621:LUT:H201	1.85	0.41
1:a:67:VAL:HG12	5:d:312:GLU:HG3	2.02	0.41
31:a:405:CLA:H141	31:a:405:CLA:H162	1.84	0.41
31:b:608:CLA:HBC1	33:b:618:BCR:H10C	2.02	0.41
5:d:123:ILE:HD11	35:h:102:LMG:H402	2.01	0.41
20:n:138:TYR:HB2	20:n:145:ILE:HG12	2.02	0.41
2:B1:384:ARG:HA	14:O1:220:THR:HG22	2.02	0.41
31:B1:610:CLA:C3B	46:H1:101:RRX:H6	2.50	0.41
31:B1:613:CLA:H171	31:B1:613:CLA:H13	1.88	0.41
31:C1:503:CLA:H61	31:C1:503:CLA:H41	1.66	0.41
31:C1:506:CLA:H152	31:C1:506:CLA:H111	1.74	0.41
33:C1:517:BCR:H282	11:K1:39:TRP:CZ3	2.55	0.41
40:C1:520:DGD:HB22	10:J1:31:PHE:HZ	1.84	0.41
41:D1:409:LHG:HC62	16:T1:24:ARG:HD3	2.02	0.41
54:K1:101:4RF:H85	54:K1:101:4RF:H34	2.02	0.41
41:L1:101:LHG:H271	26:M1:22:LEU:HD13	2.01	0.41
20:N1:88:LEU:HD12	47:N1:609:CHL:HED3	2.02	0.41
20:N1:160:LEU:HD13	50:N1:623:NEX:C34	2.50	0.41
31:R1:612:CLA:HBA1	31:R1:612:CLA:H3A	1.58	0.41
1:a1:139:MET:SD	5:d1:221:THR:HA	2.60	0.41
34:a1:412:SQD:H351	31:c1:508:CLA:H101	2.02	0.41
31:b1:604:CLA:H152	31:b1:604:CLA:H111	1.69	0.41
31:b1:613:CLA:H61	31:b1:613:CLA:H102	1.76	0.41
31:c1:504:CLA:H62	31:c1:504:CLA:H41	1.74	0.41
31:c1:505:CLA:H41	33:c1:515:BCR:H343	2.01	0.41
31:c1:512:CLA:H193	34:c1:526:SQD:H271	2.02	0.41
14:o1:183:THR:HG21	14:o1:203:PRO:HD2	2.02	0.41
2:B:28:ALA:O	2:B:104:SER:OG	2.36	0.41
31:B:605:CLA:H41	31:B:605:CLA:H62	1.73	0.41
31:B:607:CLA:H111	31:B:607:CLA:H151	1.65	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:398:VAL:HG12	4:C:400:THR:H	1.86	0.41
5:D:279:LEU:HD11	31:D:402:CLA:HBA1	2.01	0.41
21:G:121:GLN:HG3	21:G:128:LEU:HD13	2.01	0.41
48:G:620:LUT:H11	48:G:620:LUT:H191	1.78	0.41
23:S:61:LEU:HD23	23:S:61:LEU:HA	1.94	0.41
47:Y:601:CHL:H41	47:Y:601:CHL:H61	1.76	0.41
31:Y:612:CLA:H122	31:Y:612:CLA:H161	1.79	0.41
32:a:408:PHO:H8	32:a:408:PHO:H121	1.74	0.41
2:b:366:PHE:HB3	2:b:425:GLN:HE22	1.84	0.41
4:c:163:LEU:HD11	31:c:501:CLA:C2D	2.49	0.41
7:f:40:GLN:HG3	10:j:29:ILE:HG22	2.02	0.41
48:n:620:LUT:H15	48:n:620:LUT:H201	1.90	0.41
50:n:623:NEX:H15	50:n:623:NEX:H201	1.89	0.41
31:g:613:CLA:H93	41:g:624:LHG:H301	2.01	0.41
48:g:621:LUT:H35	48:g:621:LUT:H401	1.75	0.41
22:r:139:ILE:HD13	22:r:202:ARG:HH12	1.85	0.41
31:y:613:CLA:H141	31:y:613:CLA:H161	1.82	0.41
1:A1:121:LEU:HD21	31:C1:505:CLA:H162	2.03	0.41
1:A1:172:MET:HE2	1:A1:179:THR:HG23	2.02	0.41
2:B1:209:GLY:HA3	31:B1:606:CLA:H201	2.02	0.41
2:B1:384:ARG:NH2	5:D1:343:GLU:OE2	2.53	0.41
34:B1:621:SQD:H292	34:M1:101:SQD:H161	2.01	0.41
4:C1:68:PRO:HG2	4:C1:71:GLU:HG3	2.02	0.41
31:C1:501:CLA:H191	31:C1:507:CLA:HBB1	2.01	0.41
31:C1:503:CLA:H172	31:C1:510:CLA:HBB2	2.02	0.41
5:D1:198:MET:SD	12:L1:35:TYR:OH	2.79	0.41
11:K1:29:PRO:HA	11:K1:32:PHE:CD2	2.55	0.41
54:K1:101:4RF:H47	54:K1:101:4RF:H43	1.69	0.41
21:G1:91:LEU:O	21:G1:95:GLY:N	2.50	0.41
21:G1:150:VAL:HA	47:G1:609:CHL:HBB2	2.02	0.41
31:G1:602:CLA:H141	31:G1:602:CLA:H202	2.02	0.41
31:S1:614:CLA:HBA2	31:S1:614:CLA:H3A	1.78	0.41
4:c1:27:ASN:ND2	31:c1:510:CLA:O1A	2.53	0.41
33:c1:516:BCR:H402	11:k1:37:PHE:HE2	1.86	0.41
5:d1:239:GLN:NE2	5:d1:243:THR:HG22	2.35	0.41
14:o1:184:ILE:HD12	14:o1:184:ILE:HA	1.92	0.41
20:n1:125:LYS:HD2	47:n1:607:CHL:HED2	2.01	0.41
31:n1:610:CLA:H51	48:n1:620:LUT:H30	2.02	0.41
27:r1:135:GLU:HG2	31:r1:609:CLA:HED3	2.01	0.41
1:A:310:ASN:O	15:P:89:SER:OG	2.37	0.41
31:A:410:CLA:HAA2	35:A:413:LMG:H122	2.02	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:78:PRO:HB2	4:C:290:TYR:CZ	2.55	0.41
31:C:505:CLA:H152	31:C:505:CLA:H112	1.64	0.41
5:D:202:ALA:HB2	44:D:405:PL9:H353	2.00	0.41
5:D:246:MET:SD	5:D:246:MET:N	2.93	0.41
21:G:71:ASP:OD1	21:G:72:PRO:HD2	2.20	0.41
31:G:610:CLA:H62	31:G:610:CLA:H41	1.80	0.41
24:Y:94:ALA:HB1	24:Y:212:GLY:HA3	2.03	0.41
33:a:411:BCR:HC31	9:i:15:PHE:HE1	1.84	0.41
4:c:260:LEU:HD23	4:c:260:LEU:HA	1.89	0.41
31:c:504:CLA:H71	40:c:519:DGD:HB72	2.02	0.41
20:n:155:ALA:HA	31:y:613:CLA:H201	2.03	0.41
47:n:605:CHL:H71	31:s:612:CLA:HBB2	2.03	0.41
23:s:246:VAL:HA	23:s:249:PHE:CD2	2.54	0.41
24:y:124:TRP:HE3	48:y:621:LUT:H21	1.84	0.41
24:y:184:TYR:CZ	24:y:205:LYS:HE2	2.55	0.41
2:B1:29:LEU:HD21	33:B1:618:BCR:H19C	2.02	0.41
2:B1:40:PHE:HA	52:B1:624:3PH:H382	2.03	0.41
2:B1:347:LYS:HD3	2:B1:353:GLU:HA	2.02	0.41
31:B1:603:CLA:H92	8:H1:65:LEU:HB2	2.01	0.41
31:B1:609:CLA:H2	38:B1:625:DGA:HB81	2.01	0.41
41:D1:409:LHG:H152	41:L1:101:LHG:H191	2.01	0.41
6:E1:78:LYS:HG3	6:E1:79:LEU:HD12	2.01	0.41
14:O1:111:PRO:HA	14:O1:292:GLY:HA3	2.01	0.41
14:O1:259:VAL:HG13	14:O1:266:ILE:HG22	2.02	0.41
31:G1:602:CLA:H151	48:G1:621:LUT:H393	2.01	0.41
31:G1:603:CLA:H91	31:G1:603:CLA:H111	1.86	0.41
47:S1:608:CHL:H101	50:S1:623:NEX:H401	2.02	0.41
2:b1:9:HIS:HB2	31:b1:612:CLA:HAA2	2.01	0.41
2:b1:370:LEU:HD12	2:b1:379:ALA:HB3	2.03	0.41
47:g1:608:CHL:HBB2	50:g1:623:NEX:H191	2.02	0.41
23:s1:125:GLN:HB2	23:s1:131:ILE:HB	2.01	0.41
23:s1:224:ASP:HB3	23:s1:227:VAL:HG22	2.03	0.41
48:s1:621:LUT:H35	48:s1:621:LUT:H401	1.71	0.41
31:y1:612:CLA:H142	31:y1:612:CLA:H111	1.78	0.41
1:A:14:TRP:HH2	9:I:25:SER:HB3	1.85	0.41
1:A:36:ILE:HA	31:A:410:CLA:CBB	2.50	0.41
1:A:334:ARG:HH22	5:D:349:GLY:N	2.18	0.41
2:B:108:PHE:HZ	34:B:621:SQD:H142	1.85	0.41
2:B:127:ARG:HG3	2:B:128:THR:HG23	2.02	0.41
2:B:243:ALA:HB2	2:B:466:HIS:CE1	2.55	0.41
4:C:71:GLU:OE2	4:C:386:HIS:NE2	2.53	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:C:150:GLY:HA2	4:C:236:GLY:HA2	2.03	0.41
8:H:65:LEU:HD11	35:H:102:LMG:H302	2.02	0.41
50:R:622:NEX:H11	50:R:622:NEX:H191	1.88	0.41
31:S:610:CLA:H201	31:S:617:CLA:HBB2	2.03	0.41
1:a:92:HIS:CE1	4:c:208:GLY:HA2	2.55	0.41
1:a:337:HIS:CD2	5:d:352:LEU:HD13	2.56	0.41
4:c:256:GLY:O	31:c:509:CLA:HBC1	2.21	0.41
4:c:365:LEU:HA	4:c:368:LEU:HD12	2.01	0.41
4:c:385:THR:HG22	4:c:386:HIS:H	1.85	0.41
20:n:211:ARG:HA	20:n:214:MET:HB2	2.02	0.41
47:n:601:CHL:H2	41:n:624:LHG:H151	2.02	0.41
47:g:601:CHL:H93	47:g:601:CHL:H61	1.96	0.41
23:s:107:HIS:CE1	48:s:621:LUT:H201	2.55	0.41
31:s:614:CLA:HBC1	41:s:624:LHG:H362	2.02	0.41
1:A1:68:SER:OG	1:A1:69:GLY:N	2.54	0.41
31:B1:603:CLA:H202	35:H1:102:LMG:H371	2.03	0.41
31:B1:607:CLA:OBD	40:B1:623:DGD:O3D	2.38	0.41
4:C1:249:ARG:HA	4:C1:254:TRP:HZ2	1.84	0.41
40:C1:518:DGD:HA72	40:C1:518:DGD:HA42	1.84	0.41
5:D1:203:GLY:O	5:D1:207:ALA:N	2.47	0.41
11:K1:40:GLN:HA	11:K1:43:VAL:HG22	2.02	0.41
14:O1:117:LYS:HB3	14:O1:117:LYS:HE2	1.92	0.41
23:S1:75:LEU:HD21	23:S1:97:VAL:HG11	2.01	0.41
24:Y1:73:THR:N	48:Y1:621:LUT:O23	2.46	0.41
1:a1:129:ARG:NH2	5:d1:255:GLN:O	2.53	0.41
31:b1:605:CLA:HAB	31:b1:608:CLA:HAB	2.02	0.41
31:b1:608:CLA:H93	31:b1:608:CLA:H61	1.78	0.41
5:d1:43:PHE:HA	33:d1:404:BCR:H343	2.01	0.41
6:e1:47:PHE:CD2	6:e1:49:SER:HB2	2.55	0.41
14:o1:208:SER:HA	14:o1:245:TYR:HE2	1.85	0.41
14:o1:208:SER:HB3	14:o1:219:ALA:HB2	2.02	0.41
15:p1:75:PHE:CG	15:p1:86:LEU:HD13	2.56	0.41
31:s1:602:CLA:CBB	48:s1:621:LUT:H32	2.50	0.41
31:s1:603:CLA:HBC3	31:s1:609:CLA:H13	2.02	0.41
1:A:14:TRP:HB2	17:W:95:ILE:HG22	2.03	0.41
1:A:276:ALA:HB2	5:D:215:GLY:HA3	2.02	0.41
2:B:242:ILE:HG23	2:B:462:PHE:HD1	1.85	0.41
4:C:327:LYS:HE2	4:C:327:LYS:HB2	1.89	0.41
33:C:515:BCR:H351	33:C:515:BCR:H15C	1.77	0.41
24:Y:76:LEU:HD12	31:Y:602:CLA:H42	2.01	0.41
2:b:386:ALA:HA	15:p:148:GLN:HA	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
3:v:25:LEU:O	3:v:29:ARG:HB2	2.21	0.41
33:c:516:BCR:H21C	11:k:38:VAL:HG23	2.02	0.41
31:d:402:CLA:H41	31:d:402:CLA:H62	1.49	0.41
20:n:170:ASN:C	20:n:170:ASN:HD22	2.28	0.41
20:n:238:HIS:HE1	20:n:246:ASN:HA	1.86	0.41
49:r:622:XAT:H11	49:r:622:XAT:H191	1.93	0.41
41:y:624:LHG:H383	41:y:624:LHG:H352	1.83	0.41
2:B1:464:PHE:HB2	5:D1:280:TRP:CZ2	2.56	0.41
33:B1:619:BCR:H16C	52:B1:624:3PH:H2E1	2.03	0.41
4:C1:227:TRP:HZ3	57:Y1:626:PTY:H211	1.86	0.41
33:C1:515:BCR:H351	33:C1:515:BCR:H15C	1.65	0.41
5:D1:67:TYR:HE1	35:D1:411:LMG:HC1	1.85	0.41
5:D1:191:TRP:CZ2	5:D1:197:HIS:HB2	2.55	0.41
7:F1:36:ILE:HA	7:F1:39:MET:HG2	2.01	0.41
9:I1:21:PHE:HA	9:I1:24:LEU:HB2	2.01	0.41
31:G1:604:CLA:C2B	48:G1:621:LUT:H183	2.51	0.41
48:R1:620:LUT:H15	48:R1:620:LUT:H201	1.82	0.41
31:Y1:613:CLA:H93	31:Y1:613:CLA:H61	1.93	0.41
1:a1:321:ILE:O	1:a1:325:ASN:N	2.48	0.41
2:b1:158:VAL:HG23	2:b1:199:PRO:HB3	2.02	0.41
4:c1:154:ILE:HA	4:c1:233:ILE:HD13	2.02	0.41
31:c1:513:CLA:NB	33:c1:514:BCR:H383	2.36	0.41
33:c1:515:BCR:H351	33:c1:515:BCR:H15C	1.72	0.41
8:h1:31:ARG:HA	8:h1:31:ARG:HD2	1.83	0.41
14:o1:91:THR:OG1	14:o1:96:GLU:OE2	2.35	0.41
48:y1:621:LUT:H11	48:y1:621:LUT:H191	1.93	0.41
2:B:173:GLY:HA3	2:B:312:TYR:HE2	1.85	0.41
2:B:315:ILE:O	2:B:318:ASN:HB3	2.19	0.41
31:B:611:CLA:HAB	46:H:101:RRX:H13	2.03	0.41
4:C:323:THR:OG1	14:O:206:ARG:NH1	2.53	0.41
31:C:507:CLA:H161	31:C:507:CLA:H141	1.71	0.41
31:D:403:CLA:H141	31:D:403:CLA:H161	1.88	0.41
14:O:114:PHE:CD1	17:W:61:VAL:HG11	2.56	0.41
17:W:65:MET:SD	17:W:65:MET:N	2.90	0.41
20:N:191:GLY:O	20:N:193:ALA:N	2.49	0.41
31:S:603:CLA:HAB	31:S:609:CLA:CBC	2.51	0.41
47:S:606:CHL:HBB2	47:S:607:CHL:CBB	2.51	0.41
31:S:613:CLA:H93	41:S:624:LHG:H142	2.03	0.41
1:a:291:SER:HB3	4:c:419:PHE:CE2	2.55	0.41
31:a:406:CLA:HBA2	31:a:406:CLA:H93	2.02	0.41
31:b:605:CLA:H201	31:r:609:CLA:H143	2.01	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:287:SER:HA	4:c:411:ARG:HH21	1.86	0.41
12:l:18:LEU:HD22	13:m:26:TYR:CG	2.55	0.41
14:o:236:GLU:O	14:o:240:LEU:N	2.45	0.41
17:w:101:LYS:O	17:w:103:LEU:N	2.54	0.41
20:n:221:PHE:HE2	48:n:621:LUT:H14	1.86	0.41
31:n:603:CLA:HBC1	47:n:609:CHL:HAC2	2.02	0.41
21:g:94:LEU:HD12	21:g:94:LEU:HA	1.91	0.41
31:g:610:CLA:H143	31:g:610:CLA:H161	1.90	0.41
22:r:144:ALA:HB2	49:r:622:XAT:H203	2.03	0.41
23:s:52:TRP:HZ3	41:s:624:LHG:HC32	1.86	0.41
1:A1:97:TRP:NE1	9:I1:5:LYS:HE3	2.35	0.41
1:A1:321:ILE:HD11	5:D1:176:ALA:HB1	2.03	0.41
1:A1:338:ASN:HB2	4:C1:341:GLY:HA2	2.03	0.41
31:B1:605:CLA:H143	31:R1:609:CLA:H141	2.02	0.41
4:C1:104:VAL:HG11	33:C1:514:BCR:HC32	2.02	0.41
31:C1:510:CLA:HED1	31:C1:510:CLA:H102	2.02	0.41
34:M1:101:SQD:H82	34:M1:101:SQD:H112	1.86	0.41
21:G1:190:PRO:HA	21:G1:193:PHE:HB3	2.03	0.41
23:S1:251:ILE:HD11	31:S1:613:CLA:HHD	2.01	0.41
48:S1:620:LUT:H15	48:S1:620:LUT:H201	1.96	0.41
24:Y1:62:THR:OG1	24:Y1:64:GLU:OE1	2.29	0.41
24:Y1:151:ILE:HG23	24:Y1:152:LEU:HD22	2.03	0.41
2:b1:256:MET:O	2:b1:448:ARG:NH1	2.38	0.41
2:b1:362:PHE:HB3	5:d1:188:PHE:CD2	2.56	0.41
31:c1:513:CLA:H101	33:c1:514:BCR:H23C	2.02	0.41
5:d1:148:ALA:HB2	5:d1:276:VAL:HG13	2.02	0.41
5:d1:285:GLY:O	5:d1:289:LEU:N	2.50	0.41
27:r1:247:MET:HB2	49:r1:621:XAT:H35	2.01	0.41
4:C:221:ILE:HG22	4:C:222:ILE:HD13	2.02	0.41
5:D:125:PHE:O	5:D:128:ARG:HB3	2.21	0.41
5:D:273:PHE:HZ	41:D:408:LHG:H132	1.86	0.41
8:H:57:PHE:CE2	46:H:101:RRX:C23	3.04	0.41
20:N:90:LEU:HD21	20:N:94:ARG:HH21	1.85	0.41
47:N:607:CHL:C2C	47:Y:601:CHL:H143	2.51	0.41
31:N:613:CLA:H93	31:N:613:CLA:H61	1.84	0.41
23:S:80:ALA:O	23:S:101:ARG:NH1	2.48	0.41
24:Y:71:TRP:CD1	48:Y:621:LUT:H383	2.56	0.41
24:Y:139:TYR:HB2	24:Y:146:ILE:HD13	2.03	0.41
2:b:445:SER:HB3	2:b:450:TRP:NE1	2.36	0.41
4:c:51:TRP:HB2	31:c:510:CLA:HAC2	2.01	0.41
4:c:122:LEU:HD21	31:c:511:CLA:H12	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
4:c:245:TRP:CE2	31:c:506:CLA:HED2	2.55	0.41
33:c:517:BCR:H391	11:k:36:ALA:HB2	2.02	0.41
40:c:519:DGD:HB92	35:c:521:LMG:H421	2.01	0.41
21:g:202:LYS:NZ	31:g:611:CLA:O1D	2.40	0.41
48:g:621:LUT:H15	48:g:621:LUT:H201	1.82	0.41
24:y:109:LEU:HG	24:y:234:ILE:HD13	2.01	0.41
24:y:194:LEU:HD23	31:y:610:CLA:H12	2.02	0.41
1:A1:237:TYR:HE1	1:A1:241:GLN:HG2	1.85	0.41
32:A1:408:PHO:H2	32:A1:408:PHO:H61	1.64	0.41
53:A1:414:SPH:H131	34:b1:626:SQD:H202	2.02	0.41
2:B1:257:TRP:CE3	5:D1:291:LEU:HD13	2.55	0.41
33:B1:618:BCR:H342	52:B1:624:3PH:H271	2.03	0.41
31:C1:512:CLA:H12	31:C1:512:CLA:HBA2	1.75	0.41
2:b1:40:PHE:HD1	52:b1:624:3PH:H381	1.85	0.41
31:b1:602:CLA:H143	31:b1:602:CLA:H111	1.80	0.41
31:b1:617:CLA:H51	31:b1:617:CLA:H11	1.73	0.41
34:b1:621:SQD:H251	34:b1:621:SQD:H132	2.02	0.41
4:c1:128:LEU:HB3	4:c1:132:TYR:HB2	2.02	0.41
4:c1:248:ALA:O	4:c1:252:PHE:HB2	2.21	0.41
4:c1:320:GLN:HB3	14:o1:165:TYR:CE1	2.56	0.41
31:c1:510:CLA:H102	31:c1:510:CLA:H61	1.80	0.41
35:c1:523:LMG:HC1	31:y1:611:CLA:H3A	2.02	0.41
5:d1:250:ASN:O	5:d1:254:SER:OG	2.22	0.41
6:e1:68:ASP:HA	25:u1:109:LEU:HD23	2.02	0.41
7:f1:30:ILE:HA	7:f1:33:LEU:HB2	2.02	0.41
9:i1:9:TYR:HE2	17:w1:76:VAL:HG12	1.85	0.41
14:o1:70:LEU:HD22	14:o1:74:GLN:HG3	2.02	0.41
47:s1:608:CHL:H142	31:s1:610:CLA:H201	2.01	0.41
31:y1:604:CLA:HED2	31:y1:604:CLA:H2A	2.02	0.41
1:A:174:LEU:HD22	32:A:408:PHO:H151	2.03	0.41
2:B:247:TRP:CD1	31:B:603:CLA:H142	2.56	0.41
2:B:347:LYS:HE3	2:B:347:LYS:HB3	1.69	0.41
31:B:605:CLA:H12	31:B:606:CLA:C4D	2.50	0.41
31:B:608:CLA:H141	12:L:28:LEU:HD12	2.03	0.41
4:C:285:TYR:HD1	4:C:290:TYR:CE2	2.39	0.41
5:D:85:LEU:HD13	6:E:69:ARG:HG2	2.01	0.41
41:D:409:LHG:H112	41:D:409:LHG:H262	2.03	0.41
14:O:152:ASP:OD1	14:O:152:ASP:N	2.53	0.41
31:N:613:CLA:H91	31:N:613:CLA:H112	1.85	0.41
31:G:602:CLA:H18	47:Y:609:CHL:H42	2.02	0.41
41:S:624:LHG:H332	41:S:624:LHG:H302	1.86	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
24:Y:77:SER:HB3	24:Y:83:PHE:CD1	2.56	0.41
31:Y:603:CLA:HAC1	47:Y:607:CHL:CBB	2.50	0.41
31:Y:610:CLA:H72	31:Y:610:CLA:HBB1	2.02	0.41
2:b:282:GLN:HE21	25:u:107:LYS:HD2	1.86	0.41
4:c:408:VAL:N	40:c:519:DGD:O3E	2.51	0.41
31:c:506:CLA:H93	31:c:506:CLA:H61	1.76	0.41
31:c:507:CLA:H161	31:c:507:CLA:H141	1.74	0.41
40:c:520:DGD:HB92	40:c:520:DGD:HB61	1.78	0.41
5:d:36:LEU:O	5:d:40:CYS:HB2	2.20	0.41
6:e:8:ARG:O	7:f:18:ARG:NH2	2.54	0.41
14:o:228:LEU:HA	14:o:229:PRO:HD3	1.87	0.41
23:s:176:LEU:HA	23:s:179:VAL:HG12	2.03	0.41
2:B1:34:ALA:O	2:B1:38:THR:OG1	2.27	0.41
2:B1:54:PRO:HD2	2:B1:57:ARG:HG3	2.03	0.41
2:B1:91:TRP:HE1	40:B1:623:DGD:HD2	1.85	0.41
2:B1:441:GLY:HA2	14:O1:230:ALA:HB3	2.03	0.41
2:B1:462:PHE:CE1	31:B1:612:CLA:HAB	2.55	0.41
31:B1:616:CLA:H8	31:B1:617:CLA:HBB1	2.01	0.41
4:C1:46:GLY:O	4:C1:50:PHE:N	2.50	0.41
4:C1:197:ILE:HG13	4:C1:227:TRP:CD1	2.56	0.41
4:C1:413:TRP:CZ3	31:C1:504:CLA:H2	2.52	0.41
4:C1:435:ARG:NH1	31:C1:508:CLA:HED2	2.35	0.41
15:P1:231:ASP:OD1	15:P1:231:ASP:N	2.53	0.41
31:N1:604:CLA:H152	47:N1:608:CHL:HBA1	2.03	0.41
50:N1:623:NEX:H15	50:N1:623:NEX:H201	1.87	0.41
31:S1:604:CLA:HBB1	48:S1:621:LUT:H181	2.02	0.41
24:Y1:219:CYS:HB3	48:Y1:621:LUT:H12	2.01	0.41
1:a1:223:LEU:HD23	1:a1:246:TYR:HB3	2.02	0.41
4:c1:80:ILE:HG22	4:c1:85:TYR:HB2	2.02	0.41
31:c1:511:CLA:H152	31:c1:511:CLA:H111	1.77	0.41
5:d1:55:VAL:O	5:d1:66:SER:HB3	2.21	0.41
5:d1:111:TRP:HH2	5:d1:170:ALA:HB3	1.86	0.41
8:h1:26:LEU:HD12	8:h1:29:LEU:HD13	2.03	0.41
20:n1:101:LEU:HA	20:n1:104:VAL:HG22	2.02	0.41
47:r1:606:CHL:HBC2	47:r1:607:CHL:HAC2	2.03	0.41
31:y1:610:CLA:HBB2	48:y1:620:LUT:H34	2.03	0.41
1:A:47:VAL:HG21	1:A:114:LEU:HD23	2.03	0.41
1:A:91:LEU:HD11	40:C:518:DGD:O2D	2.21	0.41
1:A:184:ILE:HG23	1:A:328:MET:SD	2.61	0.41
2:B:462:PHE:HA	31:B:612:CLA:HMC2	2.03	0.41
31:B:604:CLA:H141	31:B:604:CLA:H161	1.76	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:B:606:CLA:H101	31:B:606:CLA:H13	1.99	0.41
35:B:622:LMG:H351	13:M:14:PHE:HB2	2.02	0.41
4:C:87:VAL:HG21	4:C:289:PHE:CZ	2.55	0.41
4:C:292:PRO:HB3	4:C:296:GLU:HG3	2.03	0.41
31:C:506:CLA:H61	31:C:506:CLA:H93	1.76	0.41
12:L:1:MET:HE2	12:L:1:MET:HB3	1.95	0.41
12:L:37:PHE:CZ	16:T:5:VAL:HG21	2.56	0.41
20:N:55:ASN:ND2	21:G:161:ALA:O	2.35	0.41
21:G:160:ARG:HH21	47:G:608:CHL:CHA	2.34	0.41
21:G:209:PHE:HZ	41:G:630:LHG:H151	1.85	0.41
31:G:604:CLA:NB	50:G:623:NEX:H242	2.36	0.41
48:G:620:LUT:H201	48:G:620:LUT:H15	1.81	0.41
24:Y:168:PHE:CD2	31:Y:608:CLA:HAB	2.55	0.41
31:Y:603:CLA:C3C	47:Y:607:CHL:H152	2.51	0.41
31:Y:614:CLA:H142	31:Y:614:CLA:H112	1.89	0.41
49:Y:622:XAT:H15	49:Y:622:XAT:H201	1.64	0.41
1:a:43:THR:O	1:a:47:VAL:HG22	2.21	0.41
1:a:83:VAL:HG22	5:d:314:PHE:HE2	1.86	0.41
1:a:227:THR:HA	1:a:232:SER:HA	2.02	0.41
1:a:302:PHE:HE1	4:c:393:ASN:HD22	1.67	0.41
2:b:65:PHE:CE2	31:b:605:CLA:H2A	2.55	0.41
31:b:610:CLA:H193	31:b:610:CLA:H162	1.89	0.41
3:v:33:LEU:C	11:k:39:TRP:HE1	2.29	0.41
4:c:104:VAL:HG13	33:c:517:BCR:H332	2.03	0.41
4:c:198:PHE:O	4:c:202:VAL:HG22	2.20	0.41
4:c:335:GLY:HA3	14:o:82:ASN:HB2	2.03	0.41
33:c:515:BCR:H332	9:i:20:ILE:HD13	2.01	0.41
40:c:519:DGD:HA71	35:c:521:LMG:H362	2.03	0.41
5:d:182:ILE:HG23	31:d:402:CLA:HAC1	2.02	0.41
12:l:24:LEU:HD12	41:l:101:LHG:H141	2.02	0.41
20:n:226:VAL:HG21	31:n:613:CLA:HMD2	2.03	0.41
31:n:613:CLA:H92	41:n:624:LHG:H161	2.03	0.41
48:g:620:LUT:H11	48:g:620:LUT:H191	1.80	0.41
22:r:145:MET:HA	22:r:148:THR:HG22	2.03	0.41
1:A1:196:PRO:O	1:A1:199:MET:HB3	2.21	0.41
2:B1:15:ASP:HB3	2:B1:18:ARG:HB2	2.03	0.41
2:B1:155:ALA:HB2	2:B1:203:ILE:HG12	2.02	0.41
2:B1:441:GLY:HA3	14:O1:228:LEU:HD12	2.03	0.41
31:B1:606:CLA:H142	31:B1:611:CLA:H51	2.02	0.41
38:B1:625:DGA:HBH1	8:H1:54:ILE:HD12	2.02	0.41
31:C1:501:CLA:H162	31:C1:507:CLA:HMB3	2.03	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
31:C1:504:CLA:H203	31:C1:504:CLA:H161	1.75	0.41
31:C1:508:CLA:H8	31:C1:510:CLA:H52	2.03	0.41
31:C1:513:CLA:H111	41:C1:525:LHG:H192	2.03	0.41
41:D1:409:LHG:H172	41:L1:101:LHG:H191	2.03	0.41
8:H1:44:TRP:O	8:H1:47:THR:OG1	2.36	0.41
10:J1:27:LEU:HD13	10:J1:30:PHE:HD2	1.86	0.41
11:K1:29:PRO:HA	11:K1:32:PHE:HD2	1.86	0.41
54:K1:101:4RF:H50	54:K1:101:4RF:H55	1.84	0.41
14:O1:63:THR:OG1	14:O1:66:GLU:OE1	2.38	0.41
20:N1:183:PRO:HB3	47:N1:608:CHL:HBC2	2.03	0.41
23:S1:80:ALA:HB3	23:S1:101:ARG:HH12	1.86	0.41
31:Y1:612:CLA:H111	31:Y1:612:CLA:H142	1.79	0.41
1:a1:142:TRP:CZ3	41:d1:410:LHG:HC41	2.55	0.41
1:a1:195:HIS:CD2	1:a1:293:MET:HE1	2.56	0.41
31:a1:406:CLA:H62	31:a1:406:CLA:H92	1.78	0.41
2:b1:24:LEU:HD23	2:b1:24:LEU:HA	1.91	0.41
2:b1:39:LEU:HG	2:b1:97:ALA:HB1	2.03	0.41
2:b1:103:LEU:HB2	31:b1:607:CLA:H71	2.03	0.41
31:b1:605:CLA:H18	31:r1:603:CLA:H91	2.02	0.41
31:b1:609:CLA:H62	31:b1:610:CLA:H101	2.03	0.41
31:b1:610:CLA:H91	31:b1:610:CLA:H112	1.86	0.41
4:c1:29:ARG:NH1	31:c1:511:CLA:OBD	2.53	0.41
4:c1:337:ILE:H	4:c1:362:GLY:HA3	1.86	0.41
4:c1:342:GLU:O	4:c1:345:ARG:HG2	2.21	0.41
31:c1:511:CLA:H112	33:c1:517:BCR:H24C	2.03	0.41
33:c1:516:BCR:H351	33:c1:516:BCR:H15C	1.67	0.41
5:d1:224:GLU:HG3	5:d1:226:GLY:N	2.36	0.41
6:e1:12:ASP:OD1	6:e1:12:ASP:N	2.54	0.41
48:n1:621:LUT:H35	48:n1:621:LUT:H401	1.76	0.41
48:g1:621:LUT:H372	31:y1:603:CLA:HED3	2.03	0.41
27:r1:219:ASP:OD1	48:r1:620:LUT:O23	2.30	0.41
23:s1:244:ILE:HG13	41:s1:624:LHG:H271	2.03	0.41
24:y1:95:ARG:NE	24:y1:208:GLU:OE2	2.40	0.41
24:y1:136:GLY:HA3	24:y1:149:GLN:HE21	1.85	0.41
24:y1:214:LEU:HD11	31:y1:611:CLA:HHD	2.03	0.41
50:y1:623:NEX:H15	50:y1:623:NEX:H201	1.95	0.41
32:A:408:PHO:CAD	5:D:213:ILE:HD11	2.51	0.41
2:B:334:ASP:N	2:B:334:ASP:OD1	2.54	0.41
31:C:501:CLA:HMB2	33:C:515:BCR:H23C	2.03	0.41
31:C:509:CLA:O1A	31:C:510:CLA:HBB1	2.21	0.41
5:D:93:TRP:CG	18:X:75:SER:HG	2.38	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:N:620:LUT:H35	48:N:620:LUT:H401	1.74	0.41
21:G:142:ILE:HA	21:G:145:THR:HG22	2.03	0.41
23:S:58:LYS:HE2	41:S:624:LHG:HC12	2.03	0.41
23:S:209:LYS:HZ2	23:S:209:LYS:HG3	1.65	0.41
1:a:141:PRO:HG3	4:c:434:GLY:C	2.45	0.41
1:a:333:GLU:HB2	1:a:337:HIS:NE2	2.36	0.41
2:b:3:LEU:HD23	2:b:3:LEU:HA	1.87	0.41
2:b:108:PHE:O	2:b:111:SER:OG	2.33	0.41
2:b:243:ALA:HA	2:b:246:PHE:CE2	2.56	0.41
2:b:371:ILE:HG13	25:u:100:PRO:HB3	2.01	0.41
31:b:605:CLA:H12	31:b:606:CLA:C4D	2.51	0.41
4:c:333:PRO:HB3	14:o:135:ARG:CZ	2.51	0.41
33:c:517:BCR:H312	19:z:9:LEU:HD21	2.03	0.41
14:o:278:THR:HG22	14:o:285:ALA:HB2	2.03	0.41
22:r:210:LYS:HE3	22:r:215:GLY:H	1.85	0.41
23:s:260:PRO:HA	23:s:263:ASN:HB2	2.03	0.41
48:y:621:LUT:H15	48:y:621:LUT:H201	1.88	0.41
1:A1:125:CYS:O	1:A1:129:ARG:N	2.51	0.41
1:A1:186:PHE:CE2	1:A1:293:MET:HE3	2.56	0.41
1:A1:331:MET:HA	5:D1:349:GLY:N	2.35	0.41
1:A1:340:PRO:HB2	15:P1:224:LYS:HD2	2.02	0.41
2:B1:12:VAL:HG12	2:B1:18:ARG:HD3	2.03	0.41
2:B1:226:TYR:CE2	27:R1:87:ILE:HG21	2.56	0.41
2:B1:242:ILE:HA	2:B1:245:VAL:HG12	2.03	0.41
2:B1:283:GLU:OE2	2:B1:287:ARG:NH2	2.54	0.41
2:B1:288:VAL:HG23	2:B1:305:ILE:HD11	2.03	0.41
2:B1:453:PHE:CZ	5:D1:293:LEU:HB3	2.56	0.41
14:O1:160:ASP:OD1	14:O1:161:GLU:N	2.51	0.41
20:N1:238:HIS:CE1	31:N1:613:CLA:HBA1	2.56	0.41
47:G1:605:CHL:HMA2	47:G1:605:CHL:HAA1	1.98	0.41
31:G1:613:CLA:H51	31:G1:613:CLA:NC	2.35	0.41
24:Y1:95:ARG:NH2	24:Y1:208:GLU:OE2	2.52	0.41
24:Y1:213:ARG:HA	24:Y1:216:MET:HE2	2.03	0.41
2:b1:238:LEU:HD13	31:b1:613:CLA:C1D	2.51	0.41
5:d1:203:GLY:HA2	44:d1:405:PL9:H23	2.02	0.41
41:n1:624:LHG:H201	41:n1:624:LHG:H172	1.81	0.41
21:g1:53:LEU:HD11	21:g1:64:ASP:HB2	2.02	0.41
21:g1:242:PHE:HB3	24:y1:132:PHE:CZ	2.56	0.41
31:s1:605:CLA:H42	31:s1:610:CLA:H18	2.02	0.41
48:s1:621:LUT:H15	48:s1:621:LUT:H201	1.91	0.41
52:s1:626:3PH:H342	52:s1:626:3PH:H371	1.67	0.41

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:B:356:VAL:HG12	2:B:370:LEU:HG	2.03	0.40
12:L:12:GLU:HG2	13:M:29:THR:HG23	2.03	0.40
15:P:128:ILE:HG23	15:P:209:VAL:HG12	2.03	0.40
20:N:255:THR:HG21	21:G:117:LYS:NZ	2.36	0.40
23:S:271:PRO:HB2	31:S:614:CLA:HMA2	2.03	0.40
31:S:605:CLA:CHA	31:S:605:CLA:HBA1	2.50	0.40
24:Y:221:GLY:O	24:Y:225:GLN:HB2	2.20	0.40
1:a:40:THR:HG23	31:a:410:CLA:HBB1	2.03	0.40
2:b:52:LEU:HD13	2:b:307:GLU:HG3	2.03	0.40
2:b:268:PHE:HB3	2:b:448:ARG:CG	2.51	0.40
31:c:513:CLA:H3A	31:c:513:CLA:HBA2	1.77	0.40
5:d:21:TRP:NE1	18:x:93:VAL:O	2.54	0.40
6:e:7:GLU:O	7:f:18:ARG:NH2	2.54	0.40
31:n:613:CLA:H112	31:n:613:CLA:H91	1.91	0.40
22:r:240:ILE:HD12	22:r:240:ILE:HA	1.96	0.40
23:s:92:LYS:HD2	23:s:96:GLN:HG2	2.02	0.40
31:s:613:CLA:H62	31:s:613:CLA:H41	1.86	0.40
31:s:614:CLA:HBA2	31:s:614:CLA:H3A	1.71	0.40
31:y:603:CLA:H91	31:y:603:CLA:H112	1.85	0.40
49:y:622:XAT:H35	49:y:622:XAT:H401	1.88	0.40
1:A1:61:ASP:HB2	1:A1:63:ILE:HG12	2.03	0.40
1:A1:195:HIS:HD2	1:A1:197:PHE:H	1.69	0.40
31:B1:603:CLA:H92	31:B1:603:CLA:H61	1.86	0.40
31:B1:605:CLA:H61	31:B1:605:CLA:H93	1.94	0.40
31:B1:612:CLA:H101	31:B1:614:CLA:H151	2.02	0.40
31:C1:511:CLA:H92	31:C1:511:CLA:H62	1.76	0.40
40:C1:519:DGD:HB72	35:C1:521:LMG:H421	2.02	0.40
14:O1:252:ALA:HA	14:O1:272:SER:HA	2.02	0.40
49:N1:622:XAT:H30	41:Y1:624:LHG:H371	2.03	0.40
56:R1:626:ERG:H192	56:R1:626:ERG:H111	1.86	0.40
24:Y1:213:ARG:NH2	31:Y1:602:CLA:O2D	2.51	0.40
2:b1:259:GLY:HA3	8:h1:81:TRP:CH2	2.57	0.40
31:b1:615:CLA:H3A	31:b1:615:CLA:HBA2	1.57	0.40
33:c1:514:BCR:H281	41:c1:525:LHG:HC82	2.01	0.40
33:c1:517:BCR:H392	11:k1:32:PHE:CZ	2.56	0.40
34:c1:526:SQD:H441	34:c1:526:SQD:H2	1.85	0.40
5:d1:9:GLN:HB2	5:d1:11:LYS:HE3	2.03	0.40
16:t1:25:GLU:HA	16:t1:26:PRO:HD3	1.95	0.40
47:n1:601:CHL:H202	47:g1:607:CHL:H152	2.04	0.40
47:n1:601:CHL:HED2	41:n1:624:LHG:H141	2.03	0.40
47:n1:605:CHL:H41	31:s1:611:CLA:H171	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
48:g1:621:LUT:H362	47:y1:609:CHL:H11	2.03	0.40
23:s1:57:ARG:O	23:s1:68:ARG:NH2	2.35	0.40
23:s1:111:ALA:HA	23:s1:114:ALA:HB3	2.03	0.40
31:B:609:CLA:H92	31:B:609:CLA:H62	1.83	0.40
31:C:513:CLA:CAB	33:C:514:BCR:H24C	2.50	0.40
5:D:141:TYR:CD1	5:D:144:ILE:HD12	2.56	0.40
22:R:208:LEU:O	22:R:212:ILE:HG12	2.20	0.40
31:R:604:CLA:HMA2	47:R:606:CHL:C3C	2.52	0.40
31:S:604:CLA:HBB1	48:S:621:LUT:H181	2.04	0.40
24:Y:169:ARG:NH2	47:Y:609:CHL:O1D	2.45	0.40
1:a:160:ILE:HD11	40:c:518:DGD:HBE2	2.03	0.40
2:b:369:VAL:HG12	2:b:380:ASP:HB3	2.03	0.40
2:b:388:SER:OG	2:b:389:LYS:N	2.54	0.40
31:b:614:CLA:H62	31:b:614:CLA:H41	1.73	0.40
4:c:23:TRP:CD1	4:c:23:TRP:H	2.39	0.40
4:c:141:ASP:OD1	4:c:145:MET:HE2	2.21	0.40
4:c:146:THR:O	4:c:239:HIS:HB3	2.20	0.40
4:c:296:GLU:C	4:c:298:SER:H	2.29	0.40
4:c:367:LYS:HG3	4:c:371:ASP:HB2	2.03	0.40
31:c:508:CLA:H143	31:c:510:CLA:H18	2.03	0.40
5:d:19:ASP:OD1	5:d:32:TRP:NE1	2.54	0.40
41:d:409:LHG:H212	41:d:409:LHG:H181	1.80	0.40
22:r:83:VAL:HG23	22:r:109:ARG:HA	2.02	0.40
2:B1:462:PHE:CE2	31:B1:605:CLA:HAC2	2.56	0.40
33:C1:516:BCR:H17C	11:K1:35:LEU:CD2	2.50	0.40
5:D1:19:ASP:OD1	5:D1:32:TRP:NE1	2.37	0.40
14:O1:135:ARG:O	14:O1:137:THR:N	2.53	0.40
20:N1:232:ILE:HA	20:N1:235:LEU:HB3	2.03	0.40
21:G1:163:GLY:HA2	47:G1:608:CHL:HAC1	2.02	0.40
24:Y1:50:LEU:HB2	24:Y1:54:SER:HA	2.03	0.40
24:Y1:137:LEU:HD22	47:Y1:606:CHL:HAC1	2.03	0.40
2:b1:23:HIS:ND1	31:b1:616:CLA:OBD	2.42	0.40
31:b1:603:CLA:HAC2	46:h1:101:RRX:H29	2.03	0.40
4:c1:238:TRP:HB2	53:y1:625:SPH:H162	2.04	0.40
31:c1:511:CLA:H162	31:c1:511:CLA:H141	1.85	0.40
8:h1:53:ALA:O	46:h1:101:RRX:H21	2.21	0.40
23:s1:61:LEU:HD22	23:s1:65:LEU:HD12	2.04	0.40
1:A:184:ILE:HA	31:A:405:CLA:HBC1	2.02	0.40
1:A:297:LEU:HD12	1:A:297:LEU:HA	1.90	0.40
2:B:41:GLU:HA	2:B:44:VAL:HG22	2.03	0.40
4:C:425:PHE:HA	31:C:508:CLA:HMC2	2.03	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
5:D:107:LEU:HA	5:D:107:LEU:HD23	1.90	0.40
7:F:16:THR:HG23	7:F:19:TRP:H	1.87	0.40
46:H:101:RRX:H36	46:H:101:RRX:H40	1.89	0.40
14:O:111:PRO:HA	14:O:292:GLY:HA3	2.03	0.40
21:G:96:ILE:HD13	48:G:621:LUT:H41	2.03	0.40
23:S:65:LEU:HD12	23:S:65:LEU:HA	1.95	0.40
31:S:602:CLA:H72	48:S:621:LUT:H28	2.02	0.40
1:a:174:LEU:HD22	32:a:408:PHO:H151	2.03	0.40
2:b:248:ALA:HB2	31:b:604:CLA:H61	2.04	0.40
31:b:612:CLA:H62	31:b:612:CLA:H41	1.48	0.40
40:c:518:DGD:O4E	40:c:518:DGD:O5E	2.36	0.40
5:d:236:ASN:HD21	5:d:238:THR:HB	1.87	0.40
14:o:196:PHE:HE1	14:o:256:VAL:HG23	1.85	0.40
16:t:28:ARG:HA	16:t:28:ARG:HD3	1.86	0.40
19:z:59:SER:HB3	23:s:281:GLN:HA	2.03	0.40
20:n:95:TRP:NE1	47:n:608:CHL:HED3	2.36	0.40
31:n:602:CLA:H143	31:n:602:CLA:H111	1.86	0.40
49:r:622:XAT:H31	49:r:622:XAT:H391	1.91	0.40
24:y:216:MET:SD	31:y:602:CLA:HMC3	2.60	0.40
2:B1:115:TRP:CD2	33:B1:618:BCR:H291	2.55	0.40
2:B1:394:GLN:HG2	15:P1:147:ARG:HD2	2.03	0.40
4:C1:264:LEU:HD21	31:C1:508:CLA:CAB	2.52	0.40
31:C1:505:CLA:CMD	31:C1:507:CLA:HAB	2.51	0.40
5:D1:193:LEU:O	12:L1:35:TYR:OH	2.32	0.40
5:D1:269:PHE:HZ	41:D1:408:LHG:HC5	1.86	0.40
6:E1:12:ASP:OD1	6:E1:12:ASP:N	2.54	0.40
20:N1:84:ARG:HD2	24:Y1:75:GLY:HA3	2.03	0.40
23:S1:175:LEU:HD13	50:S1:623:NEX:H34	2.03	0.40
53:Y1:625:SPH:H161	53:Y1:625:SPH:H131	1.84	0.40
2:b1:186:GLY:HA2	31:b1:602:CLA:C4D	2.52	0.40
31:b1:603:CLA:H91	31:b1:603:CLA:H112	1.94	0.40
4:c1:281:ASN:HA	40:c1:518:DGD:HE5	2.03	0.40
14:o1:265:GLU:HA	14:o1:297:GLN:HA	2.02	0.40
15:p1:192:ARG:HA	15:p1:192:ARG:HD2	1.82	0.40
31:g1:613:CLA:H201	24:y1:156:ALA:HA	2.03	0.40
31:s1:602:CLA:H41	31:s1:602:CLA:H62	1.85	0.40
47:s1:606:CHL:HBB2	47:s1:607:CHL:CBB	2.51	0.40
48:s1:620:LUT:H11	48:s1:620:LUT:H191	1.80	0.40
1:A:88:ALA:HA	4:C:344:MET:HE2	2.03	0.40
34:A:412:SQD:H62	5:D:232:PHE:HB3	2.03	0.40
31:C:501:CLA:H201	31:C:507:CLA:H171	2.04	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
10:J:31:PHE:O	10:J:34:SER:OG	2.37	0.40
12:L:18:LEU:HD22	13:M:26:TYR:CG	2.56	0.40
31:N:613:CLA:C4C	31:N:613:CLA:H51	2.52	0.40
31:R:602:CLA:H61	31:R:602:CLA:H41	1.72	0.40
23:S:192:PHE:H	23:S:198:LYS:HA	1.86	0.40
48:S:621:LUT:H35	48:S:621:LUT:H401	1.78	0.40
24:Y:166:GLU:HA	24:Y:169:ARG:HB3	2.03	0.40
1:a:97:TRP:CZ3	9:i:8:VAL:HG11	2.57	0.40
1:a:205:VAL:HG22	5:d:204:VAL:HG12	2.03	0.40
4:c:14:ARG:HD2	4:c:19:THR:HG23	2.04	0.40
4:c:58:PHE:CZ	11:k:26:PRO:HD3	2.56	0.40
31:c:513:CLA:H93	33:c:514:BCR:H271	2.03	0.40
5:d:158:LEU:HD13	35:h:102:LMG:H351	2.03	0.40
47:n:601:CHL:H92	47:n:601:CHL:H112	1.81	0.40
23:s:90:LEU:HD12	48:s:621:LUT:H221	2.04	0.40
31:s:611:CLA:H41	31:s:611:CLA:H61	1.82	0.40
24:y:159:VAL:HA	47:y:609:CHL:HBB2	2.03	0.40
24:y:243:ASP:OD1	24:y:243:ASP:N	2.54	0.40
1:A1:29:TYR:CG	1:A1:133:LEU:HD13	2.56	0.40
1:A1:159:ILE:O	1:A1:163:ILE:HG13	2.21	0.40
2:B1:99:SER:HB2	31:B1:607:CLA:H62	2.03	0.40
2:B1:247:TRP:CD1	31:B1:604:CLA:H101	2.57	0.40
3:V1:8:GLN:NE2	11:K1:23:ASP:OD2	2.55	0.40
4:C1:16:GLN:HG2	5:D1:233:ARG:NH1	2.37	0.40
4:C1:197:ILE:HG13	4:C1:227:TRP:HD1	1.86	0.40
4:C1:418:HIS:CE1	31:C1:502:CLA:HED2	2.57	0.40
31:C1:513:CLA:H62	31:C1:513:CLA:H41	1.78	0.40
33:C1:516:BCR:H17C	11:K1:35:LEU:HD22	2.03	0.40
12:L1:23:LEU:O	12:L1:27:VAL:N	2.49	0.40
26:M1:23:LEU:HA	26:M1:26:TYR:HB3	2.04	0.40
14:O1:98:LYS:H	14:O1:98:LYS:HG2	1.70	0.40
14:O1:158:ARG:NH1	14:O1:159:GLU:O	2.55	0.40
15:P1:117:TYR:HE2	15:P1:119:ILE:HD11	1.86	0.40
31:N1:610:CLA:H3A	31:N1:610:CLA:HBA2	1.63	0.40
31:G1:603:CLA:HAC1	47:G1:607:CHL:HBB2	2.04	0.40
31:S1:603:CLA:HMA3	31:S1:609:CLA:HBA2	2.03	0.40
31:Y1:614:CLA:HAB	57:Y1:626:PTY:H232	2.02	0.40
1:a1:127:MET:HG2	1:a1:127:MET:H	1.74	0.40
2:b1:224:ARG:HD2	8:h1:44:TRP:CZ3	2.56	0.40
31:b1:610:CLA:H92	31:b1:610:CLA:H61	1.79	0.40
3:v1:8:GLN:NE2	11:k1:20:PRO:HA	2.36	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
20:n1:57:PRO:HG2	20:n1:71:ASP:HB3	2.03	0.40
20:n1:141:ASN:OD1	20:n1:141:ASN:N	2.55	0.40
48:n1:620:LUT:H35	48:n1:620:LUT:H401	1.87	0.40
21:g1:76:ALA:O	21:g1:80:GLU:HG3	2.21	0.40
47:g1:601:CHL:H152	41:g1:624:LHG:H223	2.04	0.40
31:g1:611:CLA:H151	31:g1:612:CLA:HBC2	2.02	0.40
23:s1:209:LYS:HG3	23:s1:210:LEU:HG	2.03	0.40
31:y1:602:CLA:HBA1	48:y1:621:LUT:H382	2.04	0.40
48:y1:620:LUT:H401	48:y1:620:LUT:H35	1.83	0.40
31:B:610:CLA:H141	31:B:610:CLA:H161	1.79	0.40
6:E:70:PHE:HB2	25:U:110:ARG:NH1	2.37	0.40
9:I:9:TYR:HD2	17:W:85:ILE:HD11	1.86	0.40
20:N:48:TRP:HD1	20:N:68:TYR:O	2.04	0.40
31:N:604:CLA:H91	31:N:604:CLA:H112	1.87	0.40
47:N:605:CHL:HAA1	52:S:626:3PH:H3A1	2.04	0.40
21:G:209:PHE:CD2	41:G:630:LHG:H272	2.56	0.40
49:G:622:XAT:H201	49:G:622:XAT:H15	1.72	0.40
48:S:621:LUT:H15	48:S:621:LUT:H201	1.86	0.40
24:Y:99:LEU:HB3	31:Y:604:CLA:CAB	2.51	0.40
31:Y:604:CLA:H141	22:r:152:ILE:HG23	2.02	0.40
2:b:242:ILE:HA	2:b:245:VAL:HG22	2.04	0.40
31:b:616:CLA:H92	31:b:616:CLA:H61	1.86	0.40
41:c:625:LHG:H261	47:s:601:CHL:HAC1	2.04	0.40
20:n:236:THR:HA	20:n:239:LEU:HG	2.04	0.40
41:g:624:LHG:HC92	49:y:622:XAT:H393	2.04	0.40
23:s:183:ARG:HG2	47:s:608:CHL:CHD	2.52	0.40
2:B1:37:MET:HB3	2:B1:37:MET:HE3	1.83	0.40
2:B1:224:ARG:HD2	2:B1:224:ARG:HA	1.89	0.40
52:B1:624:3PH:H2B1	52:B1:624:3PH:H281	1.79	0.40
38:B1:625:DGA:HAV1	18:X1:83:LEU:HD21	2.03	0.40
31:C1:506:CLA:H8	31:C1:506:CLA:H122	1.77	0.40
5:D1:81:PRO:HB3	5:D1:85:LEU:HD12	2.03	0.40
21:G1:232:HIS:ND1	21:G1:239:ASN:O	2.35	0.40
31:G1:610:CLA:H52	48:G1:620:LUT:H30	2.04	0.40
48:R1:620:LUT:H11	48:R1:620:LUT:H191	1.89	0.40
24:Y1:240:HIS:CG	31:Y1:613:CLA:HAA2	2.55	0.40
1:a1:224:ILE:O	5:d1:265:ARG:NH2	2.38	0.40
1:a1:258:LEU:HA	5:d1:128:ARG:HE	1.87	0.40
1:a1:340:PRO:HB2	15:p1:224:LYS:HD3	2.03	0.40
31:a1:405:CLA:H152	32:a1:408:PHO:H3A	2.03	0.40
2:b1:73:GLN:HB3	2:b1:85:SER:HB2	2.02	0.40

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Atom-1	Atom-2	Interatomic distance (Å)	Clash overlap (Å)
2:b1:385:LYS:HB2	15:p1:150:TRP:NE1	2.35	0.40
31:b1:606:CLA:H192	31:b1:610:CLA:HAB	2.04	0.40
35:b1:622:LMG:H171	35:b1:622:LMG:H142	1.80	0.40
4:c1:53:GLY:HA2	4:c1:103:GLY:HA2	2.03	0.40
31:c1:504:CLA:H203	31:c1:504:CLA:H161	1.78	0.40
5:d1:111:TRP:CH2	5:d1:170:ALA:HB3	2.57	0.40
6:e1:64:PRO:HB3	6:e1:79:LEU:HD23	2.03	0.40
7:f1:19:TRP:HE3	7:f1:20:LEU:HD22	1.85	0.40
14:o1:228:LEU:HA	14:o1:229:PRO:HD3	1.85	0.40
17:w1:73:PRO:O	17:w1:76:VAL:HG22	2.22	0.40
31:n1:602:CLA:CAB	48:n1:621:LUT:H32	2.51	0.40
48:n1:621:LUT:H11	48:n1:621:LUT:H191	1.92	0.40
48:g1:620:LUT:H15	48:g1:620:LUT:H201	1.82	0.40
27:r1:268:LEU:HD23	48:r1:620:LUT:H21	2.03	0.40
48:y1:620:LUT:H11	48:y1:620:LUT:H191	1.87	0.40

There are no symmetry-related clashes.

5.3 Torsion angles (i)

5.3.1 Protein backbone (i)

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

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

Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles
1	A	335/336 (100%)	304 (91%)	30 (9%)	1 (0%)	36 70
1	A1	335/336 (100%)	313 (93%)	22 (7%)	0	100 100
1	a	335/336 (100%)	313 (93%)	22 (7%)	0	100 100
1	a1	335/336 (100%)	316 (94%)	19 (6%)	0	100 100
2	B	482/484 (100%)	460 (95%)	21 (4%)	1 (0%)	43 75
2	B1	482/484 (100%)	459 (95%)	23 (5%)	0	100 100
2	b	482/484 (100%)	454 (94%)	28 (6%)	0	100 100
2	b1	482/484 (100%)	462 (96%)	20 (4%)	0	100 100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	V	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
3	V1	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
3	v	30/32 (94%)	28 (93%)	2 (7%)	0	100	100
3	v1	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
4	C	447/449 (100%)	410 (92%)	34 (8%)	3 (1%)	18	54
4	C1	447/449 (100%)	427 (96%)	20 (4%)	0	100	100
4	c	447/449 (100%)	413 (92%)	31 (7%)	3 (1%)	18	54
4	c1	447/449 (100%)	425 (95%)	22 (5%)	0	100	100
5	D	346/348 (99%)	330 (95%)	15 (4%)	1 (0%)	36	70
5	D1	346/348 (99%)	332 (96%)	14 (4%)	0	100	100
5	d	346/348 (99%)	332 (96%)	13 (4%)	1 (0%)	36	70
5	d1	346/348 (99%)	331 (96%)	15 (4%)	0	100	100
6	E	74/76 (97%)	70 (95%)	4 (5%)	0	100	100
6	E1	74/76 (97%)	69 (93%)	5 (7%)	0	100	100
6	e	74/76 (97%)	67 (90%)	7 (10%)	0	100	100
6	e1	74/76 (97%)	72 (97%)	2 (3%)	0	100	100
7	F	29/31 (94%)	29 (100%)	0	0	100	100
7	F1	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
7	f	29/31 (94%)	29 (100%)	0	0	100	100
7	f1	29/31 (94%)	29 (100%)	0	0	100	100
8	H	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
8	H1	65/67 (97%)	61 (94%)	4 (6%)	0	100	100
8	h	65/67 (97%)	64 (98%)	1 (2%)	0	100	100
8	h1	65/67 (97%)	62 (95%)	3 (5%)	0	100	100
9	I	33/35 (94%)	33 (100%)	0	0	100	100
9	I1	33/35 (94%)	32 (97%)	1 (3%)	0	100	100
9	i	33/35 (94%)	33 (100%)	0	0	100	100
9	i1	33/35 (94%)	32 (97%)	1 (3%)	0	100	100
10	J	34/36 (94%)	34 (100%)	0	0	100	100
10	J1	34/36 (94%)	34 (100%)	0	0	100	100
10	j	34/36 (94%)	34 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	j1	34/36 (94%)	34 (100%)	0	0	100	100
11	K	35/37 (95%)	35 (100%)	0	0	100	100
11	K1	35/37 (95%)	35 (100%)	0	0	100	100
11	k	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	k1	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
12	L	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	L1	36/38 (95%)	35 (97%)	1 (3%)	0	100	100
12	l	36/38 (95%)	36 (100%)	0	0	100	100
13	M	30/32 (94%)	29 (97%)	0	1 (3%)	3	24
13	m	30/32 (94%)	28 (93%)	1 (3%)	1 (3%)	3	24
14	O	236/238 (99%)	210 (89%)	25 (11%)	1 (0%)	30	65
14	O1	236/238 (99%)	214 (91%)	21 (9%)	1 (0%)	30	65
14	o	236/238 (99%)	215 (91%)	20 (8%)	1 (0%)	30	65
14	o1	236/238 (99%)	217 (92%)	18 (8%)	1 (0%)	30	65
15	P	185/187 (99%)	167 (90%)	17 (9%)	1 (0%)	24	60
15	P1	185/187 (99%)	175 (95%)	10 (5%)	0	100	100
15	p	185/187 (99%)	173 (94%)	12 (6%)	0	100	100
15	p1	185/187 (99%)	171 (92%)	14 (8%)	0	100	100
16	T	28/30 (93%)	26 (93%)	1 (4%)	1 (4%)	2	23
16	T1	28/30 (93%)	27 (96%)	0	1 (4%)	2	23
16	t	28/30 (93%)	27 (96%)	0	1 (4%)	2	23
16	t1	28/30 (93%)	28 (100%)	0	0	100	100
17	W	42/44 (96%)	40 (95%)	2 (5%)	0	100	100
17	W1	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
17	w	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
17	w1	42/44 (96%)	41 (98%)	1 (2%)	0	100	100
18	X	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
18	X1	28/30 (93%)	28 (100%)	0	0	100	100
18	x	28/30 (93%)	26 (93%)	2 (7%)	0	100	100
18	x1	28/30 (93%)	28 (100%)	0	0	100	100
19	Z	59/61 (97%)	59 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Z1	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
19	z	59/61 (97%)	58 (98%)	1 (2%)	0	100	100
19	z1	59/61 (97%)	59 (100%)	0	0	100	100
20	N	220/222 (99%)	204 (93%)	15 (7%)	1 (0%)	24	60
20	N1	220/222 (99%)	201 (91%)	18 (8%)	1 (0%)	24	60
20	n	220/222 (99%)	201 (91%)	17 (8%)	2 (1%)	14	48
20	n1	218/222 (98%)	198 (91%)	19 (9%)	1 (0%)	24	60
21	G	219/221 (99%)	203 (93%)	15 (7%)	1 (0%)	24	60
21	G1	219/221 (99%)	201 (92%)	18 (8%)	0	100	100
21	g	219/221 (99%)	209 (95%)	9 (4%)	1 (0%)	24	60
21	g1	219/221 (99%)	202 (92%)	17 (8%)	0	100	100
22	R	198/202 (98%)	188 (95%)	10 (5%)	0	100	100
22	r	198/202 (98%)	181 (91%)	17 (9%)	0	100	100
23	S	240/243 (99%)	218 (91%)	20 (8%)	2 (1%)	16	52
23	S1	241/243 (99%)	221 (92%)	17 (7%)	3 (1%)	10	42
23	s	239/243 (98%)	219 (92%)	18 (8%)	2 (1%)	16	52
23	s1	241/243 (99%)	219 (91%)	20 (8%)	2 (1%)	16	52
24	Y	220/222 (99%)	208 (94%)	11 (5%)	1 (0%)	24	60
24	Y1	220/222 (99%)	205 (93%)	14 (6%)	1 (0%)	24	60
24	y	220/222 (99%)	209 (95%)	10 (4%)	1 (0%)	24	60
24	y1	220/222 (99%)	208 (94%)	11 (5%)	1 (0%)	24	60
25	U	25/27 (93%)	25 (100%)	0	0	100	100
25	U1	25/27 (93%)	25 (100%)	0	0	100	100
25	u	25/27 (93%)	25 (100%)	0	0	100	100
25	u1	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
26	M1	29/31 (94%)	29 (100%)	0	0	100	100
26	m1	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
27	R1	191/202 (95%)	183 (96%)	8 (4%)	0	100	100
27	r1	191/202 (95%)	181 (95%)	10 (5%)	0	100	100
All	All	14651/14872 (98%)	13772 (94%)	839 (6%)	40 (0%)	37	70

All (40) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
4	C	257	GLU
4	C	395	VAL
14	O	94	VAL
4	c	257	GLU
4	c	395	VAL
5	d	60	THR
16	t	29	ILE
23	s	92	LYS
14	O1	205	TYR
14	o1	205	TYR
23	s1	284	ASP
5	D	60	THR
15	P	126	SER
16	T	29	ILE
20	N	145	ILE
4	c	173	VAL
14	o	205	TYR
20	n	145	ILE
24	y	146	ILE
4	C	173	VAL
23	S	92	LYS
24	Y	146	ILE
24	Y1	146	ILE
20	n1	145	ILE
23	s1	92	LYS
24	y1	146	ILE
13	M	3	VAL
21	G	137	ILE
13	m	3	VAL
21	g	137	ILE
20	N1	145	ILE
2	B	401	PHE
1	A	298	ASN
23	s	284	ASP
23	S1	92	LYS
23	S1	284	ASP
23	S	158	VAL
20	n	183	PRO
16	T1	29	ILE
23	S1	158	VAL

5.3.2 Protein sidechains (i)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	276/275 (100%)	276 (100%)	0	100	100
1	A1	276/275 (100%)	276 (100%)	0	100	100
1	a	276/275 (100%)	276 (100%)	0	100	100
1	a1	276/275 (100%)	276 (100%)	0	100	100
2	B	388/388 (100%)	388 (100%)	0	100	100
2	B1	388/388 (100%)	388 (100%)	0	100	100
2	b	388/388 (100%)	388 (100%)	0	100	100
2	b1	388/388 (100%)	388 (100%)	0	100	100
3	V	25/25 (100%)	25 (100%)	0	100	100
3	V1	25/25 (100%)	25 (100%)	0	100	100
3	v	25/25 (100%)	25 (100%)	0	100	100
3	v1	25/25 (100%)	25 (100%)	0	100	100
4	C	350/350 (100%)	350 (100%)	0	100	100
4	C1	350/350 (100%)	350 (100%)	0	100	100
4	c	350/350 (100%)	350 (100%)	0	100	100
4	c1	350/350 (100%)	350 (100%)	0	100	100
5	D	279/279 (100%)	279 (100%)	0	100	100
5	D1	279/279 (100%)	279 (100%)	0	100	100
5	d	279/279 (100%)	279 (100%)	0	100	100
5	d1	279/279 (100%)	279 (100%)	0	100	100
6	E	68/68 (100%)	68 (100%)	0	100	100
6	E1	68/68 (100%)	68 (100%)	0	100	100
6	e	68/68 (100%)	68 (100%)	0	100	100
6	e1	68/68 (100%)	68 (100%)	0	100	100
7	F	25/25 (100%)	25 (100%)	0	100	100
7	F1	25/25 (100%)	25 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
7	f	25/25 (100%)	25 (100%)	0	100	100
7	f1	25/25 (100%)	25 (100%)	0	100	100
8	H	56/56 (100%)	56 (100%)	0	100	100
8	H1	56/56 (100%)	56 (100%)	0	100	100
8	h	56/56 (100%)	56 (100%)	0	100	100
8	h1	56/56 (100%)	56 (100%)	0	100	100
9	I	31/31 (100%)	31 (100%)	0	100	100
9	I1	31/31 (100%)	31 (100%)	0	100	100
9	i	31/31 (100%)	31 (100%)	0	100	100
9	i1	31/31 (100%)	31 (100%)	0	100	100
10	J	27/27 (100%)	27 (100%)	0	100	100
10	J1	27/27 (100%)	27 (100%)	0	100	100
10	j	27/27 (100%)	27 (100%)	0	100	100
10	j1	27/27 (100%)	27 (100%)	0	100	100
11	K	33/33 (100%)	33 (100%)	0	100	100
11	K1	33/33 (100%)	33 (100%)	0	100	100
11	k	33/33 (100%)	33 (100%)	0	100	100
11	k1	33/33 (100%)	33 (100%)	0	100	100
12	L	35/35 (100%)	35 (100%)	0	100	100
12	L1	35/35 (100%)	35 (100%)	0	100	100
12	l	35/35 (100%)	35 (100%)	0	100	100
13	M	27/27 (100%)	27 (100%)	0	100	100
13	m	27/27 (100%)	27 (100%)	0	100	100
14	O	195/195 (100%)	195 (100%)	0	100	100
14	O1	195/195 (100%)	195 (100%)	0	100	100
14	o	195/195 (100%)	195 (100%)	0	100	100
14	o1	195/195 (100%)	195 (100%)	0	100	100
15	P	151/151 (100%)	151 (100%)	0	100	100
15	P1	151/151 (100%)	151 (100%)	0	100	100
15	p	151/151 (100%)	151 (100%)	0	100	100
15	p1	151/151 (100%)	151 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
16	T	26/26 (100%)	26 (100%)	0	100	100
16	T1	26/26 (100%)	26 (100%)	0	100	100
16	t	26/26 (100%)	26 (100%)	0	100	100
16	t1	26/26 (100%)	26 (100%)	0	100	100
17	W	34/34 (100%)	34 (100%)	0	100	100
17	W1	34/34 (100%)	34 (100%)	0	100	100
17	w	34/34 (100%)	34 (100%)	0	100	100
17	w1	34/34 (100%)	34 (100%)	0	100	100
18	X	21/21 (100%)	21 (100%)	0	100	100
18	X1	21/21 (100%)	21 (100%)	0	100	100
18	x	21/21 (100%)	21 (100%)	0	100	100
18	x1	21/21 (100%)	21 (100%)	0	100	100
19	Z	50/50 (100%)	50 (100%)	0	100	100
19	Z1	50/50 (100%)	50 (100%)	0	100	100
19	z	50/50 (100%)	50 (100%)	0	100	100
19	z1	50/50 (100%)	50 (100%)	0	100	100
20	N	171/171 (100%)	171 (100%)	0	100	100
20	N1	171/171 (100%)	171 (100%)	0	100	100
20	n	171/171 (100%)	171 (100%)	0	100	100
20	n1	171/171 (100%)	171 (100%)	0	100	100
21	G	168/168 (100%)	168 (100%)	0	100	100
21	G1	168/168 (100%)	168 (100%)	0	100	100
21	g	168/168 (100%)	168 (100%)	0	100	100
21	g1	168/168 (100%)	168 (100%)	0	100	100
22	R	158/158 (100%)	158 (100%)	0	100	100
22	r	158/158 (100%)	158 (100%)	0	100	100
23	S	189/190 (100%)	189 (100%)	0	100	100
23	S1	190/190 (100%)	190 (100%)	0	100	100
23	s	190/190 (100%)	190 (100%)	0	100	100
23	s1	190/190 (100%)	190 (100%)	0	100	100
24	Y	167/167 (100%)	167 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
24	Y1	167/167 (100%)	167 (100%)	0	100	100
24	y	167/167 (100%)	167 (100%)	0	100	100
24	y1	167/167 (100%)	167 (100%)	0	100	100
25	U	26/26 (100%)	26 (100%)	0	100	100
25	U1	26/26 (100%)	26 (100%)	0	100	100
25	u	26/26 (100%)	26 (100%)	0	100	100
25	u1	26/26 (100%)	25 (96%)	1 (4%)	29	51
26	M1	26/26 (100%)	26 (100%)	0	100	100
26	m1	26/26 (100%)	26 (100%)	0	100	100
27	R1	151/157 (96%)	151 (100%)	0	100	100
27	r1	151/157 (96%)	151 (100%)	0	100	100
All	All	11856/11865 (100%)	11855 (100%)	1 (0%)	100	100

All (1) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
25	u1	89	GLN

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (133) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	10	ASN
1	A	165	GLN
1	A	230	ASN
1	A	252	HIS
1	A	267	ASN
1	A	301	ASN
1	A	322	ASN
2	B	73	GLN
2	B	318	ASN
2	B	407	ASN
4	C	143	ASN
4	C	147	ASN
4	C	310	GLN
4	C	315	ASN
4	C	403	ASN
5	D	230	ASN

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Mol	Chain	Res	Type
6	E	75	GLN
9	I	26	ASN
12	L	7	ASN
14	O	68	GLN
14	O	82	ASN
14	O	93	ASN
19	Z	31	ASN
20	N	39	GLN
20	N	209	ASN
20	N	223	GLN
20	N	234	ASN
21	G	129	ASN
21	G	228	ASN
22	R	99	ASN
22	R	178	GLN
22	R	256	GLN
23	S	127	ASN
24	Y	113	ASN
24	Y	158	GLN
1	a	92	HIS
1	a	108	ASN
1	a	298	ASN
1	a	303	ASN
1	a	332	HIS
2	b	317	ASN
2	b	394	GLN
2	b	425	GLN
4	c	16	GLN
4	c	56	ASN
4	c	225	HIS
4	c	282	ASN
5	d	189	HIS
5	d	220	ASN
5	d	230	ASN
5	d	236	ASN
5	d	255	GLN
8	h	34	ASN
8	h	79	ASN
9	i	31	ASN
11	k	40	GLN
14	o	238	GLN
15	p	115	ASN

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Mol	Chain	Res	Type
15	p	148	GLN
15	p	197	ASN
19	z	31	ASN
20	n	46	ASN
20	n	146	HIS
20	n	170	ASN
21	g	133	ASN
23	s	107	HIS
23	s	281	GLN
1	A1	10	ASN
1	A1	234	ASN
1	A1	247	ASN
1	A1	301	ASN
1	A1	338	ASN
2	B1	343	HIS
2	B1	349	GLN
4	C1	27	ASN
4	C1	315	ASN
5	D1	137	ASN
5	D1	164	GLN
5	D1	186	GLN
5	D1	322	ASN
5	D1	336	HIS
5	D1	350	ASN
12	L1	7	ASN
12	L1	9	GLN
14	O1	144	ASN
15	P1	109	ASN
15	P1	129	GLN
15	P1	153	GLN
17	W1	66	ASN
21	G1	73	GLN
21	G1	129	ASN
23	S1	263	ASN
24	Y1	138	ASN
24	Y1	144	ASN
24	Y1	149	GLN
24	Y1	158	GLN
24	Y1	248	ASN
1	a1	26	ASN
1	a1	92	HIS
1	a1	187	GLN

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Mol	Chain	Res	Type
1	a1	322	ASN
2	b1	73	GLN
2	b1	157	HIS
2	b1	274	GLN
2	b1	277	GLN
2	b1	290	GLN
3	v1	8	GLN
4	c1	16	GLN
4	c1	56	ASN
4	c1	143	ASN
4	c1	152	HIS
4	c1	406	ASN
4	c1	429	HIS
5	d1	194	ASN
5	d1	230	ASN
5	d1	239	GLN
5	d1	292	ASN
5	d1	336	HIS
7	f1	40	GLN
14	o1	150	ASN
14	o1	242	ASN
15	p1	163	ASN
15	p1	203	GLN
20	n1	39	GLN
21	g1	73	GLN
21	g1	129	ASN
21	g1	217	GLN
21	g1	228	ASN
21	g1	239	ASN
23	s1	96	GLN
23	s1	161	ASN
23	s1	263	ASN
24	y1	149	GLN

5.3.3 RNA

There are no RNA molecules in this entry.

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

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	$\#\|Z\| > 2$
27	SEP	R1	84	27	8,9,10	1.62	1 (12%)	7,12,14	1.53	1 (14%)
27	SEP	r1	84	27	8,9,10	1.62	1 (12%)	7,12,14	1.09	0

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
27	SEP	R1	84	27	-	3/6/8/10	-
27	SEP	r1	84	27	-	3/6/8/10	-

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	r1	84	SEP	P-O1P	3.55	1.61	1.50
27	R1	84	SEP	P-O1P	3.52	1.61	1.50

All (1) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
27	R1	84	SEP	OG-CB-CA	3.54	111.59	108.14

There are no chirality outliers.

All (6) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
27	R1	84	SEP	CB-OG-P-O1P
27	R1	84	SEP	CB-OG-P-O2P
27	R1	84	SEP	CB-OG-P-O3P
27	r1	84	SEP	CB-OG-P-O2P
27	r1	84	SEP	CB-OG-P-O1P
27	r1	84	SEP	CB-OG-P-O3P

There are no ring outliers.

1 monomer is involved in 1 short contact:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
27	r1	84	SEP	1	0

5.5 Carbohydrates (i)

There are no oligosaccharides in this entry.

5.6 Ligand geometry (i)

Of 703 ligands modelled in this entry, 16 are monoatomic - leaving 687 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	$\#\|Z\| > 2$
48	LUT	s	620	-	42,43,43	2.49	1 (2%)	51,60,60	2.27	19 (37%)
31	CLA	c	508	-	69,73,73	1.36	7 (10%)	82,113,113	1.89	15 (18%)
31	CLA	g	613	-	69,73,73	1.37	8 (11%)	82,113,113	1.91	19 (23%)
47	CHL	g1	607	-	60,74,74	1.21	8 (13%)	58,114,114	1.77	12 (20%)
33	BCR	C1	514	-	41,41,41	1.62	4 (9%)	56,56,56	4.61	16 (28%)
47	CHL	s1	601	23	40,54,74	1.62	7 (17%)	34,90,114	2.28	10 (29%)
31	CLA	c	507	-	69,73,73	1.37	7 (10%)	82,113,113	1.93	19 (23%)
47	CHL	n1	609	-	60,74,74	1.25	8 (13%)	58,114,114	1.64	10 (17%)
31	CLA	D1	403	-	69,73,73	1.36	7 (10%)	82,113,113	1.91	18 (21%)
52	3PH	t1	101	-	47,47,47	0.88	4 (8%)	50,52,52	1.14	2 (4%)
31	CLA	A	406	-	69,73,73	1.35	6 (8%)	82,113,113	1.94	14 (17%)
33	BCR	D1	404	-	41,41,41	1.59	4 (9%)	56,56,56	4.34	13 (23%)
35	LMG	A	413	-	48,48,55	1.12	5 (10%)	56,56,63	1.15	3 (5%)
31	CLA	Y	612	-	69,73,73	1.37	8 (11%)	82,113,113	1.90	19 (23%)
47	CHL	G	605	21	42,56,74	1.48	7 (16%)	36,92,114	2.10	11 (30%)
48	LUT	s	621	-	42,43,43	2.43	1 (2%)	51,60,60	1.82	14 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	y1	612	-	69,73,73	1.36	8 (11%)	82,113,113	1.88	17 (20%)
48	LUT	N	621	-	42,43,43	2.46	1 (2%)	51,60,60	1.95	12 (23%)
48	LUT	r1	620	-	42,43,43	2.47	1 (2%)	51,60,60	2.12	15 (29%)
31	CLA	R	613	-	50,54,73	1.58	7 (14%)	59,90,113	2.12	17 (28%)
35	LMG	h	102	-	48,48,55	1.13	5 (10%)	56,56,63	1.11	3 (5%)
35	LMG	C1	521	-	51,51,55	1.20	6 (11%)	59,59,63	1.12	4 (6%)
32	PHO	A	408	-	58,69,69	2.13	10 (17%)	55,99,99	1.50	7 (12%)
33	BCR	c	517	-	41,41,41	1.64	4 (9%)	56,56,56	4.50	14 (25%)
31	CLA	R1	610	-	64,68,73	1.39	7 (10%)	76,107,113	1.91	19 (25%)
31	CLA	c1	511	-	69,73,73	1.36	7 (10%)	82,113,113	2.03	23 (28%)
31	CLA	a1	405	-	69,73,73	1.35	6 (8%)	82,113,113	1.97	22 (26%)
31	CLA	C	509	-	69,73,73	1.36	7 (10%)	82,113,113	1.88	16 (19%)
31	CLA	Y1	610	-	69,73,73	1.33	6 (8%)	82,113,113	1.96	18 (21%)
45	HEM	F1	101	6	50,50,50	1.42	7 (14%)	67,82,82	1.04	1 (1%)
41	LHG	D	408	-	43,43,48	0.42	0	46,49,54	1.08	3 (6%)
47	CHL	y	601	24	60,74,74	1.30	9 (15%)	58,114,114	1.66	13 (22%)
47	CHL	y1	606	-	60,74,74	1.38	8 (13%)	58,114,114	1.63	12 (20%)
31	CLA	r	608	-	64,68,73	1.41	7 (10%)	76,107,113	1.95	16 (21%)
50	NEX	y	623	-	40,46,46	2.62	10 (25%)	50,70,70	1.89	14 (28%)
35	LMG	b	622	-	44,44,55	0.98	3 (6%)	52,52,63	1.12	3 (5%)
31	CLA	b	605	-	69,73,73	1.36	6 (8%)	82,113,113	2.01	17 (20%)
31	CLA	c	510	-	69,73,73	1.36	8 (11%)	82,113,113	1.93	18 (21%)
47	CHL	R1	607	-	44,58,74	1.54	8 (18%)	37,94,114	2.10	12 (32%)
31	CLA	y1	613	-	69,73,73	1.33	6 (8%)	82,113,113	1.89	18 (21%)
31	CLA	b1	616	-	69,73,73	1.37	7 (10%)	82,113,113	1.83	16 (19%)
31	CLA	G1	602	-	69,73,73	1.36	7 (10%)	82,113,113	1.92	18 (21%)
38	DGA	B	625	-	43,43,43	1.16	2 (4%)	45,45,45	1.50	3 (6%)
31	CLA	b1	606	-	69,73,73	1.37	7 (10%)	82,113,113	1.86	17 (20%)
44	PL9	D1	405	-	55,55,55	1.01	5 (9%)	68,69,69	1.59	11 (16%)
31	CLA	r	604	-	53,57,73	1.53	8 (15%)	61,93,113	2.15	17 (27%)
46	RRX	H1	101	-	42,42,42	4.97	24 (57%)	56,58,58	2.72	19 (33%)
31	CLA	b	608	-	69,73,73	1.36	6 (8%)	82,113,113	1.90	17 (20%)
55	LMT	R1	625	-	36,36,36	1.14	5 (13%)	47,47,47	1.01	2 (4%)
39	GOL	b	625	-	5,5,5	0.59	0	5,5,5	0.34	0
31	CLA	g1	603	-	69,73,73	1.35	8 (11%)	82,113,113	1.92	21 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	s	604	-	59,63,73	1.45	6 (10%)	70,101,113	2.04	19 (27%)
34	SQD	A1	412	-	49,51,54	0.81	1 (2%)	59,62,65	0.86	2 (3%)
31	CLA	y	611	-	69,73,73	1.35	7 (10%)	82,113,113	1.87	18 (21%)
31	CLA	b1	610	-	69,73,73	1.36	7 (10%)	82,113,113	1.89	14 (17%)
31	CLA	B1	605	-	69,73,73	1.33	6 (8%)	82,113,113	1.99	21 (25%)
31	CLA	n1	613	-	69,73,73	1.36	7 (10%)	82,113,113	2.00	21 (25%)
31	CLA	b1	602	-	69,73,73	1.36	6 (8%)	82,113,113	1.89	17 (20%)
31	CLA	S	614	-	59,63,73	1.47	6 (10%)	70,101,113	1.96	16 (22%)
40	DGD	C	518	-	56,56,67	1.07	4 (7%)	70,70,81	1.02	3 (4%)
31	CLA	S1	605	-	54,58,73	1.55	7 (12%)	64,95,113	2.16	19 (29%)
47	CHL	Y1	606	-	60,74,74	1.50	7 (11%)	58,114,114	1.75	12 (20%)
31	CLA	g1	611	-	69,73,73	1.35	6 (8%)	82,113,113	1.88	18 (21%)
50	NEX	g1	623	-	40,46,46	2.71	11 (27%)	50,70,70	2.30	13 (26%)
31	CLA	B	617	-	69,73,73	1.37	6 (8%)	82,113,113	4.00	18 (21%)
31	CLA	R1	608	-	64,68,73	1.42	8 (12%)	76,107,113	1.92	19 (25%)
31	CLA	B1	603	-	69,73,73	1.35	6 (8%)	82,113,113	1.90	21 (25%)
31	CLA	Y1	608	-	54,58,73	1.55	8 (14%)	64,95,113	2.11	17 (26%)
34	SQD	A	412	-	49,51,54	0.80	0	59,62,65	0.86	2 (3%)
31	CLA	S1	603	-	69,73,73	1.36	6 (8%)	82,113,113	2.00	21 (25%)
56	ERG	r1	626	-	32,32,32	7.98	20 (62%)	45,50,50	3.30	16 (35%)
48	LUT	n1	620	-	42,43,43	2.53	1 (2%)	51,60,60	1.70	12 (23%)
31	CLA	R1	604	-	53,57,73	1.53	7 (13%)	61,93,113	2.23	15 (24%)
33	BCR	a	411	-	41,41,41	1.63	5 (12%)	56,56,56	4.50	14 (25%)
35	LMG	B	622	-	44,44,55	0.96	3 (6%)	52,52,63	1.03	2 (3%)
31	CLA	A	407	-	53,57,73	1.55	7 (13%)	61,93,113	2.13	16 (26%)
31	CLA	b1	615	-	69,73,73	1.37	6 (8%)	82,113,113	1.86	18 (21%)
47	CHL	Y1	601	24	60,74,74	1.37	9 (15%)	58,114,114	1.90	12 (20%)
40	DGD	C	520	-	60,60,67	1.17	6 (10%)	74,74,81	1.00	2 (2%)
31	CLA	B1	614	-	69,73,73	1.35	6 (8%)	82,113,113	1.82	18 (21%)
41	LHG	G	630	-	48,48,48	0.39	0	51,54,54	1.07	3 (5%)
31	CLA	b	602	-	69,73,73	1.36	7 (10%)	82,113,113	1.92	19 (23%)
31	CLA	b	615	-	69,73,73	1.37	8 (11%)	82,113,113	2.06	19 (23%)
31	CLA	Y	613	-	69,73,73	1.36	7 (10%)	82,113,113	1.92	18 (21%)
31	CLA	b1	612	-	69,73,73	1.36	6 (8%)	82,113,113	1.91	16 (19%)
48	LUT	n1	621	-	42,43,43	2.50	1 (2%)	51,60,60	2.05	14 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
47	CHL	n1	606	-	60,74,74	1.15	7 (11%)	58,114,114	1.77	11 (18%)
38	DGA	b1	625	-	43,43,43	1.16	3 (6%)	45,45,45	1.47	3 (6%)
31	CLA	s1	603	-	69,73,73	1.36	8 (11%)	82,113,113	2.00	18 (21%)
31	CLA	b	613	-	69,73,73	1.38	6 (8%)	82,113,113	1.80	13 (15%)
33	BCR	d1	404	-	41,41,41	1.62	5 (12%)	56,56,56	4.37	16 (28%)
31	CLA	g	603	-	69,73,73	1.36	7 (10%)	82,113,113	1.96	18 (21%)
41	LHG	n1	624	-	48,48,48	0.39	0	51,54,54	1.09	3 (5%)
31	CLA	A1	406	-	69,73,73	1.36	7 (10%)	82,113,113	1.91	18 (21%)
33	BCR	b1	619	-	41,41,41	1.61	4 (9%)	56,56,56	4.54	13 (23%)
44	PL9	d1	405	-	55,55,55	1.01	2 (3%)	68,69,69	1.54	12 (17%)
31	CLA	G1	614	-	53,57,73	1.55	7 (13%)	61,93,113	2.17	16 (26%)
55	LMT	r1	625	-	36,36,36	1.15	6 (16%)	47,47,47	1.00	2 (4%)
47	CHL	y1	601	24	60,74,74	1.43	9 (15%)	58,114,114	1.90	11 (18%)
31	CLA	b	606	-	69,73,73	1.34	7 (10%)	82,113,113	1.96	13 (15%)
35	LMG	c1	523	-	55,55,55	1.28	6 (10%)	63,63,63	1.03	2 (3%)
31	CLA	C1	504	-	69,73,73	1.34	6 (8%)	82,113,113	1.95	16 (19%)
31	CLA	r1	612	-	64,68,73	1.43	8 (12%)	76,107,113	1.92	20 (26%)
49	XAT	G	622	-	41,47,47	0.71	1 (2%)	54,74,74	1.91	14 (25%)
42	LMK	C	527	-	39,39,53	1.55	3 (7%)	39,46,60	1.30	2 (5%)
41	LHG	d	410	-	38,38,48	0.43	0	41,44,54	1.19	3 (7%)
31	CLA	B	609	-	69,73,73	1.39	7 (10%)	82,113,113	1.97	20 (24%)
31	CLA	C	506	-	69,73,73	1.37	7 (10%)	82,113,113	1.91	19 (23%)
31	CLA	b	610	-	69,73,73	1.36	7 (10%)	82,113,113	1.84	15 (18%)
31	CLA	g	604	-	53,57,73	1.57	8 (15%)	61,93,113	2.17	18 (29%)
47	CHL	y1	607	-	60,74,74	1.07	7 (11%)	58,114,114	1.90	12 (20%)
54	4RF	i1	101	-	56,56,56	1.06	3 (5%)	59,59,59	0.93	3 (5%)
31	CLA	b	612	-	69,73,73	1.37	7 (10%)	82,113,113	1.86	18 (21%)
31	CLA	B1	606	-	69,73,73	1.36	7 (10%)	82,113,113	1.98	17 (20%)
31	CLA	B1	608	-	69,73,73	1.37	6 (8%)	82,113,113	1.92	17 (20%)
31	CLA	C	510	-	69,73,73	1.36	7 (10%)	82,113,113	1.89	19 (23%)
47	CHL	r1	606	-	38,52,74	1.82	8 (21%)	31,87,114	2.26	10 (32%)
48	LUT	g1	621	-	42,43,43	2.49	1 (2%)	51,60,60	1.77	11 (21%)
31	CLA	Y1	613	-	69,73,73	1.35	7 (10%)	82,113,113	1.97	17 (20%)
31	CLA	r1	609	-	64,68,73	1.41	6 (9%)	76,107,113	1.96	16 (21%)
31	CLA	B	607	-	69,73,73	1.37	8 (11%)	82,113,113	1.86	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
40	DGD	C	519	-	63,63,67	1.23	7 (11%)	77,77,81	1.10	5 (6%)
31	CLA	n	602	-	69,73,73	1.36	7 (10%)	82,113,113	1.93	21 (25%)
41	LHG	D1	409	-	48,48,48	0.39	0	51,54,54	1.11	5 (9%)
47	CHL	N1	605	20	60,74,74	1.44	8 (13%)	58,114,114	1.64	12 (20%)
31	CLA	b	614	-	69,73,73	1.34	6 (8%)	82,113,113	1.83	18 (21%)
52	3PH	S1	626	-	47,47,47	0.87	4 (8%)	50,52,52	4.53	4 (8%)
31	CLA	c	504	-	69,73,73	1.34	6 (8%)	82,113,113	2.02	20 (24%)
31	CLA	S1	610	-	69,73,73	1.38	7 (10%)	82,113,113	1.90	21 (25%)
41	LHG	d1	409	-	48,48,48	0.41	0	51,54,54	1.00	2 (3%)
45	HEM	f	101	6,7	50,50,50	1.44	6 (12%)	67,82,82	1.33	10 (14%)
47	CHL	g1	608	-	38,52,74	1.68	8 (21%)	31,87,114	2.24	11 (35%)
31	CLA	s	603	-	69,73,73	1.37	8 (11%)	82,113,113	1.82	17 (20%)
31	CLA	Y1	602	-	69,73,73	1.37	7 (10%)	82,113,113	1.85	19 (23%)
45	HEM	F	101	6,7	50,50,50	1.40	6 (12%)	67,82,82	1.30	8 (11%)
47	CHL	s	608	-	55,69,74	1.33	8 (14%)	52,108,114	1.74	13 (25%)
49	XAT	r	622	-	41,47,47	0.70	1 (2%)	54,74,74	2.12	18 (33%)
31	CLA	G	612	-	47,51,73	1.65	7 (14%)	55,86,113	2.13	14 (25%)
50	NEX	R1	622	-	40,46,46	2.67	11 (27%)	50,70,70	1.83	11 (22%)
47	CHL	g1	609	-	60,74,74	1.42	10 (16%)	58,114,114	1.56	12 (20%)
49	XAT	G1	622	-	41,47,47	0.73	1 (2%)	54,74,74	1.88	14 (25%)
31	CLA	s1	611	-	69,73,73	1.38	7 (10%)	82,113,113	1.90	20 (24%)
31	CLA	c1	507	-	69,73,73	1.38	8 (11%)	82,113,113	1.83	18 (21%)
47	CHL	G1	601	21	60,74,74	1.25	8 (13%)	58,114,114	1.70	12 (20%)
54	4RF	I1	102	-	56,56,56	1.08	3 (5%)	59,59,59	0.97	3 (5%)
31	CLA	C1	506	-	69,73,73	1.36	6 (8%)	82,113,113	1.87	19 (23%)
31	CLA	G	602	-	69,73,73	1.35	6 (8%)	82,113,113	1.90	21 (25%)
31	CLA	a1	407	-	53,57,73	1.53	6 (11%)	61,93,113	2.22	20 (32%)
41	LHG	n	624	-	48,48,48	0.39	0	51,54,54	1.06	3 (5%)
32	PHO	a1	408	-	58,69,69	2.21	10 (17%)	55,99,99	1.50	8 (14%)
49	XAT	g1	622	-	41,47,47	0.74	1 (2%)	54,74,74	1.85	13 (24%)
31	CLA	y	612	-	69,73,73	1.37	6 (8%)	82,113,113	1.89	14 (17%)
31	CLA	B1	616	-	69,73,73	1.35	6 (8%)	82,113,113	1.85	17 (20%)
41	LHG	D1	408	-	43,43,48	0.41	0	46,49,54	1.09	4 (8%)
31	CLA	n	612	-	49,53,73	1.61	6 (12%)	58,89,113	1.98	18 (31%)
50	NEX	Y	623	-	40,46,46	2.63	11 (27%)	50,70,70	2.03	14 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
50	NEX	G1	623	-	40,46,46	2.69	11 (27%)	50,70,70	1.84	12 (24%)
35	LMG	W1	201	-	39,39,55	0.95	2 (5%)	47,47,63	1.22	2 (4%)
48	LUT	S1	621	-	42,43,43	2.46	1 (2%)	51,60,60	1.93	13 (25%)
31	CLA	N1	611	-	53,57,73	1.55	6 (11%)	61,93,113	2.11	16 (26%)
39	GOL	I1	101	-	5,5,5	0.57	0	5,5,5	0.28	0
50	NEX	s1	623	-	40,46,46	2.78	14 (35%)	50,70,70	1.86	10 (20%)
31	CLA	D1	402	-	69,73,73	1.38	6 (8%)	82,113,113	1.83	17 (20%)
47	CHL	Y1	609	-	60,74,74	1.34	8 (13%)	58,114,114	1.62	12 (20%)
34	SQD	b1	626	-	52,54,54	0.79	0	62,65,65	0.84	2 (3%)
31	CLA	c1	512	-	69,73,73	1.38	6 (8%)	82,113,113	1.88	17 (20%)
31	CLA	C1	509	-	69,73,73	1.33	6 (8%)	82,113,113	1.89	16 (19%)
47	CHL	S	607	-	37,51,74	1.57	8 (21%)	30,86,114	2.34	11 (36%)
33	BCR	B1	619	-	41,41,41	1.63	4 (9%)	56,56,56	4.58	14 (25%)
31	CLA	c	512	-	69,73,73	1.37	7 (10%)	82,113,113	1.82	19 (23%)
31	CLA	y	602	-	69,73,73	1.33	7 (10%)	82,113,113	2.02	20 (24%)
51	LPX	s	625	-	29,29,29	1.04	2 (6%)	31,33,33	0.97	1 (3%)
47	CHL	R	606	-	38,52,74	1.76	9 (23%)	31,87,114	2.22	9 (29%)
31	CLA	r	612	-	64,68,73	1.42	8 (12%)	76,107,113	1.89	18 (23%)
47	CHL	G1	606	-	44,58,74	1.51	8 (18%)	37,94,114	2.19	11 (29%)
41	LHG	G1	624	-	48,48,48	0.40	0	51,54,54	0.99	3 (5%)
31	CLA	b	607	-	69,73,73	1.37	7 (10%)	82,113,113	2.02	20 (24%)
31	CLA	Y	603	-	69,73,73	1.34	7 (10%)	82,113,113	1.95	22 (26%)
31	CLA	y	613	-	69,73,73	1.35	7 (10%)	82,113,113	1.92	17 (20%)
31	CLA	n	604	-	69,73,73	1.34	6 (8%)	82,113,113	2.00	19 (23%)
31	CLA	y1	603	-	69,73,73	1.35	6 (8%)	82,113,113	1.95	21 (25%)
57	PTY	Y1	627	-	18,18,49	1.32	3 (16%)	21,23,54	1.43	2 (9%)
37	C7Z	b	620	-	43,43,43	5.52	26 (60%)	56,60,60	2.19	15 (26%)
31	CLA	g	612	-	47,51,73	1.64	7 (14%)	55,86,113	2.16	17 (30%)
31	CLA	C1	501	-	69,73,73	1.36	8 (11%)	82,113,113	1.91	19 (23%)
47	CHL	S1	607	-	37,51,74	1.67	8 (21%)	30,86,114	2.20	10 (33%)
31	CLA	G1	604	-	53,57,73	1.56	8 (15%)	61,93,113	2.10	20 (32%)
47	CHL	g	609	-	60,74,74	1.48	10 (16%)	58,114,114	1.61	10 (17%)
47	CHL	s	601	23	40,54,74	1.69	8 (20%)	34,90,114	2.17	10 (29%)
31	CLA	S1	617	23	54,58,73	1.53	7 (12%)	64,95,113	2.13	19 (29%)
43	BCT	d	401	29	3,3,3	1.12	0	2,3,3	4.18	2 (100%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	r	613	-	50,54,73	1.59	6 (12%)	59,90,113	2.12	15 (25%)
47	CHL	s	606	-	38,52,74	1.66	8 (21%)	31,87,114	2.16	10 (32%)
31	CLA	c	502	-	69,73,73	1.36	7 (10%)	82,113,113	1.93	18 (21%)
31	CLA	Y	610	-	69,73,73	1.35	7 (10%)	82,113,113	1.94	20 (24%)
33	BCR	c1	517	-	41,41,41	1.64	4 (9%)	56,56,56	4.64	21 (37%)
31	CLA	c	505	-	69,73,73	1.37	7 (10%)	82,113,113	1.90	15 (18%)
31	CLA	B1	612	-	69,73,73	1.35	7 (10%)	82,113,113	1.85	17 (20%)
31	CLA	s1	610	-	69,73,73	1.36	6 (8%)	82,113,113	1.87	17 (20%)
31	CLA	N1	614	-	53,57,73	1.54	7 (13%)	61,93,113	2.23	20 (32%)
31	CLA	n1	603	-	69,73,73	1.35	7 (10%)	82,113,113	1.95	19 (23%)
31	CLA	g1	610	-	69,73,73	1.36	7 (10%)	82,113,113	1.89	20 (24%)
35	LMG	H	102	-	48,48,55	1.13	5 (10%)	56,56,63	1.09	2 (3%)
49	XAT	g	622	-	41,47,47	0.70	1 (2%)	54,74,74	1.96	13 (24%)
31	CLA	b	609	-	69,73,73	1.42	7 (10%)	82,113,113	1.98	19 (23%)
31	CLA	Y1	612	-	69,73,73	1.36	6 (8%)	82,113,113	1.89	21 (25%)
40	DGD	c	523	-	67,67,67	1.29	7 (10%)	81,81,81	0.96	2 (2%)
48	LUT	r	620	-	42,43,43	2.46	1 (2%)	51,60,60	2.08	10 (19%)
31	CLA	y	608	-	54,58,73	1.54	7 (12%)	64,95,113	2.11	18 (28%)
40	DGD	c	519	-	63,63,67	1.21	7 (11%)	77,77,81	1.05	3 (3%)
40	DGD	b1	623	-	44,44,67	0.88	2 (4%)	58,58,81	1.17	4 (6%)
47	CHL	G	607	-	44,58,74	1.38	7 (15%)	37,94,114	2.15	10 (27%)
35	LMG	D	411	-	46,46,55	1.02	4 (8%)	54,54,63	1.18	4 (7%)
48	LUT	S	620	-	42,43,43	2.48	1 (2%)	51,60,60	1.91	13 (25%)
31	CLA	b	604	-	69,73,73	1.37	7 (10%)	82,113,113	1.84	17 (20%)
31	CLA	c1	505	-	69,73,73	1.38	8 (11%)	82,113,113	1.86	16 (19%)
49	XAT	r1	621	-	41,47,47	0.69	1 (2%)	54,74,74	1.93	15 (27%)
47	CHL	N	608	-	44,58,74	1.49	7 (15%)	37,94,114	2.11	11 (29%)
31	CLA	y	614	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	18 (21%)
35	LMG	D1	411	-	46,46,55	1.04	4 (8%)	54,54,63	1.08	2 (3%)
47	CHL	y	606	-	60,74,74	1.43	8 (13%)	58,114,114	1.73	12 (20%)
31	CLA	b1	607	-	69,73,73	1.34	6 (8%)	82,113,113	1.88	19 (23%)
50	NEX	N	623	-	40,46,46	2.73	11 (27%)	50,70,70	2.07	13 (26%)
31	CLA	d1	402	-	69,73,73	1.38	8 (11%)	82,113,113	1.79	19 (23%)
34	SQD	a	412	-	49,51,54	0.80	0	59,62,65	0.85	2 (3%)
31	CLA	C	505	-	69,73,73	1.36	7 (10%)	82,113,113	1.90	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	R	611	-	50,54,73	1.60	8 (16%)	59,90,113	2.10	16 (27%)
31	CLA	S	617	-	54,58,73	1.54	8 (14%)	64,95,113	2.10	18 (28%)
48	LUT	S1	620	-	42,43,43	2.43	1 (2%)	51,60,60	2.01	10 (19%)
57	PTY	y1	626	-	49,49,49	0.90	4 (8%)	52,54,54	1.07	2 (3%)
31	CLA	c	509	-	69,73,73	1.39	6 (8%)	82,113,113	1.88	14 (17%)
31	CLA	y1	614	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	18 (21%)
31	CLA	c	503	-	69,73,73	1.37	7 (10%)	82,113,113	1.97	21 (25%)
42	LMK	C1	527	-	39,39,53	1.53	2 (5%)	39,46,60	1.46	2 (5%)
47	CHL	N	606	-	60,74,74	1.36	8 (13%)	58,114,114	1.74	13 (22%)
35	LMG	w1	201	-	39,39,55	0.95	2 (5%)	47,47,63	1.21	4 (8%)
45	HEM	f1	101	-	50,50,50	1.45	9 (18%)	67,82,82	1.10	2 (2%)
31	CLA	G	614	-	53,57,73	1.53	7 (13%)	61,93,113	2.17	18 (29%)
31	CLA	N1	602	-	69,73,73	1.32	7 (10%)	82,113,113	1.90	19 (23%)
31	CLA	N1	613	-	69,73,73	1.37	8 (11%)	82,113,113	1.87	17 (20%)
49	XAT	y1	622	-	41,47,47	0.71	1 (2%)	54,74,74	3.69	14 (25%)
54	4RF	K1	101	-	56,56,56	1.06	4 (7%)	59,59,59	0.86	3 (5%)
31	CLA	S	613	-	59,63,73	1.48	6 (10%)	70,101,113	2.23	19 (27%)
47	CHL	n1	608	-	44,58,74	1.38	7 (15%)	37,94,114	2.17	11 (29%)
50	NEX	S1	623	-	40,46,46	2.69	12 (30%)	50,70,70	1.83	12 (24%)
54	4RF	k1	101	-	56,56,56	1.06	3 (5%)	59,59,59	0.91	3 (5%)
57	PTY	Y1	626	-	49,49,49	0.89	4 (8%)	52,54,54	1.06	2 (3%)
47	CHL	S	601	-	40,54,74	1.74	9 (22%)	34,90,114	2.18	11 (32%)
31	CLA	s	617	-	54,58,73	1.52	8 (14%)	64,95,113	2.12	20 (31%)
34	SQD	c	626	-	52,54,54	0.78	0	62,65,65	0.83	2 (3%)
31	CLA	s	611	-	69,73,73	1.36	6 (8%)	82,113,113	1.92	19 (23%)
31	CLA	N1	610	-	69,73,73	1.36	7 (10%)	82,113,113	1.90	15 (18%)
47	CHL	r	607	-	44,58,74	1.58	8 (18%)	37,94,114	2.18	12 (32%)
31	CLA	B1	615	-	69,73,73	1.38	8 (11%)	82,113,113	1.88	16 (19%)
49	XAT	N1	622	-	41,47,47	0.67	1 (2%)	54,74,74	2.03	12 (22%)
41	LHG	C	525	-	46,46,48	0.39	0	49,52,54	1.08	3 (6%)
46	RRX	h1	101	-	42,42,42	5.04	24 (57%)	56,58,58	2.60	20 (35%)
48	LUT	R1	620	-	42,43,43	2.44	1 (2%)	51,60,60	2.22	14 (27%)
39	GOL	B	627	-	5,5,5	0.57	0	5,5,5	0.29	0
33	BCR	C	515	-	41,41,41	1.62	4 (9%)	56,56,56	4.45	14 (25%)
40	DGD	c1	518	-	56,56,67	1.08	4 (7%)	70,70,81	0.97	3 (4%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	B1	613	-	69,73,73	1.35	6 (8%)	82,113,113	1.86	16 (19%)
47	CHL	s1	607	-	37,51,74	1.67	7 (18%)	30,86,114	2.37	11 (36%)
31	CLA	B	605	-	69,73,73	1.35	7 (10%)	82,113,113	2.04	20 (24%)
31	CLA	y1	602	-	69,73,73	1.35	7 (10%)	82,113,113	1.90	18 (21%)
31	CLA	B	616	-	69,73,73	1.36	6 (8%)	82,113,113	1.89	22 (26%)
31	CLA	g1	612	-	47,51,73	1.63	6 (12%)	55,86,113	2.12	15 (27%)
33	BCR	A	411	-	41,41,41	1.61	4 (9%)	56,56,56	4.42	11 (19%)
48	LUT	S	621	-	42,43,43	2.44	1 (2%)	51,60,60	1.97	16 (31%)
31	CLA	r	609	-	64,68,73	1.40	6 (9%)	76,107,113	1.93	18 (23%)
35	LMG	H1	102	-	48,48,55	1.13	6 (12%)	56,56,63	1.10	2 (3%)
31	CLA	s1	614	-	59,63,73	1.47	6 (10%)	70,101,113	1.92	14 (20%)
41	LHG	Y	624	-	48,48,48	0.38	0	51,54,54	1.06	3 (5%)
41	LHG	S	624	-	44,44,48	0.42	0	47,50,54	1.15	3 (6%)
31	CLA	G1	613	-	69,73,73	1.35	6 (8%)	82,113,113	1.93	18 (21%)
31	CLA	s1	609	-	64,68,73	1.41	8 (12%)	76,107,113	1.97	19 (25%)
47	CHL	N	609	-	60,74,74	1.27	8 (13%)	58,114,114	1.69	11 (18%)
48	LUT	R	620	-	42,43,43	2.43	1 (2%)	51,60,60	2.15	12 (23%)
31	CLA	g	614	-	53,57,73	1.55	7 (13%)	61,93,113	2.17	17 (27%)
31	CLA	Y	602	24	69,73,73	1.37	7 (10%)	82,113,113	1.80	15 (18%)
31	CLA	B	608	-	69,73,73	1.36	7 (10%)	82,113,113	1.84	17 (20%)
31	CLA	s1	602	-	64,68,73	1.40	7 (10%)	76,107,113	1.91	21 (27%)
31	CLA	y1	610	-	69,73,73	1.35	6 (8%)	82,113,113	1.86	16 (19%)
49	XAT	n1	622	-	41,47,47	0.71	1 (2%)	54,74,74	1.89	13 (24%)
31	CLA	C	511	-	69,73,73	1.37	8 (11%)	82,113,113	1.95	18 (21%)
40	DGD	C1	518	-	56,56,67	1.06	4 (7%)	70,70,81	0.94	2 (2%)
31	CLA	s	614	-	59,63,73	1.45	6 (10%)	70,101,113	2.10	17 (24%)
31	CLA	a	410	-	64,68,73	1.41	7 (10%)	76,107,113	2.03	19 (25%)
31	CLA	Y	604	-	69,73,73	1.35	8 (11%)	82,113,113	1.95	19 (23%)
31	CLA	s1	604	-	59,63,73	1.47	8 (13%)	70,101,113	2.06	19 (27%)
47	CHL	n	605	-	60,74,74	1.46	9 (15%)	58,114,114	1.61	10 (17%)
41	LHG	d1	410	-	38,38,48	0.42	0	41,44,54	1.18	3 (7%)
47	CHL	N1	609	-	60,74,74	1.21	8 (13%)	58,114,114	1.80	11 (18%)
52	3PH	B1	624	-	47,47,47	0.87	4 (8%)	50,52,52	1.13	2 (4%)
33	BCR	B1	618	-	41,41,41	1.62	4 (9%)	56,56,56	4.67	17 (30%)
47	CHL	s	607	-	37,51,74	1.55	7 (18%)	30,86,114	2.27	10 (33%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
48	LUT	G1	620	-	42,43,43	2.44	1 (2%)	51,60,60	1.94	12 (23%)
31	CLA	a	406	-	69,73,73	1.36	6 (8%)	82,113,113	1.91	14 (17%)
51	LPX	S1	625	-	29,29,29	1.06	2 (6%)	31,33,33	0.97	1 (3%)
47	CHL	N	607	-	60,74,74	1.16	7 (11%)	58,114,114	1.84	13 (22%)
31	CLA	C	507	-	69,73,73	1.38	7 (10%)	82,113,113	1.84	18 (21%)
47	CHL	g	601	21	60,74,74	1.37	8 (13%)	58,114,114	1.67	12 (20%)
31	CLA	A1	410	-	64,68,73	1.40	7 (10%)	76,107,113	2.03	21 (27%)
31	CLA	R1	602	-	64,68,73	1.40	6 (9%)	76,107,113	2.04	21 (27%)
38	DGA	J1	101	-	28,28,43	1.32	3 (10%)	30,30,45	1.28	2 (6%)
31	CLA	r1	610	-	64,68,73	1.42	8 (12%)	76,107,113	1.89	21 (27%)
35	LMG	C	521	-	51,51,55	1.20	6 (11%)	59,59,63	1.09	4 (6%)
48	LUT	G1	621	-	42,43,43	2.46	1 (2%)	51,60,60	2.02	13 (25%)
31	CLA	S	605	-	54,58,73	1.53	6 (11%)	64,95,113	2.24	20 (31%)
47	CHL	g	607	-	44,58,74	1.34	7 (15%)	37,94,114	2.06	12 (32%)
31	CLA	s	605	-	54,58,73	1.56	8 (14%)	64,95,113	2.19	21 (32%)
34	SQD	B1	626	-	52,54,54	0.79	0	62,65,65	0.84	2 (3%)
47	CHL	r1	607	-	44,58,74	1.53	8 (18%)	37,94,114	2.15	12 (32%)
47	CHL	s1	608	-	55,69,74	1.45	8 (14%)	52,108,114	1.69	12 (23%)
31	CLA	n1	612	-	49,53,73	1.61	7 (14%)	58,89,113	2.02	16 (27%)
49	XAT	N	622	-	41,47,47	0.70	1 (2%)	54,74,74	1.90	12 (22%)
31	CLA	c	513	-	69,73,73	1.38	7 (10%)	82,113,113	1.87	17 (20%)
31	CLA	Y	614	-	69,73,73	1.36	6 (8%)	82,113,113	1.90	17 (20%)
35	LMG	d1	411	-	46,46,55	1.03	4 (8%)	54,54,63	1.18	2 (3%)
47	CHL	g	608	-	38,52,74	1.64	8 (21%)	31,87,114	2.27	11 (35%)
31	CLA	r	603	-	64,68,73	1.41	7 (10%)	76,107,113	1.92	16 (21%)
31	CLA	S	603	-	69,73,73	1.37	8 (11%)	82,113,113	1.83	16 (19%)
35	LMG	A1	413	-	48,48,55	1.13	5 (10%)	56,56,63	1.18	4 (7%)
31	CLA	B1	617	-	69,73,73	1.37	7 (10%)	82,113,113	1.84	20 (24%)
31	CLA	n1	614	-	53,57,73	1.55	7 (13%)	61,93,113	2.18	19 (31%)
47	CHL	g1	606	-	44,58,74	1.71	9 (20%)	37,94,114	2.14	12 (32%)
31	CLA	B1	611	-	69,73,73	1.35	6 (8%)	82,113,113	1.89	20 (24%)
31	CLA	C1	502	-	69,73,73	1.37	7 (10%)	82,113,113	1.90	18 (21%)
31	CLA	b1	604	-	69,73,73	1.33	6 (8%)	82,113,113	1.92	20 (24%)
47	CHL	R	607	-	44,58,74	1.52	8 (18%)	37,94,114	2.17	12 (32%)
31	CLA	c1	513	-	69,73,73	1.36	7 (10%)	82,113,113	1.97	22 (26%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	A	405	-	69,73,73	1.37	6 (8%)	82,113,113	1.86	16 (19%)
28	OEX	A	401	4,1	0,15,15	-	-	-		
31	CLA	R	612	-	64,68,73	1.41	7 (10%)	76,107,113	1.94	21 (27%)
31	CLA	b1	609	-	69,73,73	1.39	7 (10%)	82,113,113	1.94	20 (24%)
31	CLA	r1	608	-	64,68,73	1.43	7 (10%)	76,107,113	1.93	16 (21%)
41	LHG	C1	525	-	46,46,48	0.40	0	49,52,54	1.12	2 (4%)
31	CLA	C1	505	-	69,73,73	1.35	7 (10%)	82,113,113	1.90	16 (19%)
37	C7Z	b1	620	-	43,43,43	5.43	26 (60%)	56,60,60	2.28	21 (37%)
48	LUT	G	620	-	42,43,43	2.45	1 (2%)	51,60,60	1.93	10 (19%)
31	CLA	B1	609	-	69,73,73	1.38	6 (8%)	82,113,113	1.92	17 (20%)
32	PHO	a	408	-	58,69,69	2.16	10 (17%)	55,99,99	1.55	7 (12%)
37	C7Z	B	620	-	43,43,43	5.50	26 (60%)	56,60,60	2.19	14 (25%)
47	CHL	n	606	-	60,74,74	1.42	8 (13%)	58,114,114	1.75	12 (20%)
31	CLA	c	501	-	69,73,73	1.35	8 (11%)	82,113,113	1.92	19 (23%)
31	CLA	R1	603	-	64,68,73	1.42	8 (12%)	76,107,113	1.87	16 (21%)
43	BCT	D1	401	-	3,3,3	1.11	0	2,3,3	4.27	2 (100%)
31	CLA	Y1	603	-	69,73,73	1.37	7 (10%)	82,113,113	1.98	20 (24%)
47	CHL	G	606	-	44,58,74	1.58	9 (20%)	37,94,114	2.09	12 (32%)
35	LMG	a1	413	-	48,48,55	1.13	5 (10%)	56,56,63	1.06	2 (3%)
35	LMG	b1	622	-	44,44,55	0.97	3 (6%)	52,52,63	1.17	3 (5%)
31	CLA	N	614	-	53,57,73	1.54	7 (13%)	61,93,113	2.16	19 (31%)
47	CHL	n1	607	-	60,74,74	1.14	7 (11%)	58,114,114	1.82	12 (20%)
31	CLA	Y	611	-	69,73,73	1.36	6 (8%)	82,113,113	1.82	15 (18%)
31	CLA	D	403	-	69,73,73	1.35	7 (10%)	82,113,113	1.91	21 (25%)
31	CLA	s	609	-	64,68,73	1.42	8 (12%)	76,107,113	1.92	17 (22%)
44	PL9	D	405	-	55,55,55	1.25	4 (7%)	68,69,69	1.52	12 (17%)
50	NEX	N1	623	-	40,46,46	2.69	11 (27%)	50,70,70	1.69	11 (22%)
38	DGA	j1	101	-	28,28,43	1.32	3 (10%)	30,30,45	1.31	2 (6%)
31	CLA	B	615	-	69,73,73	1.35	6 (8%)	82,113,113	2.03	17 (20%)
47	CHL	S	608	-	55,69,74	1.32	8 (14%)	52,108,114	1.78	12 (23%)
41	LHG	L	101	-	48,48,48	0.41	0	51,54,54	0.97	2 (3%)
47	CHL	y1	609	-	60,74,74	1.30	8 (13%)	58,114,114	1.71	12 (20%)
48	LUT	n	620	-	42,43,43	2.45	1 (2%)	51,60,60	2.07	13 (25%)
33	BCR	c	514	-	41,41,41	1.65	4 (9%)	56,56,56	4.67	19 (33%)
48	LUT	n	621	-	42,43,43	2.49	1 (2%)	51,60,60	1.90	12 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	g1	602	-	69,73,73	1.36	7 (10%)	82,113,113	1.88	21 (25%)
31	CLA	r	611	-	50,54,73	1.59	8 (16%)	59,90,113	2.07	15 (25%)
31	CLA	G	613	-	69,73,73	1.37	8 (11%)	82,113,113	2.01	24 (29%)
35	LMG	J	101	-	45,45,55	1.00	3 (6%)	53,53,63	1.09	3 (5%)
31	CLA	S	610	-	69,73,73	1.39	8 (11%)	82,113,113	1.88	17 (20%)
31	CLA	y1	604	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	19 (23%)
33	BCR	b	618	-	41,41,41	1.61	4 (9%)	56,56,56	4.50	14 (25%)
34	SQD	c1	526	-	52,54,54	0.78	0	62,65,65	0.83	2 (3%)
33	BCR	C1	515	-	41,41,41	1.60	4 (9%)	56,56,56	4.52	14 (25%)
31	CLA	y1	611	-	69,73,73	1.38	7 (10%)	82,113,113	1.87	16 (19%)
47	CHL	S1	608	-	55,69,74	1.34	8 (14%)	52,108,114	1.83	13 (25%)
48	LUT	y1	620	-	42,43,43	2.49	1 (2%)	51,60,60	1.83	10 (19%)
47	CHL	y1	605	-	40,54,74	1.49	8 (20%)	34,90,114	2.24	11 (32%)
50	NEX	r	623	-	40,46,46	2.66	11 (27%)	50,70,70	1.65	7 (14%)
38	DGA	c	524	-	43,43,43	1.16	3 (6%)	45,45,45	1.51	3 (6%)
41	LHG	L1	101	-	48,48,48	0.38	0	51,54,54	4.52	5 (9%)
48	LUT	N1	620	-	42,43,43	2.50	1 (2%)	51,60,60	1.73	13 (25%)
34	SQD	C	526	-	52,54,54	0.78	1 (1%)	62,65,65	0.83	2 (3%)
47	CHL	n1	601	20	60,74,74	1.25	8 (13%)	58,114,114	1.80	12 (20%)
31	CLA	C1	507	-	69,73,73	1.35	7 (10%)	82,113,113	1.93	18 (21%)
47	CHL	g1	605	-	42,56,74	1.58	7 (16%)	36,92,114	2.10	11 (30%)
32	PHO	a1	409	-	58,69,69	2.14	9 (15%)	55,99,99	1.79	11 (20%)
31	CLA	S1	602	-	64,68,73	1.40	7 (10%)	76,107,113	1.99	21 (27%)
50	NEX	y1	623	-	40,46,46	2.71	11 (27%)	50,70,70	1.98	12 (24%)
41	LHG	d	408	-	43,43,48	0.41	0	46,49,54	1.14	3 (6%)
31	CLA	b	617	-	69,73,73	1.36	6 (8%)	82,113,113	3.98	18 (21%)
47	CHL	G1	605	-	42,56,74	1.49	8 (19%)	36,92,114	2.13	11 (30%)
34	SQD	B	621	-	52,54,54	0.78	0	62,65,65	0.84	2 (3%)
31	CLA	R	604	-	53,57,73	1.55	6 (11%)	61,93,113	2.14	16 (26%)
31	CLA	y	610	-	69,73,73	1.38	7 (10%)	82,113,113	1.93	18 (21%)
41	LHG	c	625	-	46,46,48	0.41	0	49,52,54	1.05	4 (8%)
48	LUT	y	620	-	42,43,43	2.43	1 (2%)	51,60,60	2.03	14 (27%)
48	LUT	N1	621	-	42,43,43	2.44	1 (2%)	51,60,60	1.91	11 (21%)
49	XAT	y	622	-	41,47,47	0.69	1 (2%)	54,74,74	3.73	18 (33%)
31	CLA	d	402	-	69,73,73	1.37	7 (10%)	82,113,113	1.79	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	LMG	c1	521	-	51,51,55	1.21	6 (11%)	59,59,63	1.14	3 (5%)
31	CLA	C	508	-	69,73,73	1.37	6 (8%)	82,113,113	1.84	17 (20%)
50	NEX	r1	622	-	40,46,46	2.75	12 (30%)	50,70,70	2.34	11 (22%)
31	CLA	S1	609	-	64,68,73	1.40	7 (10%)	76,107,113	1.99	20 (26%)
31	CLA	B	612	-	69,73,73	1.38	7 (10%)	82,113,113	1.81	15 (18%)
41	LHG	s1	624	-	44,44,48	0.41	0	47,50,54	1.03	3 (6%)
31	CLA	a1	406	-	69,73,73	1.34	6 (8%)	82,113,113	1.92	17 (20%)
31	CLA	c	506	-	69,73,73	1.38	7 (10%)	82,113,113	1.92	20 (24%)
31	CLA	G1	603	-	69,73,73	1.36	7 (10%)	82,113,113	1.91	17 (20%)
41	LHG	g	624	-	48,48,48	0.39	0	51,54,54	1.10	3 (5%)
50	NEX	Y1	623	-	40,46,46	2.76	11 (27%)	50,70,70	1.98	12 (24%)
33	BCR	c	515	-	41,41,41	1.64	5 (12%)	56,56,56	4.43	18 (32%)
47	CHL	n1	605	-	60,74,74	1.23	8 (13%)	58,114,114	1.67	12 (20%)
47	CHL	G1	608	-	38,52,74	1.65	8 (21%)	31,87,114	2.20	11 (35%)
35	LMG	a	413	-	48,48,55	1.13	5 (10%)	56,56,63	1.22	4 (7%)
38	DGA	b	623	-	43,43,43	1.15	2 (4%)	45,45,45	1.53	3 (6%)
52	3PH	T1	101	-	47,47,47	0.86	4 (8%)	50,52,52	1.12	2 (4%)
57	PTY	y1	627	-	18,18,49	1.33	3 (16%)	21,23,54	1.46	2 (9%)
31	CLA	B	613	-	69,73,73	1.37	7 (10%)	82,113,113	1.89	15 (18%)
48	LUT	s1	621	-	42,43,43	2.43	1 (2%)	51,60,60	2.12	13 (25%)
32	PHO	A1	408	-	58,69,69	2.17	10 (17%)	55,99,99	1.53	7 (12%)
31	CLA	c1	502	-	69,73,73	1.34	6 (8%)	82,113,113	1.95	21 (25%)
31	CLA	B	602	-	69,73,73	1.36	6 (8%)	82,113,113	1.92	18 (21%)
31	CLA	S	602	23	64,68,73	1.40	6 (9%)	76,107,113	1.91	17 (22%)
47	CHL	G	601	-	60,74,74	1.77	9 (15%)	58,114,114	1.63	11 (18%)
31	CLA	G1	610	-	69,73,73	1.34	6 (8%)	82,113,113	1.91	19 (23%)
47	CHL	G	609	-	60,74,74	1.62	9 (15%)	58,114,114	1.56	12 (20%)
52	3PH	s1	626	-	47,47,47	0.89	4 (8%)	50,52,52	4.52	4 (8%)
33	BCR	c1	515	-	41,41,41	1.63	5 (12%)	56,56,56	4.46	16 (28%)
33	BCR	b	619	-	41,41,41	1.64	4 (9%)	56,56,56	4.59	19 (33%)
31	CLA	g	611	-	49,53,73	1.61	7 (14%)	58,89,113	2.16	16 (27%)
31	CLA	C	502	-	69,73,73	1.35	7 (10%)	82,113,113	1.94	19 (23%)
31	CLA	N	612	-	49,53,73	1.62	7 (14%)	58,89,113	2.05	12 (20%)
31	CLA	c1	508	-	69,73,73	1.35	7 (10%)	82,113,113	1.83	15 (18%)
31	CLA	b	603	-	69,73,73	1.36	8 (11%)	82,113,113	1.92	21 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
34	SQD	m1	101	-	40,42,54	0.89	0	50,53,65	0.90	2 (4%)
33	BCR	C	517	-	41,41,41	1.62	4 (9%)	56,56,56	4.40	11 (19%)
31	CLA	S1	612	-	49,53,73	1.60	6 (12%)	58,89,113	2.09	15 (25%)
47	CHL	n	601	-	60,74,74	1.34	9 (15%)	58,114,114	1.75	12 (20%)
32	PHO	A1	409	-	58,69,69	2.13	9 (15%)	55,99,99	1.63	8 (14%)
49	XAT	Y1	622	-	41,47,47	0.69	1 (2%)	54,74,74	3.78	19 (35%)
31	CLA	G	611	-	49,53,73	1.61	6 (12%)	58,89,113	2.13	18 (31%)
31	CLA	s1	605	23	54,58,73	1.56	7 (12%)	64,95,113	2.15	18 (28%)
31	CLA	B	611	-	69,73,73	1.35	7 (10%)	82,113,113	1.85	18 (21%)
31	CLA	S	611	-	69,73,73	1.36	7 (10%)	82,113,113	1.88	18 (21%)
31	CLA	B1	610	-	69,73,73	1.37	7 (10%)	82,113,113	1.85	18 (21%)
31	CLA	C1	512	-	69,73,73	1.37	7 (10%)	82,113,113	1.95	21 (25%)
40	DGD	C	523	-	67,67,67	1.29	7 (10%)	81,81,81	1.07	3 (3%)
47	CHL	Y	605	24	40,54,74	1.74	7 (17%)	34,90,114	2.09	10 (29%)
50	NEX	g	623	-	40,46,46	2.68	11 (27%)	50,70,70	2.27	14 (28%)
31	CLA	b	611	-	69,73,73	1.37	8 (11%)	82,113,113	1.92	21 (25%)
34	SQD	B1	621	-	40,42,54	0.86	0	50,53,65	0.88	2 (4%)
31	CLA	A	410	-	64,68,73	1.42	7 (10%)	76,107,113	2.02	19 (25%)
31	CLA	C	512	-	69,73,73	1.36	7 (10%)	82,113,113	1.79	17 (20%)
31	CLA	n	603	-	69,73,73	1.35	6 (8%)	82,113,113	2.00	19 (23%)
52	3PH	i	101	-	47,47,47	0.87	4 (8%)	50,52,52	1.20	2 (4%)
42	LMK	c	627	-	39,39,53	1.53	3 (7%)	39,46,60	1.39	2 (5%)
49	XAT	n	622	-	41,47,47	0.70	1 (2%)	54,74,74	1.93	10 (18%)
31	CLA	c1	510	-	69,73,73	1.37	6 (8%)	82,113,113	1.85	16 (19%)
31	CLA	g1	614	-	53,57,73	1.55	8 (15%)	61,93,113	2.18	17 (27%)
31	CLA	N	603	-	69,73,73	1.34	7 (10%)	82,113,113	1.96	20 (24%)
31	CLA	r	610	-	64,68,73	1.42	7 (10%)	76,107,113	1.95	22 (28%)
31	CLA	G	603	-	69,73,73	1.33	6 (8%)	82,113,113	2.00	21 (25%)
33	BCR	B	618	-	41,41,41	1.60	4 (9%)	56,56,56	4.57	14 (25%)
31	CLA	N	604	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	20 (24%)
43	BCT	d1	401	-	3,3,3	1.15	0	2,3,3	4.40	2 (100%)
31	CLA	a	405	-	69,73,73	1.36	6 (8%)	82,113,113	1.89	19 (23%)
41	LHG	N1	624	-	48,48,48	0.39	0	51,54,54	1.10	4 (7%)
47	CHL	Y	601	-	60,74,74	1.37	9 (15%)	58,114,114	1.70	11 (18%)
46	RRX	h	101	-	42,42,42	5.03	24 (57%)	56,58,58	1.97	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
35	LMG	h1	102	-	48,48,55	1.13	5 (10%)	56,56,63	1.11	2 (3%)
31	CLA	N1	603	-	69,73,73	1.35	6 (8%)	82,113,113	1.95	19 (23%)
31	CLA	b1	613	-	69,73,73	1.36	6 (8%)	82,113,113	1.92	15 (18%)
34	SQD	M1	101	-	40,42,54	0.87	0	50,53,65	0.89	2 (4%)
47	CHL	G1	607	-	60,74,74	1.25	8 (13%)	58,114,114	1.79	13 (22%)
50	NEX	S	622	-	40,46,46	2.68	11 (27%)	50,70,70	1.91	12 (24%)
41	LHG	S1	624	-	44,44,48	0.41	0	47,50,54	1.12	4 (8%)
31	CLA	B	610	-	69,73,73	1.37	7 (10%)	82,113,113	1.88	16 (19%)
31	CLA	s1	617	-	54,58,73	1.52	7 (12%)	64,95,113	2.12	20 (31%)
47	CHL	r	606	-	38,52,74	1.73	9 (23%)	31,87,114	2.27	10 (32%)
31	CLA	n1	611	-	53,57,73	1.53	7 (13%)	61,93,113	2.18	17 (27%)
40	DGD	C1	519	-	63,63,67	1.24	7 (11%)	77,77,81	1.00	3 (3%)
31	CLA	y	603	-	69,73,73	1.34	6 (8%)	82,113,113	1.97	20 (24%)
31	CLA	g	610	-	69,73,73	1.34	6 (8%)	82,113,113	1.91	19 (23%)
31	CLA	G	604	-	53,57,73	1.56	8 (15%)	61,93,113	2.19	17 (27%)
31	CLA	S1	604	-	59,63,73	1.48	6 (10%)	70,101,113	2.11	19 (27%)
33	BCR	c1	516	-	41,41,41	1.59	4 (9%)	56,56,56	4.60	16 (28%)
31	CLA	d1	403	-	69,73,73	1.37	8 (11%)	82,113,113	1.93	19 (23%)
31	CLA	R	603	-	64,68,73	1.42	8 (12%)	76,107,113	2.01	18 (23%)
47	CHL	y	609	-	60,74,74	1.31	9 (15%)	58,114,114	1.70	12 (20%)
50	NEX	s	623	-	40,46,46	2.75	14 (35%)	50,70,70	1.80	12 (24%)
34	SQD	b	621	-	52,54,54	0.78	0	62,65,65	0.83	2 (3%)
56	ERG	R1	626	-	32,32,32	7.93	20 (62%)	45,50,50	2.88	20 (44%)
40	DGD	C1	520	-	60,60,67	1.17	6 (10%)	74,74,81	1.00	4 (5%)
50	NEX	G	623	-	40,46,46	2.74	11 (27%)	50,70,70	1.82	11 (22%)
49	XAT	R1	621	-	41,47,47	0.65	1 (2%)	54,74,74	1.88	13 (24%)
31	CLA	a1	410	-	64,68,73	1.41	6 (9%)	76,107,113	1.92	18 (23%)
31	CLA	S1	614	-	59,63,73	1.46	6 (10%)	70,101,113	1.99	17 (24%)
33	BCR	C	516	-	41,41,41	1.62	4 (9%)	56,56,56	4.52	15 (26%)
32	PHO	A	409	-	58,69,69	2.15	9 (15%)	55,99,99	1.63	8 (14%)
41	LHG	y1	624	-	48,48,48	0.40	0	51,54,54	0.99	2 (3%)
47	CHL	G1	609	-	60,74,74	1.43	8 (13%)	58,114,114	1.62	12 (20%)
31	CLA	b1	614	-	69,73,73	1.37	8 (11%)	82,113,113	1.81	18 (21%)
51	LPX	S	625	-	29,29,29	1.03	2 (6%)	31,33,33	0.97	1 (3%)
31	CLA	n	611	-	53,57,73	1.56	7 (13%)	61,93,113	2.22	18 (29%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
33	BCR	a1	411	-	41,41,41	1.60	4 (9%)	56,56,56	4.60	14 (25%)
31	CLA	n	610	-	69,73,73	1.36	6 (8%)	82,113,113	1.96	19 (23%)
47	CHL	G	608	-	38,52,74	1.76	9 (23%)	31,87,114	2.25	10 (32%)
31	CLA	B	614	-	69,73,73	1.35	6 (8%)	82,113,113	1.84	17 (20%)
31	CLA	D	402	-	69,73,73	1.35	7 (10%)	82,113,113	1.89	18 (21%)
33	BCR	b1	618	-	41,41,41	1.61	4 (9%)	56,56,56	4.65	18 (32%)
33	BCR	d	404	-	41,41,41	1.59	4 (9%)	56,56,56	4.28	17 (30%)
35	LMG	j	101	-	45,45,55	1.00	4 (8%)	53,53,63	1.06	2 (3%)
41	LHG	D	409	-	48,48,48	0.40	0	51,54,54	1.08	3 (5%)
47	CHL	Y	606	-	60,74,74	1.31	8 (13%)	58,114,114	1.76	13 (22%)
31	CLA	c1	504	-	69,73,73	1.35	6 (8%)	82,113,113	1.91	20 (24%)
39	GOL	b	624	-	5,5,5	0.59	0	5,5,5	0.26	0
31	CLA	g1	604	-	53,57,73	1.55	7 (13%)	61,93,113	2.13	20 (32%)
31	CLA	r	602	-	64,68,73	1.43	8 (12%)	76,107,113	1.94	19 (25%)
47	CHL	n	607	-	60,74,74	1.17	7 (11%)	58,114,114	1.85	13 (22%)
31	CLA	C	503	-	69,73,73	1.37	8 (11%)	82,113,113	1.91	19 (23%)
47	CHL	N1	608	-	44,58,74	1.74	7 (15%)	37,94,114	2.01	12 (32%)
31	CLA	G1	611	-	69,73,73	1.35	6 (8%)	82,113,113	1.91	18 (21%)
34	SQD	C1	526	-	52,54,54	0.77	0	62,65,65	0.85	2 (3%)
48	LUT	Y	620	-	42,43,43	2.48	1 (2%)	51,60,60	1.90	13 (25%)
46	RRX	H	101	-	42,42,42	7.86	26 (61%)	56,58,58	6.26	22 (39%)
50	NEX	n	623	-	40,46,46	2.69	11 (27%)	50,70,70	1.80	13 (26%)
47	CHL	y	605	24	40,54,74	1.59	7 (17%)	34,90,114	2.06	10 (29%)
48	LUT	y	621	-	42,43,43	2.40	1 (2%)	51,60,60	1.87	13 (25%)
38	DGA	c1	524	-	43,43,43	1.16	3 (6%)	45,45,45	1.53	4 (8%)
33	BCR	A1	411	-	41,41,41	1.61	4 (9%)	56,56,56	4.57	13 (23%)
41	LHG	Y1	624	-	48,48,48	0.39	0	51,54,54	1.01	3 (5%)
31	CLA	S	604	-	59,63,73	1.45	6 (10%)	70,101,113	2.05	19 (27%)
31	CLA	R1	612	-	64,68,73	1.42	8 (12%)	76,107,113	1.97	20 (26%)
31	CLA	g	602	-	69,73,73	1.34	7 (10%)	82,113,113	1.92	21 (25%)
38	DGA	C	524	-	43,43,43	1.15	3 (6%)	45,45,45	1.52	3 (6%)
47	CHL	N1	601	20	60,74,74	1.38	8 (13%)	58,114,114	1.63	13 (22%)
31	CLA	s	610	-	69,73,73	1.37	6 (8%)	82,113,113	1.90	18 (21%)
38	DGA	B1	625	-	43,43,43	1.16	2 (4%)	45,45,45	1.45	3 (6%)
31	CLA	C1	508	-	69,73,73	1.34	6 (8%)	82,113,113	1.85	17 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
41	LHG	N	624	-	48,48,48	0.37	0	51,54,54	1.17	3 (5%)
47	CHL	R1	606	-	38,52,74	1.91	9 (23%)	31,87,114	2.31	11 (35%)
50	NEX	n1	623	-	40,46,46	2.64	11 (27%)	50,70,70	1.72	10 (20%)
31	CLA	n	613	-	69,73,73	1.36	8 (11%)	82,113,113	1.98	21 (25%)
31	CLA	Y1	614	-	69,73,73	1.38	8 (11%)	82,113,113	1.83	18 (21%)
40	DGD	c1	519	-	63,63,67	1.23	7 (11%)	77,77,81	0.99	5 (6%)
31	CLA	B1	602	-	69,73,73	1.35	7 (10%)	82,113,113	1.88	17 (20%)
31	CLA	R1	609	-	64,68,73	1.40	7 (10%)	76,107,113	4.17	22 (28%)
47	CHL	N	605	-	60,74,74	1.38	9 (15%)	58,114,114	1.63	10 (17%)
31	CLA	N	613	-	69,73,73	1.36	7 (10%)	82,113,113	1.88	18 (21%)
31	CLA	b1	617	-	69,73,73	1.39	7 (10%)	82,113,113	1.91	16 (19%)
47	CHL	n	609	-	60,74,74	1.45	9 (15%)	58,114,114	1.70	14 (24%)
35	LMG	c	521	-	51,51,55	1.21	6 (11%)	59,59,63	1.20	4 (6%)
52	3PH	b1	624	-	47,47,47	0.87	4 (8%)	50,52,52	1.18	2 (4%)
48	LUT	G	621	-	42,43,43	2.46	1 (2%)	51,60,60	2.05	16 (31%)
31	CLA	s	613	-	59,63,73	1.47	6 (10%)	70,101,113	2.18	14 (20%)
31	CLA	R	610	-	64,68,73	1.41	7 (10%)	76,107,113	1.97	20 (26%)
37	C7Z	B1	620	-	43,43,43	5.46	26 (60%)	56,60,60	2.36	19 (33%)
31	CLA	b1	608	-	69,73,73	1.36	6 (8%)	82,113,113	1.86	18 (21%)
40	DGD	c1	520	-	60,60,67	1.17	6 (10%)	74,74,81	1.01	3 (4%)
47	CHL	y	607	-	60,74,74	1.12	7 (11%)	58,114,114	1.79	13 (22%)
35	LMG	d	411	-	46,46,55	1.02	4 (8%)	54,54,63	1.21	3 (5%)
31	CLA	y	604	-	69,73,73	1.36	6 (8%)	82,113,113	1.86	16 (19%)
31	CLA	d	403	-	69,73,73	1.37	6 (8%)	82,113,113	1.91	17 (20%)
31	CLA	Y1	604	-	69,73,73	1.35	7 (10%)	82,113,113	1.88	22 (26%)
39	GOL	y	626	-	5,5,5	0.54	0	5,5,5	0.37	0
33	BCR	C1	517	-	41,41,41	1.66	4 (9%)	56,56,56	4.76	16 (28%)
31	CLA	B	604	-	69,73,73	1.41	9 (13%)	82,113,113	1.83	18 (21%)
48	LUT	N	620	-	42,43,43	2.46	1 (2%)	51,60,60	2.00	16 (31%)
41	LHG	l	101	-	48,48,48	0.40	0	51,54,54	0.97	2 (3%)
31	CLA	c1	501	-	69,73,73	1.36	7 (10%)	82,113,113	1.92	20 (24%)
33	BCR	B	619	-	41,41,41	1.62	4 (9%)	56,56,56	4.51	19 (33%)
41	LHG	d	409	-	48,48,48	0.40	0	51,54,54	0.99	2 (3%)
31	CLA	S	609	-	64,68,73	1.42	8 (12%)	76,107,113	1.91	20 (26%)
31	CLA	c1	506	-	69,73,73	1.35	6 (8%)	82,113,113	1.85	16 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	C	513	-	69,73,73	1.36	7 (10%)	82,113,113	1.92	19 (23%)
31	CLA	B	603	-	69,73,73	1.35	6 (8%)	82,113,113	1.96	20 (24%)
41	LHG	c1	525	-	46,46,48	0.40	0	49,52,54	1.03	3 (6%)
31	CLA	C	501	-	69,73,73	1.36	7 (10%)	82,113,113	1.99	19 (23%)
38	DGA	C1	524	-	43,43,43	1.16	3 (6%)	45,45,45	1.52	3 (6%)
40	DGD	c	520	-	60,60,67	1.16	6 (10%)	74,74,81	1.03	2 (2%)
31	CLA	n1	610	-	69,73,73	1.35	6 (8%)	82,113,113	1.91	18 (21%)
31	CLA	r1	603	-	64,68,73	1.43	7 (10%)	76,107,113	1.89	15 (19%)
53	SPH	y	625	-	19,20,20	0.66	0	18,21,21	1.15	2 (11%)
31	CLA	R	608	-	64,68,73	1.41	7 (10%)	76,107,113	1.92	16 (21%)
31	CLA	a	407	-	53,57,73	1.56	7 (13%)	61,93,113	2.14	18 (29%)
31	CLA	r1	602	-	64,68,73	1.41	7 (10%)	76,107,113	1.97	22 (28%)
31	CLA	Y	608	-	54,58,73	1.54	9 (16%)	64,95,113	2.07	17 (26%)
31	CLA	r1	604	-	53,57,73	1.53	6 (11%)	61,93,113	2.20	18 (29%)
31	CLA	A1	405	-	69,73,73	1.41	7 (10%)	82,113,113	2.03	20 (24%)
47	CHL	g	605	-	42,56,74	1.58	8 (19%)	36,92,114	2.11	11 (30%)
28	OEX	A1	401	4,1	0,15,15	-	-	-		
31	CLA	C1	511	-	69,73,73	1.35	6 (8%)	82,113,113	1.90	17 (20%)
31	CLA	c1	503	-	69,73,73	1.36	6 (8%)	82,113,113	1.97	23 (28%)
31	CLA	y1	608	-	54,58,73	1.53	8 (14%)	64,95,113	2.11	19 (29%)
31	CLA	B1	604	-	69,73,73	1.38	8 (11%)	82,113,113	1.82	19 (23%)
31	CLA	C1	510	-	69,73,73	1.37	6 (8%)	82,113,113	1.85	16 (19%)
31	CLA	G1	612	-	47,51,73	1.65	8 (17%)	55,86,113	2.10	14 (25%)
31	CLA	b1	605	-	69,73,73	1.34	6 (8%)	82,113,113	2.16	21 (25%)
47	CHL	N	601	20	60,74,74	1.46	8 (13%)	58,114,114	1.73	11 (18%)
49	XAT	Y	622	-	41,47,47	0.70	1 (2%)	54,74,74	3.76	16 (29%)
41	LHG	s	624	-	44,44,48	0.41	0	47,50,54	1.13	3 (6%)
31	CLA	A1	407	-	54,58,73	1.53	7 (12%)	64,95,113	2.10	22 (34%)
35	LMG	B1	622	-	44,44,55	0.97	3 (6%)	52,52,63	1.14	3 (5%)
31	CLA	G	610	-	69,73,73	1.34	6 (8%)	82,113,113	1.98	20 (24%)
31	CLA	S1	611	-	69,73,73	1.36	6 (8%)	82,113,113	1.91	18 (21%)
31	CLA	s	612	-	49,53,73	1.61	7 (14%)	58,89,113	2.10	16 (27%)
31	CLA	N	610	-	69,73,73	1.38	7 (10%)	82,113,113	1.95	20 (24%)
33	BCR	c1	514	-	41,41,41	1.60	4 (9%)	56,56,56	4.60	16 (28%)
47	CHL	Y	609	-	60,74,74	1.29	9 (15%)	58,114,114	1.72	12 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
31	CLA	B	606	-	69,73,73	1.36	8 (11%)	82,113,113	1.88	19 (23%)
31	CLA	b	616	-	69,73,73	1.37	6 (8%)	82,113,113	1.85	17 (20%)
33	BCR	C1	516	-	41,41,41	1.53	5 (12%)	56,56,56	4.46	18 (32%)
33	BCR	C	514	-	41,41,41	1.62	4 (9%)	56,56,56	4.55	13 (23%)
52	3PH	S	626	-	47,47,47	0.88	4 (8%)	50,52,52	1.12	2 (4%)
31	CLA	N1	604	-	69,73,73	1.37	7 (10%)	82,113,113	1.95	20 (24%)
53	SPH	A1	414	-	19,20,20	0.68	1 (5%)	18,21,21	0.92	0
48	LUT	y1	621	-	42,43,43	2.48	1 (2%)	51,60,60	1.90	13 (25%)
52	3PH	s	626	-	47,47,47	0.87	4 (8%)	50,52,52	1.14	2 (4%)
31	CLA	s	602	-	64,68,73	1.39	6 (9%)	76,107,113	1.94	19 (25%)
44	PL9	d	405	-	55,55,55	1.26	6 (10%)	68,69,69	1.47	13 (19%)
31	CLA	c1	509	-	69,73,73	1.36	6 (8%)	82,113,113	1.84	16 (19%)
41	LHG	y	624	-	48,48,48	0.39	0	51,54,54	1.09	3 (5%)
43	BCT	D	401	29	3,3,3	1.16	0	2,3,3	4.58	2 (100%)
41	LHG	D	410	-	38,38,48	0.44	0	41,44,54	1.04	2 (4%)
47	CHL	n	608	-	44,58,74	1.31	8 (18%)	37,94,114	2.16	11 (29%)
31	CLA	s1	612	-	49,53,73	1.59	6 (12%)	58,89,113	2.14	16 (27%)
48	LUT	Y	621	-	42,43,43	2.39	1 (2%)	51,60,60	1.88	14 (27%)
41	LHG	g1	624	-	48,48,48	0.39	0	51,54,54	1.06	3 (5%)
31	CLA	R	602	-	64,68,73	1.42	7 (10%)	76,107,113	1.92	20 (26%)
31	CLA	n	614	-	53,57,73	1.54	7 (13%)	61,93,113	2.16	19 (31%)
31	CLA	g1	613	-	69,73,73	1.34	7 (10%)	82,113,113	1.92	21 (25%)
47	CHL	N1	607	-	60,74,74	1.08	7 (11%)	58,114,114	1.77	14 (24%)
49	XAT	R	621	-	41,47,47	0.71	1 (2%)	54,74,74	2.02	13 (24%)
31	CLA	C1	503	-	69,73,73	1.36	7 (10%)	82,113,113	1.91	18 (21%)
32	PHO	a	409	-	58,69,69	2.14	9 (15%)	55,99,99	1.71	8 (14%)
47	CHL	s1	606	-	38,52,74	1.61	7 (18%)	31,87,114	2.22	9 (29%)
50	NEX	R	622	-	40,46,46	2.82	13 (32%)	50,70,70	1.93	10 (20%)
40	DGD	B1	623	-	44,44,67	0.84	1 (2%)	58,58,81	1.25	4 (6%)
47	CHL	g	606	-	44,58,74	1.44	8 (18%)	37,94,114	2.19	11 (29%)
31	CLA	s1	613	-	59,63,73	1.49	7 (11%)	70,101,113	2.02	16 (22%)
28	OEX	a	401	4,1	0,15,15	-	-	-		
48	LUT	g1	620	-	42,43,43	2.46	1 (2%)	51,60,60	1.84	11 (21%)
42	LMK	c1	527	-	39,39,53	1.55	3 (7%)	39,46,60	1.35	2 (5%)
47	CHL	S	606	-	38,52,74	1.63	8 (21%)	31,87,114	2.21	11 (35%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
48	LUT	g	620	-	42,43,43	2.47	1 (2%)	51,60,60	1.98	12 (23%)
31	CLA	N	611	-	53,57,73	1.56	8 (15%)	61,93,113	2.22	18 (29%)
31	CLA	b1	611	-	69,73,73	1.35	7 (10%)	82,113,113	1.84	18 (21%)
34	SQD	a1	412	-	49,51,54	0.80	0	59,62,65	0.84	2 (3%)
31	CLA	n1	602	-	69,73,73	1.35	6 (8%)	82,113,113	1.92	19 (23%)
53	SPH	Y1	625	-	19,20,20	0.66	0	18,21,21	1.07	1 (5%)
48	LUT	s1	620	-	42,43,43	2.48	1 (2%)	51,60,60	1.94	13 (25%)
31	CLA	c	511	-	69,73,73	1.38	8 (11%)	82,113,113	1.93	21 (25%)
34	SQD	b1	621	-	40,42,54	0.87	0	50,53,65	0.88	2 (4%)
31	CLA	C	504	-	69,73,73	1.33	7 (10%)	82,113,113	1.96	19 (23%)
31	CLA	n1	604	-	69,73,73	1.35	6 (8%)	82,113,113	1.87	21 (25%)
33	BCR	D	404	-	41,41,41	1.60	4 (9%)	56,56,56	4.34	19 (33%)
48	LUT	g	621	-	42,43,43	2.45	1 (2%)	51,60,60	1.98	9 (17%)
53	SPH	a1	414	-	19,20,20	0.68	0	18,21,21	1.04	1 (5%)
47	CHL	S1	606	-	38,52,74	1.87	9 (23%)	31,87,114	2.19	9 (29%)
53	SPH	y1	625	-	19,20,20	0.66	0	18,21,21	1.06	1 (5%)
41	LHG	D1	410	-	38,38,48	0.43	0	41,44,54	1.10	3 (7%)
31	CLA	S1	613	-	59,63,73	1.47	6 (10%)	70,101,113	2.02	16 (22%)
41	LHG	d1	408	-	43,43,48	0.42	0	46,49,54	1.07	3 (6%)
31	CLA	R	609	-	64,68,73	1.41	7 (10%)	76,107,113	1.93	18 (23%)
48	LUT	Y1	620	-	42,43,43	2.46	1 (2%)	51,60,60	1.88	14 (27%)
31	CLA	Y1	611	-	69,73,73	1.35	6 (8%)	82,113,113	1.84	15 (18%)
47	CHL	S1	601	23	40,54,74	1.66	8 (20%)	34,90,114	2.19	11 (32%)
33	BCR	c	516	-	41,41,41	1.58	4 (9%)	56,56,56	4.43	19 (33%)
51	LPX	s1	625	-	29,29,29	1.06	2 (6%)	31,33,33	0.97	1 (3%)
53	SPH	Y	625	-	19,20,20	0.63	0	18,21,21	1.14	1 (5%)
31	CLA	C1	513	-	69,73,73	1.36	8 (11%)	82,113,113	1.92	21 (25%)
31	CLA	N1	612	-	49,53,73	1.60	7 (14%)	58,89,113	2.07	15 (25%)
31	CLA	B1	607	-	69,73,73	1.37	7 (10%)	82,113,113	1.81	17 (20%)
31	CLA	S	612	-	49,53,73	1.63	6 (12%)	58,89,113	2.05	15 (25%)
47	CHL	Y1	607	-	60,74,74	1.11	7 (11%)	58,114,114	1.77	11 (18%)
47	CHL	g1	601	-	60,74,74	1.29	8 (13%)	58,114,114	1.71	12 (20%)
28	OEX	a1	401	4,1	0,15,15	-	-	-		
31	CLA	N	602	-	69,73,73	1.36	8 (11%)	82,113,113	1.87	20 (24%)
31	CLA	b1	603	-	69,73,73	1.37	7 (10%)	82,113,113	2.05	18 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	$\#\|Z\|>2$	Counts	RMSZ	$\#\|Z\|>2$
47	CHL	Y1	605	24	40,54,74	1.53	8 (20%)	34,90,114	2.19	10 (29%)
40	DGD	c	518	-	56,56,67	1.06	4 (7%)	70,70,81	0.98	2 (2%)
47	CHL	Y	607	-	60,74,74	1.12	7 (11%)	58,114,114	1.73	11 (18%)
48	LUT	Y1	621	-	42,43,43	2.47	1 (2%)	51,60,60	1.80	11 (21%)
35	LMG	C1	523	-	55,55,55	1.27	6 (10%)	63,63,63	1.11	3 (4%)
47	CHL	N1	606	-	60,74,74	1.34	8 (13%)	58,114,114	1.66	12 (20%)

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
48	LUT	s	620	-	1/1/12/27	2/29/67/67	0/2/2/2
31	CLA	c	508	-	1/1/15/20	11/39/115/115	-
31	CLA	g	613	-	1/1/15/20	19/39/115/115	-
47	CHL	g1	607	-	4/4/20/26	8/39/137/137	-
33	BCR	C1	514	-	-	15/29/63/63	0/2/2/2
47	CHL	s1	601	23	3/3/16/26	5/15/113/137	-
31	CLA	c	507	-	1/1/15/20	21/39/115/115	-
47	CHL	n1	609	-	4/4/20/26	3/39/137/137	-
31	CLA	D1	403	-	1/1/15/20	19/39/115/115	-
52	3PH	t1	101	-	-	27/49/49/49	-
31	CLA	A	406	-	1/1/15/20	14/39/115/115	-
33	BCR	D1	404	-	-	11/29/63/63	0/2/2/2
35	LMG	A	413	-	-	12/43/63/70	0/1/1/1
31	CLA	Y	612	-	1/1/15/20	11/39/115/115	-
47	CHL	G	605	21	3/3/16/26	1/18/116/137	-
48	LUT	s	621	-	-	1/29/67/67	0/2/2/2
31	CLA	y1	612	-	1/1/15/20	15/39/115/115	-
48	LUT	N	621	-	-	3/29/67/67	0/2/2/2
48	LUT	r1	620	-	-	6/29/67/67	0/2/2/2
31	CLA	R	613	-	1/1/11/20	10/17/93/115	-
35	LMG	h	102	-	-	13/43/63/70	0/1/1/1
35	LMG	C1	521	-	-	12/46/66/70	0/1/1/1
32	PHO	A	408	-	-	5/37/103/103	0/5/6/6

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	BCR	c	517	-	-	9/29/63/63	0/2/2/2
31	CLA	R1	610	-	1/1/14/20	11/33/109/115	-
31	CLA	c1	511	-	1/1/15/20	14/39/115/115	-
31	CLA	a1	405	-	1/1/15/20	13/39/115/115	-
31	CLA	C	509	-	1/1/15/20	11/39/115/115	-
31	CLA	Y1	610	-	1/1/15/20	15/39/115/115	-
47	CHL	y	601	24	4/4/20/26	6/39/137/137	-
41	LHG	D	408	-	-	29/48/48/53	-
47	CHL	y1	606	-	4/4/20/26	7/39/137/137	-
45	HEM	F1	101	6	-	1/14/54/54	-
31	CLA	r	608	-	1/1/14/20	16/33/109/115	-
50	NEX	y	623	-	-	5/27/83/83	0/3/3/3
35	LMG	b	622	-	-	12/39/59/70	0/1/1/1
31	CLA	b	605	-	1/1/15/20	17/39/115/115	-
31	CLA	c	510	-	1/1/15/20	13/39/115/115	-
47	CHL	R1	607	-	3/3/16/26	4/20/118/137	-
31	CLA	y1	613	-	1/1/15/20	23/39/115/115	-
31	CLA	b1	616	-	1/1/15/20	9/39/115/115	-
31	CLA	G1	602	-	1/1/15/20	18/39/115/115	-
46	RRX	H1	101	-	1/1/11/25	4/29/65/65	0/2/2/2
31	CLA	b1	606	-	1/1/15/20	9/39/115/115	-
38	DGA	B	625	-	-	25/45/45/45	-
31	CLA	r	604	-	1/1/11/20	10/20/96/115	-
44	PL9	D1	405	-	-	17/53/73/73	0/1/1/1
31	CLA	b	608	-	1/1/15/20	25/39/115/115	-
55	LMT	R1	625	-	-	9/21/61/61	0/2/2/2
39	GOL	b	625	-	-	2/4/4/4	-
31	CLA	g1	603	-	1/1/15/20	23/39/115/115	-
31	CLA	s	604	-	1/1/13/20	11/27/103/115	-
34	SQD	A1	412	-	-	15/46/66/69	0/1/1/1
31	CLA	y	611	-	1/1/15/20	18/39/115/115	-
31	CLA	b1	610	-	1/1/15/20	15/39/115/115	-
31	CLA	B1	605	-	1/1/15/20	14/39/115/115	-
31	CLA	n1	613	-	1/1/15/20	21/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	b1	602	-	1/1/15/20	17/39/115/115	-
31	CLA	S	614	-	1/1/13/20	10/27/103/115	-
40	DGD	C	518	-	-	12/44/84/95	0/2/2/2
31	CLA	S1	605	-	1/1/12/20	8/21/97/115	-
47	CHL	Y1	606	-	4/4/20/26	6/39/137/137	-
31	CLA	g1	611	-	1/1/15/20	16/39/115/115	-
50	NEX	g1	623	-	-	3/27/83/83	0/3/3/3
31	CLA	B	617	-	1/1/15/20	15/39/115/115	-
31	CLA	R1	608	-	1/1/14/20	13/33/109/115	-
31	CLA	B1	603	-	1/1/15/20	15/39/115/115	-
31	CLA	Y1	608	-	1/1/12/20	9/21/97/115	-
34	SQD	A	412	-	-	17/46/66/69	0/1/1/1
31	CLA	S1	603	-	1/1/15/20	17/39/115/115	-
56	ERG	r1	626	-	5/5/11/15	8/13/71/71	0/4/4/4
48	LUT	n1	620	-	-	4/29/67/67	0/2/2/2
31	CLA	R1	604	-	1/1/11/20	10/20/96/115	-
33	BCR	a	411	-	-	10/29/63/63	0/2/2/2
35	LMG	B	622	-	-	11/39/59/70	0/1/1/1
31	CLA	A	407	-	1/1/11/20	4/20/96/115	-
31	CLA	b1	615	-	1/1/15/20	18/39/115/115	-
47	CHL	Y1	601	24	4/4/20/26	0/39/137/137	-
40	DGD	C	520	-	-	13/48/88/95	0/2/2/2
31	CLA	B1	614	-	1/1/15/20	11/39/115/115	-
41	LHG	G	630	-	-	29/53/53/53	-
31	CLA	b	602	-	1/1/15/20	22/39/115/115	-
31	CLA	b	615	-	1/1/15/20	11/39/115/115	-
31	CLA	Y	613	-	1/1/15/20	16/39/115/115	-
31	CLA	b1	612	-	1/1/15/20	10/39/115/115	-
48	LUT	n1	621	-	-	3/29/67/67	0/2/2/2
47	CHL	n1	606	-	4/4/20/26	5/39/137/137	-
38	DGA	b1	625	-	-	23/45/45/45	-
31	CLA	s1	603	-	1/1/15/20	19/39/115/115	-
31	CLA	b	613	-	1/1/15/20	17/39/115/115	-
33	BCR	d1	404	-	-	12/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	g	603	-	1/1/15/20	17/39/115/115	-
41	LHG	n1	624	-	-	34/53/53/53	-
31	CLA	A1	406	-	1/1/15/20	12/39/115/115	-
33	BCR	b1	619	-	-	5/29/63/63	0/2/2/2
44	PL9	d1	405	-	-	22/53/73/73	0/1/1/1
31	CLA	G1	614	-	1/1/11/20	11/20/96/115	-
55	LMT	r1	625	-	-	9/21/61/61	0/2/2/2
47	CHL	y1	601	24	4/4/20/26	0/39/137/137	-
31	CLA	b	606	-	1/1/15/20	14/39/115/115	-
35	LMG	c1	523	-	-	14/50/70/70	0/1/1/1
31	CLA	C1	504	-	1/1/15/20	15/39/115/115	-
31	CLA	r1	612	-	1/1/14/20	17/33/109/115	-
49	XAT	G	622	-	2/2/12/26	0/31/93/93	0/4/4/4
42	LMK	C	527	-	1/1/6/6	12/46/46/60	-
41	LHG	d	410	-	-	32/43/43/53	-
31	CLA	B	609	-	1/1/15/20	19/39/115/115	-
31	CLA	C	506	-	1/1/15/20	21/39/115/115	-
31	CLA	b	610	-	1/1/15/20	16/39/115/115	-
31	CLA	g	604	-	1/1/11/20	8/20/96/115	-
47	CHL	y1	607	-	4/4/20/26	6/39/137/137	-
54	4RF	i1	101	-	-	28/59/59/59	-
31	CLA	b	612	-	1/1/15/20	18/39/115/115	-
31	CLA	B1	606	-	1/1/15/20	8/39/115/115	-
31	CLA	B1	608	-	1/1/15/20	25/39/115/115	-
31	CLA	C	510	-	1/1/15/20	18/39/115/115	-
47	CHL	r1	606	-	3/3/15/26	2/13/111/137	-
48	LUT	g1	621	-	1/1/12/27	3/29/67/67	0/2/2/2
31	CLA	Y1	613	-	1/1/15/20	19/39/115/115	-
31	CLA	r1	609	-	1/1/14/20	13/33/109/115	-
31	CLA	B	607	-	1/1/15/20	20/39/115/115	-
40	DGD	C	519	-	-	18/51/91/95	0/2/2/2
31	CLA	n	602	-	1/1/15/20	18/39/115/115	-
47	CHL	N1	605	20	4/4/20/26	5/39/137/137	-
41	LHG	D1	409	-	-	29/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	b	614	-	1/1/15/20	14/39/115/115	-
52	3PH	S1	626	-	-	22/49/49/49	-
31	CLA	c	504	-	1/1/15/20	13/39/115/115	-
31	CLA	S1	610	-	1/1/15/20	20/39/115/115	-
47	CHL	g1	608	-	3/3/15/26	1/13/111/137	-
41	LHG	d1	409	-	-	31/53/53/53	-
45	HEM	f	101	6,7	-	2/14/54/54	-
31	CLA	s	603	-	1/1/15/20	16/39/115/115	-
31	CLA	Y1	602	-	1/1/15/20	22/39/115/115	-
45	HEM	F	101	6,7	-	3/14/54/54	-
47	CHL	s	608	-	4/4/19/26	2/33/131/137	-
49	XAT	r	622	-	1/1/12/26	12/31/93/93	0/4/4/4
31	CLA	G	612	-	1/1/10/20	6/13/89/115	-
50	NEX	R1	622	-	-	6/27/83/83	0/3/3/3
47	CHL	g1	609	-	4/4/20/26	7/39/137/137	-
49	XAT	G1	622	-	1/1/12/26	1/31/93/93	0/4/4/4
31	CLA	s1	611	-	1/1/15/20	16/39/115/115	-
31	CLA	c1	507	-	1/1/15/20	20/39/115/115	-
47	CHL	G1	601	21	4/4/20/26	10/39/137/137	-
54	4RF	I1	102	-	-	35/59/59/59	-
31	CLA	C1	506	-	1/1/15/20	18/39/115/115	-
31	CLA	G	602	-	1/1/15/20	21/39/115/115	-
31	CLA	a1	407	-	1/1/11/20	8/20/96/115	-
49	XAT	g1	622	-	2/2/12/26	0/31/93/93	0/4/4/4
32	PHO	a1	408	-	-	4/37/103/103	0/5/6/6
41	LHG	n	624	-	-	30/53/53/53	-
31	CLA	y	612	-	1/1/15/20	14/39/115/115	-
31	CLA	B1	616	-	1/1/15/20	10/39/115/115	-
41	LHG	D1	408	-	-	30/48/48/53	-
31	CLA	n	612	-	1/1/11/20	4/15/91/115	-
50	NEX	Y	623	-	-	2/27/83/83	0/3/3/3
50	NEX	G1	623	-	-	2/27/83/83	0/3/3/3
35	LMG	W1	201	-	-	16/34/54/70	0/1/1/1
48	LUT	S1	621	-	-	2/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	N1	611	-	1/1/11/20	9/20/96/115	-
39	GOL	I1	101	-	-	0/4/4/4	-
50	NEX	s1	623	-	-	3/27/83/83	0/3/3/3
31	CLA	D1	402	-	1/1/15/20	22/39/115/115	-
47	CHL	Y1	609	-	4/4/20/26	6/39/137/137	-
34	SQD	b1	626	-	-	23/49/69/69	0/1/1/1
31	CLA	c1	512	-	1/1/15/20	18/39/115/115	-
31	CLA	C1	509	-	1/1/15/20	14/39/115/115	-
47	CHL	S	607	-	4/4/15/26	1/12/110/137	-
33	BCR	B1	619	-	-	8/29/63/63	0/2/2/2
31	CLA	c	512	-	1/1/15/20	20/39/115/115	-
31	CLA	y	602	-	1/1/15/20	24/39/115/115	-
51	LPX	s	625	-	-	13/31/31/31	-
47	CHL	R	606	-	3/3/15/26	3/13/111/137	-
31	CLA	r	612	-	1/1/14/20	14/33/109/115	-
47	CHL	G1	606	-	3/3/16/26	2/20/118/137	-
41	LHG	G1	624	-	-	29/53/53/53	-
31	CLA	b	607	-	1/1/15/20	18/39/115/115	-
31	CLA	Y	603	-	1/1/15/20	18/39/115/115	-
31	CLA	y	613	-	1/1/15/20	18/39/115/115	-
31	CLA	n	604	-	1/1/15/20	14/39/115/115	-
31	CLA	y1	603	-	1/1/15/20	17/39/115/115	-
57	PTY	Y1	627	-	-	10/20/20/53	-
37	C7Z	b	620	-	1/1/12/26	8/29/67/67	0/2/2/2
31	CLA	g	612	-	1/1/10/20	8/13/89/115	-
31	CLA	C1	501	-	1/1/15/20	12/39/115/115	-
47	CHL	S1	607	-	3/3/15/26	0/12/110/137	-
31	CLA	G1	604	-	1/1/11/20	7/20/96/115	-
47	CHL	g	609	-	4/4/20/26	5/39/137/137	-
47	CHL	s	601	23	3/3/16/26	4/15/113/137	-
31	CLA	S1	617	23	1/1/12/20	8/21/97/115	-
47	CHL	s	606	-	3/3/15/26	0/13/111/137	-
31	CLA	r	613	-	1/1/11/20	10/17/93/115	-
31	CLA	c	502	-	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	Y	610	-	1/1/15/20	18/39/115/115	-
33	BCR	c1	517	-	-	8/29/63/63	0/2/2/2
31	CLA	c	505	-	1/1/15/20	18/39/115/115	-
31	CLA	B1	612	-	1/1/15/20	9/39/115/115	-
31	CLA	s1	610	-	1/1/15/20	18/39/115/115	-
31	CLA	N1	614	-	1/1/11/20	7/20/96/115	-
31	CLA	n1	603	-	1/1/15/20	18/39/115/115	-
31	CLA	g1	610	-	1/1/15/20	16/39/115/115	-
35	LMG	H	102	-	-	10/43/63/70	0/1/1/1
49	XAT	g	622	-	2/2/12/26	1/31/93/93	0/4/4/4
31	CLA	b	609	-	1/1/15/20	11/39/115/115	-
31	CLA	Y1	612	-	1/1/15/20	15/39/115/115	-
40	DGD	c	523	-	-	17/55/95/95	0/2/2/2
48	LUT	r	620	-	-	8/29/67/67	0/2/2/2
31	CLA	y	608	-	1/1/12/20	6/21/97/115	-
47	CHL	G	607	-	3/3/16/26	3/20/118/137	-
48	LUT	S	620	-	1/1/12/27	3/29/67/67	0/2/2/2
40	DGD	c	519	-	-	22/51/91/95	0/2/2/2
35	LMG	D	411	-	-	9/41/61/70	0/1/1/1
40	DGD	b1	623	-	-	11/32/72/95	0/2/2/2
31	CLA	b	604	-	1/1/15/20	19/39/115/115	-
31	CLA	c1	505	-	1/1/15/20	17/39/115/115	-
49	XAT	r1	621	-	1/1/12/26	2/31/93/93	0/4/4/4
47	CHL	N	608	-	3/3/16/26	4/20/118/137	-
31	CLA	y	614	-	1/1/15/20	15/39/115/115	-
47	CHL	y	606	-	4/4/20/26	8/39/137/137	-
35	LMG	D1	411	-	-	11/41/61/70	0/1/1/1
31	CLA	b1	607	-	1/1/15/20	15/39/115/115	-
50	NEX	N	623	-	-	7/27/83/83	0/3/3/3
31	CLA	d1	402	-	1/1/15/20	14/39/115/115	-
34	SQD	a	412	-	-	12/46/66/69	0/1/1/1
31	CLA	C	505	-	1/1/15/20	15/39/115/115	-
31	CLA	R	611	-	1/1/11/20	6/17/93/115	-
31	CLA	S	617	-	1/1/12/20	7/21/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	LUT	S1	620	-	-	2/29/67/67	0/2/2/2
57	PTY	y1	626	-	-	22/53/53/53	-
31	CLA	c	509	-	1/1/15/20	15/39/115/115	-
31	CLA	y1	614	-	1/1/15/20	14/39/115/115	-
31	CLA	c	503	-	1/1/15/20	20/39/115/115	-
42	LMK	C1	527	-	2/2/6/6	16/46/46/60	-
47	CHL	N	606	-	4/4/20/26	6/39/137/137	-
35	LMG	w1	201	-	-	16/34/54/70	0/1/1/1
45	HEM	f1	101	-	-	0/14/54/54	-
31	CLA	G	614	-	1/1/11/20	9/20/96/115	-
31	CLA	N1	602	-	1/1/15/20	11/39/115/115	-
31	CLA	N1	613	-	1/1/15/20	18/39/115/115	-
49	XAT	y1	622	-	-	4/31/93/93	0/4/4/4
54	4RF	K1	101	-	-	29/59/59/59	-
31	CLA	S	613	-	1/1/13/20	13/27/103/115	-
47	CHL	n1	608	-	3/3/16/26	3/20/118/137	-
50	NEX	S1	623	-	-	3/27/83/83	0/3/3/3
54	4RF	k1	101	-	-	35/59/59/59	-
57	PTY	Y1	626	-	-	18/53/53/53	-
47	CHL	S	601	-	3/3/16/26	4/15/113/137	-
31	CLA	s	617	-	1/1/12/20	9/21/97/115	-
34	SQD	c	626	-	-	19/49/69/69	0/1/1/1
31	CLA	s	611	-	1/1/15/20	16/39/115/115	-
31	CLA	N1	610	-	1/1/15/20	18/39/115/115	-
47	CHL	r	607	-	3/3/16/26	4/20/118/137	-
31	CLA	B1	615	-	1/1/15/20	18/39/115/115	-
49	XAT	N1	622	-	1/1/12/26	1/31/93/93	0/4/4/4
41	LHG	C	525	-	-	28/51/51/53	-
46	RRX	h1	101	-	1/1/11/25	9/29/65/65	0/2/2/2
48	LUT	R1	620	-	1/1/12/27	5/29/67/67	0/2/2/2
39	GOL	B	627	-	-	0/4/4/4	-
33	BCR	C	515	-	-	11/29/63/63	0/2/2/2
40	DGD	c1	518	-	-	16/44/84/95	0/2/2/2
31	CLA	B1	613	-	1/1/15/20	17/39/115/115	-
47	CHL	s1	607	-	3/3/15/26	2/12/110/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	B	605	-	1/1/15/20	17/39/115/115	-
31	CLA	y1	602	-	1/1/15/20	17/39/115/115	-
31	CLA	B	616	-	1/1/15/20	15/39/115/115	-
31	CLA	g1	612	-	1/1/10/20	6/13/89/115	-
33	BCR	A	411	-	-	11/29/63/63	0/2/2/2
48	LUT	S	621	-	-	1/29/67/67	0/2/2/2
31	CLA	r	609	-	1/1/14/20	17/33/109/115	-
35	LMG	H1	102	-	-	13/43/63/70	0/1/1/1
31	CLA	s1	614	-	1/1/13/20	11/27/103/115	-
41	LHG	Y	624	-	-	31/53/53/53	-
41	LHG	S	624	-	-	27/49/49/53	-
31	CLA	G1	613	-	1/1/15/20	13/39/115/115	-
31	CLA	s1	609	-	1/1/14/20	16/33/109/115	-
47	CHL	N	609	-	4/4/20/26	10/39/137/137	-
48	LUT	R	620	-	-	9/29/67/67	0/2/2/2
31	CLA	g	614	-	1/1/11/20	10/20/96/115	-
31	CLA	Y	602	24	1/1/15/20	18/39/115/115	-
31	CLA	B	608	-	1/1/15/20	19/39/115/115	-
31	CLA	s1	602	-	1/1/14/20	12/33/109/115	-
31	CLA	y1	610	-	1/1/15/20	11/39/115/115	-
49	XAT	n1	622	-	1/1/12/26	5/31/93/93	0/4/4/4
31	CLA	C	511	-	1/1/15/20	9/39/115/115	-
40	DGD	C1	518	-	-	14/44/84/95	0/2/2/2
31	CLA	s	614	-	1/1/13/20	11/27/103/115	-
31	CLA	a	410	-	1/1/14/20	7/33/109/115	-
31	CLA	Y	604	-	1/1/15/20	17/39/115/115	-
31	CLA	s1	604	-	1/1/13/20	14/27/103/115	-
47	CHL	n	605	-	4/4/20/26	5/39/137/137	-
47	CHL	N1	609	-	4/4/20/26	6/39/137/137	-
41	LHG	d1	410	-	-	25/43/43/53	-
52	3PH	B1	624	-	-	23/49/49/49	-
33	BCR	B1	618	-	-	11/29/63/63	0/2/2/2
47	CHL	s	607	-	4/4/15/26	3/12/110/137	-
48	LUT	G1	620	-	-	4/29/67/67	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	a	406	-	1/1/15/20	9/39/115/115	-
51	LPX	S1	625	-	-	9/31/31/31	-
47	CHL	N	607	-	4/4/20/26	6/39/137/137	-
31	CLA	C	507	-	1/1/15/20	18/39/115/115	-
47	CHL	g	601	21	4/4/20/26	5/39/137/137	-
31	CLA	A1	410	-	1/1/14/20	8/33/109/115	-
31	CLA	R1	602	-	1/1/14/20	15/33/109/115	-
38	DGA	J1	101	-	-	10/30/30/45	-
31	CLA	r1	610	-	1/1/14/20	16/33/109/115	-
35	LMG	C	521	-	-	20/46/66/70	0/1/1/1
48	LUT	G1	621	-	-	4/29/67/67	0/2/2/2
31	CLA	S	605	-	1/1/12/20	12/21/97/115	-
47	CHL	g	607	-	3/3/16/26	3/20/118/137	-
31	CLA	s	605	-	1/1/12/20	10/21/97/115	-
34	SQD	B1	626	-	-	25/49/69/69	0/1/1/1
47	CHL	r1	607	-	3/3/16/26	4/20/118/137	-
47	CHL	s1	608	-	4/4/19/26	4/33/131/137	-
31	CLA	n1	612	-	1/1/11/20	8/15/91/115	-
49	XAT	N	622	-	1/1/12/26	3/31/93/93	0/4/4/4
31	CLA	c	513	-	1/1/15/20	21/39/115/115	-
31	CLA	Y	614	-	1/1/15/20	13/39/115/115	-
47	CHL	g	608	-	3/3/15/26	1/13/111/137	-
35	LMG	d1	411	-	-	11/41/61/70	0/1/1/1
31	CLA	r	603	-	1/1/14/20	16/33/109/115	-
31	CLA	S	603	-	1/1/15/20	12/39/115/115	-
35	LMG	A1	413	-	-	15/43/63/70	0/1/1/1
31	CLA	B1	617	-	1/1/15/20	17/39/115/115	-
31	CLA	n1	614	-	1/1/11/20	7/20/96/115	-
47	CHL	g1	606	-	3/3/16/26	4/20/118/137	-
31	CLA	B1	611	-	1/1/15/20	15/39/115/115	-
31	CLA	C1	502	-	1/1/15/20	13/39/115/115	-
31	CLA	b1	604	-	1/1/15/20	17/39/115/115	-
47	CHL	R	607	-	3/3/16/26	2/20/118/137	-
31	CLA	c1	513	-	1/1/15/20	21/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	A	405	-	1/1/15/20	11/39/115/115	-
31	CLA	R	612	-	1/1/14/20	13/33/109/115	-
31	CLA	b1	609	-	1/1/15/20	11/39/115/115	-
31	CLA	r1	608	-	1/1/14/20	22/33/109/115	-
41	LHG	C1	525	-	-	32/51/51/53	-
31	CLA	C1	505	-	1/1/15/20	21/39/115/115	-
37	C7Z	b1	620	-	1/1/12/26	15/29/67/67	0/2/2/2
48	LUT	G	620	-	-	3/29/67/67	0/2/2/2
31	CLA	B1	609	-	1/1/15/20	17/39/115/115	-
32	PHO	a	408	-	-	12/37/103/103	0/5/6/6
37	C7Z	B	620	-	1/1/12/26	11/29/67/67	0/2/2/2
47	CHL	n	606	-	4/4/20/26	6/39/137/137	-
31	CLA	c	501	-	1/1/15/20	17/39/115/115	-
31	CLA	R1	603	-	1/1/14/20	11/33/109/115	-
31	CLA	Y1	603	-	1/1/15/20	21/39/115/115	-
47	CHL	G	606	-	4/4/16/26	5/20/118/137	-
35	LMG	a1	413	-	-	15/43/63/70	0/1/1/1
35	LMG	b1	622	-	-	15/39/59/70	0/1/1/1
31	CLA	N	614	-	1/1/11/20	8/20/96/115	-
47	CHL	n1	607	-	4/4/20/26	7/39/137/137	-
31	CLA	Y	611	-	1/1/15/20	15/39/115/115	-
31	CLA	D	403	-	1/1/15/20	17/39/115/115	-
31	CLA	s	609	-	1/1/14/20	14/33/109/115	-
44	PL9	D	405	-	-	22/53/73/73	0/1/1/1
50	NEX	N1	623	-	-	5/27/83/83	0/3/3/3
38	DGA	j1	101	-	-	15/30/30/45	-
31	CLA	B	615	-	1/1/15/20	8/39/115/115	-
47	CHL	S	608	-	4/4/19/26	4/33/131/137	-
41	LHG	L	101	-	-	32/53/53/53	-
47	CHL	y1	609	-	4/4/20/26	7/39/137/137	-
48	LUT	n	620	-	-	6/29/67/67	0/2/2/2
48	LUT	n	621	-	1/1/12/27	4/29/67/67	0/2/2/2
33	BCR	c	514	-	-	12/29/63/63	0/2/2/2
31	CLA	g1	602	-	1/1/15/20	23/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	r	611	-	1/1/11/20	7/17/93/115	-
31	CLA	G	613	-	1/1/15/20	17/39/115/115	-
35	LMG	J	101	-	-	14/40/60/70	0/1/1/1
31	CLA	S	610	-	1/1/15/20	14/39/115/115	-
31	CLA	y1	604	-	1/1/15/20	17/39/115/115	-
33	BCR	b	618	-	-	10/29/63/63	0/2/2/2
34	SQD	c1	526	-	-	17/49/69/69	0/1/1/1
33	BCR	C1	515	-	-	10/29/63/63	0/2/2/2
31	CLA	y1	611	-	1/1/15/20	14/39/115/115	-
47	CHL	S1	608	-	4/4/19/26	8/33/131/137	-
48	LUT	y1	620	-	-	3/29/67/67	0/2/2/2
47	CHL	y1	605	-	3/3/16/26	1/15/113/137	-
50	NEX	r	623	-	-	8/27/83/83	0/3/3/3
38	DGA	c	524	-	-	22/45/45/45	-
41	LHG	L1	101	-	-	34/53/53/53	-
48	LUT	N1	620	-	-	5/29/67/67	0/2/2/2
47	CHL	n1	601	20	4/4/20/26	8/39/137/137	-
34	SQD	C	526	-	-	17/49/69/69	0/1/1/1
31	CLA	C1	507	-	1/1/15/20	18/39/115/115	-
47	CHL	g1	605	-	4/4/16/26	4/18/116/137	-
32	PHO	a1	409	-	-	11/37/103/103	0/5/6/6
31	CLA	S1	602	-	1/1/14/20	19/33/109/115	-
50	NEX	y1	623	-	-	7/27/83/83	0/3/3/3
41	LHG	d	408	-	-	28/48/48/53	-
31	CLA	b	617	-	1/1/15/20	14/39/115/115	-
47	CHL	G1	605	-	4/4/16/26	3/18/116/137	-
34	SQD	B	621	-	-	18/49/69/69	0/1/1/1
31	CLA	R	604	-	1/1/11/20	10/20/96/115	-
31	CLA	y	610	-	1/1/15/20	15/39/115/115	-
41	LHG	c	625	-	-	33/51/51/53	-
48	LUT	y	620	-	-	0/29/67/67	0/2/2/2
48	LUT	N1	621	-	-	5/29/67/67	0/2/2/2
49	XAT	y	622	-	-	3/31/93/93	0/4/4/4
31	CLA	d	402	-	1/1/15/20	18/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	LMG	c1	521	-	-	12/46/66/70	0/1/1/1
31	CLA	C	508	-	1/1/15/20	11/39/115/115	-
50	NEX	r1	622	-	-	9/27/83/83	0/3/3/3
31	CLA	S1	609	-	1/1/14/20	14/33/109/115	-
31	CLA	B	612	-	1/1/15/20	21/39/115/115	-
41	LHG	s1	624	-	-	22/49/49/53	-
31	CLA	a1	406	-	1/1/15/20	13/39/115/115	-
31	CLA	c	506	-	1/1/15/20	22/39/115/115	-
31	CLA	G1	603	-	1/1/15/20	18/39/115/115	-
41	LHG	g	624	-	-	27/53/53/53	-
50	NEX	Y1	623	-	-	8/27/83/83	0/3/3/3
47	CHL	n1	605	-	4/4/20/26	9/39/137/137	-
33	BCR	c	515	-	-	10/29/63/63	0/2/2/2
47	CHL	G1	608	-	3/3/15/26	3/13/111/137	-
35	LMG	a	413	-	-	18/43/63/70	0/1/1/1
38	DGA	b	623	-	-	27/45/45/45	-
52	3PH	T1	101	-	-	28/49/49/49	-
57	PTY	y1	627	-	-	14/20/20/53	-
31	CLA	B	613	-	1/1/15/20	14/39/115/115	-
48	LUT	s1	621	-	-	2/29/67/67	0/2/2/2
32	PHO	A1	408	-	-	6/37/103/103	0/5/6/6
31	CLA	c1	502	-	1/1/15/20	13/39/115/115	-
31	CLA	B	602	-	1/1/15/20	21/39/115/115	-
31	CLA	S	602	23	1/1/14/20	13/33/109/115	-
47	CHL	G	601	-	4/4/20/26	3/39/137/137	-
31	CLA	G1	610	-	1/1/15/20	14/39/115/115	-
47	CHL	G	609	-	4/4/20/26	10/39/137/137	-
52	3PH	s1	626	-	-	24/49/49/49	-
33	BCR	c1	515	-	-	13/29/63/63	0/2/2/2
33	BCR	b	619	-	-	9/29/63/63	0/2/2/2
31	CLA	g	611	-	1/1/11/20	7/15/91/115	-
31	CLA	C	502	-	1/1/15/20	18/39/115/115	-
31	CLA	N	612	-	1/1/11/20	7/15/91/115	-
31	CLA	c1	508	-	1/1/15/20	12/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	b	603	-	1/1/15/20	19/39/115/115	-
34	SQD	m1	101	-	-	21/37/57/69	0/1/1/1
33	BCR	C	517	-	-	8/29/63/63	0/2/2/2
31	CLA	S1	612	-	1/1/11/20	6/15/91/115	-
47	CHL	n	601	-	4/4/20/26	5/39/137/137	-
32	PHO	A1	409	-	-	13/37/103/103	0/5/6/6
49	XAT	Y1	622	-	2/2/12/26	2/31/93/93	0/4/4/4
31	CLA	G	611	-	1/1/11/20	6/15/91/115	-
31	CLA	s1	605	23	1/1/12/20	9/21/97/115	-
31	CLA	B	611	-	1/1/15/20	10/39/115/115	-
31	CLA	S	611	-	1/1/15/20	15/39/115/115	-
31	CLA	B1	610	-	1/1/15/20	14/39/115/115	-
31	CLA	C1	512	-	1/1/15/20	18/39/115/115	-
40	DGD	C	523	-	-	16/55/95/95	0/2/2/2
47	CHL	Y	605	24	3/3/16/26	0/15/113/137	-
50	NEX	g	623	-	-	4/27/83/83	0/3/3/3
31	CLA	b	611	-	1/1/15/20	10/39/115/115	-
34	SQD	B1	621	-	-	13/37/57/69	0/1/1/1
31	CLA	A	410	-	1/1/14/20	12/33/109/115	-
31	CLA	C	512	-	1/1/15/20	16/39/115/115	-
31	CLA	n	603	-	1/1/15/20	24/39/115/115	-
52	3PH	i	101	-	-	21/49/49/49	-
42	LMK	c	627	-	1/1/6/6	11/46/46/60	-
49	XAT	n	622	-	-	1/31/93/93	0/4/4/4
31	CLA	c1	510	-	1/1/15/20	17/39/115/115	-
31	CLA	g1	614	-	1/1/11/20	11/20/96/115	-
31	CLA	N	603	-	1/1/15/20	16/39/115/115	-
31	CLA	r	610	-	1/1/14/20	15/33/109/115	-
31	CLA	G	603	-	1/1/15/20	21/39/115/115	-
33	BCR	B	618	-	-	11/29/63/63	0/2/2/2
31	CLA	N	604	-	1/1/15/20	17/39/115/115	-
31	CLA	a	405	-	1/1/15/20	15/39/115/115	-
41	LHG	N1	624	-	-	39/53/53/53	-
47	CHL	Y	601	-	4/4/20/26	5/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
46	RRX	h	101	-	1/1/11/25	7/29/65/65	0/2/2/2
35	LMG	h1	102	-	-	14/43/63/70	0/1/1/1
31	CLA	N1	603	-	1/1/15/20	17/39/115/115	-
31	CLA	b1	613	-	1/1/15/20	20/39/115/115	-
34	SQD	M1	101	-	-	17/37/57/69	0/1/1/1
47	CHL	G1	607	-	4/4/20/26	12/39/137/137	-
50	NEX	S	622	-	-	12/27/83/83	0/3/3/3
41	LHG	S1	624	-	-	25/49/49/53	-
31	CLA	B	610	-	1/1/15/20	20/39/115/115	-
31	CLA	s1	617	-	1/1/12/20	10/21/97/115	-
47	CHL	r	606	-	3/3/15/26	1/13/111/137	-
31	CLA	n1	611	-	1/1/11/20	10/20/96/115	-
40	DGD	C1	519	-	-	21/51/91/95	0/2/2/2
31	CLA	y	603	-	1/1/15/20	10/39/115/115	-
31	CLA	g	610	-	1/1/15/20	12/39/115/115	-
31	CLA	G	604	-	1/1/11/20	9/20/96/115	-
31	CLA	S1	604	-	1/1/13/20	9/27/103/115	-
33	BCR	c1	516	-	-	12/29/63/63	0/2/2/2
31	CLA	d1	403	-	1/1/15/20	11/39/115/115	-
31	CLA	R	603	-	1/1/14/20	16/33/109/115	-
47	CHL	y	609	-	4/4/20/26	4/39/137/137	-
50	NEX	s	623	-	-	7/27/83/83	0/3/3/3
56	ERG	R1	626	-	5/5/11/15	7/13/71/71	0/4/4/4
34	SQD	b	621	-	-	18/49/69/69	0/1/1/1
40	DGD	C1	520	-	-	14/48/88/95	0/2/2/2
50	NEX	G	623	-	-	4/27/83/83	0/3/3/3
49	XAT	R1	621	-	-	2/31/93/93	0/4/4/4
31	CLA	a1	410	-	1/1/14/20	9/33/109/115	-
31	CLA	S1	614	-	1/1/13/20	11/27/103/115	-
33	BCR	C	516	-	-	15/29/63/63	0/2/2/2
32	PHO	A	409	-	-	8/37/103/103	0/5/6/6
41	LHG	y1	624	-	-	26/53/53/53	-
47	CHL	G1	609	-	4/4/20/26	7/39/137/137	-
31	CLA	b1	614	-	1/1/15/20	11/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
51	LPX	S	625	-	-	12/31/31/31	-
31	CLA	n	611	-	1/1/11/20	15/20/96/115	-
47	CHL	G	608	-	3/3/15/26	0/13/111/137	-
31	CLA	n	610	-	1/1/15/20	13/39/115/115	-
33	BCR	a1	411	-	-	13/29/63/63	0/2/2/2
31	CLA	B	614	-	1/1/15/20	13/39/115/115	-
31	CLA	D	402	-	1/1/15/20	17/39/115/115	-
47	CHL	Y	606	-	4/4/20/26	6/39/137/137	-
33	BCR	d	404	-	-	11/29/63/63	0/2/2/2
33	BCR	b1	618	-	-	8/29/63/63	0/2/2/2
35	LMG	j	101	-	-	14/40/60/70	0/1/1/1
41	LHG	D	409	-	-	31/53/53/53	-
31	CLA	c1	504	-	1/1/15/20	16/39/115/115	-
39	GOL	b	624	-	-	1/4/4/4	-
31	CLA	g1	604	-	1/1/11/20	10/20/96/115	-
31	CLA	r	602	-	1/1/14/20	7/33/109/115	-
47	CHL	n	607	-	4/4/20/26	9/39/137/137	-
31	CLA	C	503	-	1/1/15/20	20/39/115/115	-
47	CHL	N1	608	-	3/3/16/26	3/20/118/137	-
31	CLA	G1	611	-	1/1/15/20	16/39/115/115	-
34	SQD	C1	526	-	-	24/49/69/69	0/1/1/1
48	LUT	Y	620	-	-	6/29/67/67	0/2/2/2
46	RRX	H	101	-	1/1/11/25	10/29/65/65	0/2/2/2
50	NEX	n	623	-	-	5/27/83/83	0/3/3/3
47	CHL	y	605	24	3/3/16/26	5/15/113/137	-
48	LUT	y	621	-	-	3/29/67/67	0/2/2/2
38	DGA	c1	524	-	-	22/45/45/45	-
33	BCR	A1	411	-	-	11/29/63/63	0/2/2/2
41	LHG	Y1	624	-	-	25/53/53/53	-
31	CLA	S	604	-	1/1/13/20	11/27/103/115	-
31	CLA	R1	612	-	1/1/14/20	15/33/109/115	-
31	CLA	g	602	-	1/1/15/20	21/39/115/115	-
47	CHL	N1	601	20	4/4/20/26	2/39/137/137	-
38	DGA	C	524	-	-	26/45/45/45	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	s	610	-	1/1/15/20	21/39/115/115	-
38	DGA	B1	625	-	-	23/45/45/45	-
31	CLA	C1	508	-	1/1/15/20	11/39/115/115	-
47	CHL	R1	606	-	3/3/15/26	1/13/111/137	-
41	LHG	N	624	-	-	24/53/53/53	-
50	NEX	n1	623	-	-	5/27/83/83	1/3/3/3
31	CLA	n	613	-	1/1/15/20	17/39/115/115	-
31	CLA	Y1	614	-	1/1/15/20	16/39/115/115	-
40	DGD	c1	519	-	-	18/51/91/95	0/2/2/2
31	CLA	B1	602	-	1/1/15/20	22/39/115/115	-
31	CLA	R1	609	-	1/1/14/20	10/33/109/115	-
47	CHL	N	605	-	4/4/20/26	8/39/137/137	-
31	CLA	N	613	-	1/1/15/20	18/39/115/115	-
31	CLA	b1	617	-	1/1/15/20	18/39/115/115	-
47	CHL	n	609	-	4/4/20/26	12/39/137/137	-
35	LMG	c	521	-	-	20/46/66/70	0/1/1/1
52	3PH	b1	624	-	-	19/49/49/49	-
48	LUT	G	621	-	1/1/12/27	6/29/67/67	0/2/2/2
31	CLA	s	613	-	1/1/13/20	12/27/103/115	-
31	CLA	R	610	-	1/1/14/20	13/33/109/115	-
37	C7Z	B1	620	-	1/1/12/26	11/29/67/67	0/2/2/2
31	CLA	b1	608	-	1/1/15/20	21/39/115/115	-
40	DGD	c1	520	-	-	12/48/88/95	0/2/2/2
47	CHL	y	607	-	4/4/20/26	9/39/137/137	-
35	LMG	d	411	-	-	10/41/61/70	0/1/1/1
31	CLA	y	604	-	1/1/15/20	19/39/115/115	-
31	CLA	d	403	-	1/1/15/20	13/39/115/115	-
31	CLA	Y1	604	-	1/1/15/20	17/39/115/115	-
39	GOL	y	626	-	-	0/4/4/4	-
33	BCR	C1	517	-	-	12/29/63/63	0/2/2/2
31	CLA	B	604	-	1/1/15/20	17/39/115/115	-
48	LUT	N	620	-	-	4/29/67/67	0/2/2/2
41	LHG	l	101	-	-	28/53/53/53	-
31	CLA	c1	501	-	1/1/15/20	15/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
33	BCR	B	619	-	-	3/29/63/63	0/2/2/2
41	LHG	d	409	-	-	27/53/53/53	-
31	CLA	S	609	-	1/1/14/20	12/33/109/115	-
31	CLA	c1	506	-	1/1/15/20	17/39/115/115	-
31	CLA	C	513	-	1/1/15/20	20/39/115/115	-
31	CLA	B	603	-	1/1/15/20	18/39/115/115	-
41	LHG	c1	525	-	-	33/51/51/53	-
31	CLA	C	501	-	1/1/15/20	17/39/115/115	-
38	DGA	C1	524	-	-	35/45/45/45	-
40	DGD	c	520	-	-	15/48/88/95	0/2/2/2
31	CLA	n1	610	-	1/1/15/20	16/39/115/115	-
31	CLA	r1	603	-	1/1/14/20	13/33/109/115	-
53	SPH	y	625	-	-	13/21/21/21	-
31	CLA	R	608	-	1/1/14/20	18/33/109/115	-
31	CLA	a	407	-	1/1/11/20	5/20/96/115	-
31	CLA	r1	602	-	1/1/14/20	15/33/109/115	-
31	CLA	Y	608	-	1/1/12/20	8/21/97/115	-
31	CLA	r1	604	-	1/1/11/20	8/20/96/115	-
31	CLA	A1	405	-	1/1/15/20	12/39/115/115	-
47	CHL	g	605	-	3/3/16/26	1/18/116/137	-
31	CLA	C1	511	-	1/1/15/20	10/39/115/115	-
31	CLA	c1	503	-	1/1/15/20	18/39/115/115	-
31	CLA	y1	608	-	1/1/12/20	9/21/97/115	-
31	CLA	B1	604	-	1/1/15/20	21/39/115/115	-
31	CLA	C1	510	-	1/1/15/20	18/39/115/115	-
31	CLA	G1	612	-	1/1/10/20	7/13/89/115	-
31	CLA	b1	605	-	1/1/15/20	20/39/115/115	-
47	CHL	N	601	20	4/4/20/26	3/39/137/137	-
49	XAT	Y	622	-	1/1/12/26	3/31/93/93	0/4/4/4
41	LHG	s	624	-	-	26/49/49/53	-
31	CLA	A1	407	-	1/1/12/20	6/21/97/115	-
35	LMG	B1	622	-	-	17/39/59/70	0/1/1/1
31	CLA	G	610	-	1/1/15/20	13/39/115/115	-
31	CLA	S1	611	-	1/1/15/20	17/39/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
31	CLA	s	612	-	1/1/11/20	10/15/91/115	-
31	CLA	N	610	-	1/1/15/20	9/39/115/115	-
33	BCR	c1	514	-	-	13/29/63/63	0/2/2/2
47	CHL	Y	609	-	4/4/20/26	9/39/137/137	-
31	CLA	B	606	-	1/1/15/20	15/39/115/115	-
31	CLA	b	616	-	1/1/15/20	11/39/115/115	-
33	BCR	C1	516	-	-	15/29/63/63	0/2/2/2
33	BCR	C	514	-	-	9/29/63/63	0/2/2/2
52	3PH	S	626	-	-	19/49/49/49	-
31	CLA	N1	604	-	1/1/15/20	14/39/115/115	-
53	SPH	A1	414	-	-	13/21/21/21	-
48	LUT	y1	621	-	-	4/29/67/67	0/2/2/2
52	3PH	s	626	-	-	30/49/49/49	-
31	CLA	s	602	-	1/1/14/20	12/33/109/115	-
44	PL9	d	405	-	-	10/53/73/73	0/1/1/1
31	CLA	c1	509	-	1/1/15/20	15/39/115/115	-
41	LHG	y	624	-	-	28/53/53/53	-
41	LHG	D	410	-	-	27/43/43/53	-
47	CHL	n	608	-	3/3/16/26	4/20/118/137	-
31	CLA	s1	612	-	1/1/11/20	6/15/91/115	-
48	LUT	Y	621	-	1/1/12/27	2/29/67/67	0/2/2/2
41	LHG	g1	624	-	-	29/53/53/53	-
31	CLA	R	602	-	1/1/14/20	12/33/109/115	-
31	CLA	n	614	-	1/1/11/20	7/20/96/115	-
31	CLA	g1	613	-	1/1/15/20	15/39/115/115	-
47	CHL	N1	607	-	4/4/20/26	6/39/137/137	-
49	XAT	R	621	-	1/1/12/26	14/31/93/93	0/4/4/4
31	CLA	C1	503	-	1/1/15/20	14/39/115/115	-
32	PHO	a	409	-	-	9/37/103/103	0/5/6/6
47	CHL	s1	606	-	3/3/15/26	1/13/111/137	-
50	NEX	R	622	-	-	11/27/83/83	0/3/3/3
40	DGD	B1	623	-	-	16/32/72/95	0/2/2/2
47	CHL	g	606	-	3/3/16/26	4/20/118/137	-
31	CLA	s1	613	-	1/1/13/20	9/27/103/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	LUT	g1	620	-	-	3/29/67/67	0/2/2/2
42	LMK	c1	527	-	2/2/6/6	13/46/46/60	-
47	CHL	S	606	-	3/3/15/26	1/13/111/137	-
48	LUT	g	620	-	-	6/29/67/67	0/2/2/2
31	CLA	N	611	-	1/1/11/20	12/20/96/115	-
31	CLA	b1	611	-	1/1/15/20	11/39/115/115	-
34	SQD	a1	412	-	-	18/46/66/69	0/1/1/1
31	CLA	n1	602	-	1/1/15/20	21/39/115/115	-
53	SPH	Y1	625	-	-	11/21/21/21	-
48	LUT	s1	620	-	-	4/29/67/67	0/2/2/2
31	CLA	c	511	-	1/1/15/20	15/39/115/115	-
34	SQD	b1	621	-	-	18/37/57/69	0/1/1/1
31	CLA	C	504	-	1/1/15/20	15/39/115/115	-
31	CLA	n1	604	-	1/1/15/20	15/39/115/115	-
33	BCR	D	404	-	-	12/29/63/63	0/2/2/2
48	LUT	g	621	-	-	3/29/67/67	0/2/2/2
53	SPH	a1	414	-	-	12/21/21/21	-
47	CHL	S1	606	-	3/3/15/26	2/13/111/137	-
53	SPH	y1	625	-	-	11/21/21/21	-
41	LHG	D1	410	-	-	23/43/43/53	-
31	CLA	S1	613	-	1/1/13/20	8/27/103/115	-
41	LHG	d1	408	-	-	28/48/48/53	-
31	CLA	R	609	-	1/1/14/20	17/33/109/115	-
48	LUT	Y1	620	-	-	3/29/67/67	0/2/2/2
31	CLA	Y1	611	-	1/1/15/20	14/39/115/115	-
47	CHL	S1	601	23	3/3/16/26	0/15/113/137	-
33	BCR	c	516	-	-	11/29/63/63	0/2/2/2
51	LPX	s1	625	-	-	14/31/31/31	-
53	SPH	Y	625	-	-	12/21/21/21	-
31	CLA	C1	513	-	1/1/15/20	18/39/115/115	-
31	CLA	N1	612	-	1/1/11/20	9/15/91/115	-
31	CLA	B1	607	-	1/1/15/20	15/39/115/115	-
31	CLA	S	612	-	1/1/11/20	6/15/91/115	-
47	CHL	Y1	607	-	4/4/20/26	10/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
47	CHL	g1	601	-	4/4/20/26	14/39/137/137	-
31	CLA	N	602	-	1/1/15/20	14/39/115/115	-
31	CLA	b1	603	-	1/1/15/20	15/39/115/115	-
47	CHL	Y1	605	24	3/3/16/26	1/15/113/137	-
40	DGD	c	518	-	-	9/44/84/95	0/2/2/2
47	CHL	Y	607	-	4/4/20/26	7/39/137/137	-
48	LUT	Y1	621	-	-	2/29/67/67	0/2/2/2
35	LMG	C1	523	-	-	16/50/70/70	0/1/1/1
47	CHL	N1	606	-	4/4/20/26	13/39/137/137	-

All (4002) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	H	101	RRX	C21-C22	38.28	2.24	1.35
56	R1	626	ERG	C1-C10	-24.08	1.10	1.54
56	r1	626	ERG	C1-C10	-23.87	1.10	1.54
56	r1	626	ERG	C10-C9	-21.39	1.28	1.55
56	R1	626	ERG	C10-C9	-20.86	1.29	1.55
37	b	620	C7Z	C25-C26	16.66	1.62	1.34
37	B	620	C7Z	C25-C26	16.46	1.62	1.34
46	h	101	RRX	C26-C25	16.29	1.61	1.34
37	b1	620	C7Z	C25-C26	16.19	1.61	1.34
37	B1	620	C7Z	C25-C26	16.10	1.61	1.34
46	H1	101	RRX	C26-C25	15.79	1.61	1.34
46	h1	101	RRX	C26-C25	15.70	1.60	1.34
37	B	620	C7Z	C5-C6	15.68	1.60	1.34
37	b	620	C7Z	C5-C6	15.66	1.60	1.34
46	H	101	RRX	C26-C25	15.64	1.60	1.34
48	n1	620	LUT	C24-C25	15.63	1.51	1.33
48	n1	621	LUT	C24-C25	15.43	1.51	1.33
48	N1	620	LUT	C24-C25	15.43	1.51	1.33
48	s	620	LUT	C24-C25	15.39	1.51	1.33
37	B1	620	C7Z	C5-C6	15.37	1.60	1.34
48	y1	620	LUT	C24-C25	15.35	1.51	1.33
48	S	620	LUT	C24-C25	15.34	1.51	1.33
48	g1	621	LUT	C24-C25	15.33	1.51	1.33
48	g	620	LUT	C24-C25	15.33	1.51	1.33
46	h1	101	RRX	C5-C6	15.30	1.60	1.34
48	n	621	LUT	C24-C25	15.29	1.51	1.33
48	s1	620	LUT	C24-C25	15.29	1.51	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	y1	621	LUT	C24-C25	15.29	1.51	1.33
48	Y	620	LUT	C24-C25	15.24	1.51	1.33
48	S1	621	LUT	C24-C25	15.24	1.51	1.33
46	H1	101	RRX	C5-C6	15.24	1.60	1.34
37	b1	620	C7Z	C5-C6	15.23	1.60	1.34
48	r1	620	LUT	C24-C25	15.20	1.51	1.33
48	Y1	621	LUT	C24-C25	15.20	1.51	1.33
48	r	620	LUT	C24-C25	15.20	1.51	1.33
48	g1	620	LUT	C24-C25	15.19	1.51	1.33
46	h	101	RRX	C5-C6	15.17	1.59	1.34
48	Y1	620	LUT	C24-C25	15.16	1.51	1.33
48	G1	621	LUT	C24-C25	15.16	1.51	1.33
48	n	620	LUT	C24-C25	15.14	1.51	1.33
48	G	620	LUT	C24-C25	15.13	1.51	1.33
48	N	621	LUT	C24-C25	15.12	1.51	1.33
48	N	620	LUT	C24-C25	15.12	1.51	1.33
48	G1	620	LUT	C24-C25	15.10	1.51	1.33
48	N1	621	LUT	C24-C25	15.08	1.51	1.33
48	g	621	LUT	C24-C25	15.07	1.51	1.33
48	G	621	LUT	C24-C25	15.05	1.51	1.33
48	s	621	LUT	C24-C25	15.03	1.51	1.33
48	S	621	LUT	C24-C25	15.02	1.51	1.33
46	H	101	RRX	C5-C6	15.01	1.59	1.34
48	S1	620	LUT	C24-C25	14.99	1.51	1.33
48	y	620	LUT	C24-C25	14.99	1.51	1.33
48	R1	620	LUT	C24-C25	14.99	1.51	1.33
48	s1	621	LUT	C24-C25	14.92	1.50	1.33
48	R	620	LUT	C24-C25	14.88	1.50	1.33
48	y	621	LUT	C24-C25	14.80	1.50	1.33
48	Y	621	LUT	C24-C25	14.59	1.50	1.33
56	r1	626	ERG	C10-C5	-14.42	1.25	1.52
56	R1	626	ERG	C10-C5	-14.37	1.25	1.52
56	r1	626	ERG	C4-C3	-13.95	1.27	1.52
56	R1	626	ERG	C4-C3	-13.47	1.28	1.52
37	B1	620	C7Z	C24-C23	12.33	1.73	1.52
56	r1	626	ERG	C2-C3	-11.71	1.24	1.51
37	b	620	C7Z	C24-C23	11.56	1.72	1.52
56	R1	626	ERG	C2-C3	-11.43	1.25	1.51
37	b	620	C7Z	C22-C23	-11.42	1.36	1.52
37	B	620	C7Z	C24-C23	11.38	1.72	1.52
37	b1	620	C7Z	C24-C23	11.29	1.72	1.52
37	B	620	C7Z	C22-C23	-11.17	1.36	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	h1	101	RRX	C29-C28	-10.63	1.37	1.52
37	b1	620	C7Z	C22-C23	-10.54	1.37	1.52
37	b	620	C7Z	C2-C3	-10.47	1.37	1.52
37	b1	620	C7Z	C2-C3	-10.44	1.37	1.52
46	H1	101	RRX	C29-C28	-10.43	1.37	1.52
37	B1	620	C7Z	C2-C3	-10.42	1.37	1.52
37	B	620	C7Z	C2-C3	-10.33	1.37	1.52
46	h	101	RRX	C29-C28	-10.24	1.37	1.52
46	H	101	RRX	C29-C28	-10.08	1.38	1.52
37	B1	620	C7Z	C22-C23	-10.02	1.38	1.52
32	A1	408	PHO	C1B-C2B	9.54	1.50	1.39
32	a1	408	PHO	C1B-C2B	9.46	1.49	1.39
56	r1	626	ERG	C12-C13	9.45	1.70	1.54
56	R1	626	ERG	C12-C13	9.38	1.70	1.54
56	R1	626	ERG	O1-C3	9.33	1.70	1.43
32	a	408	PHO	C1B-C2B	9.33	1.49	1.39
32	A	409	PHO	C1B-C2B	9.32	1.49	1.39
56	r1	626	ERG	O1-C3	9.28	1.70	1.43
32	a1	409	PHO	C1B-C2B	9.23	1.49	1.39
32	A	408	PHO	C1B-C2B	9.22	1.49	1.39
32	a1	408	PHO	C3B-C4B	9.15	1.50	1.41
32	a	409	PHO	C1B-C2B	8.94	1.49	1.39
32	A1	409	PHO	C3B-C4B	8.93	1.50	1.41
32	A	409	PHO	C3B-C4B	8.81	1.50	1.41
47	G	601	CHL	C3A-C2A	-8.81	1.47	1.54
32	A1	408	PHO	C3B-C4B	8.80	1.50	1.41
32	a1	409	PHO	C3B-C4B	8.76	1.50	1.41
32	a	409	PHO	C3B-C4B	8.75	1.50	1.41
32	a	408	PHO	C3B-C4B	8.70	1.50	1.41
32	A1	409	PHO	C1B-C2B	8.69	1.49	1.39
32	A	408	PHO	C3B-C4B	8.67	1.50	1.41
37	b1	620	C7Z	C4-C3	8.55	1.67	1.52
56	R1	626	ERG	C6-C5	8.54	1.54	1.34
56	r1	626	ERG	C6-C5	8.51	1.54	1.34
37	B1	620	C7Z	C4-C3	8.49	1.67	1.52
37	B	620	C7Z	C4-C3	8.44	1.67	1.52
37	b	620	C7Z	C4-C3	8.22	1.66	1.52
46	H	101	RRX	C27-C28	7.98	1.66	1.52
46	h	101	RRX	C27-C28	7.97	1.66	1.52
46	H	101	RRX	C23-C22	7.80	1.62	1.46
46	h1	101	RRX	C27-C28	7.73	1.65	1.52
47	G	609	CHL	C3A-C2A	-7.60	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	H1	101	RRX	C27-C28	7.56	1.65	1.52
47	N1	608	CHL	C3A-C2A	-7.50	1.48	1.54
42	C1	527	LMK	O3-C4	7.38	1.44	1.22
42	C	527	LMK	O3-C4	7.34	1.43	1.22
42	c1	527	LMK	O3-C4	7.32	1.43	1.22
42	c	627	LMK	O3-C4	7.30	1.43	1.22
47	Y1	606	CHL	C3A-C2A	-7.06	1.48	1.54
47	n	609	CHL	C3A-C2A	-6.93	1.48	1.54
50	r1	622	NEX	C7-C8	6.82	1.43	1.31
46	h	101	RRX	C2-C3	-6.71	1.36	1.52
46	h1	101	RRX	C2-C3	-6.65	1.36	1.52
46	H1	101	RRX	C2-C3	-6.63	1.36	1.52
46	H	101	RRX	C2-C3	-6.62	1.36	1.52
46	H	101	RRX	C1-C6	-6.60	1.45	1.53
50	s	623	NEX	C35-C15	-6.59	1.18	1.36
47	G	601	CHL	C3B-C4B	6.58	1.47	1.41
50	n	623	NEX	C35-C15	-6.58	1.18	1.36
47	N	601	CHL	C3A-C2A	-6.58	1.49	1.54
31	r1	612	CLA	MG-NA	6.55	2.21	2.06
31	s1	611	CLA	MG-NA	6.55	2.21	2.06
31	c	509	CLA	MG-NA	6.52	2.21	2.06
50	g1	623	NEX	C35-C15	-6.52	1.18	1.36
50	Y1	623	NEX	C11-C12	-6.52	1.17	1.34
50	r	623	NEX	C35-C15	-6.50	1.18	1.36
50	N	623	NEX	C35-C15	-6.50	1.18	1.36
31	b1	616	CLA	MG-NA	6.49	2.21	2.06
31	s1	613	CLA	MG-NA	6.49	2.21	2.06
50	G	623	NEX	C11-C12	-6.49	1.17	1.34
31	r	612	CLA	MG-NA	6.49	2.21	2.06
31	R	611	CLA	MG-NA	6.49	2.21	2.06
31	s1	605	CLA	MG-NA	6.48	2.21	2.06
31	b	616	CLA	MG-NA	6.48	2.21	2.06
31	c	513	CLA	MG-NA	6.48	2.21	2.06
31	R1	608	CLA	MG-NA	6.48	2.21	2.06
31	s	609	CLA	MG-NA	6.48	2.21	2.06
31	s	605	CLA	MG-NA	6.47	2.21	2.06
50	r1	622	NEX	C11-C12	-6.47	1.17	1.34
50	R	622	NEX	C35-C15	-6.46	1.18	1.36
31	b1	602	CLA	MG-NA	6.46	2.21	2.06
50	G1	623	NEX	C35-C15	-6.46	1.18	1.36
31	N1	613	CLA	MG-NA	6.46	2.21	2.06
31	n1	612	CLA	MG-NA	6.46	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	S1	603	CLA	MG-NA	6.46	2.21	2.06
31	R1	612	CLA	MG-NA	6.45	2.21	2.06
31	B	616	CLA	MG-NA	6.45	2.21	2.06
50	s1	623	NEX	C35-C15	-6.45	1.18	1.36
50	N1	623	NEX	C35-C15	-6.45	1.18	1.36
31	c1	513	CLA	MG-NA	6.45	2.21	2.06
31	g1	614	CLA	MG-NA	6.45	2.21	2.06
31	n	611	CLA	MG-NA	6.45	2.21	2.06
31	r1	608	CLA	MG-NA	6.45	2.21	2.06
31	B1	615	CLA	MG-NA	6.44	2.21	2.06
31	N	611	CLA	MG-NA	6.44	2.21	2.06
31	r	611	CLA	MG-NA	6.44	2.21	2.06
31	g	611	CLA	MG-NA	6.44	2.21	2.06
31	r	603	CLA	MG-NA	6.44	2.21	2.06
50	G	623	NEX	C35-C15	-6.44	1.18	1.36
50	S	622	NEX	C35-C15	-6.43	1.18	1.36
31	S	617	CLA	MG-NA	6.43	2.21	2.06
31	g	613	CLA	MG-NA	6.43	2.21	2.06
31	R	603	CLA	MG-NA	6.42	2.21	2.06
46	H1	101	RRX	C1-C6	-6.42	1.45	1.53
47	N1	605	CHL	C3A-C2A	-6.42	1.49	1.54
31	b1	609	CLA	MG-NA	6.42	2.21	2.06
31	C1	512	CLA	MG-NA	6.41	2.21	2.06
50	g	623	NEX	C35-C15	-6.41	1.18	1.36
31	s	611	CLA	MG-NA	6.41	2.21	2.06
50	R1	622	NEX	C11-C12	-6.41	1.17	1.34
31	g1	603	CLA	MG-NA	6.41	2.21	2.06
31	s	617	CLA	MG-NA	6.41	2.21	2.06
50	R1	622	NEX	C35-C15	-6.41	1.18	1.36
31	g1	612	CLA	MG-NA	6.41	2.21	2.06
50	r1	622	NEX	C35-C15	-6.41	1.18	1.36
31	R1	603	CLA	MG-NA	6.41	2.21	2.06
31	s1	603	CLA	MG-NA	6.41	2.21	2.06
31	Y1	608	CLA	MG-NA	6.40	2.21	2.06
50	Y	623	NEX	C35-C15	-6.40	1.18	1.36
31	B	607	CLA	MG-NA	6.40	2.21	2.06
31	s1	609	CLA	MG-NA	6.40	2.21	2.06
31	R	610	CLA	MG-NA	6.40	2.21	2.06
31	R	608	CLA	MG-NA	6.40	2.21	2.06
50	S1	623	NEX	C35-C15	-6.40	1.18	1.36
31	s	603	CLA	MG-NA	6.40	2.21	2.06
31	c1	505	CLA	MG-NA	6.40	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	602	CLA	MG-NA	6.40	2.21	2.06
31	G	613	CLA	MG-NA	6.40	2.21	2.06
31	n1	614	CLA	MG-NA	6.40	2.21	2.06
31	s	612	CLA	MG-NA	6.39	2.21	2.06
31	R	612	CLA	MG-NA	6.39	2.21	2.06
47	n	605	CHL	C3A-C2A	-6.39	1.49	1.54
31	b1	615	CLA	MG-NA	6.39	2.21	2.06
31	b	602	CLA	MG-NA	6.39	2.21	2.06
31	G1	614	CLA	MG-NA	6.38	2.21	2.06
31	B	609	CLA	MG-NA	6.38	2.21	2.06
31	r	613	CLA	MG-NA	6.38	2.21	2.06
31	g	612	CLA	MG-NA	6.38	2.21	2.06
31	c1	512	CLA	MG-NA	6.38	2.21	2.06
31	R	613	CLA	MG-NA	6.37	2.21	2.06
31	s	613	CLA	MG-NA	6.37	2.21	2.06
31	b	608	CLA	MG-NA	6.37	2.21	2.06
31	s	610	CLA	MG-NA	6.37	2.21	2.06
31	S	612	CLA	MG-NA	6.37	2.21	2.06
31	R	602	CLA	MG-NA	6.37	2.21	2.06
50	R	622	NEX	C11-C12	-6.37	1.18	1.34
31	r	610	CLA	MG-NA	6.37	2.21	2.06
31	n	614	CLA	MG-NA	6.37	2.21	2.06
31	g	604	CLA	MG-NA	6.37	2.21	2.06
31	s1	604	CLA	MG-NA	6.37	2.21	2.06
31	c	503	CLA	MG-NA	6.36	2.21	2.06
31	y	608	CLA	MG-NA	6.36	2.21	2.06
50	n1	623	NEX	C35-C15	-6.36	1.18	1.36
31	g	614	CLA	MG-NA	6.36	2.21	2.06
31	r	602	CLA	MG-NA	6.36	2.21	2.06
50	Y1	623	NEX	C35-C15	-6.36	1.18	1.36
50	y	623	NEX	C35-C15	-6.36	1.18	1.36
31	B	604	CLA	MG-NA	6.36	2.21	2.06
31	C	512	CLA	MG-NA	6.36	2.21	2.06
50	N	623	NEX	C11-C12	-6.36	1.18	1.34
31	Y	608	CLA	MG-NA	6.36	2.21	2.06
31	S	602	CLA	MG-NA	6.35	2.21	2.06
31	d1	402	CLA	MG-NA	6.35	2.21	2.06
50	y1	623	NEX	C35-C15	-6.35	1.18	1.36
31	G1	612	CLA	MG-NA	6.35	2.21	2.06
31	N	612	CLA	MG-NA	6.35	2.21	2.06
31	Y	611	CLA	MG-NA	6.35	2.21	2.06
31	b	609	CLA	MG-NA	6.35	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	N	613	CLA	MG-NA	6.35	2.21	2.06
31	n	602	CLA	MG-NA	6.35	2.21	2.06
31	b1	614	CLA	MG-NA	6.35	2.21	2.06
31	c	512	CLA	MG-NA	6.35	2.21	2.06
31	C	503	CLA	MG-NA	6.35	2.21	2.06
31	B1	609	CLA	MG-NA	6.35	2.21	2.06
31	G	612	CLA	MG-NA	6.34	2.21	2.06
31	d	403	CLA	MG-NA	6.34	2.21	2.06
31	B	610	CLA	MG-NA	6.34	2.21	2.06
31	S	609	CLA	MG-NA	6.34	2.21	2.06
31	r1	602	CLA	MG-NA	6.34	2.21	2.06
31	b1	603	CLA	MG-NA	6.34	2.21	2.06
31	r1	603	CLA	MG-NA	6.34	2.21	2.06
31	B	611	CLA	MG-NA	6.34	2.21	2.06
31	N1	611	CLA	MG-NA	6.33	2.21	2.06
31	c1	501	CLA	MG-NA	6.33	2.21	2.06
31	n1	613	CLA	MG-NA	6.33	2.21	2.06
31	y1	608	CLA	MG-NA	6.33	2.21	2.06
31	y1	611	CLA	MG-NA	6.33	2.21	2.06
31	G	611	CLA	MG-NA	6.33	2.21	2.06
31	g1	604	CLA	MG-NA	6.33	2.21	2.06
31	B1	602	CLA	MG-NA	6.33	2.21	2.06
31	s1	617	CLA	MG-NA	6.33	2.21	2.06
50	N1	623	NEX	C11-C12	-6.33	1.18	1.34
31	Y1	603	CLA	MG-NA	6.33	2.21	2.06
31	c1	507	CLA	MG-NA	6.33	2.21	2.06
31	c1	506	CLA	MG-NA	6.33	2.21	2.06
31	b	611	CLA	MG-NA	6.33	2.21	2.06
31	S1	609	CLA	MG-NA	6.33	2.21	2.06
31	g1	611	CLA	MG-NA	6.33	2.21	2.06
31	D	403	CLA	MG-NA	6.32	2.21	2.06
31	b1	617	CLA	MG-NA	6.32	2.21	2.06
50	g	623	NEX	C7-C8	6.32	1.42	1.31
31	C	507	CLA	MG-NA	6.32	2.21	2.06
31	R1	602	CLA	MG-NA	6.32	2.21	2.06
31	N	614	CLA	MG-NA	6.32	2.21	2.06
31	S	603	CLA	MG-NA	6.32	2.21	2.06
31	n	612	CLA	MG-NA	6.32	2.21	2.06
31	C	511	CLA	MG-NA	6.32	2.21	2.06
31	G1	604	CLA	MG-NA	6.32	2.21	2.06
31	c1	509	CLA	MG-NA	6.32	2.21	2.06
31	s1	614	CLA	MG-NA	6.31	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	604	CLA	MG-NA	6.31	2.21	2.06
31	B1	608	CLA	MG-NA	6.31	2.21	2.06
31	r	608	CLA	MG-NA	6.31	2.21	2.06
31	b1	608	CLA	MG-NA	6.31	2.21	2.06
31	S	611	CLA	MG-NA	6.31	2.21	2.06
31	n	613	CLA	MG-NA	6.31	2.21	2.06
31	N	610	CLA	MG-NA	6.31	2.21	2.06
31	C1	503	CLA	MG-NA	6.31	2.21	2.06
31	g1	610	CLA	MG-NA	6.31	2.21	2.06
31	S	605	CLA	MG-NA	6.31	2.21	2.06
31	A1	407	CLA	MG-NA	6.31	2.21	2.06
31	Y	614	CLA	MG-NA	6.30	2.21	2.06
31	y	612	CLA	MG-NA	6.30	2.21	2.06
31	C1	502	CLA	MG-NA	6.30	2.21	2.06
31	n1	603	CLA	MG-NA	6.30	2.21	2.06
31	S	613	CLA	MG-NA	6.30	2.21	2.06
31	G	604	CLA	MG-NA	6.29	2.21	2.06
31	S1	604	CLA	MG-NA	6.29	2.21	2.06
31	y1	612	CLA	MG-NA	6.29	2.21	2.06
31	A1	405	CLA	MG-NA	6.29	2.21	2.06
31	N1	612	CLA	MG-NA	6.29	2.21	2.06
31	S1	605	CLA	MG-NA	6.29	2.21	2.06
31	Y	612	CLA	MG-NA	6.29	2.21	2.06
31	Y	613	CLA	MG-NA	6.29	2.21	2.06
31	Y1	602	CLA	MG-NA	6.29	2.21	2.06
31	S1	617	CLA	MG-NA	6.29	2.21	2.06
31	a1	407	CLA	MG-NA	6.28	2.21	2.06
31	r1	609	CLA	MG-NA	6.28	2.21	2.06
31	r	609	CLA	MG-NA	6.28	2.21	2.06
31	B1	604	CLA	MG-NA	6.28	2.21	2.06
31	B1	613	CLA	MG-NA	6.28	2.21	2.06
31	b1	611	CLA	MG-NA	6.28	2.21	2.06
31	Y1	614	CLA	MG-NA	6.28	2.21	2.06
31	B	612	CLA	MG-NA	6.28	2.21	2.06
31	R	609	CLA	MG-NA	6.28	2.21	2.06
31	c1	511	CLA	MG-NA	6.28	2.21	2.06
31	n1	604	CLA	MG-NA	6.28	2.21	2.06
31	y1	614	CLA	MG-NA	6.28	2.21	2.06
50	G	623	NEX	C7-C8	6.27	1.42	1.31
31	N	604	CLA	MG-NA	6.27	2.21	2.06
31	c	506	CLA	MG-NA	6.27	2.21	2.06
31	y	610	CLA	MG-NA	6.27	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	a1	410	CLA	MG-NA	6.27	2.21	2.06
50	R	622	NEX	C31-C32	-6.27	1.18	1.34
31	R1	609	CLA	MG-NA	6.27	2.21	2.06
31	s1	610	CLA	MG-NA	6.27	2.21	2.06
46	h	101	RRX	C1-C6	-6.27	1.45	1.53
31	a1	405	CLA	MG-NA	6.27	2.21	2.06
31	y1	604	CLA	MG-NA	6.27	2.21	2.06
50	s1	623	NEX	C11-C12	-6.27	1.18	1.34
31	b	615	CLA	MG-NA	6.27	2.21	2.06
31	S	604	CLA	MG-NA	6.27	2.21	2.06
31	G1	603	CLA	MG-NA	6.27	2.21	2.06
31	c	507	CLA	MG-NA	6.27	2.21	2.06
31	r1	610	CLA	MG-NA	6.27	2.21	2.06
31	a	407	CLA	MG-NA	6.26	2.21	2.06
31	n1	611	CLA	MG-NA	6.26	2.21	2.06
31	B1	607	CLA	MG-NA	6.26	2.21	2.06
31	y	614	CLA	MG-NA	6.26	2.21	2.06
31	c	511	CLA	MG-NA	6.26	2.21	2.06
50	n	623	NEX	C31-C32	-6.26	1.18	1.34
31	G1	613	CLA	MG-NA	6.26	2.21	2.06
31	S1	614	CLA	MG-NA	6.26	2.21	2.06
31	R1	610	CLA	MG-NA	6.26	2.21	2.06
31	C1	511	CLA	MG-NA	6.26	2.21	2.06
31	B1	611	CLA	MG-NA	6.26	2.21	2.06
31	R	604	CLA	MG-NA	6.25	2.21	2.06
31	c1	510	CLA	MG-NA	6.25	2.21	2.06
31	B	608	CLA	MG-NA	6.25	2.21	2.06
47	g1	606	CHL	C3A-C2A	-6.25	1.49	1.54
31	B1	614	CLA	MG-NA	6.25	2.21	2.06
31	Y1	612	CLA	MG-NA	6.25	2.21	2.06
31	D1	403	CLA	MG-NA	6.25	2.21	2.06
31	c	502	CLA	MG-NA	6.25	2.21	2.06
50	G1	623	NEX	C11-C12	-6.25	1.18	1.34
31	g	603	CLA	MG-NA	6.25	2.21	2.06
31	S1	612	CLA	MG-NA	6.25	2.21	2.06
31	b1	610	CLA	MG-NA	6.24	2.21	2.06
31	g1	613	CLA	MG-NA	6.24	2.21	2.06
31	A	407	CLA	MG-NA	6.24	2.21	2.06
50	s1	623	NEX	C31-C32	-6.24	1.18	1.34
31	a	410	CLA	MG-NA	6.24	2.21	2.06
50	Y1	623	NEX	C31-C32	-6.24	1.18	1.34
31	g	602	CLA	MG-NA	6.24	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	G	614	CLA	MG-NA	6.24	2.21	2.06
31	G1	611	CLA	MG-NA	6.24	2.21	2.06
31	b	603	CLA	MG-NA	6.23	2.21	2.06
31	g1	602	CLA	MG-NA	6.23	2.21	2.06
31	d1	403	CLA	MG-NA	6.23	2.21	2.06
31	b1	606	CLA	MG-NA	6.23	2.21	2.06
31	B	606	CLA	MG-NA	6.23	2.21	2.06
31	R1	604	CLA	MG-NA	6.23	2.21	2.06
31	b	607	CLA	MG-NA	6.23	2.21	2.06
31	B	614	CLA	MG-NA	6.23	2.21	2.06
31	y	611	CLA	MG-NA	6.23	2.21	2.06
31	B	613	CLA	MG-NA	6.22	2.21	2.06
31	S1	613	CLA	MG-NA	6.22	2.21	2.06
31	y1	603	CLA	MG-NA	6.22	2.21	2.06
31	C	510	CLA	MG-NA	6.22	2.21	2.06
31	C	502	CLA	MG-NA	6.22	2.21	2.06
31	Y1	604	CLA	MG-NA	6.22	2.21	2.06
31	B1	616	CLA	MG-NA	6.22	2.21	2.06
56	r1	626	ERG	C16-C17	-6.22	1.41	1.54
31	c	505	CLA	MG-NA	6.22	2.21	2.06
31	c1	503	CLA	MG-NA	6.22	2.21	2.06
50	N1	623	NEX	C31-C32	-6.21	1.18	1.34
31	y1	602	CLA	MG-NA	6.21	2.21	2.06
50	r	623	NEX	C31-C32	-6.21	1.18	1.34
31	A1	406	CLA	MG-NA	6.21	2.21	2.06
50	n	623	NEX	C11-C12	-6.21	1.18	1.34
31	C1	501	CLA	MG-NA	6.21	2.21	2.06
31	C	506	CLA	MG-NA	6.21	2.21	2.06
31	S1	611	CLA	MG-NA	6.21	2.21	2.06
31	G	603	CLA	MG-NA	6.21	2.21	2.06
50	N	623	NEX	C31-C32	-6.21	1.18	1.34
31	s	604	CLA	MG-NA	6.20	2.21	2.06
31	Y1	611	CLA	MG-NA	6.20	2.21	2.06
31	B1	610	CLA	MG-NA	6.20	2.21	2.06
31	B	603	CLA	MG-NA	6.20	2.21	2.06
31	c1	504	CLA	MG-NA	6.20	2.21	2.06
31	S	614	CLA	MG-NA	6.20	2.21	2.06
31	n1	602	CLA	MG-NA	6.20	2.21	2.06
31	s1	612	CLA	MG-NA	6.20	2.21	2.06
31	N	602	CLA	MG-NA	6.20	2.21	2.06
31	b	617	CLA	MG-NA	6.19	2.21	2.06
31	B1	606	CLA	MG-NA	6.19	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C1	507	CLA	MG-NA	6.19	2.21	2.06
31	N1	603	CLA	MG-NA	6.19	2.21	2.06
31	N	603	CLA	MG-NA	6.19	2.21	2.06
31	S1	602	CLA	MG-NA	6.19	2.21	2.06
31	b1	613	CLA	MG-NA	6.19	2.21	2.06
31	b	612	CLA	MG-NA	6.19	2.21	2.06
50	g1	623	NEX	C31-C32	-6.19	1.18	1.34
31	N1	614	CLA	MG-NA	6.19	2.21	2.06
50	r	623	NEX	C11-C12	-6.19	1.18	1.34
31	A	410	CLA	MG-NA	6.19	2.21	2.06
31	Y	603	CLA	MG-NA	6.19	2.21	2.06
31	B1	617	CLA	MG-NA	6.19	2.21	2.06
31	G	602	CLA	MG-NA	6.19	2.21	2.06
31	c	501	CLA	MG-NA	6.19	2.21	2.06
50	S1	623	NEX	C31-C32	-6.18	1.18	1.34
50	s	623	NEX	C31-C32	-6.18	1.18	1.34
31	B1	603	CLA	MG-NA	6.18	2.21	2.06
31	y	613	CLA	MG-NA	6.18	2.21	2.06
56	R1	626	ERG	C16-C17	-6.18	1.41	1.54
31	r	604	CLA	MG-NA	6.18	2.20	2.06
50	N	623	NEX	C7-C8	6.18	1.41	1.31
31	S1	610	CLA	MG-NA	6.18	2.20	2.06
31	C1	513	CLA	MG-NA	6.17	2.20	2.06
31	G1	602	CLA	MG-NA	6.17	2.20	2.06
50	R1	622	NEX	C31-C32	-6.17	1.18	1.34
50	S1	623	NEX	C11-C12	-6.17	1.18	1.34
31	C	509	CLA	MG-NA	6.17	2.20	2.06
31	g	610	CLA	MG-NA	6.17	2.20	2.06
50	g	623	NEX	C11-C12	-6.17	1.18	1.34
31	N1	604	CLA	MG-NA	6.16	2.20	2.06
31	y1	613	CLA	MG-NA	6.16	2.20	2.06
50	G1	623	NEX	C31-C32	-6.16	1.18	1.34
31	B	605	CLA	MG-NA	6.16	2.20	2.06
31	Y	604	CLA	MG-NA	6.16	2.20	2.06
47	y	606	CHL	C3A-C2A	-6.16	1.49	1.54
31	C	501	CLA	MG-NA	6.16	2.20	2.06
50	S	622	NEX	C11-C12	-6.16	1.18	1.34
31	A1	410	CLA	MG-NA	6.15	2.20	2.06
50	G	623	NEX	C31-C32	-6.15	1.18	1.34
31	b1	604	CLA	MG-NA	6.15	2.20	2.06
31	d	402	CLA	MG-NA	6.15	2.20	2.06
31	c	510	CLA	MG-NA	6.15	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	r1	604	CLA	MG-NA	6.15	2.20	2.06
47	n	606	CHL	C3B-C4B	6.15	1.47	1.41
31	B	617	CLA	MG-NA	6.15	2.20	2.06
31	b	605	CLA	MG-NA	6.15	2.20	2.06
31	C	513	CLA	MG-NA	6.14	2.20	2.06
31	S	610	CLA	MG-NA	6.14	2.20	2.06
31	C1	505	CLA	MG-NA	6.14	2.20	2.06
47	Y	605	CHL	C3A-C2A	-6.14	1.49	1.54
31	Y1	613	CLA	MG-NA	6.14	2.20	2.06
31	y	604	CLA	MG-NA	6.14	2.20	2.06
31	A	406	CLA	MG-NA	6.14	2.20	2.06
33	c1	517	BCR	C24-C23	6.13	1.51	1.33
50	r1	622	NEX	C31-C32	-6.13	1.18	1.34
50	Y	623	NEX	C31-C32	-6.13	1.18	1.34
31	Y	610	CLA	MG-NA	6.13	2.20	2.06
31	B1	612	CLA	MG-NA	6.12	2.20	2.06
31	n	603	CLA	MG-NA	6.12	2.20	2.06
31	a	406	CLA	MG-NA	6.12	2.20	2.06
31	b1	607	CLA	MG-NA	6.12	2.20	2.06
31	b	614	CLA	MG-NA	6.12	2.20	2.06
31	c1	502	CLA	MG-NA	6.12	2.20	2.06
50	g	623	NEX	C31-C32	-6.12	1.18	1.34
31	n1	610	CLA	MG-NA	6.11	2.20	2.06
31	y1	610	CLA	MG-NA	6.11	2.20	2.06
31	a	405	CLA	MG-NA	6.11	2.20	2.06
31	C1	506	CLA	MG-NA	6.11	2.20	2.06
31	b	610	CLA	MG-NA	6.10	2.20	2.06
37	b1	620	C7Z	C1-C6	-6.10	1.46	1.53
31	Y	602	CLA	MG-NA	6.10	2.20	2.06
33	b	619	BCR	C24-C23	6.09	1.51	1.33
31	c	504	CLA	MG-NA	6.09	2.20	2.06
31	s	614	CLA	MG-NA	6.09	2.20	2.06
50	s	623	NEX	C11-C12	-6.09	1.18	1.34
31	s1	602	CLA	MG-NA	6.09	2.20	2.06
31	C	505	CLA	MG-NA	6.09	2.20	2.06
31	C1	510	CLA	MG-NA	6.08	2.20	2.06
47	S1	606	CHL	C3A-C2A	-6.08	1.49	1.54
50	y1	623	NEX	C31-C32	-6.08	1.18	1.34
47	R1	606	CHL	C3B-C4B	6.08	1.47	1.41
46	H	101	RRX	C37-C22	6.08	1.63	1.50
31	y	603	CLA	MG-NA	6.08	2.20	2.06
31	c1	508	CLA	MG-NA	6.07	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B	615	CLA	MG-NA	6.07	2.20	2.06
31	b1	612	CLA	MG-NA	6.07	2.20	2.06
31	C	508	CLA	MG-NA	6.07	2.20	2.06
31	b	606	CLA	MG-NA	6.06	2.20	2.06
31	B1	605	CLA	MG-NA	6.06	2.20	2.06
50	S	622	NEX	C31-C32	-6.06	1.18	1.34
31	a1	406	CLA	MG-NA	6.05	2.20	2.06
31	c	508	CLA	MG-NA	6.04	2.20	2.06
31	C1	509	CLA	MG-NA	6.04	2.20	2.06
31	G1	610	CLA	MG-NA	6.03	2.20	2.06
50	y1	623	NEX	C11-C12	-6.03	1.18	1.34
47	s	601	CHL	C3B-C4B	6.03	1.47	1.41
31	D	402	CLA	MG-NA	6.02	2.20	2.06
50	y	623	NEX	C11-C12	-6.01	1.19	1.34
31	C1	504	CLA	MG-NA	6.01	2.20	2.06
31	A	405	CLA	MG-NA	6.01	2.20	2.06
50	y	623	NEX	C31-C32	-6.00	1.19	1.34
31	N1	602	CLA	MG-NA	6.00	2.20	2.06
47	S1	601	CHL	C3B-C4B	6.00	1.47	1.41
31	b	613	CLA	MG-NA	5.99	2.20	2.06
31	s	602	CLA	MG-NA	5.99	2.20	2.06
50	g1	623	NEX	C11-C12	-5.99	1.19	1.34
33	D	404	BCR	C24-C23	5.99	1.50	1.33
31	C1	508	CLA	MG-NA	5.97	2.20	2.06
50	Y	623	NEX	C11-C12	-5.95	1.19	1.34
31	D1	402	CLA	MG-NA	5.95	2.20	2.06
31	b1	605	CLA	MG-NA	5.95	2.20	2.06
33	B1	618	BCR	C24-C23	5.95	1.50	1.33
31	n	610	CLA	MG-NA	5.94	2.20	2.06
33	C1	516	BCR	C24-C23	5.93	1.50	1.33
31	C	504	CLA	MG-NA	5.93	2.20	2.06
33	c	514	BCR	C24-C23	5.93	1.50	1.33
33	B1	619	BCR	C24-C23	5.92	1.50	1.33
47	r	607	CHL	C3B-C4B	5.92	1.47	1.41
31	G	610	CLA	MG-NA	5.92	2.20	2.06
31	y	602	CLA	MG-NA	5.91	2.20	2.06
50	n1	623	NEX	C31-C32	-5.91	1.19	1.34
50	n1	623	NEX	C11-C12	-5.91	1.19	1.34
31	n	604	CLA	MG-NA	5.89	2.20	2.06
31	N1	610	CLA	MG-NA	5.89	2.20	2.06
33	d1	404	BCR	C24-C23	5.89	1.50	1.33
37	B1	620	C7Z	C12-C13	5.89	1.58	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	c	517	BCR	C24-C23	5.88	1.50	1.33
31	Y1	610	CLA	MG-NA	5.88	2.20	2.06
46	h	101	RRX	C30-C25	-5.87	1.46	1.53
33	b1	619	BCR	C24-C23	5.87	1.50	1.33
47	s1	607	CHL	C3B-C4B	5.85	1.47	1.41
33	D1	404	BCR	C24-C23	5.85	1.50	1.33
47	R1	607	CHL	C3B-C4B	5.84	1.47	1.41
33	b1	618	BCR	C24-C23	5.84	1.50	1.33
33	C	517	BCR	C24-C23	5.83	1.50	1.33
37	B1	620	C7Z	C1-C6	-5.83	1.46	1.53
50	N1	623	NEX	C7-C8	5.82	1.41	1.31
33	d	404	BCR	C24-C23	5.82	1.50	1.33
47	N1	601	CHL	C3A-C2A	-5.81	1.49	1.54
33	C1	514	BCR	C24-C23	5.81	1.50	1.33
33	C1	515	BCR	C24-C23	5.81	1.50	1.33
33	b	618	BCR	C24-C23	5.81	1.50	1.33
37	B	620	C7Z	C12-C13	5.81	1.58	1.46
33	B	619	BCR	C24-C23	5.81	1.50	1.33
33	c1	515	BCR	C24-C23	5.80	1.50	1.33
33	c1	516	BCR	C24-C23	5.80	1.50	1.33
33	A1	411	BCR	C24-C23	5.78	1.50	1.33
47	n	601	CHL	C3B-C4B	5.77	1.47	1.41
50	y	623	NEX	C7-C8	5.76	1.41	1.31
47	g	601	CHL	C3B-C4B	5.76	1.47	1.41
37	b1	620	C7Z	C12-C13	5.76	1.58	1.46
47	G	608	CHL	C3B-C4B	5.76	1.47	1.41
47	G1	606	CHL	C3B-C4B	5.75	1.47	1.41
46	h1	101	RRX	C1-C6	-5.74	1.46	1.53
50	y1	623	NEX	C7-C8	5.74	1.41	1.31
47	S1	606	CHL	C3B-C4B	5.74	1.47	1.41
47	g	609	CHL	C3A-C2A	-5.74	1.49	1.54
47	s1	601	CHL	C3B-C4B	5.73	1.47	1.41
33	C	516	BCR	C24-C23	5.72	1.50	1.33
33	a	411	BCR	C24-C23	5.72	1.50	1.33
50	G1	623	NEX	C7-C8	5.71	1.41	1.31
46	H	101	RRX	C30-C25	-5.71	1.46	1.53
33	C	514	BCR	C24-C23	5.71	1.50	1.33
47	g1	606	CHL	C3B-C4B	5.68	1.46	1.41
33	A	411	BCR	C24-C23	5.68	1.50	1.33
50	Y1	623	NEX	C7-C8	5.67	1.41	1.31
47	R1	606	CHL	C3A-C2A	-5.66	1.49	1.54
33	C1	517	BCR	C24-C23	5.66	1.49	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	S	601	CHL	C3B-C4B	5.66	1.46	1.41
33	a1	411	BCR	C24-C23	5.66	1.49	1.33
33	C	515	BCR	C24-C23	5.65	1.49	1.33
47	S	607	CHL	C3B-C4B	5.65	1.46	1.41
50	g1	623	NEX	C7-C8	5.65	1.41	1.31
37	b	620	C7Z	C12-C13	5.65	1.58	1.46
33	c1	514	BCR	C24-C23	5.64	1.49	1.33
33	c	516	BCR	C24-C23	5.62	1.49	1.33
33	B	618	BCR	C24-C23	5.62	1.49	1.33
56	R1	626	ERG	C1-C2	5.61	1.64	1.53
47	r1	606	CHL	C3B-C4B	5.59	1.46	1.41
47	R	607	CHL	C3B-C4B	5.56	1.46	1.41
47	r1	607	CHL	C3B-C4B	5.56	1.46	1.41
47	s	608	CHL	C3B-C4B	5.55	1.46	1.41
47	S1	607	CHL	C3B-C4B	5.55	1.46	1.41
47	r	606	CHL	C3B-C4B	5.52	1.46	1.41
47	N	606	CHL	C3B-C4B	5.52	1.46	1.41
47	Y1	606	CHL	C3B-C4B	5.50	1.46	1.41
37	B	620	C7Z	C1-C6	-5.49	1.46	1.53
56	R1	626	ERG	C13-C14	-5.48	1.47	1.56
47	Y	601	CHL	C3A-C2A	-5.48	1.50	1.54
46	H	101	RRX	C20-C21	5.48	1.60	1.43
50	S	622	NEX	C7-C8	5.47	1.40	1.31
50	Y	623	NEX	C7-C8	5.44	1.40	1.31
33	c	515	BCR	C24-C23	5.43	1.49	1.33
46	h1	101	RRX	C30-C25	-5.42	1.46	1.53
46	h1	101	RRX	C19-C18	5.42	1.57	1.46
47	y	605	CHL	C3B-C4B	5.41	1.46	1.41
46	H1	101	RRX	C30-C25	-5.40	1.46	1.53
47	g	605	CHL	C3B-C4B	5.39	1.46	1.41
56	r1	626	ERG	C1-C2	5.38	1.64	1.53
56	r1	626	ERG	C7-C6	-5.38	1.27	1.41
47	s1	608	CHL	C3B-C4B	5.37	1.46	1.41
50	n	623	NEX	C7-C8	5.36	1.40	1.31
47	g1	601	CHL	C3B-C4B	5.36	1.46	1.41
47	g1	608	CHL	C3B-C4B	5.36	1.46	1.41
47	N	601	CHL	C3B-C4B	5.36	1.46	1.41
47	g1	605	CHL	C3B-C4B	5.35	1.46	1.41
47	s1	608	CHL	C3A-C2A	-5.34	1.50	1.54
56	R1	626	ERG	C7-C6	-5.34	1.27	1.41
37	b	620	C7Z	C28-C29	5.33	1.57	1.46
47	G1	608	CHL	C3B-C4B	5.33	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	G1	609	CHL	C3A-C2A	-5.32	1.50	1.54
33	c	517	BCR	C11-C12	-5.32	1.20	1.34
47	s	606	CHL	C3B-C4B	5.32	1.46	1.41
46	h1	101	RRX	C8-C9	5.32	1.57	1.46
37	b	620	C7Z	C1-C6	-5.31	1.47	1.53
46	h1	101	RRX	C2-C1	5.31	1.66	1.54
33	C1	517	BCR	C11-C12	-5.31	1.20	1.34
50	S1	623	NEX	C7-C8	5.30	1.40	1.31
33	c	515	BCR	C11-C12	-5.29	1.20	1.34
50	R	622	NEX	C7-C8	5.29	1.40	1.31
47	S	606	CHL	C3B-C4B	5.28	1.46	1.41
50	Y1	623	NEX	C28-C29	-5.28	1.34	1.46
47	R	606	CHL	C3B-C4B	5.28	1.46	1.41
47	N1	606	CHL	C3B-C4B	5.27	1.46	1.41
47	G1	605	CHL	C3B-C4B	5.27	1.46	1.41
47	y1	606	CHL	C3A-C2A	-5.27	1.50	1.54
33	B	618	BCR	C11-C12	-5.27	1.20	1.34
33	C	517	BCR	C11-C12	-5.27	1.20	1.34
47	G	606	CHL	C3B-C4B	5.27	1.46	1.41
50	N1	623	NEX	C28-C29	-5.26	1.34	1.46
33	a	411	BCR	C11-C12	-5.26	1.20	1.34
47	s	607	CHL	C3B-C4B	5.26	1.46	1.41
47	n1	601	CHL	C3B-C4B	5.26	1.46	1.41
37	B	620	C7Z	C28-C29	5.26	1.57	1.46
56	r1	626	ERG	C13-C14	-5.26	1.47	1.56
50	N	623	NEX	C28-C29	-5.25	1.34	1.46
50	r1	622	NEX	C28-C29	-5.25	1.34	1.46
50	s	623	NEX	C28-C29	-5.25	1.34	1.46
50	n1	623	NEX	C7-C8	5.25	1.40	1.31
50	r	623	NEX	C28-C29	-5.25	1.34	1.46
47	y1	609	CHL	C3B-C4B	5.25	1.46	1.41
47	Y	605	CHL	C3B-C4B	5.23	1.46	1.41
50	R	622	NEX	C28-C29	-5.23	1.34	1.46
47	Y	606	CHL	C3B-C4B	5.23	1.46	1.41
47	g	609	CHL	C3B-C4B	5.23	1.46	1.41
47	y1	606	CHL	C3B-C4B	5.22	1.46	1.41
33	A	411	BCR	C11-C12	-5.22	1.21	1.34
50	s1	623	NEX	C28-C29	-5.22	1.34	1.46
33	C	514	BCR	C11-C12	-5.22	1.21	1.34
47	g	608	CHL	C3B-C4B	5.21	1.46	1.41
50	S1	623	NEX	C28-C29	-5.21	1.34	1.46
37	B1	620	C7Z	C28-C29	5.21	1.57	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	c1	514	BCR	C11-C12	-5.21	1.21	1.34
47	S	601	CHL	C3A-C2A	-5.20	1.50	1.54
46	H	101	RRX	C19-C18	5.20	1.57	1.46
33	c	514	BCR	C11-C12	-5.20	1.21	1.34
33	c1	515	BCR	C11-C12	-5.20	1.21	1.34
50	G	623	NEX	C28-C29	-5.20	1.34	1.46
56	r1	626	ERG	C12-C11	-5.19	1.43	1.53
33	B	619	BCR	C11-C12	-5.19	1.21	1.34
50	g	623	NEX	C28-C29	-5.19	1.34	1.46
46	H1	101	RRX	C2-C1	5.18	1.66	1.54
50	R1	622	NEX	C28-C29	-5.18	1.34	1.46
50	Y	623	NEX	C28-C29	-5.17	1.34	1.46
33	C	515	BCR	C11-C12	-5.17	1.21	1.34
50	r	623	NEX	C7-C8	5.16	1.40	1.31
50	n	623	NEX	C28-C29	-5.16	1.34	1.46
33	B1	619	BCR	C11-C12	-5.15	1.21	1.34
50	y1	623	NEX	C28-C29	-5.15	1.34	1.46
33	C	516	BCR	C11-C12	-5.14	1.21	1.34
47	y1	605	CHL	C3B-C4B	5.14	1.46	1.41
33	d1	404	BCR	C11-C12	-5.14	1.21	1.34
47	N	605	CHL	C3B-C4B	5.13	1.46	1.41
50	s1	623	NEX	C7-C8	5.13	1.40	1.31
50	S	622	NEX	C28-C29	-5.12	1.35	1.46
46	H	101	RRX	C2-C1	5.12	1.65	1.54
47	s1	606	CHL	C3B-C4B	5.11	1.46	1.41
47	N	605	CHL	C3A-C2A	-5.11	1.50	1.54
47	n	605	CHL	C3B-C4B	5.11	1.46	1.41
47	n1	605	CHL	C3B-C4B	5.11	1.46	1.41
47	Y1	605	CHL	C3B-C4B	5.10	1.46	1.41
50	R1	622	NEX	C7-C8	5.10	1.40	1.31
33	C1	514	BCR	C11-C12	-5.10	1.21	1.34
46	h	101	RRX	C2-C1	5.09	1.65	1.54
50	g1	623	NEX	C28-C29	-5.09	1.35	1.46
33	a1	411	BCR	C11-C12	-5.09	1.21	1.34
33	A1	411	BCR	C11-C12	-5.09	1.21	1.34
33	b	618	BCR	C11-C12	-5.09	1.21	1.34
50	y	623	NEX	C28-C29	-5.08	1.35	1.46
33	b1	619	BCR	C11-C12	-5.08	1.21	1.34
47	y	606	CHL	C3B-C4B	5.08	1.46	1.41
33	b	619	BCR	C11-C12	-5.08	1.21	1.34
47	N	609	CHL	C3A-C2A	-5.07	1.50	1.54
33	c1	517	BCR	C11-C12	-5.06	1.21	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	G1	623	NEX	C28-C29	-5.05	1.35	1.46
47	y1	601	CHL	C3A-C2A	-5.05	1.50	1.54
47	G	608	CHL	C3A-C2A	-5.05	1.50	1.54
47	S1	608	CHL	C3B-C4B	5.04	1.46	1.41
46	h	101	RRX	C19-C18	5.03	1.56	1.46
47	y	609	CHL	C3B-C4B	5.03	1.46	1.41
47	N	608	CHL	C3A-C2A	-5.02	1.50	1.54
33	c1	516	BCR	C11-C12	-5.01	1.21	1.34
50	n1	623	NEX	C28-C29	-5.00	1.35	1.46
56	R1	626	ERG	C12-C11	-5.00	1.43	1.53
47	G	605	CHL	C3B-C4B	5.00	1.46	1.41
33	C1	515	BCR	C11-C12	-4.99	1.21	1.34
33	b1	618	BCR	C11-C12	-4.99	1.21	1.34
47	Y1	609	CHL	C3B-C4B	4.98	1.46	1.41
37	b1	620	C7Z	C28-C29	4.98	1.56	1.46
47	y1	601	CHL	C3B-C4B	4.97	1.46	1.41
46	H1	101	RRX	C19-C18	4.96	1.56	1.46
33	D	404	BCR	C11-C12	-4.96	1.21	1.34
33	D1	404	BCR	C11-C12	-4.94	1.21	1.34
37	b1	620	C7Z	C24-C25	-4.94	1.43	1.51
33	c	516	BCR	C11-C12	-4.93	1.21	1.34
47	S	608	CHL	C3B-C4B	4.93	1.46	1.41
50	R	622	NEX	C7-C6	-4.92	1.24	1.30
37	B	620	C7Z	C32-C33	4.92	1.56	1.46
47	Y1	601	CHL	C3A-C2A	-4.88	1.50	1.54
37	b	620	C7Z	C32-C33	4.87	1.56	1.46
33	B1	618	BCR	C11-C12	-4.87	1.22	1.34
47	G1	609	CHL	C3B-C4B	4.87	1.46	1.41
47	g1	609	CHL	C3A-C2A	-4.86	1.50	1.54
47	N1	609	CHL	C3A-C2A	-4.85	1.50	1.54
37	B1	620	C7Z	C32-C33	4.84	1.56	1.46
47	y	601	CHL	C3A-C2A	-4.82	1.50	1.54
47	n	606	CHL	C3A-C2A	-4.81	1.50	1.54
33	C1	516	BCR	C11-C12	-4.79	1.22	1.34
50	s	623	NEX	C7-C6	-4.79	1.25	1.30
37	b1	620	C7Z	C32-C33	4.78	1.56	1.46
33	d	404	BCR	C11-C12	-4.78	1.22	1.34
47	g1	609	CHL	C3B-C4B	4.77	1.46	1.41
46	H1	101	RRX	C8-C9	4.77	1.56	1.46
46	h	101	RRX	C8-C9	4.77	1.56	1.46
46	H	101	RRX	C8-C9	4.75	1.56	1.46
50	s	623	NEX	C7-C8	4.75	1.39	1.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	G	609	CHL	C3B-C4B	4.74	1.46	1.41
50	s1	623	NEX	C10-C9	-4.74	1.24	1.35
47	r1	606	CHL	C3A-C2A	-4.74	1.50	1.54
47	G	607	CHL	C3B-C4B	4.73	1.46	1.41
47	R	606	CHL	C3A-C2A	-4.71	1.50	1.54
47	g	601	CHL	C3A-C2A	-4.70	1.50	1.54
47	N1	608	CHL	C3B-C4B	4.68	1.45	1.41
47	g1	605	CHL	C3A-C2A	-4.68	1.50	1.54
50	y1	623	NEX	C7-C6	-4.62	1.25	1.30
46	h1	101	RRX	C12-C13	4.62	1.55	1.46
47	N1	605	CHL	C3B-C4B	4.60	1.45	1.41
56	R1	626	ERG	C13-C17	4.60	1.63	1.55
37	B	620	C7Z	C24-C25	-4.60	1.43	1.51
37	B1	620	C7Z	C31-C30	4.58	1.57	1.43
47	N1	606	CHL	C3A-C2A	-4.57	1.50	1.54
37	b	620	C7Z	C24-C25	-4.57	1.43	1.51
37	B	620	C7Z	C31-C30	4.56	1.57	1.43
56	r1	626	ERG	C13-C17	4.56	1.63	1.55
47	n1	609	CHL	C3B-C4B	4.56	1.45	1.41
37	b	620	C7Z	C31-C30	4.56	1.57	1.43
47	N1	601	CHL	C3B-C4B	4.55	1.45	1.41
50	n	623	NEX	C10-C9	-4.54	1.25	1.35
47	Y	609	CHL	C3B-C4B	4.54	1.45	1.41
50	n1	623	NEX	C10-C9	-4.54	1.25	1.35
47	n	607	CHL	C3B-C4B	4.52	1.45	1.41
32	a1	408	PHO	C1D-C2D	4.52	1.44	1.39
50	y1	623	NEX	C10-C9	-4.51	1.25	1.35
50	r	623	NEX	C10-C9	-4.51	1.25	1.35
31	R	612	CLA	CBB-CAB	4.50	1.52	1.30
31	n	604	CLA	CBB-CAB	4.49	1.52	1.30
31	y1	602	CLA	CBB-CAB	4.49	1.52	1.30
31	b	609	CLA	MG-ND	-4.49	1.96	2.05
31	c	504	CLA	CBB-CAB	4.49	1.51	1.30
31	g	602	CLA	CBB-CAB	4.49	1.51	1.30
31	c1	509	CLA	CBB-CAB	4.48	1.51	1.30
46	h	101	RRX	C27-C26	-4.48	1.44	1.51
50	g1	623	NEX	C10-C9	-4.48	1.25	1.35
31	g	604	CLA	CBB-CAB	4.48	1.51	1.30
31	b1	609	CLA	CBB-CAB	4.48	1.51	1.30
31	c1	507	CLA	CBB-CAB	4.47	1.51	1.30
31	n1	602	CLA	CBB-CAB	4.47	1.51	1.30
31	N1	602	CLA	CBB-CAB	4.47	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	Y1	609	CHL	C3A-C2A	-4.47	1.50	1.54
47	G	606	CHL	C3A-C2A	-4.46	1.50	1.54
47	r	607	CHL	C3A-C2A	-4.46	1.50	1.54
31	c1	501	CLA	CBB-CAB	4.46	1.51	1.30
31	b1	608	CLA	CBB-CAB	4.46	1.51	1.30
31	Y1	603	CLA	CBB-CAB	4.46	1.51	1.30
31	n1	610	CLA	CBB-CAB	4.46	1.51	1.30
31	n	610	CLA	CBB-CAB	4.46	1.51	1.30
31	R	602	CLA	CBB-CAB	4.46	1.51	1.30
47	g1	608	CHL	C3A-C2A	-4.46	1.50	1.54
32	A1	409	PHO	C1D-C2D	4.46	1.44	1.39
31	s1	602	CLA	CBB-CAB	4.46	1.51	1.30
31	g	610	CLA	CBB-CAB	4.46	1.51	1.30
31	c1	508	CLA	CBB-CAB	4.45	1.51	1.30
31	R	610	CLA	CBB-CAB	4.45	1.51	1.30
31	B1	611	CLA	CBB-CAB	4.45	1.51	1.30
31	n	602	CLA	CBB-CAB	4.45	1.51	1.30
31	b1	612	CLA	CBB-CAB	4.45	1.51	1.30
31	N	604	CLA	CBB-CAB	4.45	1.51	1.30
31	G	614	CLA	CBB-CAB	4.45	1.51	1.30
31	g1	602	CLA	CBB-CAB	4.45	1.51	1.30
31	n	603	CLA	CBB-CAB	4.45	1.51	1.30
31	A	405	CLA	CBB-CAB	4.45	1.51	1.30
31	G1	602	CLA	CBB-CAB	4.45	1.51	1.30
31	S1	612	CLA	CBB-CAB	4.45	1.51	1.30
31	n	614	CLA	CBB-CAB	4.45	1.51	1.30
31	A1	407	CLA	CBB-CAB	4.45	1.51	1.30
31	B	615	CLA	CBB-CAB	4.44	1.51	1.30
37	b	620	C7Z	C4-C5	-4.44	1.44	1.51
31	A1	406	CLA	CBB-CAB	4.44	1.51	1.30
50	s1	623	NEX	C14-C13	-4.44	1.25	1.35
31	G1	603	CLA	CBB-CAB	4.44	1.51	1.30
31	A1	405	CLA	CBB-CAB	4.44	1.51	1.30
31	G	603	CLA	CBB-CAB	4.44	1.51	1.30
31	s1	613	CLA	CBB-CAB	4.44	1.51	1.30
31	C1	513	CLA	CBB-CAB	4.44	1.51	1.30
31	R1	610	CLA	CBB-CAB	4.44	1.51	1.30
50	n	623	NEX	C34-C33	-4.44	1.25	1.35
31	R1	612	CLA	CBB-CAB	4.44	1.51	1.30
37	b1	620	C7Z	C31-C30	4.44	1.56	1.43
31	B1	612	CLA	CBB-CAB	4.44	1.51	1.30
31	B1	610	CLA	CBB-CAB	4.44	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	613	CLA	CBB-CAB	4.44	1.51	1.30
37	B	620	C7Z	C8-C9	4.44	1.55	1.46
31	n1	604	CLA	CBB-CAB	4.43	1.51	1.30
31	c	508	CLA	CBB-CAB	4.43	1.51	1.30
31	a1	405	CLA	CBB-CAB	4.43	1.51	1.30
31	C	510	CLA	CBB-CAB	4.43	1.51	1.30
31	N1	614	CLA	CBB-CAB	4.43	1.51	1.30
31	b1	606	CLA	CBB-CAB	4.43	1.51	1.30
31	g	612	CLA	CBB-CAB	4.43	1.51	1.30
31	B1	608	CLA	CBB-CAB	4.43	1.51	1.30
31	s1	614	CLA	CBB-CAB	4.43	1.51	1.30
31	R1	608	CLA	CBB-CAB	4.43	1.51	1.30
31	Y1	612	CLA	CBB-CAB	4.43	1.51	1.30
31	c1	511	CLA	CBB-CAB	4.43	1.51	1.30
31	S	617	CLA	CBB-CAB	4.43	1.51	1.30
31	r	613	CLA	CBB-CAB	4.43	1.51	1.30
31	B	608	CLA	CBB-CAB	4.43	1.51	1.30
31	b1	613	CLA	CBB-CAB	4.43	1.51	1.30
31	s	609	CLA	CBB-CAB	4.43	1.51	1.30
31	c	512	CLA	CBB-CAB	4.43	1.51	1.30
31	C1	509	CLA	CBB-CAB	4.43	1.51	1.30
31	g1	610	CLA	CBB-CAB	4.43	1.51	1.30
31	G	602	CLA	CBB-CAB	4.43	1.51	1.30
31	C1	508	CLA	CBB-CAB	4.42	1.51	1.30
31	B	612	CLA	CBB-CAB	4.42	1.51	1.30
31	a1	406	CLA	CBB-CAB	4.42	1.51	1.30
31	s1	604	CLA	CBB-CAB	4.42	1.51	1.30
31	s1	609	CLA	CBB-CAB	4.42	1.51	1.30
31	r	611	CLA	CBB-CAB	4.42	1.51	1.30
31	s	610	CLA	CBB-CAB	4.42	1.51	1.30
31	c1	502	CLA	CBB-CAB	4.42	1.51	1.30
31	r	610	CLA	CBB-CAB	4.42	1.51	1.30
31	b	605	CLA	CBB-CAB	4.42	1.51	1.30
31	c1	512	CLA	CBB-CAB	4.42	1.51	1.30
31	N1	612	CLA	CBB-CAB	4.42	1.51	1.30
31	y1	612	CLA	CBB-CAB	4.42	1.51	1.30
31	C	507	CLA	CBB-CAB	4.42	1.51	1.30
31	Y	608	CLA	CBB-CAB	4.42	1.51	1.30
31	g	603	CLA	CBB-CAB	4.42	1.51	1.30
31	s	604	CLA	CBB-CAB	4.42	1.51	1.30
31	B1	605	CLA	CBB-CAB	4.42	1.51	1.30
50	G1	623	NEX	C14-C13	-4.42	1.25	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Y1	602	CLA	CBB-CAB	4.42	1.51	1.30
31	s1	605	CLA	CBB-CAB	4.42	1.51	1.30
31	N1	603	CLA	CBB-CAB	4.42	1.51	1.30
31	b1	607	CLA	CBB-CAB	4.42	1.51	1.30
31	r1	608	CLA	CBB-CAB	4.42	1.51	1.30
31	S	605	CLA	CBB-CAB	4.42	1.51	1.30
31	G1	610	CLA	CBB-CAB	4.42	1.51	1.30
31	b1	617	CLA	CBB-CAB	4.42	1.51	1.30
31	y1	610	CLA	CBB-CAB	4.42	1.51	1.30
31	B	603	CLA	CBB-CAB	4.41	1.51	1.30
31	R1	609	CLA	CBB-CAB	4.41	1.51	1.30
31	S1	602	CLA	CBB-CAB	4.41	1.51	1.30
31	B1	606	CLA	CBB-CAB	4.41	1.51	1.30
31	n1	613	CLA	CBB-CAB	4.41	1.51	1.30
31	y1	608	CLA	CBB-CAB	4.41	1.51	1.30
33	A1	411	BCR	C16-C17	-4.41	1.29	1.43
31	R	604	CLA	CBB-CAB	4.41	1.51	1.30
31	G1	612	CLA	CBB-CAB	4.41	1.51	1.30
31	B	604	CLA	CBB-CAB	4.41	1.51	1.30
31	c1	504	CLA	CBB-CAB	4.41	1.51	1.30
31	B	602	CLA	CBB-CAB	4.41	1.51	1.30
31	y	614	CLA	CBB-CAB	4.41	1.51	1.30
31	C1	501	CLA	CBB-CAB	4.41	1.51	1.30
47	g	608	CHL	C3A-C2A	-4.41	1.50	1.54
31	S1	603	CLA	CBB-CAB	4.41	1.51	1.30
31	s1	610	CLA	CBB-CAB	4.41	1.51	1.30
31	g1	611	CLA	CBB-CAB	4.41	1.51	1.30
31	N	614	CLA	CBB-CAB	4.41	1.51	1.30
31	b	612	CLA	CBB-CAB	4.41	1.51	1.30
31	r	608	CLA	CBB-CAB	4.41	1.51	1.30
31	b	610	CLA	CBB-CAB	4.41	1.51	1.30
31	d	403	CLA	CBB-CAB	4.41	1.51	1.30
31	g	614	CLA	CBB-CAB	4.41	1.51	1.30
31	N	602	CLA	CBB-CAB	4.41	1.51	1.30
31	n	611	CLA	CBB-CAB	4.41	1.51	1.30
31	c	507	CLA	CBB-CAB	4.41	1.51	1.30
31	G1	611	CLA	CBB-CAB	4.41	1.51	1.30
31	r	602	CLA	CBB-CAB	4.41	1.51	1.30
31	S1	611	CLA	CBB-CAB	4.41	1.51	1.30
33	c	515	BCR	C16-C17	-4.41	1.29	1.43
31	Y	614	CLA	CBB-CAB	4.41	1.51	1.30
31	d1	402	CLA	CBB-CAB	4.41	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C1	510	CLA	CBB-CAB	4.41	1.51	1.30
31	G	604	CLA	CBB-CAB	4.41	1.51	1.30
31	C1	512	CLA	CBB-CAB	4.41	1.51	1.30
31	S1	609	CLA	CBB-CAB	4.41	1.51	1.30
31	g1	614	CLA	CBB-CAB	4.41	1.51	1.30
31	b1	611	CLA	CBB-CAB	4.41	1.51	1.30
31	G	613	CLA	CBB-CAB	4.41	1.51	1.30
31	r1	602	CLA	CBB-CAB	4.41	1.51	1.30
47	s	606	CHL	C3A-C2A	-4.40	1.50	1.54
31	b	608	CLA	CBB-CAB	4.40	1.51	1.30
31	s	603	CLA	CBB-CAB	4.40	1.51	1.30
31	s1	603	CLA	CBB-CAB	4.40	1.51	1.30
31	y1	603	CLA	CBB-CAB	4.40	1.51	1.30
31	B	614	CLA	CBB-CAB	4.40	1.51	1.30
31	S	609	CLA	CBB-CAB	4.40	1.51	1.30
31	B1	616	CLA	CBB-CAB	4.40	1.51	1.30
31	y	610	CLA	CBB-CAB	4.40	1.51	1.30
31	D1	403	CLA	CBB-CAB	4.40	1.51	1.30
31	Y1	610	CLA	CBB-CAB	4.40	1.51	1.30
31	B1	604	CLA	CBB-CAB	4.40	1.51	1.30
31	G	610	CLA	CBB-CAB	4.40	1.51	1.30
31	R	613	CLA	CBB-CAB	4.40	1.51	1.30
31	N	611	CLA	CBB-CAB	4.40	1.51	1.30
31	n1	611	CLA	CBB-CAB	4.40	1.51	1.30
31	g1	603	CLA	CBB-CAB	4.40	1.51	1.30
31	N1	604	CLA	CBB-CAB	4.40	1.51	1.30
31	n1	603	CLA	CBB-CAB	4.40	1.51	1.30
46	H	101	RRX	C27-C26	-4.40	1.44	1.51
31	S1	610	CLA	CBB-CAB	4.40	1.51	1.30
31	N	612	CLA	CBB-CAB	4.40	1.51	1.30
31	N1	610	CLA	CBB-CAB	4.40	1.51	1.30
31	c1	513	CLA	CBB-CAB	4.40	1.51	1.30
31	g	613	CLA	CBB-CAB	4.40	1.51	1.30
31	C1	506	CLA	CBB-CAB	4.40	1.51	1.30
31	C	508	CLA	CBB-CAB	4.40	1.51	1.30
31	S1	604	CLA	CBB-CAB	4.40	1.51	1.30
31	B	610	CLA	CBB-CAB	4.40	1.51	1.30
31	c	502	CLA	CBB-CAB	4.40	1.51	1.30
31	b1	605	CLA	CBB-CAB	4.40	1.51	1.30
31	g1	612	CLA	CBB-CAB	4.40	1.51	1.30
31	C1	507	CLA	CBB-CAB	4.40	1.51	1.30
31	b1	602	CLA	CBB-CAB	4.40	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	s1	617	CLA	CBB-CAB	4.40	1.51	1.30
31	s	611	CLA	CBB-CAB	4.40	1.51	1.30
31	y1	611	CLA	CBB-CAB	4.40	1.51	1.30
31	s1	611	CLA	CBB-CAB	4.40	1.51	1.30
31	G	611	CLA	CBB-CAB	4.40	1.51	1.30
31	Y1	614	CLA	CBB-CAB	4.40	1.51	1.30
31	Y1	608	CLA	CBB-CAB	4.40	1.51	1.30
31	a1	410	CLA	CBB-CAB	4.40	1.51	1.30
31	s	605	CLA	CBB-CAB	4.40	1.51	1.30
31	B1	609	CLA	CBB-CAB	4.40	1.51	1.30
31	r1	610	CLA	CBB-CAB	4.40	1.51	1.30
31	C	506	CLA	CBB-CAB	4.40	1.51	1.30
31	B	613	CLA	CBB-CAB	4.40	1.51	1.30
31	a	405	CLA	CBB-CAB	4.39	1.51	1.30
31	S	614	CLA	CBB-CAB	4.39	1.51	1.30
31	B1	617	CLA	CBB-CAB	4.39	1.51	1.30
31	B1	613	CLA	CBB-CAB	4.39	1.51	1.30
31	S1	605	CLA	CBB-CAB	4.39	1.51	1.30
31	r	604	CLA	CBB-CAB	4.39	1.51	1.30
31	b	603	CLA	CBB-CAB	4.39	1.51	1.30
46	H1	101	RRX	C23-C22	4.39	1.55	1.46
31	R	611	CLA	CBB-CAB	4.39	1.51	1.30
31	G	612	CLA	CBB-CAB	4.39	1.51	1.30
31	r1	603	CLA	CBB-CAB	4.39	1.51	1.30
46	H1	101	RRX	C27-C26	-4.39	1.44	1.51
31	S1	614	CLA	CBB-CAB	4.39	1.51	1.30
31	y	608	CLA	CBB-CAB	4.39	1.51	1.30
31	B1	602	CLA	CBB-CAB	4.39	1.51	1.30
31	R1	602	CLA	CBB-CAB	4.39	1.51	1.30
31	r1	609	CLA	CBB-CAB	4.39	1.51	1.30
31	R	603	CLA	CBB-CAB	4.39	1.51	1.30
31	s	617	CLA	CBB-CAB	4.39	1.51	1.30
31	S1	613	CLA	CBB-CAB	4.39	1.51	1.30
31	y	611	CLA	CBB-CAB	4.39	1.51	1.30
31	n1	614	CLA	CBB-CAB	4.39	1.51	1.30
31	g1	613	CLA	CBB-CAB	4.39	1.51	1.30
31	r1	604	CLA	CBB-CAB	4.39	1.51	1.30
31	b	616	CLA	CBB-CAB	4.39	1.51	1.30
31	s	613	CLA	CBB-CAB	4.39	1.51	1.30
50	Y	623	NEX	C14-C13	-4.39	1.25	1.35
31	D1	402	CLA	CBB-CAB	4.39	1.51	1.30
31	R1	604	CLA	CBB-CAB	4.39	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Y	612	CLA	CBB-CAB	4.39	1.51	1.30
31	Y1	604	CLA	CBB-CAB	4.39	1.51	1.30
31	b	602	CLA	CBB-CAB	4.39	1.51	1.30
50	N	623	NEX	C34-C33	-4.39	1.25	1.35
31	C1	504	CLA	CBB-CAB	4.39	1.51	1.30
31	Y1	611	CLA	CBB-CAB	4.39	1.51	1.30
31	B1	607	CLA	CBB-CAB	4.39	1.51	1.30
31	y1	604	CLA	CBB-CAB	4.39	1.51	1.30
47	g	605	CHL	C3A-C2A	-4.39	1.50	1.54
31	n1	612	CLA	CBB-CAB	4.39	1.51	1.30
31	S1	617	CLA	CBB-CAB	4.39	1.51	1.30
31	c	510	CLA	CBB-CAB	4.39	1.51	1.30
31	N	613	CLA	CBB-CAB	4.39	1.51	1.30
31	S	604	CLA	CBB-CAB	4.39	1.51	1.30
31	s	602	CLA	CBB-CAB	4.39	1.51	1.30
31	B	606	CLA	CBB-CAB	4.39	1.51	1.30
31	D	402	CLA	CBB-CAB	4.38	1.51	1.30
31	B	616	CLA	CBB-CAB	4.38	1.51	1.30
31	b1	603	CLA	CBB-CAB	4.38	1.51	1.30
31	Y1	613	CLA	CBB-CAB	4.38	1.51	1.30
31	b	614	CLA	CBB-CAB	4.38	1.51	1.30
31	s	614	CLA	CBB-CAB	4.38	1.51	1.30
31	C1	503	CLA	CBB-CAB	4.38	1.51	1.30
31	D	403	CLA	CBB-CAB	4.38	1.51	1.30
31	N1	611	CLA	CBB-CAB	4.38	1.51	1.30
31	R	609	CLA	CBB-CAB	4.38	1.51	1.30
31	y	602	CLA	CBB-CAB	4.38	1.51	1.30
31	N1	613	CLA	CBB-CAB	4.38	1.51	1.30
31	b1	604	CLA	CBB-CAB	4.38	1.51	1.30
31	s1	612	CLA	CBB-CAB	4.38	1.51	1.30
31	C	512	CLA	CBB-CAB	4.38	1.51	1.30
31	S	613	CLA	CBB-CAB	4.38	1.51	1.30
31	s	612	CLA	CBB-CAB	4.38	1.51	1.30
31	y1	613	CLA	CBB-CAB	4.38	1.51	1.30
31	G1	614	CLA	CBB-CAB	4.38	1.51	1.30
31	S	602	CLA	CBB-CAB	4.38	1.51	1.30
31	Y	602	CLA	CBB-CAB	4.38	1.51	1.30
31	y	613	CLA	CBB-CAB	4.38	1.51	1.30
31	N	610	CLA	CBB-CAB	4.38	1.51	1.30
31	c1	505	CLA	CBB-CAB	4.38	1.51	1.30
31	G1	613	CLA	CBB-CAB	4.38	1.51	1.30
31	r	603	CLA	CBB-CAB	4.37	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c1	506	CLA	CBB-CAB	4.37	1.51	1.30
31	b1	616	CLA	CBB-CAB	4.37	1.51	1.30
31	r	609	CLA	CBB-CAB	4.37	1.51	1.30
31	b	611	CLA	CBB-CAB	4.37	1.51	1.30
31	r1	612	CLA	CBB-CAB	4.37	1.51	1.30
50	S1	623	NEX	C10-C9	-4.37	1.25	1.35
31	g	611	CLA	CBB-CAB	4.37	1.51	1.30
31	b1	610	CLA	CBB-CAB	4.37	1.51	1.30
31	b1	614	CLA	CBB-CAB	4.37	1.51	1.30
31	n	612	CLA	CBB-CAB	4.37	1.51	1.30
47	s1	601	CHL	C3A-C2A	-4.37	1.50	1.54
31	C	504	CLA	CBB-CAB	4.37	1.51	1.30
31	Y	604	CLA	CBB-CAB	4.37	1.51	1.30
31	a	407	CLA	CBB-CAB	4.37	1.51	1.30
31	N	603	CLA	CBB-CAB	4.37	1.51	1.30
31	Y	603	CLA	CBB-CAB	4.37	1.51	1.30
31	b	615	CLA	CBB-CAB	4.37	1.51	1.30
31	c	503	CLA	CBB-CAB	4.37	1.51	1.30
31	c	506	CLA	CBB-CAB	4.37	1.51	1.30
31	b	604	CLA	CBB-CAB	4.37	1.51	1.30
31	y	603	CLA	CBB-CAB	4.37	1.51	1.30
31	C	502	CLA	CBB-CAB	4.37	1.51	1.30
31	S	612	CLA	CBB-CAB	4.37	1.51	1.30
31	y1	614	CLA	CBB-CAB	4.37	1.51	1.30
31	C	511	CLA	CBB-CAB	4.37	1.51	1.30
33	D1	404	BCR	C10-C9	4.37	1.45	1.35
31	B1	603	CLA	CBB-CAB	4.37	1.51	1.30
31	G1	604	CLA	CBB-CAB	4.37	1.51	1.30
47	G1	601	CHL	C3B-C4B	4.36	1.45	1.41
31	C	503	CLA	CBB-CAB	4.36	1.51	1.30
37	B	620	C7Z	C11-C10	4.36	1.56	1.43
46	H	101	RRX	C3-C4	4.36	1.66	1.52
31	y	612	CLA	CBB-CAB	4.36	1.51	1.30
37	B1	620	C7Z	C11-C10	4.36	1.56	1.43
31	C1	505	CLA	CBB-CAB	4.36	1.51	1.30
31	R	608	CLA	CBB-CAB	4.36	1.51	1.30
31	C1	511	CLA	CBB-CAB	4.36	1.51	1.30
31	Y	613	CLA	CBB-CAB	4.36	1.51	1.30
40	C1	519	DGD	O1G-C1A	4.36	1.46	1.33
31	c1	503	CLA	CBB-CAB	4.36	1.51	1.30
31	B1	614	CLA	CBB-CAB	4.36	1.51	1.30
31	n	613	CLA	CBB-CAB	4.35	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	N	606	CHL	C3A-C2A	-4.35	1.51	1.54
31	a	406	CLA	CBB-CAB	4.35	1.51	1.30
31	c	509	CLA	CBB-CAB	4.35	1.51	1.30
31	B1	615	CLA	CBB-CAB	4.35	1.51	1.30
31	Y	611	CLA	CBB-CAB	4.35	1.51	1.30
31	S	603	CLA	CBB-CAB	4.35	1.51	1.30
31	A	406	CLA	CBB-CAB	4.35	1.51	1.30
31	A	407	CLA	CBB-CAB	4.35	1.51	1.30
31	B	607	CLA	CBB-CAB	4.35	1.51	1.30
50	n	623	NEX	C30-C29	-4.35	1.25	1.35
40	C	523	DGD	O1G-C1A	4.35	1.46	1.33
40	c1	518	DGD	O1G-C1A	4.35	1.46	1.33
31	g1	604	CLA	CBB-CAB	4.35	1.51	1.30
40	C	518	DGD	O1G-C1A	4.35	1.46	1.33
31	B	605	CLA	CBB-CAB	4.35	1.51	1.30
31	c1	510	CLA	CBB-CAB	4.35	1.51	1.30
31	C	509	CLA	CBB-CAB	4.35	1.51	1.30
31	C1	502	CLA	CBB-CAB	4.35	1.51	1.30
31	r	612	CLA	CBB-CAB	4.35	1.51	1.30
33	C1	517	BCR	C16-C17	-4.35	1.29	1.43
46	H1	101	RRX	C3-C4	4.34	1.66	1.52
47	G1	608	CHL	C3A-C2A	-4.34	1.51	1.54
31	d1	403	CLA	CBB-CAB	4.34	1.51	1.30
50	g1	623	NEX	C34-C33	-4.34	1.25	1.35
31	c	511	CLA	CBB-CAB	4.34	1.51	1.30
46	h1	101	RRX	C27-C26	-4.34	1.44	1.51
47	N	608	CHL	C3B-C4B	4.34	1.45	1.41
46	h1	101	RRX	C23-C22	4.34	1.55	1.46
50	N	623	NEX	C14-C13	-4.34	1.25	1.35
50	Y1	623	NEX	C30-C29	-4.34	1.25	1.35
50	s1	623	NEX	C30-C29	-4.34	1.25	1.35
50	s1	623	NEX	C7-C6	-4.34	1.25	1.30
31	b	607	CLA	CBB-CAB	4.34	1.51	1.30
46	H	101	RRX	C12-C13	4.34	1.55	1.46
46	h1	101	RRX	C3-C4	4.34	1.66	1.52
31	d	402	CLA	CBB-CAB	4.33	1.51	1.30
31	S	610	CLA	CBB-CAB	4.33	1.51	1.30
33	d	404	BCR	C10-C9	4.33	1.45	1.35
37	B1	620	C7Z	C24-C25	-4.33	1.44	1.51
47	s1	606	CHL	C3A-C2A	-4.33	1.51	1.54
33	B1	618	BCR	C10-C9	4.33	1.45	1.35
31	a1	407	CLA	CBB-CAB	4.33	1.51	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Y	610	CLA	CBB-CAB	4.33	1.51	1.30
31	C	501	CLA	CBB-CAB	4.33	1.51	1.30
31	B	611	CLA	CBB-CAB	4.32	1.51	1.30
31	C	505	CLA	CBB-CAB	4.32	1.51	1.30
47	Y	606	CHL	C3A-C2A	-4.32	1.51	1.54
37	b	620	C7Z	C8-C9	4.32	1.55	1.46
31	R1	603	CLA	CBB-CAB	4.32	1.51	1.30
37	B1	620	C7Z	C8-C9	4.31	1.55	1.46
33	a1	411	BCR	C16-C17	-4.31	1.29	1.43
31	S	611	CLA	CBB-CAB	4.31	1.51	1.30
37	b1	620	C7Z	C8-C9	4.31	1.55	1.46
50	N	623	NEX	C10-C9	-4.31	1.25	1.35
37	b1	620	C7Z	C11-C10	4.31	1.56	1.43
31	C	513	CLA	CBB-CAB	4.31	1.51	1.30
50	g	623	NEX	C10-C9	-4.31	1.25	1.35
31	y	604	CLA	CBB-CAB	4.31	1.51	1.30
31	b	606	CLA	CBB-CAB	4.30	1.51	1.30
33	A	411	BCR	C16-C17	-4.30	1.29	1.43
33	c	517	BCR	C16-C17	-4.30	1.29	1.43
50	n	623	NEX	C14-C13	-4.29	1.25	1.35
50	s	623	NEX	C34-C33	-4.29	1.25	1.35
40	c1	520	DGD	O1G-C1A	4.29	1.45	1.33
50	N1	623	NEX	C14-C13	-4.29	1.25	1.35
40	c	518	DGD	O1G-C1A	4.29	1.45	1.33
31	b1	615	CLA	CBB-CAB	4.29	1.51	1.30
50	R1	622	NEX	C30-C29	-4.29	1.25	1.35
47	Y	609	CHL	C3A-C2A	-4.29	1.51	1.54
46	h	101	RRX	C3-C4	4.28	1.65	1.52
46	h	101	RRX	C12-C13	4.28	1.55	1.46
33	C	515	BCR	C16-C17	-4.28	1.29	1.43
50	N1	623	NEX	C34-C33	-4.28	1.25	1.35
33	a	411	BCR	C16-C17	-4.27	1.29	1.43
46	h1	101	RRX	C20-C21	4.27	1.56	1.43
33	C	516	BCR	C16-C17	-4.27	1.29	1.43
31	B	609	CLA	MG-ND	-4.27	1.97	2.05
31	b	617	CLA	CBB-CAB	4.27	1.50	1.30
50	R	622	NEX	C30-C29	-4.27	1.25	1.35
31	B	617	CLA	CBB-CAB	4.27	1.50	1.30
32	A1	408	PHO	C1D-C2D	4.26	1.44	1.39
50	r	623	NEX	C30-C29	-4.26	1.26	1.35
33	c	516	BCR	C10-C9	4.25	1.45	1.35
33	c1	516	BCR	C10-C9	4.25	1.45	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	505	CLA	CBB-CAB	4.25	1.50	1.30
33	C1	517	BCR	C10-C9	4.25	1.45	1.35
40	c	523	DGD	O1G-C1A	4.25	1.45	1.33
50	N1	623	NEX	C30-C29	-4.25	1.26	1.35
31	c	513	CLA	CBB-CAB	4.25	1.50	1.30
31	B1	609	CLA	MG-ND	-4.25	1.97	2.05
50	Y	623	NEX	C30-C29	-4.24	1.26	1.35
40	b1	623	DGD	O1G-C1A	4.24	1.45	1.33
31	B	609	CLA	CBB-CAB	4.24	1.50	1.30
46	H1	101	RRX	C12-C13	4.24	1.55	1.46
50	G	623	NEX	C30-C29	-4.24	1.26	1.35
40	C	519	DGD	O1G-C1A	4.24	1.45	1.33
31	A1	410	CLA	CBB-CAB	4.24	1.50	1.30
50	N	623	NEX	C30-C29	-4.23	1.26	1.35
31	c	501	CLA	CBB-CAB	4.23	1.50	1.30
31	b	609	CLA	CBB-CAB	4.23	1.50	1.30
31	b1	609	CLA	MG-ND	-4.23	1.97	2.05
33	D	404	BCR	C10-C9	4.23	1.45	1.35
37	b1	620	C7Z	C4-C5	-4.23	1.44	1.51
33	d1	404	BCR	C16-C17	-4.23	1.30	1.43
47	g1	609	CHL	C2C-C3C	4.23	1.40	1.36
47	n1	606	CHL	C3B-C4B	4.23	1.45	1.41
40	C	520	DGD	O1G-C1A	4.23	1.45	1.33
50	r1	622	NEX	C34-C33	-4.23	1.26	1.35
33	C	517	BCR	C16-C17	-4.23	1.30	1.43
50	G1	623	NEX	C30-C29	-4.23	1.26	1.35
40	B1	623	DGD	O1G-C1A	4.23	1.45	1.33
47	y	609	CHL	C3A-C2A	-4.23	1.51	1.54
50	S1	623	NEX	C14-C13	-4.22	1.26	1.35
50	R	622	NEX	C34-C33	-4.22	1.26	1.35
47	Y1	601	CHL	C3B-C4B	4.22	1.45	1.41
33	c1	515	BCR	C10-C9	4.22	1.45	1.35
37	B	620	C7Z	C4-C5	-4.22	1.44	1.51
40	C1	520	DGD	O1G-C1A	4.22	1.45	1.33
40	c1	519	DGD	O1G-C1A	4.21	1.45	1.33
33	b1	618	BCR	C10-C9	4.21	1.45	1.35
37	b	620	C7Z	C11-C10	4.20	1.56	1.43
47	S	606	CHL	C3A-C2A	-4.20	1.51	1.54
33	C1	515	BCR	C10-C9	4.20	1.45	1.35
47	y	605	CHL	C3A-C2A	-4.20	1.51	1.54
50	R	622	NEX	C18-C5	-4.20	1.46	1.52
33	C	514	BCR	C16-C17	-4.19	1.30	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
56	R1	626	ERG	C16-C15	4.19	1.65	1.54
40	C1	518	DGD	O1G-C1A	4.19	1.45	1.33
50	r	623	NEX	C34-C33	-4.19	1.26	1.35
33	B	619	BCR	C16-C17	-4.19	1.30	1.43
50	S	622	NEX	C34-C33	-4.19	1.26	1.35
50	s	623	NEX	C14-C13	-4.19	1.26	1.35
31	N1	604	CLA	MG-ND	-4.18	1.97	2.05
50	G1	623	NEX	C34-C33	-4.18	1.26	1.35
50	S	622	NEX	C30-C29	-4.18	1.26	1.35
50	G1	623	NEX	C10-C9	-4.18	1.26	1.35
33	b	618	BCR	C16-C17	-4.18	1.30	1.43
31	A	410	CLA	CBB-CAB	4.18	1.50	1.30
50	r	623	NEX	C14-C13	-4.18	1.26	1.35
33	a1	411	BCR	C10-C9	4.18	1.45	1.35
50	r1	622	NEX	C14-C13	-4.17	1.26	1.35
31	a	410	CLA	CBB-CAB	4.17	1.50	1.30
50	g	623	NEX	C30-C29	-4.17	1.26	1.35
31	D1	402	CLA	MG-ND	-4.17	1.97	2.05
47	G	609	CHL	C2C-C3C	4.16	1.40	1.36
31	C	507	CLA	MG-ND	-4.16	1.97	2.05
50	S	622	NEX	C14-C13	-4.16	1.26	1.35
47	S1	601	CHL	C3A-C2A	-4.16	1.51	1.54
31	c	505	CLA	MG-ND	-4.16	1.97	2.05
40	c	520	DGD	O1G-C1A	4.15	1.45	1.33
50	g	623	NEX	C14-C13	-4.15	1.26	1.35
50	r1	622	NEX	C30-C29	-4.15	1.26	1.35
50	R1	622	NEX	C14-C13	-4.15	1.26	1.35
47	s	601	CHL	C3A-C2A	-4.15	1.51	1.54
50	S1	623	NEX	C30-C29	-4.15	1.26	1.35
50	Y	623	NEX	C10-C9	-4.15	1.26	1.35
31	C1	510	CLA	MG-ND	-4.14	1.97	2.05
50	r1	622	NEX	C10-C9	-4.14	1.26	1.35
50	Y1	623	NEX	C14-C13	-4.14	1.26	1.35
31	B	604	CLA	MG-ND	-4.13	1.97	2.05
50	s	623	NEX	C30-C29	-4.13	1.26	1.35
33	B1	619	BCR	C16-C17	-4.13	1.30	1.43
33	b1	619	BCR	C16-C17	-4.13	1.30	1.43
33	c1	514	BCR	C16-C17	-4.13	1.30	1.43
32	a	409	PHO	C4D-CHA	4.13	1.45	1.39
50	Y	623	NEX	C34-C33	-4.12	1.26	1.35
42	C1	527	LMK	O2-C4	4.12	1.43	1.30
47	g	606	CHL	C3B-C4B	4.12	1.45	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	h1	101	RRX	C15-C14	4.12	1.56	1.43
50	Y1	623	NEX	C34-C33	-4.12	1.26	1.35
33	b	619	BCR	C10-C9	4.12	1.45	1.35
33	C1	514	BCR	C10-C9	4.12	1.45	1.35
47	y1	609	CHL	C3A-C2A	-4.12	1.51	1.54
33	C	516	BCR	C10-C9	4.11	1.45	1.35
37	b1	620	C7Z	C22-C21	4.11	1.67	1.54
31	B	617	CLA	MG-ND	-4.11	1.97	2.05
33	C1	515	BCR	C16-C17	-4.10	1.30	1.43
47	n1	608	CHL	C3B-C4B	4.10	1.45	1.41
31	b1	617	CLA	MG-ND	-4.10	1.97	2.05
50	G	623	NEX	C14-C13	-4.10	1.26	1.35
50	s1	623	NEX	C34-C33	-4.10	1.26	1.35
50	g1	623	NEX	C30-C29	-4.10	1.26	1.35
42	c	627	LMK	O2-C4	4.10	1.43	1.30
33	b	618	BCR	C10-C9	4.10	1.45	1.35
33	C1	514	BCR	C16-C17	-4.10	1.30	1.43
50	y1	623	NEX	C30-C29	-4.10	1.26	1.35
50	G	623	NEX	C34-C33	-4.10	1.26	1.35
47	R	607	CHL	C3A-C2A	-4.09	1.51	1.54
33	B	618	BCR	C16-C17	-4.09	1.30	1.43
32	a	408	PHO	C1D-C2D	4.09	1.44	1.39
50	n1	623	NEX	C14-C13	-4.09	1.26	1.35
31	b	613	CLA	MG-ND	-4.09	1.97	2.05
50	s	623	NEX	C10-C9	-4.09	1.26	1.35
31	B	612	CLA	MG-ND	-4.09	1.97	2.05
47	n	601	CHL	C3A-C2A	-4.09	1.51	1.54
31	c1	505	CLA	MG-ND	-4.09	1.97	2.05
42	C	527	LMK	O2-C4	4.09	1.43	1.30
50	y1	623	NEX	C34-C33	-4.09	1.26	1.35
50	R1	622	NEX	C34-C33	-4.09	1.26	1.35
50	y	623	NEX	C10-C9	-4.08	1.26	1.35
33	b1	618	BCR	C16-C17	-4.08	1.30	1.43
31	c	506	CLA	MG-ND	-4.08	1.97	2.05
31	r1	603	CLA	MG-ND	-4.08	1.97	2.05
47	n1	607	CHL	C3B-C4B	4.08	1.45	1.41
33	c1	516	BCR	C16-C17	-4.07	1.30	1.43
31	Y1	614	CLA	MG-ND	-4.07	1.97	2.05
33	d	404	BCR	C16-C17	-4.07	1.30	1.43
50	G	623	NEX	C10-C9	-4.07	1.26	1.35
31	C1	506	CLA	MG-ND	-4.07	1.97	2.05
50	S1	623	NEX	C34-C33	-4.07	1.26	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	B1	619	BCR	C10-C9	4.07	1.45	1.35
31	G1	604	CLA	MG-ND	-4.07	1.97	2.05
50	R	622	NEX	C14-C13	-4.07	1.26	1.35
31	B1	604	CLA	MG-ND	-4.06	1.97	2.05
31	A1	405	CLA	MG-ND	-4.06	1.97	2.05
47	g	606	CHL	C3A-C2A	-4.06	1.51	1.54
31	s1	611	CLA	MG-ND	-4.06	1.97	2.05
31	C	505	CLA	MG-ND	-4.05	1.97	2.05
31	C	508	CLA	MG-ND	-4.05	1.97	2.05
50	Y1	623	NEX	C10-C9	-4.05	1.26	1.35
33	c	514	BCR	C10-C9	4.05	1.45	1.35
50	y	623	NEX	C34-C33	-4.05	1.26	1.35
50	g1	623	NEX	C14-C13	-4.05	1.26	1.35
31	S1	610	CLA	MG-ND	-4.04	1.97	2.05
37	B1	620	C7Z	C4-C5	-4.04	1.44	1.51
37	B1	620	C7Z	C22-C21	4.04	1.66	1.54
31	b	612	CLA	MG-ND	-4.04	1.97	2.05
33	c	514	BCR	C16-C17	-4.04	1.30	1.43
31	c1	510	CLA	MG-ND	-4.04	1.97	2.05
47	y	607	CHL	C3B-C4B	4.04	1.45	1.41
33	b1	619	BCR	C10-C9	4.04	1.45	1.35
31	d1	402	CLA	MG-ND	-4.03	1.97	2.05
50	g	623	NEX	C34-C33	-4.03	1.26	1.35
50	n1	623	NEX	C30-C29	-4.03	1.26	1.35
31	S	612	CLA	MG-ND	-4.03	1.97	2.05
31	A	410	CLA	MG-ND	-4.03	1.97	2.05
50	n1	623	NEX	C34-C33	-4.03	1.26	1.35
33	c1	517	BCR	C16-C17	-4.03	1.30	1.43
50	y	623	NEX	C30-C29	-4.03	1.26	1.35
33	B	619	BCR	C10-C9	4.03	1.45	1.35
47	r1	606	CHL	C2C-C3C	4.03	1.40	1.36
31	B	607	CLA	MG-ND	-4.02	1.97	2.05
31	S	603	CLA	MG-ND	-4.02	1.97	2.05
31	C	506	CLA	MG-ND	-4.02	1.97	2.05
50	y1	623	NEX	C14-C13	-4.02	1.26	1.35
31	B	613	CLA	MG-ND	-4.02	1.97	2.05
31	b	604	CLA	MG-ND	-4.02	1.97	2.05
33	c	516	BCR	C16-C17	-4.02	1.30	1.43
31	b1	615	CLA	MG-ND	-4.02	1.97	2.05
56	r1	626	ERG	C16-C15	4.02	1.65	1.54
31	y	604	CLA	MG-ND	-4.01	1.97	2.05
31	c	509	CLA	MG-ND	-4.01	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	S	622	NEX	C7-C6	-4.01	1.25	1.30
50	N1	623	NEX	C10-C9	-4.01	1.26	1.35
31	y1	611	CLA	MG-ND	-4.01	1.97	2.05
33	b	619	BCR	C16-C17	-4.01	1.30	1.43
33	c1	514	BCR	C10-C9	4.01	1.45	1.35
37	B	620	C7Z	C27-C26	4.01	1.58	1.45
50	R1	622	NEX	C10-C9	-4.00	1.26	1.35
47	R1	607	CHL	C3A-C2A	-4.00	1.51	1.54
31	d	402	CLA	MG-ND	-4.00	1.97	2.05
31	c1	512	CLA	MG-ND	-4.00	1.97	2.05
46	h	101	RRX	C20-C21	4.00	1.55	1.43
31	S	614	CLA	MG-ND	-4.00	1.97	2.05
31	S1	611	CLA	MG-ND	-4.00	1.97	2.05
31	Y1	608	CLA	MG-ND	-3.99	1.97	2.05
31	S	610	CLA	MG-ND	-3.99	1.97	2.05
31	b	617	CLA	MG-ND	-3.99	1.97	2.05
31	C1	502	CLA	MG-ND	-3.99	1.97	2.05
47	S1	607	CHL	C3A-C2A	-3.99	1.51	1.54
31	S1	605	CLA	MG-ND	-3.99	1.97	2.05
31	a	410	CLA	MG-ND	-3.99	1.97	2.05
42	c1	527	LMK	O2-C4	3.99	1.43	1.30
31	c	513	CLA	MG-ND	-3.98	1.97	2.05
31	d	403	CLA	MG-ND	-3.98	1.97	2.05
50	y	623	NEX	C14-C13	-3.98	1.26	1.35
31	N1	613	CLA	MG-ND	-3.98	1.97	2.05
31	R1	603	CLA	MG-ND	-3.98	1.97	2.05
33	B1	618	BCR	C16-C17	-3.98	1.30	1.43
32	A	409	PHO	C1D-C2D	3.97	1.43	1.39
32	a	409	PHO	C1D-C2D	3.97	1.43	1.39
31	c	502	CLA	MG-ND	-3.97	1.97	2.05
31	b1	612	CLA	MG-ND	-3.97	1.97	2.05
31	B1	615	CLA	MG-ND	-3.97	1.97	2.05
33	D	404	BCR	C16-C17	-3.97	1.30	1.43
31	S1	604	CLA	MG-ND	-3.97	1.97	2.05
50	S1	623	NEX	C7-C6	-3.97	1.26	1.30
31	b	605	CLA	MG-ND	-3.97	1.97	2.05
31	B1	613	CLA	MG-ND	-3.97	1.97	2.05
47	R1	606	CHL	C2C-C3C	3.97	1.40	1.36
33	D1	404	BCR	C16-C17	-3.97	1.30	1.43
46	H1	101	RRX	C20-C21	3.97	1.55	1.43
31	C1	505	CLA	MG-ND	-3.96	1.97	2.05
31	N	610	CLA	MG-ND	-3.96	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	512	CLA	MG-ND	-3.96	1.97	2.05
47	g1	607	CHL	C3B-C4B	3.96	1.45	1.41
31	s	613	CLA	MG-ND	-3.95	1.97	2.05
31	C1	503	CLA	MG-ND	-3.95	1.97	2.05
47	G1	607	CHL	C2C-C3C	3.95	1.40	1.36
31	B1	607	CLA	MG-ND	-3.95	1.98	2.05
31	s1	614	CLA	MG-ND	-3.95	1.98	2.05
31	N	612	CLA	MG-ND	-3.95	1.98	2.05
31	R	604	CLA	MG-ND	-3.95	1.98	2.05
31	N	602	CLA	MG-ND	-3.95	1.98	2.05
31	B1	606	CLA	MG-ND	-3.95	1.98	2.05
31	Y	611	CLA	MG-ND	-3.95	1.98	2.05
31	S1	617	CLA	MG-ND	-3.94	1.98	2.05
33	a	411	BCR	C10-C9	3.94	1.44	1.35
31	G1	612	CLA	MG-ND	-3.94	1.98	2.05
47	S	608	CHL	C3A-C2A	-3.94	1.51	1.54
31	B	610	CLA	MG-ND	-3.94	1.98	2.05
31	S	611	CLA	MG-ND	-3.94	1.98	2.05
31	S1	613	CLA	MG-ND	-3.94	1.98	2.05
31	C	509	CLA	MG-ND	-3.94	1.98	2.05
31	s	614	CLA	MG-ND	-3.94	1.98	2.05
31	y	612	CLA	MG-ND	-3.94	1.98	2.05
31	A	407	CLA	MG-ND	-3.93	1.98	2.05
31	b	616	CLA	MG-ND	-3.93	1.98	2.05
31	C	503	CLA	MG-ND	-3.93	1.98	2.05
31	a	407	CLA	MG-ND	-3.93	1.98	2.05
31	a	405	CLA	MG-ND	-3.93	1.98	2.05
31	b	607	CLA	MG-ND	-3.93	1.98	2.05
31	G1	614	CLA	MG-ND	-3.93	1.98	2.05
31	b1	603	CLA	MG-ND	-3.93	1.98	2.05
40	c	519	DGD	O1G-C1A	3.93	1.44	1.33
31	C1	507	CLA	MG-ND	-3.92	1.98	2.05
37	B	620	C7Z	C22-C21	3.92	1.66	1.54
31	C1	508	CLA	MG-ND	-3.92	1.98	2.05
31	b1	610	CLA	MG-ND	-3.92	1.98	2.05
31	b1	613	CLA	MG-ND	-3.92	1.98	2.05
31	c1	507	CLA	MG-ND	-3.92	1.98	2.05
31	s	605	CLA	MG-ND	-3.92	1.98	2.05
31	A1	410	CLA	MG-ND	-3.92	1.98	2.05
31	c	504	CLA	MG-ND	-3.92	1.98	2.05
31	A	405	CLA	MG-ND	-3.92	1.98	2.05
31	b	611	CLA	MG-ND	-3.92	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	N1	610	CLA	MG-ND	-3.92	1.98	2.05
31	b	603	CLA	MG-ND	-3.92	1.98	2.05
31	b	606	CLA	MG-ND	-3.92	1.98	2.05
33	C	514	BCR	C10-C9	3.92	1.44	1.35
31	b1	614	CLA	MG-ND	-3.91	1.98	2.05
31	c	511	CLA	MG-ND	-3.91	1.98	2.05
31	Y	613	CLA	MG-ND	-3.91	1.98	2.05
31	g	611	CLA	MG-ND	-3.91	1.98	2.05
31	G1	603	CLA	MG-ND	-3.91	1.98	2.05
31	c1	506	CLA	MG-ND	-3.91	1.98	2.05
31	Y1	603	CLA	MG-ND	-3.91	1.98	2.05
47	N	607	CHL	C3A-C2A	-3.91	1.51	1.54
31	c	507	CLA	MG-ND	-3.91	1.98	2.05
31	g1	604	CLA	MG-ND	-3.91	1.98	2.05
33	d1	404	BCR	C10-C9	3.90	1.44	1.35
31	n1	604	CLA	MG-ND	-3.90	1.98	2.05
31	B1	603	CLA	MG-ND	-3.90	1.98	2.05
31	B1	608	CLA	MG-ND	-3.90	1.98	2.05
31	Y1	613	CLA	MG-ND	-3.90	1.98	2.05
47	n	609	CHL	C3B-C4B	3.90	1.45	1.41
37	b1	620	C7Z	C15-C14	3.90	1.55	1.43
31	Y1	612	CLA	MG-ND	-3.90	1.98	2.05
31	r1	608	CLA	MG-ND	-3.90	1.98	2.05
37	B1	620	C7Z	C15-C14	3.90	1.55	1.43
31	Y	614	CLA	MG-ND	-3.90	1.98	2.05
31	B	605	CLA	MG-ND	-3.90	1.98	2.05
31	Y	612	CLA	MG-ND	-3.90	1.98	2.05
31	c	508	CLA	MG-ND	-3.90	1.98	2.05
31	B1	617	CLA	MG-ND	-3.90	1.98	2.05
31	r	603	CLA	MG-ND	-3.90	1.98	2.05
31	n	613	CLA	MG-ND	-3.90	1.98	2.05
31	b1	606	CLA	MG-ND	-3.90	1.98	2.05
31	c	503	CLA	MG-ND	-3.89	1.98	2.05
47	g	607	CHL	C3B-C4B	3.89	1.45	1.41
31	R	609	CLA	MG-ND	-3.89	1.98	2.05
31	S	613	CLA	MG-ND	-3.89	1.98	2.05
33	C1	516	BCR	C16-C17	-3.89	1.31	1.43
37	b	620	C7Z	C27-C26	3.89	1.58	1.45
31	s	602	CLA	MG-ND	-3.89	1.98	2.05
33	B	618	BCR	C10-C9	3.89	1.44	1.35
37	B1	620	C7Z	C27-C26	3.89	1.58	1.45
37	B	620	C7Z	C15-C14	3.89	1.55	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	c	517	BCR	C10-C9	3.89	1.44	1.35
31	b	610	CLA	MG-ND	-3.88	1.98	2.05
31	n	612	CLA	MG-ND	-3.88	1.98	2.05
31	g1	602	CLA	MG-ND	-3.88	1.98	2.05
31	Y1	611	CLA	MG-ND	-3.88	1.98	2.05
46	H	101	RRX	C15-C14	3.88	1.55	1.43
31	g	604	CLA	MG-ND	-3.88	1.98	2.05
31	n1	613	CLA	MG-ND	-3.88	1.98	2.05
31	s1	605	CLA	MG-ND	-3.88	1.98	2.05
31	c	508	CLA	C1C-NC	-3.88	1.31	1.37
31	G	611	CLA	MG-ND	-3.88	1.98	2.05
31	N	603	CLA	MG-ND	-3.87	1.98	2.05
44	d	405	PL9	C3-C4	-3.87	1.43	1.49
31	D	402	CLA	MG-ND	-3.87	1.98	2.05
31	y1	612	CLA	MG-ND	-3.87	1.98	2.05
46	h	101	RRX	C23-C22	3.87	1.54	1.46
31	y	610	CLA	MG-ND	-3.87	1.98	2.05
31	s1	610	CLA	MG-ND	-3.87	1.98	2.05
33	c	515	BCR	C10-C9	3.87	1.44	1.35
33	C	515	BCR	C10-C9	3.87	1.44	1.35
47	r1	607	CHL	C3A-C2A	-3.87	1.51	1.54
31	a	406	CLA	MG-ND	-3.87	1.98	2.05
31	G1	602	CLA	MG-ND	-3.86	1.98	2.05
31	c1	504	CLA	MG-ND	-3.86	1.98	2.05
31	B	615	CLA	MG-ND	-3.86	1.98	2.05
33	c1	515	BCR	C16-C17	-3.86	1.31	1.43
31	B	608	CLA	MG-ND	-3.86	1.98	2.05
47	n1	609	CHL	C3A-C2A	-3.86	1.51	1.54
31	g	603	CLA	MG-ND	-3.86	1.98	2.05
31	G	612	CLA	MG-ND	-3.86	1.98	2.05
37	b	620	C7Z	C2-C1	3.86	1.66	1.54
31	C1	501	CLA	MG-ND	-3.86	1.98	2.05
31	N1	611	CLA	MG-ND	-3.86	1.98	2.05
50	G	623	NEX	C7-C6	-3.86	1.26	1.30
31	C	511	CLA	MG-ND	-3.86	1.98	2.05
31	y	614	CLA	MG-ND	-3.86	1.98	2.05
50	S	622	NEX	C10-C9	-3.85	1.26	1.35
31	G	604	CLA	MG-ND	-3.85	1.98	2.05
31	a1	410	CLA	MG-ND	-3.85	1.98	2.05
31	S1	603	CLA	MG-ND	-3.85	1.98	2.05
31	Y1	602	CLA	MG-ND	-3.85	1.98	2.05
33	A	411	BCR	C10-C9	3.85	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	N1	612	CLA	MG-ND	-3.85	1.98	2.05
31	D1	403	CLA	MG-ND	-3.85	1.98	2.05
31	A1	406	CLA	MG-ND	-3.85	1.98	2.05
31	A	406	CLA	MG-ND	-3.85	1.98	2.05
31	C1	504	CLA	MG-ND	-3.85	1.98	2.05
31	r1	609	CLA	MG-ND	-3.85	1.98	2.05
47	g1	607	CHL	C2C-C3C	3.85	1.40	1.36
31	Y	608	CLA	MG-ND	-3.85	1.98	2.05
37	b	620	C7Z	C22-C21	3.85	1.66	1.54
31	C	501	CLA	MG-ND	-3.85	1.98	2.05
31	c1	511	CLA	MG-ND	-3.84	1.98	2.05
31	n	611	CLA	MG-ND	-3.84	1.98	2.05
31	Y	604	CLA	MG-ND	-3.84	1.98	2.05
46	h	101	RRX	C15-C14	3.84	1.55	1.43
37	B1	620	C7Z	C35-C34	3.84	1.55	1.43
31	C1	509	CLA	MG-ND	-3.84	1.98	2.05
35	h1	102	LMG	C19-C18	-3.83	1.32	1.51
31	b1	605	CLA	MG-ND	-3.83	1.98	2.05
31	R	603	CLA	MG-ND	-3.83	1.98	2.05
31	c	510	CLA	MG-ND	-3.83	1.98	2.05
31	s	603	CLA	MG-ND	-3.83	1.98	2.05
31	r1	612	CLA	MG-ND	-3.83	1.98	2.05
31	S1	614	CLA	MG-ND	-3.83	1.98	2.05
31	B	611	CLA	MG-ND	-3.83	1.98	2.05
50	G1	623	NEX	C7-C6	-3.83	1.26	1.30
31	r	604	CLA	MG-ND	-3.83	1.98	2.05
31	a1	407	CLA	MG-ND	-3.83	1.98	2.05
31	y1	610	CLA	MG-ND	-3.83	1.98	2.05
33	C	517	BCR	C10-C9	3.83	1.44	1.35
31	r1	610	CLA	MG-ND	-3.83	1.98	2.05
37	b	620	C7Z	C15-C14	3.83	1.55	1.43
31	b	615	CLA	MG-ND	-3.83	1.98	2.05
31	y	608	CLA	MG-ND	-3.82	1.98	2.05
31	B	606	CLA	MG-ND	-3.82	1.98	2.05
31	g	613	CLA	MG-ND	-3.82	1.98	2.05
31	s	611	CLA	MG-ND	-3.82	1.98	2.05
31	s1	613	CLA	MG-ND	-3.82	1.98	2.05
31	G1	611	CLA	MG-ND	-3.82	1.98	2.05
47	G1	609	CHL	C2C-C3C	3.82	1.40	1.36
31	B1	610	CLA	MG-ND	-3.82	1.98	2.05
31	C1	511	CLA	MG-ND	-3.82	1.98	2.05
31	C	513	CLA	MG-ND	-3.82	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c1	508	CLA	MG-ND	-3.81	1.98	2.05
47	y1	601	CHL	C2C-C3C	3.81	1.40	1.36
50	n	623	NEX	C7-C6	-3.81	1.26	1.30
31	C	512	CLA	MG-ND	-3.81	1.98	2.05
31	N	614	CLA	MG-ND	-3.81	1.98	2.05
31	n	603	CLA	MG-ND	-3.81	1.98	2.05
31	n	610	CLA	MG-ND	-3.81	1.98	2.05
31	B1	605	CLA	MG-ND	-3.81	1.98	2.05
31	Y1	610	CLA	MG-ND	-3.81	1.98	2.05
31	d1	403	CLA	MG-ND	-3.81	1.98	2.05
31	B	603	CLA	MG-ND	-3.81	1.98	2.05
31	N	604	CLA	MG-ND	-3.81	1.98	2.05
31	r	612	CLA	MG-ND	-3.81	1.98	2.05
31	Y	603	CLA	MG-ND	-3.81	1.98	2.05
31	y	611	CLA	MG-ND	-3.81	1.98	2.05
31	y	613	CLA	MG-ND	-3.81	1.98	2.05
31	S	609	CLA	MG-ND	-3.81	1.98	2.05
31	S1	612	CLA	MG-ND	-3.81	1.98	2.05
31	G	613	CLA	MG-ND	-3.80	1.98	2.05
31	n1	611	CLA	MG-ND	-3.80	1.98	2.05
37	B	620	C7Z	C2-C1	3.80	1.66	1.54
31	a1	405	CLA	MG-ND	-3.80	1.98	2.05
31	B	602	CLA	MG-ND	-3.80	1.98	2.05
31	c1	503	CLA	MG-ND	-3.80	1.98	2.05
31	s1	603	CLA	MG-ND	-3.80	1.98	2.05
31	G	602	CLA	MG-ND	-3.80	1.98	2.05
31	g1	614	CLA	MG-ND	-3.80	1.98	2.05
31	G	610	CLA	MG-ND	-3.80	1.98	2.05
31	R1	609	CLA	MG-ND	-3.80	1.98	2.05
31	s1	612	CLA	MG-ND	-3.80	1.98	2.05
31	B	616	CLA	MG-ND	-3.80	1.98	2.05
31	S	604	CLA	MG-ND	-3.80	1.98	2.05
46	H1	101	RRX	C15-C14	3.79	1.54	1.43
31	s	609	CLA	MG-ND	-3.79	1.98	2.05
31	r	609	CLA	MG-ND	-3.79	1.98	2.05
31	N1	603	CLA	MG-ND	-3.79	1.98	2.05
31	N	613	CLA	MG-ND	-3.79	1.98	2.05
31	b	614	CLA	MG-ND	-3.79	1.98	2.05
31	R1	608	CLA	MG-ND	-3.79	1.98	2.05
31	c	501	CLA	MG-ND	-3.79	1.98	2.05
31	s	604	CLA	MG-ND	-3.79	1.98	2.05
33	A1	411	BCR	C10-C9	3.79	1.44	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	g1	612	CLA	MG-ND	-3.79	1.98	2.05
35	h	102	LMG	C19-C18	-3.79	1.32	1.51
31	D	403	CLA	MG-ND	-3.79	1.98	2.05
31	g	614	CLA	MG-ND	-3.79	1.98	2.05
31	S	617	CLA	MG-ND	-3.79	1.98	2.05
31	B1	611	CLA	MG-ND	-3.79	1.98	2.05
32	A	408	PHO	C1D-C2D	3.79	1.43	1.39
31	r1	604	CLA	MG-ND	-3.78	1.98	2.05
31	N	611	CLA	MG-ND	-3.78	1.98	2.05
31	b1	608	CLA	MG-ND	-3.78	1.98	2.05
31	Y	610	CLA	MG-ND	-3.78	1.98	2.05
31	y1	608	CLA	MG-ND	-3.78	1.98	2.05
31	B1	602	CLA	MG-ND	-3.78	1.98	2.05
31	S1	609	CLA	MG-ND	-3.78	1.98	2.05
31	b1	604	CLA	MG-ND	-3.78	1.98	2.05
31	y1	604	CLA	MG-ND	-3.78	1.98	2.05
31	r	610	CLA	MG-ND	-3.78	1.98	2.05
32	A	409	PHO	C4D-CHA	3.77	1.45	1.39
31	C	504	CLA	MG-ND	-3.77	1.98	2.05
31	b1	602	CLA	MG-ND	-3.77	1.98	2.05
31	S1	602	CLA	MG-ND	-3.77	1.98	2.05
31	c1	513	CLA	MG-ND	-3.77	1.98	2.05
31	b1	611	CLA	MG-ND	-3.77	1.98	2.05
31	g	612	CLA	MG-ND	-3.77	1.98	2.05
37	B	620	C7Z	C35-C34	3.77	1.54	1.43
31	y1	602	CLA	MG-ND	-3.77	1.98	2.05
32	A1	409	PHO	C4D-CHA	3.77	1.45	1.39
31	n1	612	CLA	MG-ND	-3.77	1.98	2.05
31	r	602	CLA	MG-ND	-3.77	1.98	2.05
31	s1	602	CLA	MG-ND	-3.77	1.98	2.05
31	B1	612	CLA	MG-ND	-3.76	1.98	2.05
31	b	608	CLA	MG-ND	-3.76	1.98	2.05
31	B1	616	CLA	MG-ND	-3.76	1.98	2.05
40	C	519	DGD	CDB-CCB	-3.76	1.33	1.51
31	s1	604	CLA	MG-ND	-3.76	1.98	2.05
31	B1	614	CLA	MG-ND	-3.76	1.98	2.05
31	y1	614	CLA	MG-ND	-3.76	1.98	2.05
31	R	611	CLA	MG-ND	-3.76	1.98	2.05
31	b1	616	CLA	MG-ND	-3.76	1.98	2.05
31	r	611	CLA	MG-ND	-3.76	1.98	2.05
31	C1	512	CLA	MG-ND	-3.76	1.98	2.05
31	c1	502	CLA	MG-ND	-3.76	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b1	607	CLA	MG-ND	-3.75	1.98	2.05
37	b1	620	C7Z	C2-C1	3.75	1.66	1.54
31	a1	406	CLA	MG-ND	-3.75	1.98	2.05
31	C1	513	CLA	MG-ND	-3.75	1.98	2.05
47	r	606	CHL	C2C-C3C	3.75	1.40	1.36
31	R1	604	CLA	MG-ND	-3.75	1.98	2.05
31	R	602	CLA	MG-ND	-3.75	1.98	2.05
31	S	605	CLA	MG-ND	-3.75	1.98	2.05
37	b1	620	C7Z	C27-C26	3.75	1.57	1.45
44	D	405	PL9	C3-C4	-3.75	1.43	1.49
31	N1	602	CLA	MG-ND	-3.75	1.98	2.05
35	c1	521	LMG	C22-C21	-3.75	1.33	1.51
40	C	518	DGD	CDB-CCB	-3.75	1.33	1.51
31	n1	610	CLA	MG-ND	-3.74	1.98	2.05
31	S	602	CLA	MG-ND	-3.74	1.98	2.05
31	G1	613	CLA	MG-ND	-3.74	1.98	2.05
31	y1	613	CLA	MG-ND	-3.74	1.98	2.05
31	n1	614	CLA	MG-ND	-3.74	1.98	2.05
47	G1	601	CHL	C3A-C2A	-3.74	1.51	1.54
32	A	408	PHO	C4D-CHA	3.74	1.45	1.39
31	R	613	CLA	MG-ND	-3.74	1.98	2.05
31	C	510	CLA	MG-ND	-3.74	1.98	2.05
31	s1	609	CLA	MG-ND	-3.74	1.98	2.05
40	c	523	DGD	CGA-CFA	-3.74	1.33	1.51
50	r	623	NEX	C7-C6	-3.74	1.26	1.30
31	y	603	CLA	MG-ND	-3.74	1.98	2.05
31	n1	602	CLA	MG-ND	-3.74	1.98	2.05
40	C	520	DGD	CAB-C9B	-3.74	1.33	1.51
31	g1	613	CLA	MG-ND	-3.74	1.98	2.05
47	G1	607	CHL	C3A-C2A	-3.73	1.51	1.54
31	s	610	CLA	MG-ND	-3.73	1.98	2.05
31	n1	603	CLA	MG-ND	-3.73	1.98	2.05
32	a1	409	PHO	C4D-CHA	3.73	1.45	1.39
31	C	502	CLA	MG-ND	-3.73	1.98	2.05
31	n	614	CLA	MG-ND	-3.73	1.98	2.05
31	N1	614	CLA	MG-ND	-3.73	1.98	2.05
40	c	523	DGD	CAA-C9A	-3.73	1.33	1.51
37	B1	620	C7Z	C2-C1	3.73	1.66	1.54
31	r	613	CLA	MG-ND	-3.73	1.98	2.05
35	H	102	LMG	C37-C36	-3.73	1.33	1.51
31	y1	603	CLA	MG-ND	-3.73	1.98	2.05
40	C1	520	DGD	CAA-C9A	-3.73	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C	521	LMG	C22-C21	-3.73	1.33	1.51
35	b	622	LMG	C19-C18	-3.72	1.33	1.51
35	c	521	LMG	C40-C39	-3.72	1.33	1.51
40	c	520	DGD	CAB-C9B	-3.72	1.33	1.51
40	c	519	DGD	CDB-CCB	-3.72	1.33	1.51
40	c	519	DGD	CAB-C9B	-3.72	1.33	1.51
31	Y1	604	CLA	MG-ND	-3.72	1.98	2.05
31	g	602	CLA	MG-ND	-3.72	1.98	2.05
35	H	102	LMG	C19-C18	-3.72	1.33	1.51
32	a1	409	PHO	C1D-C2D	3.72	1.43	1.39
35	c1	521	LMG	C19-C18	-3.72	1.33	1.51
31	R	608	CLA	MG-ND	-3.72	1.98	2.05
35	c	521	LMG	C22-C21	-3.72	1.33	1.51
31	y	602	CLA	MG-ND	-3.72	1.98	2.05
47	Y1	601	CHL	C2C-C3C	3.72	1.40	1.36
31	Y	602	CLA	MG-ND	-3.72	1.98	2.05
40	c1	518	DGD	CDB-CCB	-3.71	1.33	1.51
31	n	604	CLA	MG-ND	-3.71	1.98	2.05
31	s	617	CLA	MG-ND	-3.71	1.98	2.05
31	r1	602	CLA	MG-ND	-3.71	1.98	2.05
32	a	408	PHO	C4D-CHA	3.71	1.45	1.39
40	C	520	DGD	CAA-C9A	-3.71	1.33	1.51
40	C1	518	DGD	CDB-CCB	-3.71	1.33	1.51
50	R1	622	NEX	C7-C6	-3.71	1.26	1.30
31	R1	602	CLA	MG-ND	-3.71	1.98	2.05
35	a	413	LMG	C37-C36	-3.71	1.33	1.51
31	b	605	CLA	C1C-NC	-3.71	1.32	1.37
35	c1	523	LMG	C37-C36	-3.71	1.33	1.51
40	c	523	DGD	CAB-C9B	-3.71	1.33	1.51
31	b	602	CLA	MG-ND	-3.71	1.98	2.05
31	r	608	CLA	MG-ND	-3.71	1.98	2.05
31	c1	501	CLA	MG-ND	-3.71	1.98	2.05
31	C	508	CLA	C1C-NC	-3.70	1.32	1.37
37	b	620	C7Z	C35-C34	3.70	1.54	1.43
35	b1	622	LMG	C22-C21	-3.70	1.33	1.51
40	C1	519	DGD	CAB-C9B	-3.70	1.33	1.51
40	c	520	DGD	CAA-C9A	-3.70	1.33	1.51
38	b1	625	DGA	OG2-CB1	3.70	1.44	1.34
31	s1	617	CLA	MG-ND	-3.70	1.98	2.05
40	c1	519	DGD	CAB-C9B	-3.70	1.33	1.51
31	B	614	CLA	MG-ND	-3.70	1.98	2.05
31	R1	612	CLA	MG-ND	-3.70	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	c1	519	DGD	CDA-CCA	-3.70	1.33	1.51
31	G1	610	CLA	MG-ND	-3.70	1.98	2.05
31	g1	610	CLA	MG-ND	-3.70	1.98	2.05
40	C	523	DGD	CDA-CCA	-3.70	1.33	1.51
35	B1	622	LMG	C22-C21	-3.70	1.33	1.51
35	H	102	LMG	C40-C39	-3.69	1.33	1.51
31	b1	605	CLA	C1C-NC	-3.69	1.32	1.37
35	A1	413	LMG	C40-C39	-3.69	1.33	1.51
40	C1	519	DGD	CDA-CCA	-3.69	1.33	1.51
31	G	603	CLA	MG-ND	-3.69	1.98	2.05
35	b	622	LMG	C22-C21	-3.69	1.33	1.51
35	c1	523	LMG	C40-C39	-3.69	1.33	1.51
50	Y1	623	NEX	C7-C6	-3.69	1.26	1.30
35	A	413	LMG	C37-C36	-3.69	1.33	1.51
47	n1	608	CHL	C3A-C2A	-3.69	1.51	1.54
35	h	102	LMG	C37-C36	-3.69	1.33	1.51
35	C1	523	LMG	C40-C39	-3.68	1.33	1.51
40	c	519	DGD	CDA-CCA	-3.68	1.33	1.51
35	B	622	LMG	C22-C21	-3.68	1.33	1.51
35	a1	413	LMG	C37-C36	-3.68	1.33	1.51
35	c1	523	LMG	C25-C24	-3.68	1.33	1.51
47	s1	607	CHL	C3A-C2A	-3.68	1.51	1.54
35	C1	521	LMG	C22-C21	-3.68	1.33	1.51
40	C1	520	DGD	CAB-C9B	-3.68	1.33	1.51
35	C1	523	LMG	C25-C24	-3.68	1.33	1.51
35	w1	201	LMG	C37-C36	-3.68	1.33	1.51
47	Y1	601	CHL	CBB-CAB	3.68	1.52	1.29
37	b1	620	C7Z	C35-C34	3.68	1.54	1.43
35	a1	413	LMG	C40-C39	-3.68	1.33	1.51
35	A	413	LMG	C40-C39	-3.68	1.33	1.51
35	D	411	LMG	C22-C21	-3.67	1.33	1.51
40	c	518	DGD	CDB-CCB	-3.67	1.33	1.51
35	a	413	LMG	C40-C39	-3.67	1.33	1.51
31	R	610	CLA	MG-ND	-3.67	1.98	2.05
35	h1	102	LMG	C37-C36	-3.67	1.33	1.51
40	C	523	DGD	CGA-CFA	-3.67	1.33	1.51
47	Y	607	CHL	C3A-C2A	-3.67	1.51	1.54
35	W1	201	LMG	C40-C39	-3.67	1.33	1.51
31	g1	603	CLA	MG-ND	-3.67	1.98	2.05
35	C1	523	LMG	C37-C36	-3.67	1.33	1.51
35	W1	201	LMG	C37-C36	-3.67	1.33	1.51
35	H1	102	LMG	C19-C18	-3.67	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b1	612	CLA	C1C-NC	-3.67	1.32	1.37
35	B	622	LMG	C19-C18	-3.66	1.33	1.51
40	c1	518	DGD	CAB-C9B	-3.66	1.33	1.51
31	Y1	610	CLA	C1C-NC	-3.66	1.32	1.37
35	B1	622	LMG	C19-C18	-3.66	1.33	1.51
37	B	620	C7Z	C7-C6	3.66	1.57	1.45
35	J	101	LMG	C22-C21	-3.66	1.33	1.51
35	d1	411	LMG	C19-C18	-3.66	1.33	1.51
40	C1	518	DGD	CAB-C9B	-3.66	1.33	1.51
47	N1	608	CHL	CBB-CAB	3.66	1.52	1.29
35	C1	523	LMG	C43-C42	-3.66	1.33	1.51
31	G	614	CLA	MG-ND	-3.66	1.98	2.05
35	A1	413	LMG	C37-C36	-3.66	1.33	1.51
35	a	413	LMG	C19-C18	-3.66	1.33	1.51
47	y1	601	CHL	CBB-CAB	3.66	1.52	1.29
35	C1	521	LMG	C40-C39	-3.66	1.33	1.51
35	c1	523	LMG	C22-C21	-3.66	1.33	1.51
40	C	519	DGD	CAB-C9B	-3.65	1.33	1.51
40	C	523	DGD	CAA-C9A	-3.65	1.33	1.51
31	R1	610	CLA	MG-ND	-3.65	1.98	2.05
31	A1	407	CLA	MG-ND	-3.65	1.98	2.05
35	C	521	LMG	C19-C18	-3.65	1.33	1.51
40	C	519	DGD	CDA-CCA	-3.65	1.33	1.51
31	g	610	CLA	MG-ND	-3.65	1.98	2.05
35	H1	102	LMG	C37-C36	-3.65	1.33	1.51
40	c	523	DGD	CDA-CCA	-3.65	1.33	1.51
40	c	523	DGD	CGB-CFB	-3.65	1.33	1.51
35	C1	523	LMG	C22-C21	-3.65	1.33	1.51
35	d	411	LMG	C22-C21	-3.65	1.33	1.51
35	H1	102	LMG	C40-C39	-3.65	1.33	1.51
46	h1	101	RRX	C11-C10	3.65	1.54	1.43
40	C1	519	DGD	CDB-CCB	-3.65	1.33	1.51
31	s	612	CLA	MG-ND	-3.65	1.98	2.05
31	n	602	CLA	MG-ND	-3.65	1.98	2.05
35	C1	521	LMG	C19-C18	-3.64	1.33	1.51
47	Y	601	CHL	CBB-CAB	3.64	1.52	1.29
35	D1	411	LMG	C19-C18	-3.64	1.33	1.51
35	c1	523	LMG	C43-C42	-3.64	1.33	1.51
40	c	523	DGD	CDB-CCB	-3.64	1.33	1.51
40	C	520	DGD	CDB-CCB	-3.64	1.33	1.51
40	c	518	DGD	CAB-C9B	-3.64	1.33	1.51
35	J	101	LMG	C19-C18	-3.64	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
40	C	518	DGD	CAB-C9B	-3.64	1.33	1.51
47	s1	606	CHL	CBB-CAB	3.64	1.52	1.29
45	f1	101	HEM	FE-ND	3.64	2.06	1.94
35	C	521	LMG	C40-C39	-3.64	1.33	1.51
35	d1	411	LMG	C22-C21	-3.64	1.33	1.51
47	r	606	CHL	C3A-C2A	-3.64	1.51	1.54
35	b1	622	LMG	C19-C18	-3.64	1.33	1.51
35	a1	413	LMG	C19-C18	-3.64	1.33	1.51
32	A1	408	PHO	C4D-CHA	3.64	1.45	1.39
35	h	102	LMG	C40-C39	-3.63	1.33	1.51
35	c	521	LMG	C37-C36	-3.63	1.33	1.51
35	c	521	LMG	C19-C18	-3.63	1.33	1.51
40	c1	520	DGD	CDB-CCB	-3.63	1.33	1.51
35	A	413	LMG	C19-C18	-3.63	1.33	1.51
40	c1	520	DGD	CAA-C9A	-3.63	1.33	1.51
31	b	617	CLA	C1C-NC	-3.63	1.32	1.37
35	c1	521	LMG	C40-C39	-3.63	1.33	1.51
35	j	101	LMG	C19-C18	-3.63	1.33	1.51
40	c1	519	DGD	CAA-C9A	-3.63	1.33	1.51
31	g1	611	CLA	MG-ND	-3.63	1.98	2.05
40	C1	519	DGD	CAA-C9A	-3.63	1.33	1.51
35	D1	411	LMG	C22-C21	-3.63	1.33	1.51
47	g	609	CHL	C2C-C3C	3.63	1.39	1.36
35	C	521	LMG	C37-C36	-3.63	1.33	1.51
40	C	523	DGD	CAB-C9B	-3.63	1.33	1.51
38	b	623	DGA	OG2-CB1	3.63	1.44	1.34
40	C	523	DGD	CDB-CCB	-3.63	1.33	1.51
47	Y1	607	CHL	CBB-CAB	3.62	1.52	1.29
44	d1	405	PL9	C7-C3	-3.62	1.46	1.51
47	G	609	CHL	CBB-CAB	3.62	1.52	1.29
35	A1	413	LMG	C19-C18	-3.62	1.33	1.51
47	Y	601	CHL	C3B-C4B	3.62	1.44	1.41
47	N	609	CHL	CBB-CAB	3.62	1.52	1.29
38	B	625	DGA	OG2-CB1	3.62	1.44	1.34
47	n1	609	CHL	CBB-CAB	3.62	1.52	1.29
40	c1	520	DGD	CAB-C9B	-3.62	1.33	1.51
40	C	523	DGD	CGB-CFB	-3.62	1.33	1.51
35	j	101	LMG	C22-C21	-3.62	1.33	1.51
35	c1	523	LMG	C19-C18	-3.62	1.33	1.51
35	h1	102	LMG	C40-C39	-3.62	1.33	1.51
47	n	609	CHL	CBB-CAB	3.62	1.52	1.29
31	R	612	CLA	MG-ND	-3.61	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	C1	523	LMG	C19-C18	-3.61	1.33	1.51
35	D	411	LMG	C19-C18	-3.61	1.33	1.51
40	c	520	DGD	CDB-CCB	-3.61	1.33	1.51
47	G	607	CHL	CBB-CAB	3.61	1.51	1.29
47	N	608	CHL	CBB-CAB	3.61	1.51	1.29
47	g1	605	CHL	CBB-CAB	3.61	1.51	1.29
40	c	519	DGD	CAA-C9A	-3.61	1.33	1.51
47	g	606	CHL	CBB-CAB	3.61	1.51	1.29
37	b1	620	C7Z	C38-C25	3.60	1.56	1.50
47	G1	609	CHL	CBB-CAB	3.60	1.51	1.29
47	G	605	CHL	CBB-CAB	3.60	1.51	1.29
40	C1	520	DGD	CDB-CCB	-3.60	1.33	1.51
38	B1	625	DGA	OG2-CB1	3.60	1.44	1.34
35	c1	521	LMG	C37-C36	-3.60	1.33	1.51
47	y	601	CHL	CBB-CAB	3.60	1.51	1.29
47	g	601	CHL	CBB-CAB	3.60	1.51	1.29
40	c1	519	DGD	CDB-CCB	-3.60	1.33	1.51
47	y	609	CHL	CBB-CAB	3.60	1.51	1.29
47	Y	609	CHL	CBB-CAB	3.59	1.51	1.29
40	C	519	DGD	CAA-C9A	-3.59	1.33	1.51
47	G1	605	CHL	CBB-CAB	3.59	1.51	1.29
47	g	608	CHL	CBB-CAB	3.59	1.51	1.29
47	N	607	CHL	CBB-CAB	3.59	1.51	1.29
37	b	620	C7Z	C38-C25	3.59	1.56	1.50
35	w1	201	LMG	C40-C39	-3.59	1.33	1.51
31	D1	402	CLA	C1C-NC	-3.59	1.32	1.37
35	C1	521	LMG	C37-C36	-3.58	1.33	1.51
35	d	411	LMG	C19-C18	-3.58	1.34	1.51
47	G1	607	CHL	CBB-CAB	3.58	1.51	1.29
47	n	605	CHL	CBB-CAB	3.58	1.51	1.29
47	S1	607	CHL	CBB-CAB	3.58	1.51	1.29
47	Y	605	CHL	CBB-CAB	3.58	1.51	1.29
47	y	607	CHL	CBB-CAB	3.58	1.51	1.29
47	G1	601	CHL	CBB-CAB	3.58	1.51	1.29
47	n1	607	CHL	CBB-CAB	3.57	1.51	1.29
45	F1	101	HEM	FE-ND	3.57	2.05	1.94
47	N1	605	CHL	CBB-CAB	3.57	1.51	1.29
47	S1	608	CHL	CBB-CAB	3.57	1.51	1.29
47	n1	605	CHL	CBB-CAB	3.57	1.51	1.29
47	y1	609	CHL	CBB-CAB	3.57	1.51	1.29
47	Y1	606	CHL	CBB-CAB	3.57	1.51	1.29
47	g1	607	CHL	CBB-CAB	3.57	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	g1	601	CHL	CBB-CAB	3.57	1.51	1.29
47	s1	607	CHL	CBB-CAB	3.57	1.51	1.29
47	s	607	CHL	CBB-CAB	3.57	1.51	1.29
47	n1	601	CHL	CBB-CAB	3.57	1.51	1.29
47	y	605	CHL	CBB-CAB	3.57	1.51	1.29
31	c	506	CLA	C1C-NC	-3.56	1.32	1.37
47	g1	609	CHL	CBB-CAB	3.56	1.51	1.29
47	n	601	CHL	CBB-CAB	3.56	1.51	1.29
47	n1	606	CHL	CBB-CAB	3.56	1.51	1.29
37	B1	620	C7Z	C7-C6	3.56	1.57	1.45
47	g1	606	CHL	CBB-CAB	3.56	1.51	1.29
47	Y1	605	CHL	CBB-CAB	3.56	1.51	1.29
47	g	605	CHL	CBB-CAB	3.56	1.51	1.29
47	N1	601	CHL	CBB-CAB	3.56	1.51	1.29
46	h1	101	RRX	C16-C17	3.56	1.54	1.43
47	y1	605	CHL	CBB-CAB	3.56	1.51	1.29
47	s	606	CHL	CBB-CAB	3.55	1.51	1.29
37	b	620	C7Z	C7-C6	3.55	1.57	1.45
47	n	607	CHL	CBB-CAB	3.55	1.51	1.29
31	c1	509	CLA	MG-ND	-3.55	1.98	2.05
47	s1	601	CHL	CBB-CAB	3.55	1.51	1.29
47	G	601	CHL	CBB-CAB	3.55	1.51	1.29
47	r	606	CHL	CBB-CAB	3.55	1.51	1.29
47	y	606	CHL	CBB-CAB	3.55	1.51	1.29
47	N	601	CHL	CBB-CAB	3.55	1.51	1.29
47	n1	608	CHL	CBB-CAB	3.55	1.51	1.29
31	Y	610	CLA	C1C-NC	-3.55	1.32	1.37
47	y1	606	CHL	CBB-CAB	3.55	1.51	1.29
47	s1	608	CHL	CBB-CAB	3.55	1.51	1.29
47	y1	607	CHL	CBB-CAB	3.55	1.51	1.29
47	s	608	CHL	CBB-CAB	3.54	1.51	1.29
47	G1	608	CHL	CBB-CAB	3.54	1.51	1.29
54	i1	101	4RF	O18-C16	3.54	1.43	1.33
47	S	608	CHL	CBB-CAB	3.54	1.51	1.29
32	a1	408	PHO	C4D-CHA	3.54	1.44	1.39
47	r1	607	CHL	CBB-CAB	3.54	1.51	1.29
47	S	606	CHL	CBB-CAB	3.54	1.51	1.29
47	n	608	CHL	CBB-CAB	3.54	1.51	1.29
47	R	606	CHL	CBB-CAB	3.54	1.51	1.29
47	N	605	CHL	CBB-CAB	3.54	1.51	1.29
47	G1	607	CHL	C3B-C4B	3.54	1.44	1.41
54	I1	102	4RF	O18-C16	3.53	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	Y1	609	CHL	CBB-CAB	3.53	1.51	1.29
38	j1	101	DGA	OG2-CB1	3.53	1.44	1.34
47	G	608	CHL	CBB-CAB	3.53	1.51	1.29
31	B1	617	CLA	C1C-NC	-3.53	1.32	1.37
47	Y	601	CHL	C2C-C3C	3.53	1.39	1.36
47	Y	606	CHL	CBB-CAB	3.53	1.51	1.29
47	G	605	CHL	C3A-C2A	-3.53	1.51	1.54
31	N1	610	CLA	C1C-NC	-3.52	1.32	1.37
47	r1	606	CHL	CBB-CAB	3.52	1.51	1.29
33	c1	517	BCR	C10-C9	3.52	1.43	1.35
37	B1	620	C7Z	C38-C25	3.52	1.56	1.50
47	r	607	CHL	CBB-CAB	3.52	1.51	1.29
31	n	610	CLA	C1C-NC	-3.52	1.32	1.37
47	S	607	CHL	CBB-CAB	3.51	1.51	1.29
46	h	101	RRX	C24-C25	3.51	1.57	1.45
47	R1	607	CHL	CBB-CAB	3.51	1.51	1.29
47	y	601	CHL	C2C-C3C	3.51	1.39	1.36
47	R1	606	CHL	CBB-CAB	3.51	1.51	1.29
47	g	609	CHL	CBB-CAB	3.50	1.51	1.29
47	G	606	CHL	CBB-CAB	3.50	1.51	1.29
37	b1	620	C7Z	C7-C6	3.50	1.57	1.45
37	B1	620	C7Z	C21-C26	-3.50	1.49	1.53
31	D	402	CLA	C1C-NC	-3.50	1.32	1.37
47	g1	608	CHL	CBB-CAB	3.50	1.51	1.29
44	D	405	PL9	C6-C1	-3.50	1.42	1.48
31	b	613	CLA	C1C-NC	-3.50	1.32	1.37
47	N1	606	CHL	CBB-CAB	3.50	1.51	1.29
50	N	623	NEX	C7-C6	-3.49	1.26	1.30
46	H	101	RRX	C11-C10	3.49	1.54	1.43
31	B1	616	CLA	C1C-NC	-3.48	1.32	1.37
47	R	607	CHL	CBB-CAB	3.48	1.51	1.29
31	a	406	CLA	C1C-NC	-3.48	1.32	1.37
47	N1	609	CHL	CBB-CAB	3.48	1.51	1.29
50	y	623	NEX	C7-C6	-3.48	1.26	1.30
47	S1	601	CHL	CBB-CAB	3.47	1.51	1.29
31	c1	502	CLA	C1C-NC	-3.47	1.32	1.37
46	h1	101	RRX	C24-C25	3.47	1.56	1.45
31	S1	610	CLA	C1C-NC	-3.46	1.32	1.37
31	B	617	CLA	C1C-NC	-3.45	1.32	1.37
47	G1	606	CHL	CBB-CAB	3.45	1.50	1.29
50	g1	623	NEX	C1-C6	-3.45	1.48	1.54
54	k1	101	4RF	O18-C16	3.45	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	c1	524	DGA	OG2-CB1	3.45	1.44	1.34
31	s	602	CLA	C1C-NC	-3.45	1.32	1.37
46	h	101	RRX	C11-C10	3.44	1.53	1.43
44	d	405	PL9	C6-C1	-3.44	1.42	1.48
31	B	605	CLA	C1C-NC	-3.44	1.32	1.37
31	b	612	CLA	C1C-NC	-3.44	1.32	1.37
46	H	101	RRX	C16-C17	3.43	1.53	1.43
31	b1	617	CLA	C1C-NC	-3.43	1.32	1.37
54	K1	101	4RF	O18-C16	3.42	1.43	1.33
47	g	607	CHL	CBB-CAB	3.42	1.50	1.29
31	G	610	CLA	C1C-NC	-3.42	1.32	1.37
31	y	604	CLA	C1C-NC	-3.42	1.32	1.37
31	G1	610	CLA	C1C-NC	-3.42	1.32	1.37
46	h	101	RRX	C29-C30	3.41	1.65	1.54
38	C	524	DGA	OG2-CB1	3.41	1.43	1.34
31	C	506	CLA	C1C-NC	-3.41	1.32	1.37
38	J1	101	DGA	OG2-CB1	3.41	1.43	1.34
47	N1	607	CHL	CBB-CAB	3.41	1.50	1.29
38	c	524	DGA	OG2-CB1	3.41	1.43	1.34
47	N	606	CHL	CBB-CAB	3.40	1.50	1.29
31	B	612	CLA	C1C-NC	-3.40	1.32	1.37
31	A1	405	CLA	C1C-NC	-3.40	1.32	1.37
38	C1	524	DGA	OG2-CB1	3.39	1.43	1.34
31	C	504	CLA	C1C-NC	-3.39	1.32	1.37
47	g1	601	CHL	C3A-C2A	-3.39	1.51	1.54
50	Y1	623	NEX	C1-C6	-3.39	1.48	1.54
46	H	101	RRX	C24-C25	3.39	1.56	1.45
47	R	606	CHL	C2C-C3C	3.39	1.39	1.36
31	C1	502	CLA	C1C-NC	-3.38	1.32	1.37
47	s	608	CHL	C3A-C2A	-3.38	1.51	1.54
46	H1	101	RRX	C11-C10	3.38	1.53	1.43
47	Y	607	CHL	CBB-CAB	3.38	1.50	1.29
31	C1	501	CLA	C1C-NC	-3.38	1.32	1.37
37	B	620	C7Z	C38-C25	3.38	1.56	1.50
31	b	611	CLA	C1C-NC	-3.38	1.32	1.37
47	s	601	CHL	CBB-CAB	3.37	1.50	1.29
31	y	603	CLA	C1C-NC	-3.37	1.32	1.37
47	S	601	CHL	CBB-CAB	3.37	1.50	1.29
38	J1	101	DGA	OG1-CA1	3.37	1.43	1.33
31	n	604	CLA	C1C-NC	-3.37	1.32	1.37
31	C1	504	CLA	C1C-NC	-3.37	1.32	1.37
38	c	524	DGA	OG1-CA1	3.37	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b	607	CLA	C1C-NC	-3.36	1.32	1.37
38	C1	524	DGA	OG1-CA1	3.36	1.43	1.33
31	C	510	CLA	C1C-NC	-3.36	1.32	1.37
38	C	524	DGA	OG1-CA1	3.36	1.43	1.33
31	B1	611	CLA	C1C-NC	-3.36	1.32	1.37
47	y1	607	CHL	C3B-C4B	3.36	1.44	1.41
47	g	607	CHL	C3A-C2A	-3.35	1.51	1.54
31	y1	610	CLA	C1C-NC	-3.35	1.32	1.37
31	C	505	CLA	C1C-NC	-3.35	1.32	1.37
50	n1	623	NEX	C7-C6	-3.35	1.26	1.30
47	S1	606	CHL	CBB-CAB	3.35	1.50	1.29
31	A	410	CLA	C1C-NC	-3.34	1.32	1.37
50	N1	623	NEX	C7-C6	-3.34	1.26	1.30
31	N1	604	CLA	C1C-NC	-3.34	1.32	1.37
46	H1	101	RRX	C29-C30	3.34	1.64	1.54
31	Y	602	CLA	C1C-NC	-3.34	1.32	1.37
31	C1	508	CLA	C1C-NC	-3.34	1.32	1.37
47	S1	608	CHL	C3A-C2A	-3.34	1.51	1.54
31	y	610	CLA	C1C-NC	-3.34	1.32	1.37
47	Y1	605	CHL	C3A-C2A	-3.33	1.51	1.54
31	N	610	CLA	C1C-NC	-3.33	1.32	1.37
31	C	502	CLA	C1C-NC	-3.33	1.32	1.37
38	c1	524	DGA	OG1-CA1	3.33	1.43	1.33
31	C1	506	CLA	C1C-NC	-3.33	1.32	1.37
31	c1	503	CLA	C1C-NC	-3.32	1.32	1.37
46	h	101	RRX	C16-C17	3.32	1.53	1.43
46	H1	101	RRX	C24-C25	3.32	1.56	1.45
31	c	511	CLA	C1C-NC	-3.32	1.32	1.37
38	j1	101	DGA	OG1-CA1	3.31	1.43	1.33
31	a	407	CLA	C1C-NC	-3.31	1.32	1.37
45	F	101	HEM	FE-NB	3.31	2.05	1.94
31	S	612	CLA	C1C-NC	-3.31	1.32	1.37
31	A	405	CLA	C1C-NC	-3.31	1.32	1.37
38	B	625	DGA	OG1-CA1	3.31	1.43	1.33
47	n	606	CHL	CBB-CAB	3.31	1.50	1.29
46	h1	101	RRX	C29-C30	3.31	1.64	1.54
38	B1	625	DGA	OG1-CA1	3.31	1.43	1.33
31	B	611	CLA	C1C-NC	-3.31	1.32	1.37
44	D	405	PL9	C7-C3	-3.31	1.46	1.51
31	a	405	CLA	C1C-NC	-3.30	1.32	1.37
31	A	407	CLA	C1C-NC	-3.30	1.32	1.37
31	S1	611	CLA	C1C-NC	-3.30	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
46	H1	101	RRX	C16-C17	3.30	1.53	1.43
31	r1	604	CLA	C1C-NC	-3.29	1.32	1.37
31	C	503	CLA	C1C-NC	-3.29	1.32	1.37
31	S1	613	CLA	C1C-NC	-3.29	1.32	1.37
31	c	507	CLA	C1C-NC	-3.29	1.32	1.37
31	B1	607	CLA	C1C-NC	-3.29	1.32	1.37
44	D1	405	PL9	C6-C1	-3.29	1.43	1.48
31	G	603	CLA	C1C-NC	-3.29	1.32	1.37
31	a1	406	CLA	C1C-NC	-3.29	1.32	1.37
31	A	406	CLA	C1C-NC	-3.29	1.32	1.37
31	B1	606	CLA	C1C-NC	-3.28	1.32	1.37
47	G1	606	CHL	C3A-C2A	-3.28	1.51	1.54
38	b	623	DGA	OG1-CA1	3.28	1.42	1.33
31	C1	509	CLA	C1C-NC	-3.28	1.32	1.37
31	S	610	CLA	C1C-NC	-3.28	1.32	1.37
31	b1	607	CLA	C1C-NC	-3.28	1.32	1.37
31	c1	509	CLA	C1C-NC	-3.28	1.32	1.37
31	b1	611	CLA	C1C-NC	-3.27	1.32	1.37
46	H	101	RRX	C29-C30	3.27	1.64	1.54
46	h	101	RRX	C4-C5	-3.27	1.44	1.51
31	g	603	CLA	C1C-NC	-3.27	1.32	1.37
31	Y	612	CLA	C1C-NC	-3.27	1.32	1.37
31	a	410	CLA	C1C-NC	-3.27	1.32	1.37
31	C1	510	CLA	C1C-NC	-3.27	1.32	1.37
50	R	622	NEX	C10-C9	-3.27	1.28	1.35
31	b	610	CLA	C1C-NC	-3.26	1.32	1.37
45	F1	101	HEM	CAB-C3B	3.26	1.56	1.47
31	y	612	CLA	C1C-NC	-3.26	1.32	1.37
31	C	513	CLA	C1C-NC	-3.26	1.32	1.37
31	b	606	CLA	C1C-NC	-3.26	1.32	1.37
31	y1	613	CLA	C1C-NC	-3.26	1.32	1.37
45	f1	101	HEM	CAB-C3B	3.26	1.56	1.47
47	Y1	607	CHL	C3B-C4B	3.26	1.44	1.41
45	f	101	HEM	FE-ND	3.26	2.04	1.94
31	B1	605	CLA	C1C-NC	-3.26	1.32	1.37
31	a1	407	CLA	C1C-NC	-3.25	1.32	1.37
45	f	101	HEM	FE-NA	3.25	2.05	1.95
45	f1	101	HEM	FE-NB	3.25	2.04	1.94
31	S1	605	CLA	C1C-NC	-3.25	1.32	1.37
31	a	410	CLA	C4B-NB	-3.25	1.33	1.37
31	G	604	CLA	C1C-NC	-3.25	1.32	1.37
31	Y1	603	CLA	C1C-NC	-3.25	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	y	614	CLA	C1C-NC	-3.24	1.32	1.37
47	y	601	CHL	C3B-C4B	3.24	1.44	1.41
31	R	612	CLA	C1C-NC	-3.24	1.32	1.37
31	y1	611	CLA	C1C-NC	-3.24	1.32	1.37
31	C	501	CLA	C1C-NC	-3.23	1.32	1.37
45	f1	101	HEM	CAC-C3C	3.23	1.56	1.47
31	S	613	CLA	C1C-NC	-3.23	1.32	1.37
31	r1	608	CLA	C1C-NC	-3.23	1.32	1.37
50	Y	623	NEX	C7-C6	-3.22	1.26	1.30
31	N	602	CLA	C1C-NC	-3.22	1.32	1.37
31	r1	603	CLA	C1C-NC	-3.22	1.32	1.37
31	B1	603	CLA	C1C-NC	-3.22	1.32	1.37
31	B	614	CLA	C1C-NC	-3.22	1.32	1.37
31	n1	610	CLA	C1C-NC	-3.22	1.32	1.37
31	d	403	CLA	C1C-NC	-3.21	1.32	1.37
31	y	613	CLA	C1C-NC	-3.21	1.32	1.37
31	G	612	CLA	C1C-NC	-3.21	1.32	1.37
31	A1	407	CLA	C1C-NC	-3.21	1.32	1.37
45	f	101	HEM	FE-NC	3.21	2.05	1.95
31	b1	613	CLA	C1C-NC	-3.21	1.32	1.37
31	c	509	CLA	C1C-NC	-3.21	1.32	1.37
31	b1	602	CLA	C1C-NC	-3.21	1.32	1.37
31	c	510	CLA	C1C-NC	-3.21	1.32	1.37
31	C	512	CLA	C1C-NC	-3.21	1.32	1.37
31	Y	614	CLA	C1C-NC	-3.21	1.32	1.37
31	B1	604	CLA	C1C-NC	-3.20	1.32	1.37
31	S1	602	CLA	C1C-NC	-3.20	1.32	1.37
31	B	609	CLA	C1C-NC	-3.20	1.32	1.37
31	S	602	CLA	C1C-NC	-3.20	1.32	1.37
31	n	603	CLA	C1C-NC	-3.20	1.32	1.37
31	A1	406	CLA	C1C-NC	-3.20	1.32	1.37
31	r	613	CLA	C1C-NC	-3.20	1.32	1.37
31	B1	610	CLA	C1C-NC	-3.20	1.32	1.37
31	y1	603	CLA	C1C-NC	-3.20	1.32	1.37
31	Y1	604	CLA	C1C-NC	-3.20	1.32	1.37
31	c1	510	CLA	C1C-NC	-3.19	1.32	1.37
31	c1	501	CLA	C1C-NC	-3.19	1.32	1.37
46	h1	101	RRX	C7-C6	3.19	1.56	1.45
31	B	616	CLA	C1C-NC	-3.19	1.32	1.37
31	Y1	613	CLA	C1C-NC	-3.19	1.32	1.37
31	C	511	CLA	C1C-NC	-3.19	1.32	1.37
31	N	612	CLA	C1C-NC	-3.19	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	C1	513	CLA	C1C-NC	-3.19	1.32	1.37
31	C	507	CLA	C1C-NC	-3.19	1.32	1.37
31	g	604	CLA	C1C-NC	-3.19	1.32	1.37
47	N	609	CHL	C3B-C4B	3.19	1.44	1.41
31	C	509	CLA	C1C-NC	-3.18	1.32	1.37
47	G1	605	CHL	C3A-C2A	-3.18	1.52	1.54
31	r1	609	CLA	C1C-NC	-3.18	1.32	1.37
31	y	611	CLA	C1C-NC	-3.18	1.32	1.37
31	c1	505	CLA	C1C-NC	-3.18	1.32	1.37
31	B1	615	CLA	C1C-NC	-3.18	1.32	1.37
31	S1	612	CLA	C1C-NC	-3.18	1.32	1.37
47	n1	605	CHL	C3A-C2A	-3.18	1.52	1.54
46	H	101	RRX	C4-C5	-3.18	1.45	1.51
31	c1	507	CLA	C1C-NC	-3.18	1.32	1.37
31	d	402	CLA	C1C-NC	-3.18	1.32	1.37
31	b1	610	CLA	C1C-NC	-3.17	1.32	1.37
31	G1	602	CLA	C1C-NC	-3.17	1.32	1.37
31	c	512	CLA	C1C-NC	-3.17	1.32	1.37
31	Y1	614	CLA	C1C-NC	-3.17	1.32	1.37
38	b1	625	DGA	OG1-CA1	3.17	1.42	1.33
31	s	604	CLA	C1C-NC	-3.17	1.32	1.37
31	R	604	CLA	C1C-NC	-3.17	1.32	1.37
31	S	614	CLA	C1C-NC	-3.17	1.32	1.37
31	G1	613	CLA	C1C-NC	-3.17	1.32	1.37
31	R1	602	CLA	C1C-NC	-3.17	1.32	1.37
31	B	615	CLA	C1C-NC	-3.17	1.32	1.37
31	G	602	CLA	C1C-NC	-3.17	1.32	1.37
31	Y	611	CLA	C1C-NC	-3.17	1.32	1.37
31	d1	402	CLA	C1C-NC	-3.16	1.32	1.37
31	B	602	CLA	C1C-NC	-3.16	1.32	1.37
31	s1	610	CLA	C1C-NC	-3.16	1.32	1.37
31	Y	604	CLA	C1C-NC	-3.16	1.32	1.37
31	Y1	612	CLA	C1C-NC	-3.16	1.32	1.37
45	f1	101	HEM	FE-NA	3.16	2.05	1.95
31	c	502	CLA	C1C-NC	-3.16	1.32	1.37
31	b	615	CLA	C1C-NC	-3.16	1.32	1.37
31	A1	410	CLA	C1C-NC	-3.16	1.32	1.37
31	c	504	CLA	C1C-NC	-3.15	1.32	1.37
31	B1	614	CLA	C1C-NC	-3.15	1.32	1.37
31	N	603	CLA	C1C-NC	-3.15	1.32	1.37
31	Y	613	CLA	C1C-NC	-3.15	1.32	1.37
31	c	503	CLA	C1C-NC	-3.15	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	b1	603	CLA	C1C-NC	-3.15	1.32	1.37
31	c1	504	CLA	C1C-NC	-3.15	1.32	1.37
31	s1	611	CLA	C1C-NC	-3.15	1.32	1.37
31	Y	603	CLA	C1C-NC	-3.15	1.32	1.37
31	G	611	CLA	C1C-NC	-3.15	1.32	1.37
47	N1	607	CHL	C3A-C2A	-3.14	1.52	1.54
46	H1	101	RRX	C4-C5	-3.14	1.45	1.51
31	G1	603	CLA	C1C-NC	-3.14	1.32	1.37
31	C1	511	CLA	C1C-NC	-3.14	1.32	1.37
47	N	607	CHL	C3B-C4B	3.14	1.44	1.41
31	g1	604	CLA	C1C-NC	-3.14	1.32	1.37
31	B	608	CLA	C1C-NC	-3.14	1.32	1.37
54	k1	101	4RF	O40-C41	3.14	1.42	1.33
31	D	403	CLA	C1C-NC	-3.14	1.32	1.37
31	Y1	611	CLA	C1C-NC	-3.14	1.32	1.37
31	c	513	CLA	C1C-NC	-3.14	1.32	1.37
31	C1	503	CLA	C1C-NC	-3.14	1.32	1.37
31	c	501	CLA	C1C-NC	-3.14	1.32	1.37
31	r	608	CLA	C1C-NC	-3.14	1.32	1.37
31	S1	604	CLA	C1C-NC	-3.14	1.32	1.37
31	r1	610	CLA	C1C-NC	-3.13	1.32	1.37
31	c1	512	CLA	C1C-NC	-3.13	1.32	1.37
31	r	609	CLA	C1C-NC	-3.13	1.33	1.37
31	C1	505	CLA	C1C-NC	-3.13	1.33	1.37
31	S1	609	CLA	C1C-NC	-3.13	1.33	1.37
31	b	616	CLA	C1C-NC	-3.13	1.33	1.37
31	a	406	CLA	C4B-NB	-3.13	1.33	1.37
31	B1	613	CLA	C1C-NC	-3.13	1.33	1.37
31	B	610	CLA	C1C-NC	-3.13	1.33	1.37
31	c	505	CLA	C1C-NC	-3.13	1.33	1.37
31	s1	614	CLA	C1C-NC	-3.13	1.33	1.37
31	Y1	602	CLA	C1C-NC	-3.12	1.33	1.37
31	c	507	CLA	C4B-NB	-3.12	1.33	1.37
31	G	614	CLA	C1C-NC	-3.12	1.33	1.37
31	b	614	CLA	C1C-NC	-3.12	1.33	1.37
31	S1	603	CLA	C1C-NC	-3.12	1.33	1.37
31	B	603	CLA	C1C-NC	-3.12	1.33	1.37
31	s1	612	CLA	C1C-NC	-3.12	1.33	1.37
31	y1	602	CLA	C1C-NC	-3.12	1.33	1.37
31	A1	410	CLA	C4B-NB	-3.12	1.33	1.37
31	r	610	CLA	C1C-NC	-3.12	1.33	1.37
31	Y	602	CLA	C4B-NB	-3.12	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	S1	614	CLA	C1C-NC	-3.12	1.33	1.37
31	g1	612	CLA	C1C-NC	-3.12	1.33	1.37
46	h	101	RRX	C7-C6	3.12	1.55	1.45
31	c1	508	CLA	C1C-NC	-3.12	1.33	1.37
31	n1	602	CLA	C1C-NC	-3.12	1.33	1.37
45	f	101	HEM	CAB-C3B	3.11	1.55	1.47
31	C1	507	CLA	C1C-NC	-3.11	1.33	1.37
31	R1	612	CLA	C1C-NC	-3.11	1.33	1.37
31	b	602	CLA	C1C-NC	-3.11	1.33	1.37
31	B1	609	CLA	C1C-NC	-3.11	1.33	1.37
31	G1	604	CLA	C1C-NC	-3.11	1.33	1.37
31	N1	612	CLA	C1C-NC	-3.11	1.33	1.37
31	y	602	CLA	C1C-NC	-3.11	1.33	1.37
31	N1	614	CLA	C1C-NC	-3.11	1.33	1.37
31	b	603	CLA	C1C-NC	-3.11	1.33	1.37
31	G1	611	CLA	C1C-NC	-3.11	1.33	1.37
31	s1	613	CLA	C1C-NC	-3.11	1.33	1.37
31	b	608	CLA	C1C-NC	-3.11	1.33	1.37
46	h1	101	RRX	C4-C5	-3.11	1.45	1.51
31	S	604	CLA	C1C-NC	-3.10	1.33	1.37
31	G1	612	CLA	C1C-NC	-3.10	1.33	1.37
31	G1	614	CLA	C1C-NC	-3.10	1.33	1.37
31	A	410	CLA	C4B-NB	-3.10	1.33	1.37
31	B	606	CLA	C1C-NC	-3.10	1.33	1.37
31	B1	612	CLA	C1C-NC	-3.10	1.33	1.37
31	N	613	CLA	C1C-NC	-3.10	1.33	1.37
31	B	613	CLA	C1C-NC	-3.10	1.33	1.37
31	s	610	CLA	C1C-NC	-3.10	1.33	1.37
31	B1	608	CLA	C1C-NC	-3.10	1.33	1.37
31	a1	405	CLA	C1C-NC	-3.10	1.33	1.37
31	b	604	CLA	C1C-NC	-3.09	1.33	1.37
31	N1	613	CLA	C1C-NC	-3.09	1.33	1.37
31	b	613	CLA	C4B-NB	-3.09	1.33	1.37
31	B	604	CLA	C1C-NC	-3.09	1.33	1.37
31	S1	617	CLA	C1C-NC	-3.09	1.33	1.37
31	b1	606	CLA	C1C-NC	-3.09	1.33	1.37
31	s	609	CLA	C1C-NC	-3.09	1.33	1.37
31	n	613	CLA	C1C-NC	-3.09	1.33	1.37
31	s1	602	CLA	C1C-NC	-3.09	1.33	1.37
31	g1	610	CLA	C1C-NC	-3.09	1.33	1.37
31	S	605	CLA	C1C-NC	-3.09	1.33	1.37
31	S1	610	CLA	C4B-NB	-3.08	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	n	612	CLA	C1C-NC	-3.08	1.33	1.37
31	d1	403	CLA	C1C-NC	-3.08	1.33	1.37
31	g	612	CLA	C1C-NC	-3.08	1.33	1.37
31	s	603	CLA	C1C-NC	-3.08	1.33	1.37
31	R1	604	CLA	C1C-NC	-3.08	1.33	1.37
31	n1	612	CLA	C1C-NC	-3.08	1.33	1.37
31	n	611	CLA	C1C-NC	-3.08	1.33	1.37
31	y1	614	CLA	C1C-NC	-3.08	1.33	1.37
31	R	608	CLA	C1C-NC	-3.08	1.33	1.37
31	g	610	CLA	C1C-NC	-3.08	1.33	1.37
31	N1	603	CLA	C1C-NC	-3.08	1.33	1.37
31	s1	604	CLA	C1C-NC	-3.08	1.33	1.37
31	g	611	CLA	C1C-NC	-3.08	1.33	1.37
31	b1	604	CLA	C1C-NC	-3.08	1.33	1.37
31	N	611	CLA	C1C-NC	-3.08	1.33	1.37
31	r	604	CLA	C1C-NC	-3.08	1.33	1.37
56	R1	626	ERG	C4-C5	3.08	1.57	1.51
31	N1	602	CLA	C1C-NC	-3.08	1.33	1.37
31	s1	605	CLA	C1C-NC	-3.07	1.33	1.37
45	f	101	HEM	FE-NB	3.07	2.04	1.94
50	g1	623	NEX	C7-C6	-3.07	1.27	1.30
31	N	614	CLA	C1C-NC	-3.07	1.33	1.37
47	G	601	CHL	C1A-CHA	-3.07	1.36	1.40
31	r1	602	CLA	C1C-NC	-3.07	1.33	1.37
47	n	607	CHL	C3A-C2A	-3.07	1.52	1.54
31	R1	603	CLA	C1C-NC	-3.07	1.33	1.37
54	I1	102	4RF	O40-C41	3.07	1.42	1.33
31	R1	609	CLA	C1C-NC	-3.07	1.33	1.37
45	F	101	HEM	CAC-C3C	3.07	1.55	1.47
31	R	611	CLA	C1C-NC	-3.06	1.33	1.37
31	g	614	CLA	C1C-NC	-3.06	1.33	1.37
31	s1	603	CLA	C1C-NC	-3.06	1.33	1.37
46	H1	101	RRX	C7-C6	3.06	1.55	1.45
56	R1	626	ERG	C9-C8	3.06	1.59	1.51
46	H	101	RRX	C7-C6	3.06	1.55	1.45
31	n1	603	CLA	C1C-NC	-3.06	1.33	1.37
31	C	509	CLA	C4B-NB	-3.06	1.33	1.37
31	y1	604	CLA	C1C-NC	-3.06	1.33	1.37
31	c1	511	CLA	C1C-NC	-3.06	1.33	1.37
31	g1	613	CLA	C1C-NC	-3.06	1.33	1.37
45	f	101	HEM	CAC-C3C	3.05	1.55	1.47
31	n1	604	CLA	C1C-NC	-3.05	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	n1	614	CLA	C1C-NC	-3.05	1.33	1.37
31	s	613	CLA	C1C-NC	-3.05	1.33	1.37
47	N1	608	CHL	CHB-C4A	-3.05	1.35	1.38
31	N1	611	CLA	C1C-NC	-3.05	1.33	1.37
31	b1	616	CLA	C1C-NC	-3.05	1.33	1.37
31	N1	610	CLA	C4B-NB	-3.05	1.33	1.37
31	C	513	CLA	C4B-NB	-3.05	1.33	1.37
31	a	405	CLA	C4B-NB	-3.05	1.33	1.37
31	S	610	CLA	C4B-NB	-3.04	1.33	1.37
31	c1	513	CLA	C1C-NC	-3.04	1.33	1.37
45	F1	101	HEM	CAC-C3C	3.04	1.55	1.47
31	D1	403	CLA	C1C-NC	-3.04	1.33	1.37
31	b1	615	CLA	C1C-NC	-3.04	1.33	1.37
31	g1	614	CLA	C1C-NC	-3.04	1.33	1.37
31	s	612	CLA	C1C-NC	-3.04	1.33	1.37
31	C	508	CLA	C4B-NB	-3.04	1.33	1.37
31	S	609	CLA	C1C-NC	-3.03	1.33	1.37
31	Y1	608	CLA	C1C-NC	-3.03	1.33	1.37
54	K1	101	4RF	O40-C41	3.03	1.42	1.33
31	R	610	CLA	C1C-NC	-3.03	1.33	1.37
31	N	604	CLA	C1C-NC	-3.03	1.33	1.37
31	b1	614	CLA	C1C-NC	-3.03	1.33	1.37
31	B1	602	CLA	C1C-NC	-3.03	1.33	1.37
31	S	603	CLA	C1C-NC	-3.03	1.33	1.37
31	S	611	CLA	C1C-NC	-3.03	1.33	1.37
47	Y	607	CHL	C3B-C4B	3.03	1.44	1.41
31	R	613	CLA	C1C-NC	-3.02	1.33	1.37
51	S1	625	LPX	P1-O1	3.02	1.71	1.59
31	s	614	CLA	C1C-NC	-3.02	1.33	1.37
31	b1	617	CLA	C4B-NB	-3.02	1.33	1.37
31	g1	603	CLA	C1C-NC	-3.01	1.33	1.37
31	B	607	CLA	C1C-NC	-3.01	1.33	1.37
31	g1	602	CLA	C1C-NC	-3.01	1.33	1.37
31	r	603	CLA	C1C-NC	-3.01	1.33	1.37
31	r	602	CLA	C1C-NC	-3.01	1.33	1.37
31	n1	611	CLA	C1C-NC	-3.01	1.33	1.37
31	B	617	CLA	C4B-NB	-3.01	1.33	1.37
54	i1	101	4RF	O40-C41	3.01	1.42	1.33
47	N	606	CHL	C3B-C2B	-3.01	1.36	1.40
56	r1	626	ERG	C4-C5	3.01	1.57	1.51
31	y	612	CLA	C4B-NB	-3.00	1.33	1.37
31	A	405	CLA	C4B-NB	-3.00	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	R1	608	CLA	C1C-NC	-3.00	1.33	1.37
31	c1	506	CLA	C1C-NC	-3.00	1.33	1.37
31	R	602	CLA	C1C-NC	-3.00	1.33	1.37
51	S	625	LPX	P1-O1	3.00	1.71	1.59
31	a1	410	CLA	C1C-NC	-3.00	1.33	1.37
31	y	608	CLA	C1C-NC	-2.99	1.33	1.37
31	S	612	CLA	C4B-NB	-2.99	1.33	1.37
31	C1	512	CLA	C1C-NC	-2.99	1.33	1.37
51	s1	625	LPX	P1-O1	2.99	1.71	1.59
35	J	101	LMG	C37-C36	-2.99	1.33	1.51
31	s1	617	CLA	C1C-NC	-2.99	1.33	1.37
31	n	602	CLA	C1C-NC	-2.98	1.33	1.37
31	c1	510	CLA	C4B-NB	-2.98	1.33	1.37
31	s1	609	CLA	C1C-NC	-2.98	1.33	1.37
31	C	507	CLA	C4B-NB	-2.98	1.33	1.37
51	s	625	LPX	P1-O1	2.98	1.71	1.59
31	c	508	CLA	C4B-NB	-2.98	1.33	1.37
31	S	617	CLA	C1C-NC	-2.98	1.33	1.37
31	n	610	CLA	C4B-NB	-2.98	1.33	1.37
31	g	613	CLA	C1C-NC	-2.98	1.33	1.37
47	G	601	CHL	C1D-C2D	2.98	1.42	1.39
31	G	613	CLA	C1C-NC	-2.98	1.33	1.37
31	R1	610	CLA	C1C-NC	-2.98	1.33	1.37
31	y1	608	CLA	C1C-NC	-2.98	1.33	1.37
31	b1	608	CLA	C1C-NC	-2.98	1.33	1.37
46	h1	101	RRX	C32-C1	2.98	1.59	1.53
31	s1	612	CLA	C4B-NB	-2.98	1.34	1.37
31	d1	403	CLA	C4B-NB	-2.98	1.34	1.37
31	n1	613	CLA	C1C-NC	-2.97	1.33	1.37
31	b	609	CLA	C1C-NC	-2.97	1.33	1.37
31	n	614	CLA	C1C-NC	-2.97	1.33	1.37
35	j	101	LMG	C37-C36	-2.97	1.33	1.51
31	r1	612	CLA	C1C-NC	-2.97	1.33	1.37
31	s	611	CLA	C1C-NC	-2.96	1.33	1.37
50	g	623	NEX	C7-C6	-2.96	1.27	1.30
31	R	603	CLA	C1C-NC	-2.96	1.33	1.37
31	s	605	CLA	C1C-NC	-2.96	1.33	1.37
33	C1	516	BCR	C10-C9	2.96	1.42	1.35
31	y	610	CLA	C4B-NB	-2.96	1.34	1.37
31	a	407	CLA	C4B-NB	-2.96	1.34	1.37
45	F1	101	HEM	FE-NA	2.95	2.04	1.95
45	F	101	HEM	FE-ND	2.95	2.04	1.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	Y1	607	CHL	C3A-C2A	-2.95	1.52	1.54
31	r	611	CLA	C1C-NC	-2.95	1.33	1.37
31	y	604	CLA	C4B-NB	-2.95	1.34	1.37
35	D1	411	LMG	C37-C36	-2.95	1.33	1.51
31	b	617	CLA	C4B-NB	-2.94	1.34	1.37
47	n	608	CHL	C3B-C4B	2.94	1.44	1.41
47	G	609	CHL	CHB-C4A	-2.94	1.35	1.38
31	R	609	CLA	C1C-NC	-2.94	1.33	1.37
31	g1	611	CLA	C1C-NC	-2.93	1.33	1.37
35	d	411	LMG	C37-C36	-2.93	1.33	1.51
45	F	101	HEM	FE-NC	2.93	2.04	1.95
31	Y1	610	CLA	C4B-NB	-2.92	1.34	1.37
31	B	606	CLA	C4B-NB	-2.92	1.34	1.37
31	r	612	CLA	C1C-NC	-2.92	1.33	1.37
31	C	502	CLA	C4B-NB	-2.92	1.34	1.37
47	n1	601	CHL	C3A-C2A	-2.92	1.52	1.54
31	C	512	CLA	C4B-NB	-2.92	1.34	1.37
31	Y	608	CLA	C1C-NC	-2.92	1.33	1.37
47	N1	605	CHL	C1A-CHA	-2.91	1.36	1.40
31	N1	604	CLA	C4B-NB	-2.91	1.34	1.37
45	F1	101	HEM	FE-NB	2.91	2.03	1.94
35	d1	411	LMG	C37-C36	-2.91	1.33	1.51
31	y1	612	CLA	C1C-NC	-2.91	1.33	1.37
47	y1	601	CHL	C1D-C2D	2.91	1.42	1.39
35	D	411	LMG	C37-C36	-2.91	1.33	1.51
31	c	511	CLA	C4B-NB	-2.91	1.34	1.37
45	F	101	HEM	CAB-C3B	2.90	1.55	1.47
47	G	607	CHL	CHB-C4A	-2.90	1.35	1.38
31	A	406	CLA	C4B-NB	-2.90	1.34	1.37
31	y1	611	CLA	C4B-NB	-2.90	1.34	1.37
31	b1	605	CLA	C4B-NB	-2.90	1.34	1.37
47	s	601	CHL	C1D-C2D	2.90	1.42	1.39
31	C1	507	CLA	C4B-NB	-2.90	1.34	1.37
31	b	605	CLA	C4B-NB	-2.90	1.34	1.37
31	Y1	604	CLA	C4B-NB	-2.90	1.34	1.37
31	b	615	CLA	C4B-NB	-2.89	1.34	1.37
31	c1	503	CLA	C4B-NB	-2.88	1.34	1.37
31	n1	610	CLA	C4B-NB	-2.88	1.34	1.37
47	g	609	CHL	C1D-C2D	2.88	1.42	1.39
31	c	506	CLA	C4B-NB	-2.88	1.34	1.37
31	C1	510	CLA	C4B-NB	-2.88	1.34	1.37
44	d	405	PL9	C7-C3	-2.88	1.47	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	g1	604	CLA	C4B-NB	-2.88	1.34	1.37
45	F	101	HEM	FE-NA	2.87	2.04	1.95
31	B1	610	CLA	C4B-NB	-2.87	1.34	1.37
54	I1	102	4RF	O21-C22	2.87	1.42	1.34
31	C1	503	CLA	C4B-NB	-2.87	1.34	1.37
47	n	608	CHL	C1B-C2B	2.87	1.42	1.39
46	H	101	RRX	C32-C1	2.87	1.59	1.53
31	G1	604	CLA	C4B-NB	-2.87	1.34	1.37
47	S1	606	CHL	C3B-C2B	-2.87	1.36	1.40
31	s	617	CLA	C1C-NC	-2.87	1.33	1.37
31	Y1	614	CLA	C4B-NB	-2.87	1.34	1.37
31	Y1	613	CLA	C4B-NB	-2.86	1.34	1.37
47	g	606	CHL	C1B-C2B	2.86	1.42	1.39
31	Y	612	CLA	C4B-NB	-2.86	1.34	1.37
47	g1	607	CHL	C1B-C2B	2.86	1.42	1.39
47	n	609	CHL	C1D-C2D	2.85	1.42	1.39
56	r1	626	ERG	C9-C8	2.85	1.58	1.51
31	g	602	CLA	C1C-NC	-2.85	1.33	1.37
47	y1	609	CHL	C1D-C2D	2.85	1.42	1.39
47	G	609	CHL	C1D-C2D	2.84	1.42	1.39
47	g	606	CHL	C1D-C2D	2.84	1.42	1.39
47	N	607	CHL	C1B-C2B	2.84	1.42	1.39
31	B	614	CLA	C4B-NB	-2.84	1.34	1.37
31	C	511	CLA	C4B-NB	-2.84	1.34	1.37
31	C1	505	CLA	C4B-NB	-2.84	1.34	1.37
31	S	614	CLA	C4B-NB	-2.84	1.34	1.37
31	y	613	CLA	C4B-NB	-2.84	1.34	1.37
47	S1	606	CHL	CHB-C4A	-2.84	1.35	1.38
31	C	506	CLA	C4B-NB	-2.83	1.34	1.37
31	c	510	CLA	C4B-NB	-2.83	1.34	1.37
31	B	604	CLA	C4B-NB	-2.83	1.34	1.37
47	g	601	CHL	C1D-C2D	2.83	1.42	1.39
47	y1	601	CHL	CHB-C4A	-2.83	1.35	1.38
31	A	407	CLA	C4B-NB	-2.83	1.34	1.37
46	h	101	RRX	C32-C1	2.83	1.59	1.53
31	B	609	CLA	C4B-NB	-2.83	1.34	1.37
47	y1	607	CHL	C1B-C2B	2.83	1.42	1.39
31	c	502	CLA	C4B-NB	-2.83	1.34	1.37
31	b	616	CLA	C4B-NB	-2.83	1.34	1.37
31	c	504	CLA	C4B-NB	-2.83	1.34	1.37
31	a1	407	CLA	C4B-NB	-2.83	1.34	1.37
47	Y	607	CHL	CHB-C4A	-2.82	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	n	606	CHL	CHB-C4A	-2.82	1.35	1.38
31	G1	610	CLA	C4B-NB	-2.82	1.34	1.37
47	G	605	CHL	C1B-C2B	2.82	1.42	1.39
47	G	608	CHL	C1D-C2D	2.82	1.42	1.39
47	s	601	CHL	CHB-C4A	-2.82	1.35	1.38
47	g1	608	CHL	C1B-C2B	2.82	1.42	1.39
31	Y1	611	CLA	C4B-NB	-2.82	1.34	1.37
31	b1	609	CLA	C1C-NC	-2.82	1.33	1.37
31	C	504	CLA	C4B-NB	-2.82	1.34	1.37
31	G	602	CLA	C4B-NB	-2.81	1.34	1.37
31	Y	611	CLA	C4B-NB	-2.81	1.34	1.37
31	D1	402	CLA	C4B-NB	-2.81	1.34	1.37
45	f1	101	HEM	FE-NC	2.81	2.04	1.95
47	y1	605	CHL	C1D-C2D	2.81	1.42	1.39
47	s1	606	CHL	C1D-C2D	2.81	1.42	1.39
31	B	615	CLA	C4B-NB	-2.81	1.34	1.37
32	a	409	PHO	CMC-C2C	-2.81	1.46	1.50
47	Y1	607	CHL	C1B-C2B	2.81	1.42	1.39
31	C1	509	CLA	C4B-NB	-2.81	1.34	1.37
47	N1	609	CHL	C1B-C2B	2.81	1.42	1.39
42	C	527	LMK	C3-N4	-2.81	1.48	1.54
31	c	512	CLA	C4B-NB	-2.80	1.34	1.37
31	Y	610	CLA	C4B-NB	-2.80	1.34	1.37
31	b1	615	CLA	C4B-NB	-2.80	1.34	1.37
47	G	608	CHL	CHB-C4A	-2.80	1.35	1.38
47	n1	601	CHL	C1D-C2D	2.80	1.42	1.39
31	n1	602	CLA	C4B-NB	-2.80	1.34	1.37
31	B1	609	CLA	C4B-NB	-2.80	1.34	1.37
31	B	613	CLA	C4B-NB	-2.80	1.34	1.37
49	r	622	XAT	O24-C25	-2.80	1.42	1.46
47	n1	601	CHL	C1B-C2B	2.80	1.42	1.39
47	n1	608	CHL	C1B-C2B	2.80	1.42	1.39
47	N	606	CHL	CHB-C4A	-2.79	1.35	1.38
47	y	607	CHL	C1D-C2D	2.79	1.42	1.39
47	s1	608	CHL	C1D-C2D	2.79	1.42	1.39
37	b1	620	C7Z	C21-C26	-2.79	1.50	1.53
47	n	607	CHL	C1B-C2B	2.79	1.42	1.39
42	c	627	LMK	C3-N4	-2.79	1.48	1.54
47	G1	606	CHL	C1D-C2D	2.79	1.42	1.39
31	B1	606	CLA	C4B-NB	-2.79	1.34	1.37
31	Y1	612	CLA	C4B-NB	-2.79	1.34	1.37
31	Y1	603	CLA	C4B-NB	-2.78	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	g1	605	CHL	C1D-C2D	2.78	1.42	1.39
47	N1	607	CHL	C3B-C4B	2.78	1.44	1.41
31	s	602	CLA	C4B-NB	-2.78	1.34	1.37
31	C1	506	CLA	C4B-NB	-2.78	1.34	1.37
47	Y1	601	CHL	C1B-C2B	2.78	1.42	1.39
47	g	607	CHL	CHB-C4A	-2.78	1.35	1.38
47	n1	609	CHL	C1D-C2D	2.78	1.42	1.39
31	a1	410	CLA	C4B-NB	-2.78	1.34	1.37
31	C	510	CLA	C4B-NB	-2.78	1.34	1.37
47	y1	601	CHL	C1B-C2B	2.78	1.42	1.39
47	Y1	609	CHL	CHB-C4A	-2.78	1.35	1.38
50	r1	622	NEX	C1-C6	-2.78	1.49	1.54
49	G	622	XAT	O24-C25	-2.78	1.42	1.46
54	i1	101	4RF	O21-C22	2.77	1.42	1.34
47	N1	605	CHL	C1D-C2D	2.77	1.42	1.39
47	g1	609	CHL	C1D-C2D	2.77	1.42	1.39
31	n	604	CLA	C4B-NB	-2.77	1.34	1.37
47	G	607	CHL	C1D-C2D	2.77	1.42	1.39
31	S1	604	CLA	C4B-NB	-2.77	1.34	1.37
47	G1	601	CHL	CHB-C4A	-2.77	1.35	1.38
31	C1	512	CLA	C4B-NB	-2.77	1.34	1.37
31	Y1	602	CLA	C4B-NB	-2.77	1.34	1.37
47	N	609	CHL	C1B-C2B	2.77	1.42	1.39
47	r	606	CHL	C1B-C2B	2.77	1.42	1.39
47	G	606	CHL	C1D-C2D	2.77	1.42	1.39
47	s1	606	CHL	CHB-C4A	-2.77	1.35	1.38
31	C1	511	CLA	C4B-NB	-2.77	1.34	1.37
47	n	606	CHL	C3B-C2B	-2.76	1.36	1.40
47	G	601	CHL	C1B-C2B	2.76	1.42	1.39
47	R1	607	CHL	CHB-C4A	-2.76	1.35	1.38
31	a1	406	CLA	C4B-NB	-2.76	1.34	1.37
31	c1	502	CLA	C4B-NB	-2.76	1.34	1.37
47	n	601	CHL	C1D-C2D	2.76	1.42	1.39
31	S1	612	CLA	C4B-NB	-2.76	1.34	1.37
47	S1	606	CHL	C1D-C2D	2.76	1.42	1.39
31	r1	604	CLA	C4B-NB	-2.76	1.34	1.37
31	r	602	CLA	C4B-NB	-2.76	1.34	1.37
42	c1	527	LMK	C3-N4	-2.76	1.48	1.54
47	g1	606	CHL	C1B-C2B	2.76	1.42	1.39
47	g1	609	CHL	CHB-C4A	-2.76	1.35	1.38
31	y1	613	CLA	C4B-NB	-2.76	1.34	1.37
54	k1	101	4RF	O21-C22	2.76	1.42	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	n	609	CHL	C1B-C2B	2.76	1.42	1.39
31	c	513	CLA	C4B-NB	-2.76	1.34	1.37
31	a1	405	CLA	C4B-NB	-2.76	1.34	1.37
46	H1	101	RRX	C32-C1	2.75	1.59	1.53
31	c1	512	CLA	C4B-NB	-2.75	1.34	1.37
47	g	607	CHL	C1B-C2B	2.75	1.42	1.39
47	r	606	CHL	C1D-C2D	2.75	1.42	1.39
31	D1	403	CLA	C4B-NB	-2.75	1.34	1.37
31	N	610	CLA	C4B-NB	-2.75	1.34	1.37
31	n	612	CLA	C4B-NB	-2.75	1.34	1.37
31	S1	611	CLA	C4B-NB	-2.75	1.34	1.37
47	Y	601	CHL	C1B-C2B	2.75	1.42	1.39
47	n	605	CHL	C1A-CHA	-2.75	1.36	1.40
31	A1	405	CLA	C4B-NB	-2.75	1.34	1.37
47	N	605	CHL	C1B-C2B	2.75	1.42	1.39
47	S	606	CHL	C1B-C2B	2.75	1.42	1.39
31	b	610	CLA	C4B-NB	-2.75	1.34	1.37
31	r1	609	CLA	C4B-NB	-2.75	1.34	1.37
47	S1	608	CHL	C1B-C2B	2.75	1.42	1.39
31	G	610	CLA	C4B-NB	-2.75	1.34	1.37
47	g	609	CHL	CHB-C4A	-2.74	1.35	1.38
31	c	503	CLA	C4B-NB	-2.74	1.34	1.37
32	a	408	PHO	CMC-C2C	-2.74	1.46	1.50
31	b	614	CLA	C4B-NB	-2.74	1.34	1.37
47	n	605	CHL	C1D-C2D	2.74	1.42	1.39
31	b1	613	CLA	C4B-NB	-2.74	1.34	1.37
31	C	505	CLA	C4B-NB	-2.74	1.34	1.37
47	y	601	CHL	C1B-C2B	2.74	1.42	1.39
47	S1	607	CHL	CHB-C4A	-2.74	1.35	1.38
47	N1	605	CHL	C1B-C2B	2.74	1.42	1.39
31	B1	614	CLA	C4B-NB	-2.74	1.34	1.37
47	N	609	CHL	C1D-C2D	2.74	1.42	1.39
47	y	609	CHL	C1D-C2D	2.74	1.42	1.39
47	Y1	601	CHL	C1D-C2D	2.74	1.42	1.39
47	g1	601	CHL	C1B-C2B	2.74	1.42	1.39
31	d	403	CLA	C4B-NB	-2.74	1.34	1.37
31	c1	511	CLA	C4B-NB	-2.74	1.34	1.37
47	s1	608	CHL	CHB-C4A	-2.74	1.35	1.38
50	R	622	NEX	C1-C6	-2.74	1.50	1.54
47	n	609	CHL	CHB-C4A	-2.73	1.35	1.38
47	N1	606	CHL	CHB-C4A	-2.73	1.35	1.38
31	A1	406	CLA	C4B-NB	-2.73	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a1	409	PHO	CMD-C2D	-2.73	1.46	1.51
47	N	601	CHL	C1B-C2B	2.73	1.42	1.39
47	s	606	CHL	C1D-C2D	2.73	1.42	1.39
47	s	607	CHL	C3A-C2A	-2.73	1.52	1.54
47	y	607	CHL	C1B-C2B	2.73	1.42	1.39
47	Y	607	CHL	C1D-C2D	2.73	1.42	1.39
47	S	601	CHL	CHB-C4A	-2.73	1.35	1.38
32	A	409	PHO	CMD-C2D	-2.73	1.46	1.51
47	S1	607	CHL	C1D-C2D	2.73	1.42	1.39
31	r	604	CLA	C4B-NB	-2.73	1.34	1.37
31	b1	614	CLA	C4B-NB	-2.73	1.34	1.37
49	G1	622	XAT	O24-C25	-2.73	1.42	1.46
47	N1	601	CHL	CHB-C4A	-2.73	1.35	1.38
47	n	605	CHL	C1B-C2B	2.73	1.42	1.39
31	S	611	CLA	C4B-NB	-2.72	1.34	1.37
31	b	604	CLA	C4B-NB	-2.72	1.34	1.37
31	b1	606	CLA	C4B-NB	-2.72	1.34	1.37
31	b	606	CLA	C4B-NB	-2.72	1.34	1.37
47	S1	601	CHL	CHB-C4A	-2.72	1.35	1.38
47	N	608	CHL	C1B-C2B	2.72	1.42	1.39
31	B	603	CLA	C4B-NB	-2.72	1.34	1.37
31	C1	502	CLA	C4B-NB	-2.72	1.34	1.37
47	y	605	CHL	C1B-C2B	2.72	1.42	1.39
47	G1	608	CHL	CHB-C4A	-2.72	1.35	1.38
47	y1	606	CHL	C1D-C2D	2.72	1.42	1.39
47	R	606	CHL	CHB-C4A	-2.72	1.35	1.38
31	c	505	CLA	C4B-NB	-2.72	1.34	1.37
31	C1	513	CLA	C4B-NB	-2.72	1.34	1.37
31	g1	610	CLA	C4B-NB	-2.72	1.34	1.37
47	g1	606	CHL	C1D-C2D	2.72	1.42	1.39
47	G	606	CHL	CHB-C4A	-2.72	1.35	1.38
47	G	606	CHL	C3B-C2B	-2.72	1.36	1.40
47	R1	606	CHL	C1B-C2B	2.72	1.42	1.39
47	y1	606	CHL	C1B-C2B	2.72	1.42	1.39
31	B	608	CLA	C4B-NB	-2.72	1.34	1.37
47	G1	609	CHL	C1D-C2D	2.72	1.42	1.39
47	n1	605	CHL	C1B-C2B	2.72	1.42	1.39
31	S1	602	CLA	C4B-NB	-2.71	1.34	1.37
47	g	605	CHL	C1B-C2B	2.71	1.42	1.39
47	n	607	CHL	CHB-C4A	-2.71	1.35	1.38
31	b1	610	CLA	C4B-NB	-2.71	1.34	1.37
47	r1	606	CHL	C1D-C2D	2.71	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B1	607	CLA	C4B-NB	-2.71	1.34	1.37
47	N1	601	CHL	C1D-C2D	2.71	1.42	1.39
47	Y1	609	CHL	C1B-C2B	2.71	1.42	1.39
32	A	409	PHO	CMC-C2C	-2.71	1.46	1.50
47	G1	601	CHL	C1D-C2D	2.71	1.42	1.39
54	K1	101	4RF	O21-C22	2.71	1.41	1.34
47	Y1	609	CHL	C1D-C2D	2.71	1.42	1.39
47	S	606	CHL	C1D-C2D	2.71	1.42	1.39
47	R1	606	CHL	C1D-C2D	2.71	1.42	1.39
31	R1	604	CLA	C4B-NB	-2.71	1.34	1.37
56	R1	626	ERG	C14-C8	2.71	1.58	1.51
31	n1	613	CLA	C4B-NB	-2.71	1.34	1.37
47	Y1	605	CHL	C1D-C2D	2.71	1.42	1.39
31	N	602	CLA	C4B-NB	-2.71	1.34	1.37
52	i	101	3PH	O21-C2	-2.71	1.40	1.46
47	Y1	606	CHL	C1B-C2B	2.71	1.42	1.39
45	F1	101	HEM	FE-NC	2.71	2.04	1.95
47	n1	609	CHL	CHB-C4A	-2.71	1.35	1.38
31	B	612	CLA	C4B-NB	-2.70	1.34	1.37
31	g	614	CLA	C4B-NB	-2.70	1.34	1.37
47	S1	601	CHL	C1D-C2D	2.70	1.42	1.39
31	r	609	CLA	C4B-NB	-2.70	1.34	1.37
57	y1	627	PTY	O7-C6	-2.70	1.40	1.46
47	s1	607	CHL	C1B-C2B	2.70	1.42	1.39
31	B	610	CLA	C4B-NB	-2.70	1.34	1.37
47	g	601	CHL	C1B-C2B	2.70	1.42	1.39
47	N1	606	CHL	C1D-C2D	2.70	1.42	1.39
47	Y	606	CHL	C1B-C2B	2.70	1.42	1.39
47	n1	608	CHL	C1D-C2D	2.70	1.42	1.39
47	G1	606	CHL	CHB-C4A	-2.70	1.35	1.38
47	Y	601	CHL	C1D-C2D	2.70	1.42	1.39
47	y1	605	CHL	C1B-C2B	2.70	1.42	1.39
57	Y1	626	PTY	O7-C6	-2.70	1.40	1.46
47	R	606	CHL	C1D-C2D	2.70	1.42	1.39
47	s	607	CHL	C1D-C2D	2.70	1.42	1.39
47	n1	605	CHL	C1D-C2D	2.70	1.42	1.39
49	g1	622	XAT	O24-C25	-2.70	1.42	1.46
31	B1	615	CLA	C4B-NB	-2.70	1.34	1.37
47	s1	608	CHL	C1B-C2B	2.70	1.42	1.39
47	y	609	CHL	C1B-C2B	2.70	1.42	1.39
32	a1	408	PHO	CMC-C2C	-2.70	1.46	1.50
31	b	612	CLA	C4B-NB	-2.70	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	y1	610	CLA	C4B-NB	-2.70	1.34	1.37
52	s	626	3PH	O21-C2	-2.70	1.40	1.46
31	y	611	CLA	C4B-NB	-2.70	1.34	1.37
31	S1	614	CLA	C4B-NB	-2.70	1.34	1.37
47	s	608	CHL	CHB-C4A	-2.69	1.35	1.38
31	G	614	CLA	C4B-NB	-2.69	1.34	1.37
31	s	605	CLA	C4B-NB	-2.69	1.34	1.37
47	G	607	CHL	C1B-C2B	2.69	1.42	1.39
47	g1	601	CHL	C1D-C2D	2.69	1.42	1.39
31	c1	509	CLA	C4B-NB	-2.69	1.34	1.37
47	s1	607	CHL	CHB-C4A	-2.69	1.35	1.38
31	s1	610	CLA	C4B-NB	-2.69	1.34	1.37
47	N	608	CHL	CHB-C4A	-2.69	1.35	1.38
31	r	610	CLA	C4B-NB	-2.69	1.34	1.37
47	N1	607	CHL	C1D-C2D	2.69	1.42	1.39
50	s1	623	NEX	C1-C6	-2.69	1.50	1.54
31	C	503	CLA	C4B-NB	-2.69	1.34	1.37
31	C1	508	CLA	C4B-NB	-2.69	1.34	1.37
47	N1	607	CHL	C1B-C2B	2.69	1.42	1.39
32	a1	409	PHO	CMC-C2C	-2.68	1.46	1.50
47	S	608	CHL	C1B-C2B	2.68	1.42	1.39
47	G1	609	CHL	C1B-C2B	2.68	1.42	1.39
31	C1	504	CLA	C4B-NB	-2.68	1.34	1.37
31	N1	613	CLA	C4B-NB	-2.68	1.34	1.37
47	R1	607	CHL	C1B-C2B	2.68	1.42	1.39
47	Y1	607	CHL	C1D-C2D	2.68	1.42	1.39
31	B1	605	CLA	C4B-NB	-2.68	1.34	1.37
47	N1	608	CHL	C1D-C2D	2.68	1.42	1.39
31	B1	617	CLA	C4B-NB	-2.68	1.34	1.37
31	y1	604	CLA	C4B-NB	-2.68	1.34	1.37
47	s1	606	CHL	C1B-C2B	2.68	1.42	1.39
31	S	605	CLA	C4B-NB	-2.68	1.34	1.37
31	n	613	CLA	C4B-NB	-2.68	1.34	1.37
47	g1	607	CHL	C3A-C2A	-2.68	1.52	1.54
47	y	606	CHL	CHB-C4A	-2.68	1.35	1.38
47	r1	607	CHL	C1B-C2B	2.68	1.42	1.39
47	g	608	CHL	CHB-C4A	-2.68	1.35	1.38
47	R1	606	CHL	CHB-C4A	-2.68	1.35	1.38
47	R	607	CHL	C1B-C2B	2.68	1.42	1.39
31	G1	611	CLA	C4B-NB	-2.68	1.34	1.37
47	n	601	CHL	C1B-C2B	2.68	1.42	1.39
47	G1	605	CHL	CHB-C4A	-2.68	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c1	507	CLA	C4B-NB	-2.68	1.34	1.37
31	r1	612	CLA	C4B-NB	-2.68	1.34	1.37
57	Y1	627	PTY	O7-C6	-2.68	1.40	1.46
47	R	606	CHL	C1B-C2B	2.67	1.42	1.39
47	Y1	605	CHL	C1B-C2B	2.67	1.42	1.39
31	B	607	CLA	C4B-NB	-2.67	1.34	1.37
31	b1	604	CLA	C4B-NB	-2.67	1.34	1.37
47	Y	606	CHL	CHB-C4A	-2.67	1.35	1.38
47	G1	609	CHL	CHB-C4A	-2.67	1.35	1.38
31	B1	603	CLA	C4B-NB	-2.67	1.34	1.37
47	Y	607	CHL	C1B-C2B	2.67	1.42	1.39
31	s1	602	CLA	C4B-NB	-2.67	1.34	1.37
31	B1	608	CLA	C4B-NB	-2.67	1.34	1.37
37	B	620	C7Z	C21-C26	-2.67	1.50	1.53
31	R1	609	CLA	C4B-NB	-2.67	1.34	1.37
47	S	607	CHL	C1B-C2B	2.67	1.42	1.39
47	n	606	CHL	C1D-C2D	2.67	1.42	1.39
47	S	607	CHL	C1D-C2D	2.67	1.42	1.39
47	y	607	CHL	CHB-C4A	-2.67	1.35	1.38
52	S	626	3PH	O21-C2	-2.67	1.40	1.46
31	b	607	CLA	C4B-NB	-2.67	1.34	1.37
47	Y	609	CHL	C1B-C2B	2.67	1.42	1.39
47	g	605	CHL	C1D-C2D	2.67	1.42	1.39
31	s	614	CLA	C4B-NB	-2.67	1.34	1.37
47	S	601	CHL	C1B-C2B	2.67	1.42	1.39
47	Y	605	CHL	C1D-C2D	2.67	1.42	1.39
47	G1	607	CHL	C1B-C2B	2.67	1.42	1.39
47	s1	607	CHL	C1D-C2D	2.67	1.42	1.39
47	y1	609	CHL	C1B-C2B	2.67	1.42	1.39
47	Y	605	CHL	CHB-C4A	-2.67	1.35	1.38
31	N	613	CLA	C4B-NB	-2.66	1.34	1.37
31	Y	604	CLA	C4B-NB	-2.66	1.34	1.37
31	g	603	CLA	C4B-NB	-2.66	1.34	1.37
31	Y	614	CLA	C4B-NB	-2.66	1.34	1.37
47	R1	607	CHL	C1D-C2D	2.66	1.42	1.39
31	B	616	CLA	C4B-NB	-2.66	1.34	1.37
31	G1	603	CLA	C4B-NB	-2.66	1.34	1.37
47	g	608	CHL	C1D-C2D	2.66	1.42	1.39
31	R	610	CLA	C4B-NB	-2.66	1.34	1.37
47	n	609	CHL	C2C-C3C	2.66	1.38	1.36
31	B1	613	CLA	C4B-NB	-2.66	1.34	1.37
52	s1	626	3PH	O21-C2	-2.66	1.40	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	a	409	PHO	CMB-C2B	-2.66	1.46	1.51
47	Y	609	CHL	C1D-C2D	2.66	1.42	1.39
47	G	608	CHL	C1B-C2B	2.66	1.42	1.39
47	r	606	CHL	CHB-C4A	-2.66	1.35	1.38
47	r1	607	CHL	CHB-C4A	-2.66	1.35	1.38
31	b1	612	CLA	C4B-NB	-2.65	1.34	1.37
47	Y	601	CHL	C1A-CHA	-2.65	1.37	1.40
47	g	608	CHL	C1B-C2B	2.65	1.42	1.39
31	n	603	CLA	C4B-NB	-2.65	1.34	1.37
47	Y1	601	CHL	CHB-C4A	-2.65	1.35	1.38
31	c	509	CLA	C4B-NB	-2.65	1.34	1.37
31	b1	603	CLA	C4B-NB	-2.65	1.34	1.37
47	r1	606	CHL	C1B-C2B	2.65	1.42	1.39
47	y1	607	CHL	C1D-C2D	2.65	1.42	1.39
47	N	609	CHL	C1A-CHA	-2.65	1.37	1.40
31	r1	602	CLA	C4B-NB	-2.65	1.34	1.37
47	Y	605	CHL	C1B-C2B	2.65	1.42	1.39
31	b1	608	CLA	C4B-NB	-2.65	1.34	1.37
47	N	601	CHL	C1D-C2D	2.65	1.42	1.39
47	g	607	CHL	C1D-C2D	2.65	1.42	1.39
52	B1	624	3PH	O21-C2	-2.65	1.40	1.46
31	S1	605	CLA	C4B-NB	-2.65	1.34	1.37
31	s1	614	CLA	C4B-NB	-2.65	1.34	1.37
47	r	607	CHL	CHB-C4A	-2.65	1.35	1.38
47	N1	608	CHL	C1B-C2B	2.65	1.42	1.39
31	b	603	CLA	C4B-NB	-2.65	1.34	1.37
31	S1	613	CLA	C4B-NB	-2.65	1.34	1.37
47	n1	607	CHL	C1B-C2B	2.65	1.42	1.39
47	y	605	CHL	CHB-C4A	-2.65	1.35	1.38
31	B1	604	CLA	C4B-NB	-2.65	1.34	1.37
47	N	608	CHL	C1D-C2D	2.65	1.42	1.39
31	y1	612	CLA	C4B-NB	-2.64	1.34	1.37
31	S	613	CLA	C4B-NB	-2.64	1.34	1.37
47	G	605	CHL	C1D-C2D	2.64	1.42	1.39
31	s	613	CLA	C4B-NB	-2.64	1.34	1.37
47	N	605	CHL	C1D-C2D	2.64	1.42	1.39
47	s	607	CHL	C1B-C2B	2.64	1.42	1.39
47	G1	605	CHL	C1D-C2D	2.64	1.42	1.39
47	n1	606	CHL	C3B-C2B	-2.64	1.36	1.40
31	g	604	CLA	C4B-NB	-2.64	1.34	1.37
49	R	621	XAT	O24-C25	-2.64	1.42	1.46
47	n1	601	CHL	CHB-C4A	-2.64	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	y1	601	CHL	C1A-CHA	-2.64	1.37	1.40
31	c1	513	CLA	C4B-NB	-2.64	1.34	1.37
47	G1	607	CHL	CHB-C4A	-2.64	1.35	1.38
47	s1	601	CHL	C1B-C2B	2.64	1.42	1.39
47	g1	601	CHL	CHB-C4A	-2.64	1.35	1.38
47	G1	605	CHL	C1B-C2B	2.64	1.42	1.39
32	A1	409	PHO	CMC-C2C	-2.64	1.46	1.50
47	S	601	CHL	C1D-C2D	2.64	1.42	1.39
47	r	607	CHL	C1D-C2D	2.64	1.42	1.39
47	s	608	CHL	C1B-C2B	2.64	1.42	1.39
47	s	606	CHL	C1B-C2B	2.63	1.42	1.39
31	b1	607	CLA	C4B-NB	-2.63	1.34	1.37
31	r1	610	CLA	C4B-NB	-2.63	1.34	1.37
47	n	601	CHL	CHB-C4A	-2.63	1.35	1.38
31	r1	603	CLA	C4B-NB	-2.63	1.34	1.37
47	s	608	CHL	C1D-C2D	2.63	1.42	1.39
47	n1	609	CHL	C1B-C2B	2.63	1.42	1.39
31	N1	611	CLA	C4B-NB	-2.63	1.34	1.37
47	Y1	606	CHL	C1D-C2D	2.63	1.42	1.39
31	y1	614	CLA	C4B-NB	-2.63	1.34	1.37
47	r	607	CHL	C1B-C2B	2.63	1.42	1.39
31	R	602	CLA	C4B-NB	-2.63	1.34	1.37
47	G	601	CHL	CHB-C4A	-2.63	1.35	1.38
47	N1	606	CHL	C3B-C2B	-2.63	1.36	1.40
31	G	604	CLA	C4B-NB	-2.63	1.34	1.37
31	G	611	CLA	C4B-NB	-2.63	1.34	1.37
47	s	601	CHL	C1B-C2B	2.63	1.42	1.39
47	S1	606	CHL	C1B-C2B	2.63	1.42	1.39
47	N	609	CHL	CHB-C4A	-2.63	1.35	1.38
31	R	604	CLA	C4B-NB	-2.63	1.34	1.37
31	G1	613	CLA	C4B-NB	-2.63	1.34	1.37
47	S1	608	CHL	CHB-C4A	-2.63	1.35	1.38
31	G	612	CLA	C4B-NB	-2.62	1.34	1.37
52	S1	626	3PH	O21-C2	-2.62	1.40	1.46
44	d1	405	PL9	C3-C4	-2.62	1.45	1.49
47	N	607	CHL	CHB-C4A	-2.62	1.35	1.38
47	s	607	CHL	CHB-C4A	-2.62	1.35	1.38
47	N1	607	CHL	CHB-C4A	-2.62	1.35	1.38
47	n1	607	CHL	C3A-C2A	-2.62	1.52	1.54
47	r1	606	CHL	CHB-C4A	-2.62	1.35	1.38
31	s1	617	CLA	C4B-NB	-2.62	1.34	1.37
31	S	603	CLA	C4B-NB	-2.62	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	s	603	CLA	C4B-NB	-2.62	1.34	1.37
31	R1	603	CLA	C4B-NB	-2.62	1.34	1.37
47	S	608	CHL	C1D-C2D	2.62	1.42	1.39
31	g1	613	CLA	C4B-NB	-2.62	1.34	1.37
47	n	605	CHL	CHB-C4A	-2.62	1.35	1.38
31	N	603	CLA	C4B-NB	-2.62	1.34	1.37
31	R	609	CLA	C4B-NB	-2.62	1.34	1.37
31	R1	602	CLA	C4B-NB	-2.62	1.34	1.37
31	Y1	608	CLA	C4B-NB	-2.62	1.34	1.37
47	S	606	CHL	CHB-C4A	-2.62	1.35	1.38
31	N1	614	CLA	C4B-NB	-2.62	1.34	1.37
47	R	607	CHL	CHB-C4A	-2.61	1.35	1.38
31	c	501	CLA	C4B-NB	-2.61	1.34	1.37
47	g	609	CHL	C1A-CHA	-2.61	1.37	1.40
47	g1	605	CHL	C1B-C2B	2.61	1.42	1.39
47	N1	605	CHL	CHB-C4A	-2.61	1.35	1.38
47	G1	607	CHL	C1D-C2D	2.61	1.42	1.39
47	g1	605	CHL	CHB-C4A	-2.61	1.35	1.38
31	b	608	CLA	C4B-NB	-2.61	1.34	1.37
31	r	603	CLA	C4B-NB	-2.61	1.34	1.37
31	s	612	CLA	C4B-NB	-2.61	1.34	1.37
47	y	605	CHL	C1D-C2D	2.61	1.42	1.39
31	s1	609	CLA	C4B-NB	-2.61	1.34	1.37
47	N	605	CHL	CHB-C4A	-2.61	1.35	1.38
31	A1	407	CLA	C4B-NB	-2.61	1.34	1.37
31	S1	617	CLA	C4B-NB	-2.61	1.34	1.37
47	n	607	CHL	C1D-C2D	2.61	1.42	1.39
31	r	613	CLA	C4B-NB	-2.60	1.34	1.37
47	S	607	CHL	CHB-C4A	-2.60	1.35	1.38
31	G1	602	CLA	C4B-NB	-2.60	1.34	1.37
47	G	606	CHL	C1B-C2B	2.60	1.42	1.39
52	t1	101	3PH	O21-C2	-2.60	1.40	1.46
31	B	602	CLA	C4B-NB	-2.60	1.34	1.37
37	b	620	C7Z	C21-C26	-2.60	1.50	1.53
47	N1	609	CHL	C1D-C2D	2.60	1.42	1.39
47	G1	606	CHL	C1B-C2B	2.60	1.42	1.39
47	g1	607	CHL	C1D-C2D	2.60	1.42	1.39
47	g1	609	CHL	C1B-C2B	2.60	1.42	1.39
50	r1	622	NEX	C7-C6	-2.60	1.27	1.30
31	s	604	CLA	C4B-NB	-2.60	1.34	1.37
31	B1	616	CLA	C4B-NB	-2.60	1.34	1.37
44	D	405	PL9	C53-C6	-2.60	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	N	612	CLA	C4B-NB	-2.60	1.34	1.37
47	Y1	607	CHL	CHB-C4A	-2.60	1.35	1.38
47	n1	607	CHL	C1D-C2D	2.60	1.42	1.39
31	Y	613	CLA	C4B-NB	-2.60	1.34	1.37
31	b	609	CLA	C4B-NB	-2.60	1.34	1.37
31	n1	604	CLA	C4B-NB	-2.60	1.34	1.37
47	R	607	CHL	C1D-C2D	2.59	1.42	1.39
31	g	611	CLA	C4B-NB	-2.59	1.34	1.37
32	A1	409	PHO	CMB-C2B	-2.59	1.46	1.51
47	y	606	CHL	C1D-C2D	2.59	1.42	1.39
47	G1	608	CHL	C1B-C2B	2.59	1.42	1.39
31	N	614	CLA	C4B-NB	-2.59	1.34	1.37
31	s	610	CLA	C4B-NB	-2.59	1.34	1.37
47	N	601	CHL	CHB-C4A	-2.59	1.35	1.38
47	N	606	CHL	C1D-C2D	2.59	1.42	1.39
31	c1	505	CLA	C4B-NB	-2.59	1.34	1.37
31	n1	614	CLA	C4B-NB	-2.59	1.34	1.37
47	g	609	CHL	C1B-C2B	2.59	1.42	1.39
31	s1	611	CLA	C4B-NB	-2.59	1.34	1.37
31	C	501	CLA	C4B-NB	-2.59	1.34	1.37
47	s	606	CHL	CHB-C4A	-2.59	1.35	1.38
31	y	608	CLA	C4B-NB	-2.59	1.34	1.37
31	c1	508	CLA	C4B-NB	-2.59	1.34	1.37
31	Y	603	CLA	C4B-NB	-2.59	1.34	1.37
31	n1	611	CLA	C4B-NB	-2.59	1.34	1.37
47	g1	608	CHL	CHB-C4A	-2.59	1.35	1.38
47	N1	601	CHL	C1B-C2B	2.58	1.42	1.39
47	y	601	CHL	CHB-C4A	-2.58	1.35	1.38
31	R	613	CLA	C4B-NB	-2.58	1.34	1.37
31	c1	506	CLA	C4B-NB	-2.58	1.34	1.37
47	N	605	CHL	C3B-C2B	-2.58	1.36	1.40
31	b	602	CLA	C4B-NB	-2.58	1.34	1.37
47	G1	608	CHL	C1D-C2D	2.58	1.42	1.39
32	a	408	PHO	CMD-C2D	-2.58	1.46	1.51
31	R1	610	CLA	C4B-NB	-2.58	1.34	1.37
31	y1	602	CLA	C4B-NB	-2.58	1.34	1.37
47	s	601	CHL	C3B-C2B	-2.58	1.36	1.40
47	S1	607	CHL	C1B-C2B	2.58	1.42	1.39
47	Y1	605	CHL	CHB-C4A	-2.58	1.35	1.38
47	G	609	CHL	C1B-C2B	2.58	1.42	1.39
47	S1	601	CHL	C1B-C2B	2.58	1.42	1.39
47	S1	608	CHL	C1D-C2D	2.58	1.42	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A	408	PHO	CMC-C2C	-2.58	1.46	1.50
57	y1	626	PTY	O7-C6	-2.58	1.40	1.46
49	g	622	XAT	O24-C25	-2.58	1.42	1.46
47	y	606	CHL	C1B-C2B	2.58	1.42	1.39
46	H1	101	RRX	C35-C13	2.57	1.56	1.50
37	b	620	C7Z	C18-C5	2.57	1.55	1.50
31	N1	612	CLA	C4B-NB	-2.57	1.34	1.37
31	G1	614	CLA	C4B-NB	-2.57	1.34	1.37
47	N	606	CHL	C1B-C2B	2.57	1.42	1.39
47	n	608	CHL	CHB-C4A	-2.57	1.35	1.38
47	y1	605	CHL	CHB-C4A	-2.57	1.35	1.38
31	R	611	CLA	C4B-NB	-2.57	1.34	1.37
31	g1	611	CLA	C4B-NB	-2.57	1.34	1.37
47	g	601	CHL	CHB-C4A	-2.56	1.35	1.38
31	S	609	CLA	C4B-NB	-2.56	1.34	1.37
31	G1	612	CLA	C4B-NB	-2.56	1.34	1.37
46	h1	101	RRX	C35-C13	2.56	1.56	1.50
31	y1	603	CLA	C4B-NB	-2.56	1.34	1.37
47	Y	606	CHL	C1D-C2D	2.56	1.42	1.39
31	n	614	CLA	C4B-NB	-2.56	1.34	1.37
47	Y1	609	CHL	C3B-C2B	-2.56	1.36	1.40
31	y	614	CLA	C4B-NB	-2.56	1.34	1.37
47	G1	601	CHL	C1B-C2B	2.56	1.42	1.39
47	G	605	CHL	CHB-C4A	-2.56	1.35	1.38
47	y1	609	CHL	CHB-C4A	-2.56	1.35	1.38
31	S	604	CLA	C4B-NB	-2.55	1.34	1.37
47	n	606	CHL	C1B-C2B	2.55	1.42	1.39
32	a	408	PHO	CAC-C3C	-2.55	1.47	1.51
31	c1	504	CLA	C4B-NB	-2.55	1.34	1.37
47	r1	607	CHL	C1D-C2D	2.55	1.42	1.39
49	Y1	622	XAT	O24-C25	-2.55	1.42	1.46
31	B	605	CLA	C4B-NB	-2.55	1.34	1.37
47	n	608	CHL	C1D-C2D	2.55	1.42	1.39
47	n1	605	CHL	CHB-C4A	-2.55	1.35	1.38
47	s1	601	CHL	C1D-C2D	2.54	1.42	1.39
31	G	613	CLA	C4B-NB	-2.54	1.34	1.37
37	B	620	C7Z	C18-C5	2.54	1.55	1.50
47	n1	606	CHL	C1B-C2B	2.54	1.42	1.39
31	g1	602	CLA	C4B-NB	-2.54	1.34	1.37
47	N1	606	CHL	C1B-C2B	2.54	1.42	1.39
31	N1	602	CLA	C4B-NB	-2.54	1.34	1.37
49	r1	621	XAT	O24-C25	-2.54	1.42	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	Y1	601	CHL	C1A-CHA	-2.54	1.37	1.40
47	S	608	CHL	CHB-C4A	-2.53	1.35	1.38
47	n1	607	CHL	CHB-C4A	-2.53	1.35	1.38
47	g1	608	CHL	C1D-C2D	2.53	1.42	1.39
31	s1	605	CLA	C4B-NB	-2.53	1.34	1.37
49	Y	622	XAT	O24-C25	-2.53	1.42	1.46
31	g	612	CLA	C4B-NB	-2.53	1.34	1.37
47	Y1	606	CHL	CHB-C4A	-2.53	1.35	1.38
47	y	606	CHL	C3B-C2B	-2.53	1.36	1.40
31	g	610	CLA	C4B-NB	-2.53	1.34	1.37
55	R1	625	LMT	O3'-C3'	-2.53	1.36	1.43
31	S	602	CLA	C4B-NB	-2.53	1.34	1.37
47	y1	605	CHL	C3A-C2A	-2.52	1.52	1.54
47	Y	601	CHL	CHB-C4A	-2.52	1.35	1.38
32	a1	409	PHO	CMB-C2B	-2.52	1.46	1.51
31	y	602	CLA	C4B-NB	-2.52	1.34	1.37
31	b1	609	CLA	C4B-NB	-2.52	1.34	1.37
47	y1	606	CHL	CHB-C4A	-2.52	1.35	1.38
47	N	607	CHL	C1D-C2D	2.52	1.42	1.39
31	y1	608	CLA	C4B-NB	-2.52	1.34	1.37
49	n	622	XAT	O24-C25	-2.52	1.43	1.46
31	n	611	CLA	C4B-NB	-2.52	1.34	1.37
47	g	605	CHL	CHB-C4A	-2.52	1.35	1.38
32	A1	408	PHO	CMC-C2C	-2.52	1.46	1.50
32	a	408	PHO	CMB-C2B	-2.52	1.46	1.51
31	S	617	CLA	C4B-NB	-2.51	1.34	1.37
31	r1	608	CLA	C4B-NB	-2.51	1.34	1.37
32	a	409	PHO	CMD-C2D	-2.51	1.46	1.51
47	y	601	CHL	C1D-C2D	2.51	1.42	1.39
52	t1	101	3PH	O31-C31	2.51	1.40	1.33
32	a1	409	PHO	C3D-C4D	2.51	1.44	1.41
52	B1	624	3PH	O31-C31	2.51	1.40	1.33
47	n1	608	CHL	CHB-C4A	-2.51	1.35	1.38
31	N	611	CLA	C4B-NB	-2.51	1.34	1.37
46	h	101	RRX	C35-C13	2.51	1.55	1.50
31	s	617	CLA	C4B-NB	-2.51	1.34	1.37
47	N1	609	CHL	CHB-C4A	-2.51	1.35	1.38
47	Y	609	CHL	CHB-C4A	-2.50	1.35	1.38
49	N1	622	XAT	O24-C25	-2.50	1.43	1.46
47	y1	607	CHL	CHB-C4A	-2.50	1.35	1.38
47	y	609	CHL	CHB-C4A	-2.50	1.35	1.38
47	n1	606	CHL	CHB-C4A	-2.50	1.35	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	b	620	C7Z	C20-C13	2.50	1.55	1.50
32	A1	409	PHO	C3D-C4D	2.50	1.44	1.41
49	y1	622	XAT	O24-C25	-2.49	1.43	1.46
32	A1	408	PHO	CMB-C2B	-2.49	1.46	1.51
47	G	606	CHL	C1A-CHA	-2.49	1.37	1.40
37	B1	620	C7Z	C20-C13	2.49	1.55	1.50
32	A	409	PHO	CAC-C3C	-2.49	1.47	1.51
31	r	611	CLA	C4B-NB	-2.49	1.34	1.37
31	s	611	CLA	C4B-NB	-2.49	1.34	1.37
31	s1	604	CLA	C4B-NB	-2.49	1.34	1.37
31	C1	501	CLA	C4B-NB	-2.49	1.34	1.37
31	B1	612	CLA	C4B-NB	-2.48	1.34	1.37
32	A	408	PHO	CMD-C2D	-2.48	1.46	1.51
47	g1	606	CHL	CHB-C4A	-2.48	1.35	1.38
47	g	606	CHL	CHB-C4A	-2.48	1.35	1.38
47	G	608	CHL	C1A-CHA	-2.48	1.37	1.40
31	B1	602	CLA	C4B-NB	-2.48	1.34	1.37
31	Y	608	CLA	C4B-NB	-2.48	1.34	1.37
49	N	622	XAT	O24-C25	-2.48	1.43	1.46
31	s	609	CLA	C4B-NB	-2.48	1.34	1.37
31	s1	613	CLA	C4B-NB	-2.48	1.34	1.37
31	g1	614	CLA	C4B-NB	-2.48	1.34	1.37
32	A1	408	PHO	C3D-C4D	2.48	1.44	1.41
50	n1	623	NEX	C17-C1	-2.47	1.49	1.53
32	A	408	PHO	CMB-C2B	-2.47	1.46	1.51
52	b1	624	3PH	O21-C2	-2.47	1.40	1.46
32	A1	409	PHO	CMD-C2D	-2.47	1.46	1.51
57	y1	626	PTY	O4-C30	2.47	1.40	1.33
32	A	409	PHO	CMB-C2B	-2.47	1.46	1.51
31	S1	609	CLA	C4B-NB	-2.47	1.34	1.37
47	y	607	CHL	C3A-C2A	-2.47	1.52	1.54
32	a1	408	PHO	CMD-C2D	-2.47	1.46	1.51
31	D	403	CLA	C4B-NB	-2.47	1.34	1.37
47	N1	609	CHL	C3B-C4B	2.47	1.43	1.41
31	B	611	CLA	C4B-NB	-2.47	1.34	1.37
47	n	608	CHL	C3D-C2D	-2.46	1.35	1.39
40	c1	519	DGD	CGB-CFB	-2.46	1.32	1.50
31	R1	612	CLA	C4B-NB	-2.46	1.34	1.37
31	S1	603	CLA	C4B-NB	-2.46	1.34	1.37
31	g1	612	CLA	C4B-NB	-2.46	1.34	1.37
31	N1	603	CLA	C4B-NB	-2.46	1.34	1.37
47	N1	601	CHL	C3B-C2B	-2.46	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
32	A1	408	PHO	CMD-C2D	-2.46	1.46	1.51
47	S	601	CHL	C3B-C2B	-2.45	1.37	1.40
56	r1	626	ERG	C7-C8	-2.45	1.28	1.34
31	n1	603	CLA	C4B-NB	-2.45	1.34	1.37
52	b1	624	3PH	O31-C31	2.45	1.40	1.33
49	n1	622	XAT	O24-C25	-2.45	1.43	1.46
47	n1	606	CHL	C1D-C2D	2.45	1.42	1.39
46	H	101	RRX	C35-C13	2.45	1.55	1.50
57	Y1	626	PTY	O4-C30	2.45	1.40	1.33
55	r1	625	LMT	O3'-C3'	-2.45	1.36	1.43
47	s1	601	CHL	CHB-C4A	-2.45	1.35	1.38
31	g	602	CLA	C4B-NB	-2.44	1.34	1.37
35	h1	102	LMG	C22-C21	-2.44	1.32	1.50
50	s	623	NEX	C1-C6	-2.44	1.50	1.54
51	S1	625	LPX	P1-O2	2.44	1.68	1.59
31	y	602	CLA	C1C-C2C	2.44	1.49	1.44
50	s1	623	NEX	C18-C5	2.44	1.56	1.52
32	a1	408	PHO	C3D-C4D	2.44	1.44	1.41
31	d	402	CLA	C4B-NB	-2.43	1.34	1.37
31	s1	603	CLA	C4B-NB	-2.43	1.34	1.37
52	s1	626	3PH	O31-C31	2.43	1.40	1.33
31	n1	612	CLA	C4B-NB	-2.43	1.34	1.37
47	G1	601	CHL	C3B-C2B	-2.43	1.37	1.40
31	R	603	CLA	C4B-NB	-2.43	1.34	1.37
31	n	602	CLA	C4B-NB	-2.43	1.34	1.37
37	b1	620	C7Z	C20-C13	2.42	1.55	1.50
52	s	626	3PH	O31-C31	2.42	1.40	1.33
37	b1	620	C7Z	C18-C5	2.42	1.54	1.50
47	g	601	CHL	C3B-C2B	-2.42	1.37	1.40
31	c1	501	CLA	C4B-NB	-2.42	1.34	1.37
49	y	622	XAT	O24-C25	-2.42	1.43	1.46
32	a1	408	PHO	CAC-C3C	-2.42	1.47	1.51
31	r	608	CLA	C4B-NB	-2.42	1.34	1.37
47	R	606	CHL	CHA-CBD	2.42	1.54	1.51
31	S	613	CLA	C1A-CHA	2.41	1.53	1.43
35	A	413	LMG	C22-C21	-2.41	1.33	1.50
32	a	409	PHO	C3D-C4D	2.40	1.44	1.41
35	A	413	LMG	C43-C42	-2.40	1.33	1.50
47	y	601	CHL	C1A-CHA	-2.40	1.37	1.40
52	S	626	3PH	O31-C31	2.40	1.40	1.33
50	s	623	NEX	O4-C5	-2.40	1.39	1.43
47	G	607	CHL	C3A-C2A	-2.40	1.52	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	C1	524	DGA	OG2-CG2	-2.40	1.41	1.46
31	b1	605	CLA	C1A-CHA	2.40	1.53	1.43
35	b1	622	LMG	C25-C24	-2.40	1.33	1.50
35	A1	413	LMG	C43-C42	-2.40	1.33	1.50
31	s1	603	CLA	C1A-CHA	2.39	1.53	1.43
40	C	520	DGD	CDA-CCA	-2.39	1.33	1.50
35	a1	413	LMG	C43-C42	-2.39	1.33	1.50
35	h	102	LMG	C22-C21	-2.39	1.33	1.50
35	C	521	LMG	C25-C24	-2.39	1.33	1.50
35	c	521	LMG	C43-C42	-2.39	1.33	1.50
47	G1	608	CHL	C3B-C2B	-2.39	1.37	1.40
40	c	520	DGD	CDA-CCA	-2.39	1.33	1.50
31	b1	602	CLA	C4B-NB	-2.39	1.34	1.37
40	C1	518	DGD	CGB-CFB	-2.39	1.33	1.50
47	G1	606	CHL	C3B-C2B	-2.39	1.37	1.40
40	C	518	DGD	CGB-CFB	-2.39	1.33	1.50
31	A1	405	CLA	C1C-C2C	2.39	1.49	1.44
31	b	611	CLA	C4B-NB	-2.39	1.34	1.37
40	c	518	DGD	CGB-CFB	-2.39	1.33	1.50
35	h	102	LMG	C43-C42	-2.38	1.33	1.50
51	s1	625	LPX	P1-O2	2.38	1.68	1.59
31	R1	608	CLA	C4B-NB	-2.38	1.34	1.37
40	C1	520	DGD	CDA-CCA	-2.38	1.33	1.50
40	c1	519	DGD	CGA-CFA	-2.38	1.33	1.50
40	c	519	DGD	CGB-CFB	-2.38	1.33	1.50
44	D1	405	PL9	C53-C6	-2.38	1.45	1.50
35	a	413	LMG	C22-C21	-2.38	1.33	1.50
35	D1	411	LMG	C25-C24	-2.38	1.33	1.50
40	C1	519	DGD	CGB-CFB	-2.38	1.33	1.50
35	b	622	LMG	C25-C24	-2.38	1.33	1.50
35	c1	521	LMG	C43-C42	-2.38	1.33	1.50
35	C1	521	LMG	C25-C24	-2.38	1.33	1.50
40	C	520	DGD	CGB-CFB	-2.37	1.33	1.50
35	H	102	LMG	C43-C42	-2.37	1.33	1.50
35	a1	413	LMG	C22-C21	-2.37	1.33	1.50
35	D	411	LMG	C25-C24	-2.37	1.33	1.50
47	n1	607	CHL	CHA-CBD	2.37	1.54	1.51
40	c1	518	DGD	CGB-CFB	-2.37	1.33	1.50
35	C	521	LMG	C43-C42	-2.37	1.33	1.50
40	C	519	DGD	CGB-CFB	-2.37	1.33	1.50
40	C1	520	DGD	CGB-CFB	-2.37	1.33	1.50
35	B1	622	LMG	C25-C24	-2.37	1.33	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	A1	413	LMG	C22-C21	-2.37	1.33	1.50
32	a	408	PHO	C3D-C4D	2.37	1.44	1.41
35	a	413	LMG	C43-C42	-2.37	1.33	1.50
35	H	102	LMG	C22-C21	-2.37	1.33	1.50
47	R	606	CHL	C3B-C2B	-2.37	1.37	1.40
31	b1	616	CLA	C4B-NB	-2.37	1.34	1.37
35	H1	102	LMG	C43-C42	-2.37	1.33	1.50
35	c1	521	LMG	C25-C24	-2.37	1.33	1.50
40	C1	519	DGD	CGA-CFA	-2.37	1.33	1.50
31	r	612	CLA	C4B-NB	-2.37	1.34	1.37
35	H1	102	LMG	C22-C21	-2.36	1.33	1.50
40	c	519	DGD	CGA-CFA	-2.36	1.33	1.50
47	n	605	CHL	C3B-C2B	-2.36	1.37	1.40
35	C1	521	LMG	C43-C42	-2.36	1.33	1.50
52	b1	624	3PH	O21-C21	2.36	1.41	1.34
44	d	405	PL9	C53-C6	-2.36	1.45	1.50
35	c	521	LMG	C25-C24	-2.36	1.33	1.50
57	Y1	627	PTY	O7-C8	2.36	1.40	1.35
40	c1	520	DGD	CGB-CFB	-2.36	1.33	1.50
49	R1	621	XAT	O24-C25	-2.36	1.43	1.46
40	c	520	DGD	CGB-CFB	-2.36	1.33	1.50
31	B1	611	CLA	C4B-NB	-2.36	1.34	1.37
52	i	101	3PH	O31-C31	2.36	1.40	1.33
31	b1	611	CLA	C4B-NB	-2.36	1.34	1.37
47	s1	608	CHL	C3B-C2B	-2.36	1.37	1.40
35	B	622	LMG	C25-C24	-2.36	1.33	1.50
52	T1	101	3PH	O21-C21	2.36	1.40	1.34
35	h1	102	LMG	C43-C42	-2.36	1.33	1.50
31	B1	605	CLA	C1A-CHA	2.36	1.52	1.43
52	S1	626	3PH	O31-C31	2.35	1.40	1.33
35	d	411	LMG	C25-C24	-2.35	1.33	1.50
35	d1	411	LMG	C25-C24	-2.35	1.33	1.50
32	a1	408	PHO	CMB-C2B	-2.35	1.46	1.51
31	R	608	CLA	C4B-NB	-2.35	1.34	1.37
40	C	519	DGD	CGA-CFA	-2.35	1.33	1.50
47	R1	606	CHL	CHA-CBD	2.35	1.54	1.51
51	s	625	LPX	P1-O2	2.35	1.68	1.59
47	g1	607	CHL	CHB-C4A	-2.35	1.35	1.38
31	g	613	CLA	C4B-NB	-2.35	1.34	1.37
47	g1	607	CHL	CHA-CBD	2.35	1.54	1.51
37	B1	620	C7Z	C18-C5	2.35	1.54	1.50
31	D	402	CLA	C4B-NB	-2.34	1.34	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	G	603	CLA	C4B-NB	-2.34	1.34	1.37
31	y	603	CLA	C4B-NB	-2.34	1.34	1.37
52	T1	101	3PH	O31-C31	2.34	1.40	1.33
31	s1	605	CLA	C1A-CHA	2.34	1.52	1.43
31	d1	402	CLA	C4B-NB	-2.34	1.34	1.37
47	N	601	CHL	CHA-CBD	2.34	1.54	1.51
31	B	604	CLA	C1C-C2C	2.33	1.49	1.44
38	J1	101	DGA	OG2-CG2	-2.33	1.41	1.46
31	B1	602	CLA	C1A-CHA	2.33	1.52	1.43
31	N	604	CLA	C4B-NB	-2.33	1.34	1.37
31	b	615	CLA	C1A-CHA	2.33	1.52	1.43
47	N1	609	CHL	CHA-CBD	2.33	1.54	1.51
37	B	620	C7Z	C20-C13	2.33	1.55	1.50
32	A	409	PHO	C3D-C4D	2.33	1.44	1.41
37	B	620	C7Z	C40-C33	2.32	1.55	1.50
31	R1	602	CLA	C1A-CHA	2.32	1.52	1.43
47	G	601	CHL	CHA-CBD	2.32	1.54	1.51
47	g1	605	CHL	CHA-CBD	2.32	1.54	1.51
40	c1	520	DGD	CDA-CCA	-2.32	1.33	1.50
47	g1	608	CHL	C3B-C2B	-2.32	1.37	1.40
31	c1	502	CLA	C1A-CHA	2.31	1.52	1.43
31	a1	407	CLA	C1A-CHA	2.31	1.52	1.43
47	S1	601	CHL	C3B-C2B	-2.31	1.37	1.40
31	s	613	CLA	C1A-CHA	2.31	1.52	1.43
38	c1	524	DGA	OG2-CG2	-2.31	1.41	1.46
47	s1	601	CHL	CHA-CBD	2.31	1.54	1.51
31	s1	609	CLA	C1A-CHA	2.31	1.52	1.43
31	b	611	CLA	C1C-C2C	2.31	1.49	1.44
31	b1	610	CLA	C1A-CHA	2.31	1.52	1.43
55	R1	625	LMT	O2'-C2'	-2.31	1.37	1.43
47	n1	608	CHL	CHA-CBD	2.30	1.54	1.51
51	S	625	LPX	P1-O2	2.30	1.68	1.59
31	B	616	CLA	C1A-CHA	2.30	1.52	1.43
47	r	606	CHL	CHA-CBD	2.30	1.54	1.51
31	s	605	CLA	C1A-CHA	2.30	1.52	1.43
56	r1	626	ERG	C14-C8	2.30	1.57	1.51
31	S1	603	CLA	C1A-CHA	2.30	1.52	1.43
31	S	610	CLA	C1C-C2C	2.30	1.49	1.44
31	r	610	CLA	C1A-CHA	2.30	1.52	1.43
47	y	609	CHL	CHA-CBD	2.29	1.54	1.51
31	g1	614	CLA	C1A-CHA	2.29	1.52	1.43
47	n1	601	CHL	CHA-CBD	2.29	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	g	613	CLA	C1C-C2C	2.29	1.49	1.44
47	g	608	CHL	CHA-CBD	2.29	1.54	1.51
47	s	606	CHL	CHA-CBD	2.29	1.54	1.51
56	R1	626	ERG	C7-C8	-2.29	1.29	1.34
32	a	408	PHO	C4D-ND	-2.29	1.35	1.38
31	G1	602	CLA	C1C-C2C	2.29	1.49	1.44
47	y1	607	CHL	CHA-CBD	2.29	1.54	1.51
47	s	606	CHL	C3B-C2B	-2.28	1.37	1.40
31	b1	608	CLA	C1A-CHA	2.28	1.52	1.43
31	S1	605	CLA	C1A-CHA	2.28	1.52	1.43
31	b	605	CLA	C1A-CHA	2.28	1.52	1.43
31	b1	602	CLA	C1A-CHA	2.28	1.52	1.43
32	A1	408	PHO	CAC-C3C	-2.28	1.47	1.51
47	y1	606	CHL	C3B-C2B	-2.28	1.37	1.40
55	r1	625	LMT	O3B-C3B	-2.28	1.37	1.43
47	G	607	CHL	CHA-CBD	2.28	1.54	1.51
47	S1	601	CHL	CHA-CBD	2.28	1.54	1.51
31	n1	613	CLA	C1A-CHA	2.28	1.52	1.43
47	S1	606	CHL	C1A-CHA	-2.28	1.37	1.40
47	r	607	CHL	CHA-CBD	2.28	1.54	1.51
31	c1	512	CLA	C1A-CHA	2.28	1.52	1.43
31	R1	608	CLA	C1A-CHA	2.28	1.52	1.43
31	g1	603	CLA	C4B-NB	-2.28	1.34	1.37
57	y1	627	PTY	O7-C8	2.27	1.40	1.35
47	n	606	CHL	CHA-CBD	2.27	1.54	1.51
47	g	605	CHL	CHA-CBD	2.27	1.54	1.51
32	A	408	PHO	C3D-C4D	2.27	1.44	1.41
31	b1	614	CLA	C1A-CHA	2.27	1.52	1.43
31	r	613	CLA	C1A-CHA	2.27	1.52	1.43
31	N	611	CLA	C1A-CHA	2.27	1.52	1.43
47	Y	609	CHL	C1A-CHA	-2.27	1.37	1.40
31	g	611	CLA	C1A-CHA	2.27	1.52	1.43
57	y1	626	PTY	O7-C8	2.27	1.40	1.34
47	y1	609	CHL	C3B-C2B	-2.27	1.37	1.40
31	B	605	CLA	C1A-CHA	2.27	1.52	1.43
31	r1	608	CLA	C1A-CHA	2.26	1.52	1.43
31	n1	611	CLA	C1A-CHA	2.26	1.52	1.43
47	n1	601	CHL	C3B-C2B	-2.26	1.37	1.40
31	C1	512	CLA	C1C-C2C	2.26	1.49	1.44
47	G1	607	CHL	CHA-CBD	2.26	1.54	1.51
31	n1	614	CLA	C1A-CHA	2.26	1.52	1.43
47	n	607	CHL	CHA-CBD	2.26	1.54	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	r1	607	CHL	CHA-CBD	2.26	1.54	1.51
47	Y	609	CHL	C3B-C2B	-2.26	1.37	1.40
50	R	622	NEX	O24-C25	-2.26	1.43	1.46
31	R1	612	CLA	C1A-CHA	2.26	1.52	1.43
47	y	607	CHL	CHA-CBD	2.25	1.54	1.51
31	C1	506	CLA	C1A-CHA	2.25	1.52	1.43
37	b	620	C7Z	C40-C33	2.25	1.55	1.50
47	N	601	CHL	C3B-C2B	-2.25	1.37	1.40
47	S1	608	CHL	C3B-C2B	-2.25	1.37	1.40
31	r1	602	CLA	C1C-C2C	2.25	1.49	1.44
31	B	610	CLA	C1A-CHA	2.25	1.52	1.43
31	c	512	CLA	C1A-CHA	2.25	1.52	1.43
31	s1	610	CLA	C1A-CHA	2.25	1.52	1.43
47	s1	607	CHL	CHA-CBD	2.25	1.54	1.51
31	G1	614	CLA	C1A-CHA	2.25	1.52	1.43
31	r	611	CLA	C1A-CHA	2.25	1.52	1.43
47	y1	609	CHL	CHA-CBD	2.25	1.54	1.51
31	S	611	CLA	C1A-CHA	2.25	1.52	1.43
31	s1	602	CLA	C1C-C2C	2.25	1.49	1.44
47	N1	608	CHL	CHA-CBD	2.25	1.54	1.51
37	b1	620	C7Z	C40-C33	2.25	1.55	1.50
31	R	603	CLA	C1A-CHA	2.24	1.52	1.43
31	R	608	CLA	C1A-CHA	2.24	1.52	1.43
31	R	613	CLA	C1A-CHA	2.24	1.52	1.43
31	a	406	CLA	C1A-CHA	2.24	1.52	1.43
31	n	604	CLA	C1A-CHA	2.24	1.52	1.43
47	y	605	CHL	CHA-CBD	2.24	1.54	1.51
47	g1	608	CHL	CHA-CBD	2.24	1.54	1.51
47	N1	601	CHL	CHA-CBD	2.24	1.54	1.51
31	S1	611	CLA	C1A-CHA	2.24	1.52	1.43
31	b	608	CLA	C1A-CHA	2.24	1.52	1.43
38	j1	101	DGA	OG2-CG2	-2.24	1.41	1.46
47	N	607	CHL	CHA-CBD	2.24	1.54	1.51
31	n1	603	CLA	C1A-CHA	2.24	1.52	1.43
31	y1	610	CLA	C1A-CHA	2.24	1.52	1.43
31	c1	503	CLA	C1A-CHA	2.24	1.52	1.43
47	N	608	CHL	CHA-CBD	2.24	1.54	1.51
31	c1	501	CLA	C1A-CHA	2.24	1.52	1.43
47	r	606	CHL	C3B-C2B	-2.24	1.37	1.40
47	n	605	CHL	CHA-CBD	2.24	1.54	1.51
31	a1	406	CLA	C1A-CHA	2.23	1.52	1.43
38	c	524	DGA	OG2-CG2	-2.23	1.41	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	r	607	CHL	C3B-C2B	-2.23	1.37	1.40
31	b	602	CLA	C1A-CHA	2.23	1.52	1.43
31	s	603	CLA	C1A-CHA	2.23	1.52	1.43
47	n	608	CHL	CHA-CBD	2.23	1.54	1.51
47	y1	605	CHL	CHA-CBD	2.23	1.54	1.51
31	Y	613	CLA	C1A-CHA	2.23	1.52	1.43
47	Y	605	CHL	CHA-CBD	2.23	1.54	1.51
31	b	616	CLA	C1A-CHA	2.23	1.52	1.43
31	r	602	CLA	C1A-CHA	2.23	1.52	1.43
31	B1	609	CLA	C1A-CHA	2.23	1.52	1.43
31	B	609	CLA	C1A-CHA	2.23	1.52	1.43
47	n1	606	CHL	CHA-CBD	2.23	1.54	1.51
31	b	607	CLA	C1A-CHA	2.23	1.52	1.43
31	a1	405	CLA	C1A-CHA	2.23	1.52	1.43
31	r1	612	CLA	C1A-CHA	2.23	1.52	1.43
52	S1	626	3PH	O31-C3	-2.23	1.40	1.45
56	R1	626	ERG	C11-C9	2.23	1.57	1.53
31	A1	407	CLA	C1A-CHA	2.23	1.52	1.43
47	g1	601	CHL	CHA-CBD	2.23	1.54	1.51
38	C	524	DGA	OG2-CG2	-2.23	1.41	1.46
31	A	406	CLA	C1A-CHA	2.23	1.52	1.43
31	G	613	CLA	C1A-CHA	2.23	1.52	1.43
31	B	615	CLA	C1A-CHA	2.23	1.52	1.43
37	B1	620	C7Z	C40-C33	2.23	1.55	1.50
31	S	605	CLA	C1A-CHA	2.22	1.52	1.43
31	n	611	CLA	C1A-CHA	2.22	1.52	1.43
32	A	408	PHO	CAC-C3C	-2.22	1.47	1.51
47	Y	601	CHL	CHA-CBD	2.22	1.54	1.51
31	g1	604	CLA	C1A-CHA	2.22	1.52	1.43
31	R	609	CLA	C1C-C2C	2.22	1.49	1.44
47	Y1	606	CHL	CHA-CBD	2.22	1.54	1.51
31	Y1	612	CLA	C1A-CHA	2.22	1.52	1.43
31	A1	410	CLA	C1A-CHA	2.22	1.52	1.43
50	g	623	NEX	O24-C25	-2.22	1.43	1.46
31	G1	612	CLA	C1A-CHA	2.22	1.52	1.43
31	S1	610	CLA	C1A-CHA	2.22	1.52	1.43
31	g	613	CLA	C1A-CHA	2.22	1.52	1.43
31	B1	612	CLA	C1C-C2C	2.22	1.49	1.44
47	Y1	607	CHL	CHA-CBD	2.22	1.54	1.51
31	N1	603	CLA	C1A-CHA	2.22	1.52	1.43
47	G	605	CHL	CHA-CBD	2.22	1.54	1.51
52	t1	101	3PH	O21-C21	2.22	1.40	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	Y	606	CHL	C3B-C2B	-2.22	1.37	1.40
31	c	513	CLA	C1C-C2C	2.22	1.49	1.44
31	c	505	CLA	C1A-CHA	2.22	1.52	1.43
31	d1	403	CLA	C1A-CHA	2.22	1.52	1.43
31	N1	604	CLA	C3D-C4D	-2.22	1.39	1.44
31	b	615	CLA	CHD-C1D	2.22	1.42	1.38
31	g1	611	CLA	C1A-CHA	2.22	1.52	1.43
31	r1	602	CLA	C1A-CHA	2.22	1.52	1.43
31	S	603	CLA	C1A-CHA	2.21	1.52	1.43
31	r	608	CLA	C1A-CHA	2.21	1.52	1.43
52	T1	101	3PH	O31-C3	-2.21	1.40	1.45
52	S	626	3PH	O31-C3	-2.21	1.40	1.45
31	s	609	CLA	C1C-C2C	2.21	1.49	1.44
31	B1	607	CLA	C1A-CHA	2.21	1.52	1.43
47	g1	609	CHL	CHA-CBD	2.21	1.54	1.51
31	c1	513	CLA	C1A-CHA	2.21	1.52	1.43
31	B	612	CLA	C1A-CHA	2.21	1.52	1.43
31	y1	608	CLA	C1A-CHA	2.21	1.52	1.43
47	g1	606	CHL	C1A-CHA	-2.21	1.37	1.40
31	R1	609	CLA	C1A-CHA	2.21	1.52	1.43
47	G1	609	CHL	CHA-CBD	2.21	1.54	1.51
31	S1	604	CLA	C1A-CHA	2.21	1.52	1.43
47	G	609	CHL	CHA-CBD	2.21	1.54	1.51
47	S	601	CHL	CHA-CBD	2.21	1.54	1.51
31	C1	505	CLA	C1A-CHA	2.21	1.52	1.43
31	c1	508	CLA	C1C-C2C	2.21	1.49	1.44
31	r1	612	CLA	MG-NC	2.21	2.11	2.06
47	Y1	609	CHL	CHA-CBD	2.21	1.54	1.51
31	s	611	CLA	C1A-CHA	2.21	1.52	1.43
31	y	610	CLA	C1A-CHA	2.21	1.52	1.43
50	R1	622	NEX	O24-C25	-2.21	1.43	1.46
31	B1	614	CLA	C1A-CHA	2.21	1.52	1.43
31	c	509	CLA	C1A-CHA	2.21	1.52	1.43
31	y	612	CLA	C1A-CHA	2.20	1.52	1.43
31	C	501	CLA	C3D-C4D	-2.20	1.39	1.44
32	A1	409	PHO	CAC-C3C	-2.20	1.47	1.51
47	n	609	CHL	CHA-CBD	2.20	1.54	1.51
47	s1	608	CHL	CHA-CBD	2.20	1.54	1.51
31	N	613	CLA	C1A-CHA	2.20	1.52	1.43
31	c1	509	CLA	C1A-CHA	2.20	1.52	1.43
31	g1	613	CLA	C1A-CHA	2.20	1.52	1.43
31	b	613	CLA	C3D-C4D	-2.20	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	B1	615	CLA	C1A-CHA	2.20	1.52	1.43
31	y1	613	CLA	C1A-CHA	2.20	1.52	1.43
31	s1	613	CLA	C1A-CHA	2.20	1.52	1.43
55	r1	625	LMT	O2B-C2B	-2.20	1.37	1.43
47	S	607	CHL	CHA-CBD	2.20	1.54	1.51
47	S	606	CHL	CHA-CBD	2.20	1.54	1.51
47	G1	606	CHL	CHA-CBD	2.20	1.54	1.51
47	r1	606	CHL	CHA-CBD	2.20	1.54	1.51
31	b	604	CLA	C1A-CHA	2.20	1.52	1.43
47	S	607	CHL	C3A-C2A	-2.20	1.52	1.54
31	S	604	CLA	C1A-CHA	2.20	1.52	1.43
47	N	609	CHL	CHA-CBD	2.20	1.54	1.51
31	Y	610	CLA	C1A-CHA	2.20	1.52	1.43
31	g1	612	CLA	C1A-CHA	2.20	1.52	1.43
31	s	602	CLA	C1A-CHA	2.20	1.52	1.43
47	n	601	CHL	CHA-CBD	2.20	1.54	1.51
31	r1	604	CLA	C1A-CHA	2.20	1.52	1.43
31	r	610	CLA	C1C-C2C	2.19	1.49	1.44
47	y1	605	CHL	C3B-C2B	-2.19	1.37	1.40
52	S	626	3PH	O21-C21	2.19	1.40	1.34
31	s1	614	CLA	C1A-CHA	2.19	1.52	1.43
47	R	607	CHL	CHA-CBD	2.19	1.54	1.51
31	b	607	CLA	C3D-C4D	-2.19	1.39	1.44
31	N1	614	CLA	C1A-CHA	2.19	1.52	1.43
31	s1	617	CLA	C1A-CHA	2.19	1.52	1.43
50	s1	623	NEX	C17-C1	-2.19	1.49	1.53
47	S1	608	CHL	CHA-CBD	2.19	1.54	1.51
31	b1	614	CLA	C1C-C2C	2.19	1.49	1.44
31	b1	615	CLA	C1A-CHA	2.19	1.52	1.43
31	S	609	CLA	C1C-C2C	2.19	1.49	1.44
47	s	607	CHL	CHA-CBD	2.19	1.54	1.51
47	R1	607	CHL	CHA-CBD	2.19	1.54	1.51
47	s1	606	CHL	CHA-CBD	2.19	1.54	1.51
31	n	610	CLA	C1A-CHA	2.19	1.52	1.43
31	S1	617	CLA	C1A-CHA	2.19	1.52	1.43
47	G1	605	CHL	CHA-CBD	2.19	1.54	1.51
31	y1	612	CLA	C1A-CHA	2.19	1.52	1.43
31	B1	604	CLA	C1C-C2C	2.19	1.49	1.44
32	a1	408	PHO	C4D-ND	-2.19	1.35	1.38
31	b1	611	CLA	C1C-C2C	2.19	1.49	1.44
47	G	608	CHL	CHA-CBD	2.19	1.54	1.51
31	c	501	CLA	C3D-C4D	-2.19	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	508	CLA	C1A-CHA	2.19	1.52	1.43
31	d	402	CLA	C1C-C2C	2.19	1.49	1.44
32	a1	409	PHO	CAC-C3C	-2.19	1.47	1.51
31	y1	604	CLA	C1A-CHA	2.19	1.52	1.43
31	C	511	CLA	C1A-CHA	2.19	1.52	1.43
47	N	606	CHL	CHA-CBD	2.19	1.54	1.51
47	N1	607	CHL	CHA-CBD	2.19	1.54	1.51
31	S1	609	CLA	C1A-CHA	2.19	1.52	1.43
31	r1	603	CLA	C1A-CHA	2.19	1.52	1.43
47	S	607	CHL	C3B-C2B	-2.18	1.37	1.40
31	s1	604	CLA	C1A-CHA	2.18	1.52	1.43
31	G	611	CLA	C1A-CHA	2.18	1.52	1.43
31	s	614	CLA	C1A-CHA	2.18	1.52	1.43
47	g	607	CHL	CHA-CBD	2.18	1.54	1.51
31	G	612	CLA	C1A-CHA	2.18	1.52	1.43
31	b1	613	CLA	C1A-CHA	2.18	1.52	1.43
31	y	603	CLA	C1A-CHA	2.18	1.52	1.43
47	g	606	CHL	CHA-CBD	2.18	1.54	1.51
47	s	601	CHL	CHA-CBD	2.18	1.54	1.51
31	N1	611	CLA	C1A-CHA	2.18	1.52	1.43
31	r	612	CLA	C1C-C2C	2.18	1.48	1.44
52	B1	624	3PH	O21-C21	2.18	1.40	1.34
47	n1	605	CHL	CHA-CBD	2.18	1.54	1.51
47	n1	609	CHL	CHA-CBD	2.18	1.54	1.51
31	B	613	CLA	C3D-C4D	-2.18	1.39	1.44
31	n1	610	CLA	C1A-CHA	2.18	1.52	1.43
45	F1	101	HEM	CMB-C2B	2.18	1.55	1.50
47	g1	609	CHL	C1A-CHA	-2.18	1.37	1.40
44	D1	405	PL9	C3-C4	-2.18	1.46	1.49
45	f1	101	HEM	CMB-C2B	2.18	1.55	1.50
31	r	603	CLA	C1A-CHA	2.18	1.52	1.43
31	n	614	CLA	C1A-CHA	2.18	1.52	1.43
31	Y	611	CLA	C1A-CHA	2.18	1.52	1.43
31	b1	617	CLA	C1A-CHA	2.18	1.52	1.43
31	S	612	CLA	C1A-CHA	2.18	1.52	1.43
50	G1	623	NEX	O24-C25	-2.18	1.43	1.46
31	n1	612	CLA	C1A-CHA	2.18	1.52	1.43
31	y	611	CLA	C1A-CHA	2.18	1.52	1.43
31	N1	613	CLA	C1A-CHA	2.18	1.52	1.43
47	s	608	CHL	C3B-C2B	-2.18	1.37	1.40
31	a	410	CLA	C1A-CHA	2.18	1.52	1.43
31	C1	511	CLA	C1A-CHA	2.18	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	g	612	CLA	C1A-CHA	2.17	1.52	1.43
31	n	611	CLA	C1C-C2C	2.17	1.48	1.44
47	G1	601	CHL	CHA-CBD	2.17	1.54	1.51
47	S1	607	CHL	CHA-CBD	2.17	1.54	1.51
31	s1	612	CLA	C1A-CHA	2.17	1.52	1.43
47	G1	608	CHL	CHA-CBD	2.17	1.54	1.51
31	B	602	CLA	C1A-CHA	2.17	1.52	1.43
31	y1	611	CLA	C1A-CHA	2.17	1.52	1.43
31	y	608	CLA	C1C-C2C	2.17	1.48	1.44
31	S	609	CLA	C1A-CHA	2.17	1.52	1.43
55	r1	625	LMT	O4'-C4B	-2.17	1.37	1.43
31	B1	611	CLA	C1A-CHA	2.17	1.52	1.43
31	c1	505	CLA	C1A-CHA	2.17	1.52	1.43
31	R	602	CLA	C1C-C2C	2.17	1.48	1.44
31	Y	602	CLA	C1C-C2C	2.17	1.48	1.44
31	S	602	CLA	C1A-CHA	2.17	1.52	1.43
31	B1	608	CLA	C1A-CHA	2.17	1.52	1.43
31	R1	604	CLA	C1A-CHA	2.17	1.52	1.43
31	y1	602	CLA	C1A-CHA	2.17	1.52	1.43
31	c1	504	CLA	C1A-CHA	2.17	1.52	1.43
47	y1	606	CHL	CHA-CBD	2.17	1.54	1.51
31	N1	614	CLA	C1C-C2C	2.17	1.48	1.44
31	r	612	CLA	C1A-CHA	2.17	1.52	1.43
47	Y	609	CHL	CHA-CBD	2.17	1.54	1.51
31	b1	616	CLA	C1A-CHA	2.17	1.52	1.43
31	B	614	CLA	C1A-CHA	2.17	1.52	1.43
31	c	507	CLA	C1A-CHA	2.17	1.52	1.43
52	i	101	3PH	O21-C21	2.17	1.40	1.34
31	C1	509	CLA	C1A-CHA	2.17	1.52	1.43
47	G	606	CHL	CHA-CBD	2.17	1.54	1.51
47	y	606	CHL	CHA-CBD	2.17	1.54	1.51
31	B	603	CLA	C1A-CHA	2.17	1.52	1.43
45	f1	101	HEM	CMC-C2C	2.17	1.55	1.50
55	R1	625	LMT	O2B-C2B	-2.17	1.37	1.43
31	a	407	CLA	C1A-CHA	2.17	1.52	1.43
31	g1	610	CLA	C1A-CHA	2.17	1.52	1.43
31	A	407	CLA	C1A-CHA	2.17	1.52	1.43
31	b	609	CLA	C3D-C4D	-2.17	1.39	1.44
31	B	607	CLA	C1A-CHA	2.17	1.52	1.43
55	R1	625	LMT	O3B-C3B	-2.17	1.37	1.43
31	g	614	CLA	C1A-CHA	2.17	1.52	1.43
31	C	503	CLA	C1A-CHA	2.17	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	R1	610	CLA	C1A-CHA	2.17	1.52	1.43
31	Y1	610	CLA	C1A-CHA	2.17	1.52	1.43
47	Y1	605	CHL	CHA-CBD	2.17	1.54	1.51
31	c1	506	CLA	C1A-CHA	2.16	1.52	1.43
31	R	602	CLA	C1A-CHA	2.16	1.52	1.43
47	G	609	CHL	C3B-C2B	-2.16	1.37	1.40
31	n	603	CLA	C1A-CHA	2.16	1.52	1.43
31	A	405	CLA	C3D-C4D	-2.16	1.39	1.44
31	N	612	CLA	C1A-CHA	2.16	1.52	1.43
31	s	612	CLA	C1C-C2C	2.16	1.48	1.44
56	r1	626	ERG	C11-C9	2.16	1.57	1.53
31	B1	610	CLA	C1C-C2C	2.16	1.48	1.44
31	C	512	CLA	C1A-CHA	2.16	1.52	1.43
31	b1	604	CLA	C1A-CHA	2.16	1.52	1.43
31	b1	609	CLA	C1A-CHA	2.16	1.52	1.43
31	n	613	CLA	C1C-C2C	2.16	1.48	1.44
52	i	101	3PH	O31-C3	-2.16	1.40	1.45
31	R	611	CLA	C1C-C2C	2.16	1.48	1.44
31	b	606	CLA	C1A-CHA	2.16	1.52	1.43
31	A1	406	CLA	C1A-CHA	2.16	1.52	1.43
31	C	502	CLA	C1A-CHA	2.16	1.52	1.43
31	n	612	CLA	C1C-C2C	2.16	1.48	1.44
31	g1	602	CLA	C1C-C2C	2.16	1.48	1.44
31	c1	507	CLA	C1C-C2C	2.16	1.48	1.44
31	s1	617	CLA	C1C-C2C	2.16	1.48	1.44
31	r1	609	CLA	C1A-CHA	2.16	1.52	1.43
31	B1	606	CLA	C1A-CHA	2.16	1.52	1.43
31	b1	603	CLA	C1A-CHA	2.16	1.52	1.43
47	n	608	CHL	C3A-C2A	-2.16	1.52	1.54
31	n1	604	CLA	C1A-CHA	2.16	1.52	1.43
31	n1	614	CLA	C1C-C2C	2.16	1.48	1.44
31	N	604	CLA	C1C-C2C	2.16	1.48	1.44
47	N	605	CHL	C1A-CHA	-2.16	1.37	1.40
31	A	410	CLA	C1A-CHA	2.16	1.52	1.43
31	C1	502	CLA	C1A-CHA	2.16	1.52	1.43
31	C1	512	CLA	C1A-CHA	2.16	1.52	1.43
31	G1	611	CLA	C1A-CHA	2.15	1.52	1.43
31	a1	410	CLA	C1A-CHA	2.15	1.52	1.43
31	c1	510	CLA	C1A-CHA	2.15	1.52	1.43
31	y	608	CLA	C1A-CHA	2.15	1.52	1.43
31	s	617	CLA	C1C-C2C	2.15	1.48	1.44
31	b1	612	CLA	C1A-CHA	2.15	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	503	CLA	C1A-CHA	2.15	1.52	1.43
31	R	613	CLA	C1C-C2C	2.15	1.48	1.44
31	d1	402	CLA	C1C-C2C	2.15	1.48	1.44
50	Y	623	NEX	O24-C25	-2.15	1.43	1.46
31	n	602	CLA	C1C-C2C	2.15	1.48	1.44
31	g1	610	CLA	C1C-C2C	2.15	1.48	1.44
47	N1	605	CHL	CHA-CBD	2.15	1.54	1.51
31	Y1	608	CLA	C3D-C4D	-2.15	1.39	1.44
52	s1	626	3PH	O21-C21	2.15	1.40	1.34
31	C	505	CLA	C1A-CHA	2.15	1.52	1.43
31	S1	602	CLA	C1A-CHA	2.15	1.52	1.43
47	N1	606	CHL	CHA-CBD	2.15	1.54	1.51
47	S1	606	CHL	CHA-CBD	2.15	1.54	1.51
31	G	603	CLA	C1A-CHA	2.15	1.52	1.43
52	S1	626	3PH	O21-C21	2.15	1.40	1.34
52	s	626	3PH	O21-C21	2.15	1.40	1.34
31	R	610	CLA	C1A-CHA	2.15	1.52	1.43
31	b	614	CLA	C1A-CHA	2.15	1.52	1.43
31	g1	602	CLA	C1A-CHA	2.15	1.51	1.43
47	Y	606	CHL	CHA-CBD	2.15	1.54	1.51
31	B	608	CLA	C1A-CHA	2.15	1.51	1.43
31	G	610	CLA	C1A-CHA	2.15	1.51	1.43
31	r	611	CLA	C1C-C2C	2.15	1.48	1.44
50	s	623	NEX	C16-C1	2.15	1.57	1.53
47	g1	601	CHL	C3B-C2B	-2.15	1.37	1.40
31	B1	603	CLA	C1A-CHA	2.15	1.51	1.43
31	R	612	CLA	C1A-CHA	2.15	1.51	1.43
31	s	605	CLA	C1C-C2C	2.15	1.48	1.44
31	B	609	CLA	C3D-C4D	-2.15	1.39	1.44
31	n	614	CLA	C1C-C2C	2.15	1.48	1.44
31	n	602	CLA	C1A-CHA	2.15	1.51	1.43
52	s1	626	3PH	O31-C3	-2.15	1.40	1.45
31	r	609	CLA	C1A-CHA	2.15	1.51	1.43
31	A1	405	CLA	C1A-CHA	2.15	1.51	1.43
31	g1	603	CLA	C1A-CHA	2.15	1.51	1.43
31	B1	616	CLA	C1A-CHA	2.14	1.51	1.43
31	c	513	CLA	C1A-CHA	2.14	1.51	1.43
31	s	617	CLA	C1A-CHA	2.14	1.51	1.43
31	R	611	CLA	C1A-CHA	2.14	1.51	1.43
31	R1	603	CLA	C1A-CHA	2.14	1.51	1.43
31	g	604	CLA	C1A-CHA	2.14	1.51	1.43
31	C1	504	CLA	C1A-CHA	2.14	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
47	g	601	CHL	CHA-CBD	2.14	1.54	1.51
31	G	602	CLA	C1A-CHA	2.14	1.51	1.43
31	b1	611	CLA	C1A-CHA	2.14	1.51	1.43
32	a	409	PHO	CAC-C3C	-2.14	1.48	1.51
31	Y1	611	CLA	C1A-CHA	2.14	1.51	1.43
47	G	601	CHL	C2C-C3C	2.14	1.38	1.36
31	y1	611	CLA	C3D-C4D	-2.14	1.39	1.44
31	N1	602	CLA	C1C-C2C	2.14	1.48	1.44
47	y	601	CHL	CHA-CBD	2.14	1.54	1.51
31	b1	607	CLA	C1A-CHA	2.14	1.51	1.43
52	s	626	3PH	O31-C3	-2.14	1.40	1.45
50	n	623	NEX	O24-C25	-2.14	1.43	1.46
31	G	614	CLA	C1A-CHA	2.14	1.51	1.43
31	n1	612	CLA	C1C-C2C	2.14	1.48	1.44
31	y	613	CLA	C1A-CHA	2.14	1.51	1.43
31	C	513	CLA	C1A-CHA	2.14	1.51	1.43
31	C1	510	CLA	C3D-C4D	-2.14	1.39	1.44
31	C1	513	CLA	C1A-CHA	2.14	1.51	1.43
31	s1	611	CLA	C1A-CHA	2.14	1.51	1.43
31	c	510	CLA	C3D-C4D	-2.14	1.39	1.44
31	c	511	CLA	C1C-C2C	2.14	1.48	1.44
31	N	603	CLA	C1A-CHA	2.14	1.51	1.43
31	N	604	CLA	C1A-CHA	2.14	1.51	1.43
47	g1	606	CHL	CHA-CBD	2.14	1.54	1.51
31	s1	605	CLA	MG-NC	2.14	2.11	2.06
31	G1	604	CLA	C1A-CHA	2.14	1.51	1.43
31	Y1	613	CLA	C1A-CHA	2.13	1.51	1.43
31	S	617	CLA	C1A-CHA	2.13	1.51	1.43
31	y	604	CLA	C1A-CHA	2.13	1.51	1.43
31	N1	612	CLA	C1A-CHA	2.13	1.51	1.43
31	S1	614	CLA	C1A-CHA	2.13	1.51	1.43
47	S	608	CHL	C3B-C2B	-2.13	1.37	1.40
31	b	609	CLA	C1A-CHA	2.13	1.51	1.43
52	T1	101	3PH	O21-C2	-2.13	1.41	1.46
47	N	605	CHL	CHA-CBD	2.13	1.54	1.51
31	Y	613	CLA	C1C-C2C	2.13	1.48	1.44
31	c	504	CLA	C1A-CHA	2.13	1.51	1.43
47	S	608	CHL	CHA-CBD	2.13	1.54	1.51
31	Y1	602	CLA	C1C-C2C	2.13	1.48	1.44
31	Y	608	CLA	C1A-CHA	2.13	1.51	1.43
31	r1	610	CLA	C1A-CHA	2.13	1.51	1.43
55	r1	625	LMT	O2'-C2'	-2.13	1.37	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c1	511	CLA	C1A-CHA	2.13	1.51	1.43
31	c1	511	CLA	C1C-C2C	2.13	1.48	1.44
32	A	408	PHO	C4D-ND	-2.13	1.35	1.38
32	A1	408	PHO	C4D-ND	-2.13	1.35	1.38
40	b1	623	DGD	O5D-C1E	2.13	1.43	1.40
31	C1	501	CLA	C1A-CHA	2.13	1.51	1.43
31	B	617	CLA	C3D-C4D	-2.13	1.39	1.44
31	G1	613	CLA	C1A-CHA	2.13	1.51	1.43
33	c1	515	BCR	C12-C13	-2.12	1.41	1.46
31	s	610	CLA	C1A-CHA	2.12	1.51	1.43
31	y	614	CLA	C1A-CHA	2.12	1.51	1.43
31	N	614	CLA	C1A-CHA	2.12	1.51	1.43
31	S	610	CLA	C1A-CHA	2.12	1.51	1.43
31	B1	610	CLA	C1A-CHA	2.12	1.51	1.43
31	S	617	CLA	C1C-C2C	2.12	1.48	1.44
31	D	403	CLA	C1A-CHA	2.12	1.51	1.43
31	g	603	CLA	C1A-CHA	2.12	1.51	1.43
47	y1	601	CHL	CHA-CBD	2.12	1.54	1.51
31	R1	610	CLA	C1C-C2C	2.12	1.48	1.44
31	G1	604	CLA	C1C-C2C	2.12	1.48	1.44
31	a	407	CLA	C3D-C4D	-2.12	1.39	1.44
31	D1	403	CLA	C1A-CHA	2.12	1.51	1.43
31	d	403	CLA	C1A-CHA	2.12	1.51	1.43
47	n1	609	CHL	C1A-CHA	-2.12	1.37	1.40
31	c	506	CLA	C1A-CHA	2.12	1.51	1.43
47	g	609	CHL	C3B-C2B	-2.12	1.37	1.40
31	N	611	CLA	C1C-C2C	2.12	1.48	1.44
31	r	602	CLA	C1C-C2C	2.12	1.48	1.44
47	g	609	CHL	CHA-CBD	2.12	1.54	1.51
31	s	604	CLA	C1A-CHA	2.12	1.51	1.43
31	B1	612	CLA	CHC-C1C	2.12	1.42	1.38
31	S	614	CLA	C1A-CHA	2.12	1.51	1.43
31	n	613	CLA	C1A-CHA	2.12	1.51	1.43
31	Y1	614	CLA	C3D-C4D	-2.12	1.39	1.44
31	b	603	CLA	C1A-CHA	2.11	1.51	1.43
31	Y1	604	CLA	C1A-CHA	2.11	1.51	1.43
31	b	611	CLA	C1A-CHA	2.11	1.51	1.43
31	R	609	CLA	C1A-CHA	2.11	1.51	1.43
31	C1	508	CLA	C1A-CHA	2.11	1.51	1.43
31	N	602	CLA	C1C-C2C	2.11	1.48	1.44
31	b	603	CLA	C1C-C2C	2.11	1.48	1.44
47	g1	606	CHL	C3B-C2B	-2.11	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Y1	608	CLA	C1A-CHA	2.11	1.51	1.43
31	c1	505	CLA	C1C-C2C	2.11	1.48	1.44
31	g	612	CLA	C1C-C2C	2.11	1.48	1.44
31	G	604	CLA	C1A-CHA	2.11	1.51	1.43
31	c1	507	CLA	C1A-CHA	2.11	1.51	1.43
47	Y1	605	CHL	C3B-C2B	-2.11	1.37	1.40
31	G1	612	CLA	C1C-C2C	2.11	1.48	1.44
31	B1	617	CLA	C1A-CHA	2.11	1.51	1.43
31	C1	503	CLA	C1A-CHA	2.11	1.51	1.43
50	S	622	NEX	O24-C25	-2.11	1.43	1.46
31	c	502	CLA	C1A-CHA	2.11	1.51	1.43
31	S1	613	CLA	C1A-CHA	2.11	1.51	1.43
31	G1	614	CLA	C1C-C2C	2.11	1.48	1.44
31	r	604	CLA	C1A-CHA	2.10	1.51	1.43
31	S1	609	CLA	C3D-C4D	-2.10	1.39	1.44
31	C	507	CLA	C1A-CHA	2.10	1.51	1.43
31	Y	614	CLA	C1A-CHA	2.10	1.51	1.43
31	B	604	CLA	C3D-C4D	-2.10	1.39	1.44
31	s	605	CLA	MG-NC	2.10	2.11	2.06
31	R	604	CLA	C1A-CHA	2.10	1.51	1.43
52	b1	624	3PH	O31-C3	-2.10	1.40	1.45
47	G	608	CHL	C3B-C2B	-2.10	1.37	1.40
31	C	510	CLA	C1A-CHA	2.10	1.51	1.43
31	r1	610	CLA	C1C-C2C	2.10	1.48	1.44
47	S	606	CHL	C3B-C2B	-2.10	1.37	1.40
47	s	608	CHL	CHA-CBD	2.10	1.54	1.51
31	b	606	CLA	C3D-C4D	-2.10	1.39	1.44
31	Y	604	CLA	C1A-CHA	2.10	1.51	1.43
31	R	603	CLA	MG-NC	2.10	2.11	2.06
31	c1	513	CLA	C1C-C2C	2.10	1.48	1.44
31	C	509	CLA	C1A-CHA	2.10	1.51	1.43
31	y1	603	CLA	C1A-CHA	2.10	1.51	1.43
31	S1	617	CLA	C1C-C2C	2.10	1.48	1.44
50	N	623	NEX	O24-C25	-2.10	1.43	1.46
31	N	613	CLA	C1C-C2C	2.10	1.48	1.44
31	b1	616	CLA	C1C-C2C	2.10	1.48	1.44
31	C	504	CLA	C1A-CHA	2.10	1.51	1.43
47	Y	607	CHL	CHA-CBD	2.10	1.54	1.51
31	s	612	CLA	C1A-CHA	2.10	1.51	1.43
31	c1	508	CLA	C1A-CHA	2.10	1.51	1.43
31	g1	614	CLA	C1C-C2C	2.10	1.48	1.44
31	c	502	CLA	C3D-C4D	-2.10	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	Y	612	CLA	C1A-CHA	2.10	1.51	1.43
31	R	603	CLA	C1C-C2C	2.10	1.48	1.44
31	y1	612	CLA	C1C-C2C	2.09	1.48	1.44
44	d	405	PL9	C46-C44	-2.09	1.47	1.51
31	b	612	CLA	C3D-C4D	-2.09	1.39	1.44
57	Y1	627	PTY	O4-C1	-2.09	1.40	1.45
47	y1	607	CHL	C3A-C2A	-2.09	1.52	1.54
31	N	610	CLA	C1C-C2C	2.09	1.48	1.44
31	c	507	CLA	C3D-C4D	-2.09	1.39	1.44
31	C1	503	CLA	C3D-C4D	-2.09	1.39	1.44
31	c	511	CLA	C3D-C4D	-2.09	1.39	1.44
31	B	611	CLA	C1A-CHA	2.09	1.51	1.43
31	g	604	CLA	C1C-C2C	2.09	1.48	1.44
31	Y1	603	CLA	C1A-CHA	2.09	1.51	1.43
31	c	501	CLA	C1A-CHA	2.09	1.51	1.43
31	Y1	613	CLA	C3D-C4D	-2.09	1.39	1.44
31	g1	613	CLA	C1C-C2C	2.09	1.48	1.44
31	A	410	CLA	C3D-C4D	-2.09	1.39	1.44
31	B1	604	CLA	C1A-CHA	2.09	1.51	1.43
31	A1	406	CLA	C1C-C2C	2.09	1.48	1.44
47	g	605	CHL	C1A-CHA	-2.09	1.37	1.40
31	S1	612	CLA	C1A-CHA	2.09	1.51	1.43
31	C1	501	CLA	C3D-C4D	-2.09	1.39	1.44
31	N1	610	CLA	C1A-CHA	2.09	1.51	1.43
31	C	501	CLA	C1A-CHA	2.09	1.51	1.43
31	S	603	CLA	C1C-C2C	2.09	1.48	1.44
44	d	405	PL9	C52-C5	-2.09	1.46	1.50
31	B	604	CLA	C1A-CHA	2.08	1.51	1.43
31	R	612	CLA	C4B-NB	-2.08	1.35	1.37
31	R1	608	CLA	C1C-C2C	2.08	1.48	1.44
31	Y1	614	CLA	C1A-CHA	2.08	1.51	1.43
31	b1	606	CLA	C1A-CHA	2.08	1.51	1.43
31	A	407	CLA	C3D-C4D	-2.08	1.39	1.44
31	B1	606	CLA	C3D-C4D	-2.08	1.39	1.44
31	b	617	CLA	C1A-CHA	2.08	1.51	1.43
53	A1	414	SPH	C3-C4	2.08	1.53	1.50
47	Y1	601	CHL	CHA-CBD	2.08	1.54	1.51
31	G1	603	CLA	C1A-CHA	2.08	1.51	1.43
33	c	515	BCR	C1-C6	-2.08	1.51	1.53
31	d	402	CLA	C3D-C4D	-2.08	1.39	1.44
31	G1	610	CLA	C1A-CHA	2.08	1.51	1.43
31	B1	613	CLA	C1A-CHA	2.08	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	y1	614	CLA	C3D-C4D	-2.08	1.39	1.44
31	d1	402	CLA	C1A-CHA	2.08	1.51	1.43
31	B	606	CLA	C1C-C2C	2.08	1.48	1.44
31	N	611	CLA	MG-NC	2.08	2.11	2.06
31	N1	604	CLA	C1A-CHA	2.08	1.51	1.43
31	b	610	CLA	C1A-CHA	2.08	1.51	1.43
44	D1	405	PL9	C52-C5	-2.08	1.46	1.50
50	r1	622	NEX	O24-C25	-2.08	1.43	1.46
31	g	602	CLA	C1C-C2C	2.07	1.48	1.44
31	R1	603	CLA	C1C-C2C	2.07	1.48	1.44
31	n1	613	CLA	C1C-C2C	2.07	1.48	1.44
31	C	509	CLA	C3D-C4D	-2.07	1.39	1.44
31	a	410	CLA	C3D-C4D	-2.07	1.39	1.44
31	D1	402	CLA	C3D-C4D	-2.07	1.39	1.44
31	g1	603	CLA	C1C-C2C	2.07	1.48	1.44
31	B1	604	CLA	C3D-C4D	-2.07	1.39	1.44
31	d1	403	CLA	C1C-C2C	2.07	1.48	1.44
52	t1	101	3PH	O31-C3	-2.07	1.40	1.45
57	y1	627	PTY	O4-C1	-2.07	1.40	1.45
31	s1	613	CLA	MG-NC	2.07	2.11	2.06
31	B1	615	CLA	MG-NC	2.07	2.11	2.06
47	y	609	CHL	C3B-C2B	-2.07	1.37	1.40
47	n	601	CHL	C1A-CHA	-2.07	1.37	1.40
31	n1	602	CLA	C1A-CHA	2.07	1.51	1.43
34	A1	412	SQD	O47-C45	-2.07	1.41	1.46
31	N1	613	CLA	C1C-C2C	2.07	1.48	1.44
31	N1	602	CLA	C1A-CHA	2.07	1.51	1.43
31	Y1	608	CLA	C1C-C2C	2.07	1.48	1.44
57	Y1	626	PTY	O7-C8	2.07	1.40	1.34
47	g	608	CHL	C3B-C2B	-2.07	1.37	1.40
31	c	505	CLA	C3D-C4D	-2.07	1.39	1.44
31	N	612	CLA	C1C-C2C	2.07	1.48	1.44
31	g	602	CLA	C1A-CHA	2.07	1.51	1.43
31	N1	610	CLA	C3D-C4D	-2.07	1.39	1.44
31	s1	603	CLA	C1C-C2C	2.07	1.48	1.44
31	g	614	CLA	C1C-C2C	2.07	1.48	1.44
31	C	503	CLA	C1C-C2C	2.07	1.48	1.44
31	D	402	CLA	C3D-C4D	-2.06	1.39	1.44
47	n1	605	CHL	C3B-C2B	-2.06	1.37	1.40
31	B	613	CLA	C1A-CHA	2.06	1.51	1.43
31	D1	403	CLA	C1C-C2C	2.06	1.48	1.44
31	Y1	614	CLA	C1C-C2C	2.06	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c1	501	CLA	C1C-C2C	2.06	1.48	1.44
47	y	609	CHL	C1A-CHA	-2.06	1.37	1.40
33	C1	516	BCR	C12-C13	-2.06	1.41	1.46
50	S1	623	NEX	O24-C25	-2.06	1.43	1.46
31	b	612	CLA	C1A-CHA	2.06	1.51	1.43
31	s	603	CLA	C1C-C2C	2.06	1.48	1.44
31	S	617	CLA	MG-NC	2.06	2.11	2.06
31	B1	615	CLA	C1C-C2C	2.06	1.48	1.44
31	R1	612	CLA	C1C-C2C	2.06	1.48	1.44
31	N	602	CLA	C3D-C4D	-2.06	1.39	1.44
31	Y	603	CLA	C1A-CHA	2.06	1.51	1.43
31	C	508	CLA	C3D-C4D	-2.06	1.39	1.44
31	g1	603	CLA	MG-NC	2.06	2.11	2.06
31	C	511	CLA	C1C-C2C	2.06	1.48	1.44
31	S	610	CLA	C3D-C4D	-2.06	1.39	1.44
31	n	613	CLA	MG-NC	2.06	2.11	2.06
31	c	511	CLA	C1A-CHA	2.06	1.51	1.43
47	n	601	CHL	C3B-C2B	-2.06	1.37	1.40
31	B	606	CLA	C3D-C4D	-2.06	1.39	1.44
31	d1	402	CLA	C3D-C4D	-2.06	1.39	1.44
31	A1	407	CLA	C1C-C2C	2.05	1.48	1.44
31	G1	602	CLA	C1A-CHA	2.05	1.51	1.43
31	y1	604	CLA	C1C-C2C	2.05	1.48	1.44
31	b1	606	CLA	C3D-C4D	-2.05	1.39	1.44
31	R1	608	CLA	MG-NC	2.05	2.11	2.06
50	s	623	NEX	O24-C25	-2.05	1.43	1.46
31	s1	611	CLA	C1C-C2C	2.05	1.48	1.44
50	r	623	NEX	O24-C25	-2.05	1.43	1.46
31	y1	614	CLA	C1A-CHA	2.05	1.51	1.43
31	B	611	CLA	C1C-C2C	2.05	1.48	1.44
47	S1	607	CHL	C3B-C2B	-2.05	1.37	1.40
31	G	604	CLA	C3D-C4D	-2.05	1.39	1.44
31	C1	505	CLA	C3D-C4D	-2.05	1.39	1.44
50	N1	623	NEX	O24-C25	-2.05	1.43	1.46
47	r1	607	CHL	C3B-C2B	-2.05	1.37	1.40
47	n	609	CHL	C1A-CHA	-2.05	1.37	1.40
31	n1	611	CLA	C1C-C2C	2.05	1.48	1.44
50	G	623	NEX	O24-C25	-2.05	1.43	1.46
31	B	610	CLA	C1C-C2C	2.05	1.48	1.44
31	y	602	CLA	C1A-CHA	2.05	1.51	1.43
31	s	617	CLA	MG-NC	2.05	2.11	2.06
31	C	502	CLA	C3D-C4D	-2.05	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
57	Y1	626	PTY	O4-C1	-2.05	1.40	1.45
31	S1	602	CLA	C1C-C2C	2.05	1.48	1.44
31	y1	608	CLA	C1C-C2C	2.05	1.48	1.44
31	D	403	CLA	C1C-C2C	2.05	1.48	1.44
31	Y	604	CLA	C3D-C4D	-2.05	1.39	1.44
31	G	614	CLA	C1C-C2C	2.05	1.48	1.44
31	R1	604	CLA	CHD-C1D	2.04	1.42	1.38
38	b1	625	DGA	OG2-CG2	-2.04	1.41	1.46
50	s1	623	NEX	O24-C25	-2.04	1.43	1.46
31	C	510	CLA	C3D-C4D	-2.04	1.39	1.44
31	B	606	CLA	C1A-CHA	2.04	1.51	1.43
31	G1	604	CLA	C3D-C4D	-2.04	1.39	1.44
31	R	610	CLA	C1C-C2C	2.04	1.48	1.44
31	s	609	CLA	C1A-CHA	2.04	1.51	1.43
31	b	604	CLA	C3D-C4D	-2.04	1.39	1.44
47	R	607	CHL	C3B-C2B	-2.04	1.37	1.40
31	r1	603	CLA	C1C-C2C	2.04	1.48	1.44
31	C	507	CLA	C3D-C4D	-2.04	1.39	1.44
31	y1	612	CLA	MG-NC	2.04	2.11	2.06
47	G1	605	CHL	C1A-CHA	-2.04	1.37	1.40
44	D1	405	PL9	C35-C34	-2.04	1.45	1.50
31	C1	502	CLA	C3D-C4D	-2.04	1.39	1.44
31	s1	604	CLA	MG-NC	2.04	2.11	2.06
31	N	602	CLA	C1A-CHA	2.04	1.51	1.43
31	C	511	CLA	C3D-C4D	-2.04	1.39	1.44
31	Y	610	CLA	C3D-C4D	-2.04	1.39	1.44
31	b	610	CLA	C3D-C4D	-2.04	1.39	1.44
31	C1	513	CLA	C3D-C4D	-2.04	1.39	1.44
31	g1	614	CLA	MG-NC	2.04	2.11	2.06
31	C	506	CLA	C3D-C4D	-2.04	1.39	1.44
31	y1	602	CLA	C1C-C2C	2.04	1.48	1.44
31	b1	614	CLA	MG-NC	2.04	2.11	2.06
31	y1	608	CLA	C3D-C4D	-2.03	1.39	1.44
31	c	510	CLA	C1A-CHA	2.03	1.51	1.43
31	Y	602	CLA	C3D-C4D	-2.03	1.39	1.44
31	G	604	CLA	C1C-C2C	2.03	1.48	1.44
31	Y	612	CLA	C1C-C2C	2.03	1.48	1.44
47	R1	607	CHL	C3B-C2B	-2.03	1.37	1.40
55	r1	625	LMT	O1'-C1'	-2.03	1.36	1.40
31	b1	609	CLA	CHD-C1D	2.03	1.42	1.38
31	y	613	CLA	C3D-C4D	-2.03	1.39	1.44
31	R1	612	CLA	MG-NC	2.03	2.11	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	N	614	CLA	C1C-C2C	2.03	1.48	1.44
31	g	603	CLA	C1C-C2C	2.03	1.48	1.44
31	b1	603	CLA	C1C-C2C	2.03	1.48	1.44
31	B1	607	CLA	C3D-C4D	-2.03	1.39	1.44
31	g	611	CLA	C1C-C2C	2.03	1.48	1.44
31	C1	513	CLA	C1C-C2C	2.03	1.48	1.44
50	S1	623	NEX	O4-C5	2.03	1.47	1.43
31	g	610	CLA	C1A-CHA	2.03	1.51	1.43
31	b1	610	CLA	MG-NC	2.03	2.11	2.06
31	c1	507	CLA	C3D-C4D	-2.03	1.39	1.44
31	C1	507	CLA	C1A-CHA	2.03	1.51	1.43
31	R1	603	CLA	C3D-C4D	-2.03	1.39	1.44
31	S	603	CLA	MG-NC	2.02	2.11	2.06
31	b	615	CLA	MG-NC	2.02	2.11	2.06
31	N1	612	CLA	C1C-C2C	2.02	1.48	1.44
31	s1	602	CLA	C3D-C4D	-2.02	1.39	1.44
31	G	612	CLA	C1C-C2C	2.02	1.48	1.44
31	Y	604	CLA	C1C-C2C	2.02	1.48	1.44
31	c	512	CLA	C1C-C2C	2.02	1.48	1.44
31	g	613	CLA	MG-NC	2.02	2.11	2.06
31	A1	410	CLA	C1C-C2C	2.02	1.48	1.44
31	Y1	602	CLA	C3D-C4D	-2.02	1.39	1.44
31	s	609	CLA	MG-NC	2.02	2.11	2.06
31	B	604	CLA	MG-NC	2.02	2.11	2.06
31	G	613	CLA	C1C-C2C	2.02	1.48	1.44
31	R	608	CLA	MG-NC	2.02	2.11	2.06
52	B1	624	3PH	O31-C3	-2.02	1.40	1.45
47	g	606	CHL	C1A-CHA	-2.02	1.37	1.40
31	C	503	CLA	C3D-C4D	-2.02	1.39	1.44
31	S	611	CLA	MG-NC	2.02	2.11	2.06
31	B	607	CLA	C3D-C4D	-2.02	1.39	1.44
31	r1	608	CLA	MG-NC	2.02	2.11	2.06
55	R1	625	LMT	O1'-C1'	-2.02	1.36	1.40
47	g1	609	CHL	C3B-C2B	-2.02	1.37	1.40
31	c	501	CLA	C1C-C2C	2.02	1.48	1.44
31	S1	610	CLA	C3D-C4D	-2.02	1.39	1.44
31	b	611	CLA	C3D-C4D	-2.02	1.39	1.44
31	c	506	CLA	C3D-C4D	-2.02	1.39	1.44
31	r	612	CLA	MG-NC	2.02	2.11	2.06
31	S1	605	CLA	C3D-C4D	-2.02	1.39	1.44
31	Y	608	CLA	MG-NC	2.02	2.11	2.06
31	Y	608	CLA	C1C-C2C	2.02	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	s1	604	CLA	C1C-C2C	2.02	1.48	1.44
31	N	603	CLA	C3D-C4D	-2.02	1.39	1.44
31	Y	603	CLA	C3D-C4D	-2.02	1.39	1.44
31	B	605	CLA	C3D-C4D	-2.02	1.39	1.44
33	a	411	BCR	C1-C6	-2.02	1.51	1.53
31	c	510	CLA	C1C-C2C	2.02	1.48	1.44
54	K1	101	4RF	O21-C20	-2.02	1.41	1.46
31	a	405	CLA	C3D-C4D	-2.02	1.39	1.44
31	C1	507	CLA	C3D-C4D	-2.02	1.39	1.44
31	C	504	CLA	C3D-C4D	-2.02	1.39	1.44
31	c	508	CLA	C3D-C4D	-2.02	1.39	1.44
31	d1	403	CLA	CHD-C1D	2.01	1.42	1.38
31	r	603	CLA	C1C-C2C	2.01	1.48	1.44
31	C1	501	CLA	C1C-C2C	2.01	1.48	1.44
31	c1	505	CLA	MG-NC	2.01	2.11	2.06
31	C	506	CLA	C1A-CHA	2.01	1.51	1.43
31	b	602	CLA	C3D-C4D	-2.01	1.39	1.44
31	b1	617	CLA	C3D-C4D	-2.01	1.39	1.44
31	C	513	CLA	C1C-C2C	2.01	1.48	1.44
31	B1	602	CLA	C1C-C2C	2.01	1.48	1.44
47	R1	606	CHL	C3B-C2B	-2.01	1.37	1.40
31	Y1	603	CLA	C3D-C4D	-2.01	1.39	1.44
31	C	505	CLA	C1C-C2C	2.01	1.48	1.44
31	R	612	CLA	C1C-C2C	2.01	1.48	1.44
31	r	604	CLA	C1C-C2C	2.01	1.48	1.44
50	y1	623	NEX	C17-C1	-2.01	1.50	1.53
31	c	503	CLA	C3D-C4D	-2.01	1.39	1.44
47	S	601	CHL	C3D-C2D	-2.01	1.36	1.39
31	n1	603	CLA	MG-NC	2.01	2.11	2.06
31	y	614	CLA	C3D-C4D	-2.01	1.39	1.44
31	B	608	CLA	C1C-C2C	2.01	1.48	1.44
31	S	609	CLA	MG-NC	2.01	2.11	2.06
34	C	526	SQD	O47-C45	-2.01	1.41	1.46
31	N	610	CLA	C1A-CHA	2.01	1.51	1.43
31	Y	612	CLA	C3D-C4D	-2.01	1.39	1.44
31	r1	612	CLA	C1C-C2C	2.01	1.48	1.44
31	r1	610	CLA	C3D-C4D	-2.01	1.39	1.44
31	r	602	CLA	MG-NC	2.01	2.11	2.06
31	r	611	CLA	MG-NC	2.01	2.11	2.06
33	d1	404	BCR	C12-C13	-2.01	1.41	1.46
31	R	611	CLA	MG-NC	2.01	2.11	2.06
31	r	608	CLA	C3D-C4D	-2.01	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	H1	102	LMG	O1-C1	2.01	1.43	1.40
31	R1	609	CLA	C1C-C2C	2.01	1.48	1.44
31	s1	603	CLA	MG-NC	2.01	2.11	2.06
31	G1	603	CLA	C3D-C4D	-2.01	1.39	1.44
31	Y1	604	CLA	C1C-C2C	2.01	1.48	1.44
31	s	603	CLA	MG-NC	2.01	2.11	2.06
31	g	604	CLA	C3D-C4D	-2.00	1.39	1.44
31	y	610	CLA	C1C-C2C	2.00	1.48	1.44
31	b	603	CLA	C3D-C4D	-2.00	1.39	1.44
31	r	604	CLA	C3D-C4D	-2.00	1.39	1.44
31	y	611	CLA	C3D-C4D	-2.00	1.39	1.44
31	g1	604	CLA	C1C-C2C	2.00	1.48	1.44
31	s1	609	CLA	C1C-C2C	2.00	1.48	1.44
31	G	613	CLA	MG-NC	2.00	2.11	2.06
35	j	101	LMG	O1-C1	2.00	1.43	1.40
31	N1	613	CLA	MG-NC	2.00	2.11	2.06
31	C	512	CLA	C1C-C2C	2.00	1.48	1.44
31	B	607	CLA	CHD-C1D	2.00	1.42	1.38
31	s1	609	CLA	MG-NC	2.00	2.11	2.06
45	f1	101	HEM	CMA-C3A	2.00	1.54	1.50
31	B	612	CLA	C1C-C2C	2.00	1.48	1.44
31	B1	617	CLA	C3D-C4D	-2.00	1.39	1.44
47	N1	609	CHL	C2C-C3C	2.00	1.38	1.36
31	G1	612	CLA	MG-NC	2.00	2.11	2.06
31	D	402	CLA	C1A-CHA	2.00	1.51	1.43
57	y1	626	PTY	O4-C1	-2.00	1.40	1.45
31	Y	608	CLA	C3D-C4D	-2.00	1.39	1.44

All (8887) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	H	101	RRX	C37-C22-C23	-31.76	69.57	118.09
41	L1	101	LHG	O7-C7-C8	23.31	161.90	111.48
52	S1	626	3PH	O21-C21-C22	22.43	160.00	111.48
52	s1	626	3PH	O21-C21-C22	22.34	159.81	111.48
31	R1	609	CLA	C4-C3-C5	-22.08	76.90	115.23
31	B	617	CLA	C4-C3-C5	-21.78	77.43	115.23
31	b	617	CLA	C4-C3-C5	-21.46	77.98	115.23
46	H	101	RRX	C20-C21-C22	20.46	155.97	127.28
33	c1	514	BCR	C10-C11-C12	19.27	179.03	123.20
33	C1	517	BCR	C10-C11-C12	19.13	178.63	123.20
33	B1	618	BCR	C10-C11-C12	19.08	178.49	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	C	517	BCR	C10-C11-C12	19.07	178.45	123.20
33	C1	514	BCR	C10-C11-C12	19.04	178.38	123.20
52	s1	626	3PH	O21-C21-O22	-18.80	79.75	123.70
33	b1	618	BCR	C10-C11-C12	18.80	177.66	123.20
52	S1	626	3PH	O21-C21-O22	-18.78	79.80	123.70
33	c	514	BCR	C10-C11-C12	18.75	177.54	123.20
33	b	619	BCR	C10-C11-C12	18.75	177.53	123.20
33	D	404	BCR	C10-C11-C12	18.74	177.50	123.20
33	c1	516	BCR	C10-C11-C12	18.73	177.47	123.20
33	B	619	BCR	C10-C11-C12	18.72	177.45	123.20
33	B1	619	BCR	C10-C11-C12	18.67	177.31	123.20
33	C	516	BCR	C10-C11-C12	18.67	177.30	123.20
33	b1	619	BCR	C10-C11-C12	18.66	177.28	123.20
33	B	618	BCR	C10-C11-C12	18.64	177.20	123.20
33	c	515	BCR	C10-C11-C12	18.64	177.20	123.20
33	C1	515	BCR	C10-C11-C12	18.63	177.19	123.20
41	L1	101	LHG	O7-C7-O9	-18.56	80.30	123.70
33	a1	411	BCR	C10-C11-C12	18.56	176.96	123.20
33	b	618	BCR	C10-C11-C12	18.55	176.96	123.20
33	C	515	BCR	C10-C11-C12	18.48	176.75	123.20
33	c1	515	BCR	C10-C11-C12	18.48	176.74	123.20
33	a	411	BCR	C10-C11-C12	18.47	176.71	123.20
33	C	514	BCR	C10-C11-C12	18.41	176.54	123.20
33	c	517	BCR	C10-C11-C12	18.37	176.43	123.20
33	d	404	BCR	C10-C11-C12	18.25	176.07	123.20
33	c	516	BCR	C10-C11-C12	18.18	175.87	123.20
33	A	411	BCR	C10-C11-C12	18.10	175.65	123.20
33	A1	411	BCR	C10-C11-C12	18.10	175.64	123.20
33	D1	404	BCR	C10-C11-C12	17.97	175.27	123.20
33	d1	404	BCR	C10-C11-C12	17.85	174.91	123.20
49	Y1	622	XAT	C37-C21-C36	-17.52	81.91	107.37
49	Y	622	XAT	C37-C21-C36	-17.34	82.19	107.37
33	c1	517	BCR	C10-C11-C12	17.28	173.26	123.20
33	C1	516	BCR	C10-C11-C12	17.18	172.97	123.20
49	y	622	XAT	C37-C21-C36	-17.12	82.50	107.37
49	y1	622	XAT	C37-C21-C36	-17.09	82.55	107.37
31	b	617	CLA	C5-C3-C2	17.05	159.44	121.17
31	B	617	CLA	C5-C3-C2	17.01	159.35	121.17
31	R1	609	CLA	C5-C3-C2	16.82	158.93	121.17
31	b	617	CLA	C4-C3-C2	-16.42	81.47	123.63
31	B	617	CLA	C4-C3-C2	-16.22	81.96	123.63
31	R1	609	CLA	C4-C3-C2	-16.19	82.04	123.63

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	H	101	RRX	C37-C22-C21	15.99	148.72	122.82
56	r1	626	ERG	C15-C14-C8	-15.21	99.78	120.42
33	B1	618	BCR	C16-C15-C14	14.91	154.02	123.52
33	c1	514	BCR	C16-C15-C14	14.89	153.98	123.52
33	c	514	BCR	C16-C15-C14	14.88	153.97	123.52
33	c1	517	BCR	C21-C20-C19	14.83	166.17	123.20
33	b1	618	BCR	C16-C15-C14	14.78	153.76	123.52
33	A1	411	BCR	C21-C20-C19	14.77	166.00	123.20
33	c1	517	BCR	C16-C15-C14	14.68	153.56	123.52
33	C	514	BCR	C16-C15-C14	14.62	153.44	123.52
33	C1	517	BCR	C21-C20-C19	14.61	165.54	123.20
33	D1	404	BCR	C21-C20-C19	14.55	165.35	123.20
33	a1	411	BCR	C11-C10-C9	14.52	147.64	127.28
33	B	619	BCR	C21-C20-C19	14.52	165.26	123.20
33	c1	517	BCR	C11-C10-C9	14.43	147.52	127.28
46	H	101	RRX	C23-C22-C21	14.40	141.66	119.01
33	A1	411	BCR	C11-C10-C9	14.33	147.37	127.28
33	C1	517	BCR	C16-C15-C14	14.28	152.74	123.52
33	C1	514	BCR	C16-C15-C14	14.28	152.73	123.52
33	B1	619	BCR	C16-C15-C14	14.06	152.28	123.52
33	b	619	BCR	C16-C15-C14	13.96	152.09	123.52
33	C	516	BCR	C11-C10-C9	13.96	146.86	127.28
33	C1	516	BCR	C11-C10-C9	13.90	146.78	127.28
33	c1	516	BCR	C11-C10-C9	13.90	146.78	127.28
33	b	618	BCR	C11-C10-C9	13.89	146.75	127.28
33	B	618	BCR	C16-C15-C14	13.88	151.93	123.52
33	C	517	BCR	C21-C20-C19	13.87	163.38	123.20
33	C	514	BCR	C11-C10-C9	13.83	146.67	127.28
33	a	411	BCR	C21-C20-C19	13.81	163.20	123.20
33	c	517	BCR	C21-C20-C19	13.79	163.15	123.20
33	b	619	BCR	C21-C20-C19	13.69	162.87	123.20
33	C1	515	BCR	C16-C15-C14	13.66	151.47	123.52
33	A	411	BCR	C11-C10-C9	13.66	146.43	127.28
33	C1	516	BCR	C21-C20-C19	13.66	162.77	123.20
33	c	514	BCR	C11-C10-C9	13.60	146.35	127.28
33	b1	619	BCR	C16-C15-C14	13.57	151.29	123.52
33	C1	515	BCR	C11-C10-C9	13.47	146.16	127.28
33	c1	516	BCR	C21-C20-C19	13.46	162.20	123.20
33	B	618	BCR	C11-C10-C9	13.40	146.07	127.28
33	C1	517	BCR	C11-C10-C9	13.28	145.91	127.28
33	b1	619	BCR	C21-C20-C19	13.28	161.67	123.20
33	C1	514	BCR	C11-C10-C9	13.24	145.85	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	C	514	BCR	C21-C20-C19	13.21	161.49	123.20
33	a1	411	BCR	C21-C20-C19	13.16	161.32	123.20
33	c	517	BCR	C11-C10-C9	13.15	145.72	127.28
33	a1	411	BCR	C16-C15-C14	13.11	150.35	123.52
33	b	619	BCR	C11-C10-C9	13.06	145.60	127.28
33	B1	618	BCR	C21-C20-C19	13.03	160.96	123.20
33	D	404	BCR	C11-C10-C9	13.02	145.54	127.28
33	c	514	BCR	C21-C20-C19	13.01	160.90	123.20
33	C1	516	BCR	C16-C15-C14	12.93	149.98	123.52
33	c	517	BCR	C16-C15-C14	12.92	149.95	123.52
33	B1	619	BCR	C21-C20-C19	12.90	160.57	123.20
33	D1	404	BCR	C16-C15-C14	12.89	149.90	123.52
33	d1	404	BCR	C21-C20-C19	12.86	160.46	123.20
33	a	411	BCR	C11-C10-C9	12.84	145.29	127.28
33	c1	516	BCR	C16-C15-C14	12.84	149.79	123.52
33	b1	618	BCR	C11-C10-C9	12.78	145.20	127.28
33	c	516	BCR	C11-C10-C9	12.75	145.16	127.28
33	B1	618	BCR	C11-C10-C9	12.73	145.14	127.28
33	C	515	BCR	C16-C15-C14	12.66	149.43	123.52
33	A	411	BCR	C21-C20-C19	12.66	159.89	123.20
33	c1	515	BCR	C11-C10-C9	12.66	145.03	127.28
33	C	517	BCR	C16-C15-C14	12.65	149.40	123.52
33	B1	619	BCR	C11-C10-C9	12.63	144.99	127.28
33	b	618	BCR	C21-C20-C19	12.61	159.73	123.20
33	b	618	BCR	C16-C15-C14	12.60	149.30	123.52
33	c1	514	BCR	C21-C20-C19	12.59	159.69	123.20
33	c	516	BCR	C16-C15-C14	12.59	149.28	123.52
33	c1	515	BCR	C16-C15-C14	12.58	149.25	123.52
33	A1	411	BCR	C16-C15-C14	12.56	149.21	123.52
33	b1	618	BCR	C21-C20-C19	12.46	159.30	123.20
33	b1	619	BCR	C11-C10-C9	12.41	144.69	127.28
33	C1	514	BCR	C21-C20-C19	12.41	159.16	123.20
33	c1	514	BCR	C11-C10-C9	12.40	144.67	127.28
33	C	515	BCR	C11-C10-C9	12.39	144.65	127.28
33	c	515	BCR	C16-C15-C14	12.36	148.82	123.52
49	y	622	XAT	C37-C21-C22	-12.33	87.29	108.97
33	A	411	BCR	C16-C15-C14	12.28	148.65	123.52
33	a	411	BCR	C16-C15-C14	12.26	148.60	123.52
33	c	515	BCR	C11-C10-C9	12.24	144.45	127.28
49	Y	622	XAT	C37-C21-C22	-12.20	87.53	108.97
33	B	618	BCR	C21-C20-C19	12.19	158.51	123.20
33	C	516	BCR	C16-C15-C14	12.17	148.42	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	Y1	622	XAT	C37-C21-C22	-12.10	87.70	108.97
33	B	619	BCR	C16-C15-C14	12.03	148.13	123.52
33	C	515	BCR	C21-C20-C19	11.99	157.94	123.20
49	y1	622	XAT	C37-C21-C22	-11.95	87.96	108.97
33	c1	515	BCR	C21-C20-C19	11.81	157.43	123.20
33	D	404	BCR	C16-C15-C14	11.78	147.63	123.52
33	d1	404	BCR	C16-C15-C14	11.77	147.60	123.52
56	R1	626	ERG	C15-C14-C8	-11.74	104.50	120.42
33	d1	404	BCR	C11-C10-C9	11.67	143.65	127.28
33	d	404	BCR	C16-C15-C14	11.65	147.35	123.52
33	C	515	BCR	C11-C12-C13	11.63	158.26	126.36
33	B	619	BCR	C11-C10-C9	11.58	143.52	127.28
33	C	517	BCR	C11-C10-C9	11.53	143.45	127.28
33	c	516	BCR	C21-C20-C19	11.43	156.31	123.20
33	D	404	BCR	C11-C12-C13	11.42	157.67	126.36
33	d	404	BCR	C11-C10-C9	11.40	143.26	127.28
50	r1	622	NEX	C8-C7-C6	-11.34	164.28	177.66
33	a	411	BCR	C11-C12-C13	11.34	157.46	126.36
33	B	619	BCR	C11-C12-C13	11.34	157.45	126.36
31	b1	605	CLA	C4A-NA-C1A	11.29	111.83	106.68
33	c1	515	BCR	C11-C12-C13	11.27	157.26	126.36
33	d	404	BCR	C11-C12-C13	11.27	157.25	126.36
33	a1	411	BCR	C11-C12-C13	11.20	157.08	126.36
52	s1	626	3PH	O22-C21-C22	-11.17	80.08	123.78
52	S1	626	3PH	O22-C21-C22	-11.14	80.20	123.78
33	B1	619	BCR	C11-C12-C13	11.14	156.91	126.36
33	C1	517	BCR	C11-C12-C13	11.11	156.84	126.36
33	C1	515	BCR	C21-C20-C19	11.02	155.14	123.20
33	C	516	BCR	C11-C12-C13	11.02	156.58	126.36
33	d1	404	BCR	C11-C12-C13	11.01	156.56	126.36
33	A1	411	BCR	C11-C12-C13	10.99	156.49	126.36
33	c	515	BCR	C21-C20-C19	10.84	154.61	123.20
33	c	517	BCR	C11-C12-C13	10.76	155.88	126.36
33	c1	516	BCR	C11-C12-C13	10.76	155.88	126.36
33	c	515	BCR	C11-C12-C13	10.76	155.88	126.36
33	b1	619	BCR	C11-C12-C13	10.76	155.87	126.36
41	L1	101	LHG	O9-C7-C8	-10.68	82.00	123.78
33	b	618	BCR	C11-C12-C13	10.68	155.65	126.36
33	B	618	BCR	C11-C12-C13	10.65	155.55	126.36
31	n	604	CLA	C4A-NA-C1A	10.61	111.52	106.68
33	C	517	BCR	C11-C12-C13	10.52	155.19	126.36
33	A	411	BCR	C11-C12-C13	10.49	155.12	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	605	CLA	C4A-NA-C1A	10.48	111.46	106.68
33	d	404	BCR	C21-C20-C19	10.41	153.36	123.20
33	c	516	BCR	C11-C12-C13	10.41	154.90	126.36
33	D1	404	BCR	C11-C10-C9	10.35	141.79	127.28
33	b	619	BCR	C11-C12-C13	10.30	154.60	126.36
33	C	516	BCR	C21-C20-C19	10.28	152.98	123.20
33	C1	514	BCR	C11-C12-C13	10.27	154.51	126.36
33	C	516	BCR	C20-C19-C18	10.24	154.43	126.36
33	C1	515	BCR	C11-C12-C13	10.23	154.42	126.36
31	b1	612	CLA	C4A-NA-C1A	10.17	111.32	106.68
31	B	605	CLA	C4A-NA-C1A	10.06	111.27	106.68
31	S	613	CLA	C4A-NA-C1A	10.02	111.25	106.68
31	B1	605	CLA	C4A-NA-C1A	10.02	111.25	106.68
33	b1	618	BCR	C11-C12-C13	10.00	153.77	126.36
31	Y1	610	CLA	C4A-NA-C1A	9.91	111.20	106.68
31	a1	406	CLA	C4A-NA-C1A	9.86	111.18	106.68
31	b	606	CLA	C4A-NA-C1A	9.86	111.18	106.68
33	C1	515	BCR	C20-C19-C18	9.85	153.37	126.36
33	D	404	BCR	C21-C20-C19	9.84	151.72	123.20
31	a1	405	CLA	C4A-NA-C1A	9.82	111.16	106.68
31	c1	502	CLA	C4A-NA-C1A	9.82	111.16	106.68
31	a	406	CLA	C4A-NA-C1A	9.81	111.15	106.68
33	B1	618	BCR	C11-C12-C13	9.80	153.24	126.36
31	b	615	CLA	C4A-NA-C1A	9.77	111.14	106.68
47	Y1	601	CHL	C1B-CHB-C4A	9.77	127.61	121.32
31	C	505	CLA	C4A-NA-C1A	9.72	111.11	106.68
31	C1	513	CLA	C4A-NA-C1A	9.72	111.11	106.68
33	C	514	BCR	C11-C12-C13	9.71	152.98	126.36
31	C1	509	CLA	C4A-NA-C1A	9.70	111.11	106.68
31	A1	410	CLA	C4A-NA-C1A	9.69	111.10	106.68
31	c1	511	CLA	C4A-NA-C1A	9.68	111.10	106.68
31	s	602	CLA	C4A-NA-C1A	9.68	111.10	106.68
50	g	623	NEX	C8-C7-C6	-9.68	166.24	177.66
31	G1	602	CLA	C4A-NA-C1A	9.66	111.09	106.68
31	Y	610	CLA	C4A-NA-C1A	9.65	111.08	106.68
31	b1	610	CLA	C4A-NA-C1A	9.64	111.08	106.68
31	B	615	CLA	C4A-NA-C1A	9.63	111.07	106.68
31	G	603	CLA	C4A-NA-C1A	9.61	111.06	106.68
47	y1	601	CHL	C1B-CHB-C4A	9.60	127.50	121.32
31	A	406	CLA	C4A-NA-C1A	9.59	111.06	106.68
31	n	603	CLA	C4A-NA-C1A	9.57	111.05	106.68
33	c	514	BCR	C11-C12-C13	9.57	152.61	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	c1	517	BCR	C11-C12-C13	9.57	152.61	126.36
31	y	603	CLA	C4A-NA-C1A	9.57	111.04	106.68
31	N1	603	CLA	C4A-NA-C1A	9.56	111.04	106.68
31	a	405	CLA	C4A-NA-C1A	9.52	111.02	106.68
31	s	613	CLA	C4A-NA-C1A	9.51	111.02	106.68
31	y	602	CLA	C4A-NA-C1A	9.50	111.01	106.68
31	n1	613	CLA	C4A-NA-C1A	9.50	111.01	106.68
31	b	617	CLA	C4A-NA-C1A	9.49	111.01	106.68
33	D1	404	BCR	C11-C12-C13	9.47	152.32	126.36
31	c	508	CLA	C4A-NA-C1A	9.46	111.00	106.68
31	S1	612	CLA	C4A-NA-C1A	9.45	110.99	106.68
31	g1	613	CLA	C4A-NA-C1A	9.45	110.99	106.68
31	C	513	CLA	C4A-NA-C1A	9.44	110.98	106.68
31	s1	603	CLA	C4A-NA-C1A	9.43	110.98	106.68
31	C1	511	CLA	C4A-NA-C1A	9.43	110.98	106.68
31	B	613	CLA	C4A-NA-C1A	9.43	110.98	106.68
31	C1	504	CLA	C4A-NA-C1A	9.42	110.98	106.68
31	G	610	CLA	C4A-NA-C1A	9.41	110.97	106.68
31	Y	613	CLA	C4A-NA-C1A	9.41	110.97	106.68
33	c1	514	BCR	C11-C12-C13	9.41	152.16	126.36
31	g	603	CLA	C4A-NA-C1A	9.41	110.97	106.68
31	y1	613	CLA	C4A-NA-C1A	9.40	110.97	106.68
31	c	502	CLA	C4A-NA-C1A	9.40	110.97	106.68
31	r1	604	CLA	C4A-NA-C1A	9.39	110.96	106.68
47	y1	607	CHL	C1B-CHB-C4A	9.38	127.36	121.32
31	c	505	CLA	C4A-NA-C1A	9.38	110.96	106.68
31	c1	504	CLA	C4A-NA-C1A	9.37	110.95	106.68
31	c1	503	CLA	C4A-NA-C1A	9.36	110.95	106.68
31	N1	614	CLA	C4A-NA-C1A	9.35	110.95	106.68
31	R1	602	CLA	C4A-NA-C1A	9.35	110.94	106.68
31	B1	615	CLA	C4A-NA-C1A	9.34	110.94	106.68
31	n	613	CLA	C4A-NA-C1A	9.34	110.94	106.68
31	c	504	CLA	C4A-NA-C1A	9.31	110.93	106.68
31	y1	603	CLA	C4A-NA-C1A	9.30	110.92	106.68
31	b1	617	CLA	C4A-NA-C1A	9.30	110.92	106.68
31	C	511	CLA	C4A-NA-C1A	9.29	110.92	106.68
31	N1	610	CLA	C4A-NA-C1A	9.29	110.92	106.68
31	S	602	CLA	C4A-NA-C1A	9.28	110.91	106.68
31	Y1	603	CLA	C4A-NA-C1A	9.28	110.91	106.68
31	B	610	CLA	C4A-NA-C1A	9.28	110.91	106.68
31	c	507	CLA	C4A-NA-C1A	9.27	110.91	106.68
31	N1	602	CLA	C4A-NA-C1A	9.27	110.91	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	g	613	CLA	C4A-NA-C1A	9.26	110.91	106.68
31	C1	505	CLA	C4A-NA-C1A	9.26	110.91	106.68
31	S1	604	CLA	C4A-NA-C1A	9.26	110.91	106.68
31	b1	603	CLA	C4A-NA-C1A	9.26	110.91	106.68
31	c1	509	CLA	C4A-NA-C1A	9.26	110.91	106.68
31	N	603	CLA	C4A-NA-C1A	9.26	110.90	106.68
31	G1	610	CLA	C4A-NA-C1A	9.25	110.90	106.68
31	S	605	CLA	C4A-NA-C1A	9.24	110.89	106.68
31	n	610	CLA	C4A-NA-C1A	9.24	110.89	106.68
31	b	608	CLA	C4A-NA-C1A	9.23	110.89	106.68
31	S1	613	CLA	C4A-NA-C1A	9.23	110.89	106.68
31	b	607	CLA	C4A-NA-C1A	9.23	110.89	106.68
31	b1	604	CLA	C4A-NA-C1A	9.23	110.89	106.68
31	C	504	CLA	C4A-NA-C1A	9.22	110.89	106.68
31	y	612	CLA	C4A-NA-C1A	9.22	110.89	106.68
31	b1	613	CLA	C4A-NA-C1A	9.22	110.89	106.68
31	C1	502	CLA	C4A-NA-C1A	9.21	110.88	106.68
31	y	613	CLA	C4A-NA-C1A	9.21	110.88	106.68
31	B1	613	CLA	C4A-NA-C1A	9.21	110.88	106.68
31	S1	609	CLA	C4A-NA-C1A	9.20	110.88	106.68
31	B1	603	CLA	C4A-NA-C1A	9.19	110.87	106.68
31	C1	508	CLA	C4A-NA-C1A	9.19	110.87	106.68
31	g	611	CLA	C4A-NA-C1A	9.19	110.87	106.68
31	Y1	613	CLA	C4A-NA-C1A	9.18	110.87	106.68
31	S1	611	CLA	C4A-NA-C1A	9.17	110.86	106.68
31	c1	508	CLA	C4A-NA-C1A	9.17	110.86	106.68
31	B1	606	CLA	C4A-NA-C1A	9.16	110.86	106.68
31	c1	512	CLA	C4A-NA-C1A	9.16	110.86	106.68
31	s1	612	CLA	C4A-NA-C1A	9.16	110.86	106.68
31	C	502	CLA	C4A-NA-C1A	9.15	110.86	106.68
33	C1	516	BCR	C11-C12-C13	9.15	151.44	126.36
31	A1	407	CLA	C4A-NA-C1A	9.14	110.85	106.68
31	s1	614	CLA	C4A-NA-C1A	9.14	110.85	106.68
31	B1	602	CLA	C4A-NA-C1A	9.14	110.85	106.68
31	S1	603	CLA	C4A-NA-C1A	9.14	110.85	106.68
31	b	610	CLA	C4A-NA-C1A	9.14	110.85	106.68
31	G1	613	CLA	C4A-NA-C1A	9.14	110.85	106.68
31	n1	610	CLA	C4A-NA-C1A	9.14	110.85	106.68
31	A1	406	CLA	C4A-NA-C1A	9.14	110.85	106.68
31	S	612	CLA	C4A-NA-C1A	9.12	110.84	106.68
31	C1	512	CLA	C4A-NA-C1A	9.12	110.84	106.68
31	G1	612	CLA	C4A-NA-C1A	9.12	110.84	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	N	613	CLA	C4A-NA-C1A	9.11	110.84	106.68
31	r	613	CLA	C4A-NA-C1A	9.10	110.83	106.68
31	s1	613	CLA	C4A-NA-C1A	9.10	110.83	106.68
31	r1	602	CLA	C4A-NA-C1A	9.10	110.83	106.68
31	c	503	CLA	C4A-NA-C1A	9.09	110.83	106.68
31	B1	608	CLA	C4A-NA-C1A	9.08	110.82	106.68
31	R1	604	CLA	C4A-NA-C1A	9.08	110.82	106.68
31	R1	608	CLA	C4A-NA-C1A	9.08	110.82	106.68
31	b1	607	CLA	C4A-NA-C1A	9.08	110.82	106.68
31	R	603	CLA	C4A-NA-C1A	9.08	110.82	106.68
31	G1	614	CLA	C4A-NA-C1A	9.07	110.82	106.68
31	S1	605	CLA	C4A-NA-C1A	9.07	110.82	106.68
31	Y1	612	CLA	C4A-NA-C1A	9.06	110.81	106.68
31	G	602	CLA	C4A-NA-C1A	9.06	110.81	106.68
31	B1	610	CLA	C4A-NA-C1A	9.06	110.81	106.68
31	B	614	CLA	C4A-NA-C1A	9.05	110.81	106.68
31	S	604	CLA	C4A-NA-C1A	9.05	110.81	106.68
31	s1	617	CLA	C4A-NA-C1A	9.05	110.81	106.68
31	D	402	CLA	C4A-NA-C1A	9.05	110.81	106.68
31	S1	617	CLA	C4A-NA-C1A	9.04	110.81	106.68
31	b1	602	CLA	C4A-NA-C1A	9.04	110.81	106.68
33	c	515	BCR	C20-C19-C18	9.04	151.15	126.36
31	A	405	CLA	C4A-NA-C1A	9.04	110.80	106.68
31	G	613	CLA	C4A-NA-C1A	9.03	110.80	106.68
31	B1	614	CLA	C4A-NA-C1A	9.03	110.80	106.68
31	s1	609	CLA	C4A-NA-C1A	9.03	110.80	106.68
31	b1	606	CLA	C4A-NA-C1A	9.02	110.80	106.68
31	s	612	CLA	C4A-NA-C1A	9.02	110.79	106.68
33	c1	515	BCR	C20-C19-C18	9.02	151.09	126.36
31	b	613	CLA	C4A-NA-C1A	9.01	110.79	106.68
31	N1	604	CLA	C4A-NA-C1A	9.01	110.79	106.68
31	g1	602	CLA	C4A-NA-C1A	9.00	110.78	106.68
31	n1	611	CLA	C4A-NA-C1A	8.99	110.78	106.68
31	N	611	CLA	C4A-NA-C1A	8.98	110.78	106.68
31	R	608	CLA	C4A-NA-C1A	8.98	110.78	106.68
31	r	604	CLA	C4A-NA-C1A	8.98	110.78	106.68
31	R	613	CLA	C4A-NA-C1A	8.98	110.78	106.68
31	Y	603	CLA	C4A-NA-C1A	8.98	110.77	106.68
31	y1	608	CLA	C4A-NA-C1A	8.98	110.77	106.68
31	n1	603	CLA	C4A-NA-C1A	8.97	110.77	106.68
31	C	501	CLA	C4A-NA-C1A	8.96	110.77	106.68
31	S1	610	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	A	410	CLA	C4A-NA-C1A	8.96	110.77	106.68
31	B	602	CLA	C4A-NA-C1A	8.96	110.77	106.68
31	r	609	CLA	C4A-NA-C1A	8.96	110.77	106.68
31	G	612	CLA	C4A-NA-C1A	8.95	110.76	106.68
31	a	410	CLA	C4A-NA-C1A	8.95	110.76	106.68
31	S1	602	CLA	C4A-NA-C1A	8.95	110.76	106.68
31	b	604	CLA	C4A-NA-C1A	8.95	110.76	106.68
31	Y	604	CLA	C4A-NA-C1A	8.95	110.76	106.68
31	N1	612	CLA	C4A-NA-C1A	8.95	110.76	106.68
31	B	603	CLA	C4A-NA-C1A	8.94	110.76	106.68
31	g	612	CLA	C4A-NA-C1A	8.93	110.75	106.68
31	C	510	CLA	C4A-NA-C1A	8.93	110.75	106.68
31	Y1	604	CLA	C4A-NA-C1A	8.92	110.75	106.68
31	r	603	CLA	C4A-NA-C1A	8.92	110.75	106.68
31	s	604	CLA	C4A-NA-C1A	8.92	110.75	106.68
31	g	610	CLA	C4A-NA-C1A	8.90	110.74	106.68
31	N	614	CLA	C4A-NA-C1A	8.90	110.74	106.68
31	y	604	CLA	C4A-NA-C1A	8.89	110.74	106.68
31	b1	608	CLA	C4A-NA-C1A	8.89	110.73	106.68
31	c	506	CLA	C4A-NA-C1A	8.89	110.73	106.68
31	n1	602	CLA	C4A-NA-C1A	8.89	110.73	106.68
31	b	602	CLA	C4A-NA-C1A	8.88	110.73	106.68
31	s	614	CLA	C4A-NA-C1A	8.88	110.73	106.68
31	R	611	CLA	C4A-NA-C1A	8.87	110.73	106.68
31	B1	611	CLA	C4A-NA-C1A	8.86	110.72	106.68
31	R1	612	CLA	C4A-NA-C1A	8.86	110.72	106.68
31	g	604	CLA	C4A-NA-C1A	8.86	110.72	106.68
33	b1	618	BCR	C20-C19-C18	8.85	150.63	126.36
31	D	403	CLA	C4A-NA-C1A	8.84	110.71	106.68
31	r	610	CLA	C4A-NA-C1A	8.84	110.71	106.68
31	r1	609	CLA	C4A-NA-C1A	8.84	110.71	106.68
31	C1	506	CLA	C4A-NA-C1A	8.84	110.71	106.68
31	N1	613	CLA	C4A-NA-C1A	8.84	110.71	106.68
31	s1	605	CLA	C4A-NA-C1A	8.84	110.71	106.68
31	s	605	CLA	C4A-NA-C1A	8.84	110.71	106.68
31	B1	617	CLA	C4A-NA-C1A	8.84	110.71	106.68
31	s1	604	CLA	C4A-NA-C1A	8.84	110.71	106.68
31	g	602	CLA	C4A-NA-C1A	8.83	110.71	106.68
31	c	509	CLA	C4A-NA-C1A	8.83	110.71	106.68
31	Y	614	CLA	C4A-NA-C1A	8.83	110.71	106.68
31	C	509	CLA	C4A-NA-C1A	8.81	110.70	106.68
31	g1	611	CLA	C4A-NA-C1A	8.81	110.70	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c1	501	CLA	C4A-NA-C1A	8.81	110.70	106.68
31	a1	407	CLA	C4A-NA-C1A	8.80	110.70	106.68
31	g1	614	CLA	C4A-NA-C1A	8.80	110.69	106.68
31	r	602	CLA	C4A-NA-C1A	8.80	110.69	106.68
31	C1	503	CLA	C4A-NA-C1A	8.80	110.69	106.68
31	s1	610	CLA	C4A-NA-C1A	8.79	110.69	106.68
31	b	603	CLA	C4A-NA-C1A	8.79	110.69	106.68
31	B	612	CLA	C4A-NA-C1A	8.78	110.69	106.68
31	b	612	CLA	C4A-NA-C1A	8.78	110.69	106.68
31	G	604	CLA	C4A-NA-C1A	8.78	110.69	106.68
31	n	611	CLA	C4A-NA-C1A	8.78	110.69	106.68
31	y1	610	CLA	C4A-NA-C1A	8.78	110.68	106.68
31	S	617	CLA	C4A-NA-C1A	8.78	110.68	106.68
31	B	608	CLA	C4A-NA-C1A	8.77	110.68	106.68
31	N	612	CLA	C4A-NA-C1A	8.76	110.68	106.68
31	c	501	CLA	C4A-NA-C1A	8.76	110.68	106.68
31	B	609	CLA	C4A-NA-C1A	8.75	110.67	106.68
31	g	614	CLA	C4A-NA-C1A	8.75	110.67	106.68
31	n1	614	CLA	C4A-NA-C1A	8.75	110.67	106.68
33	B	618	BCR	C20-C19-C18	8.75	150.35	126.36
31	B1	609	CLA	C4A-NA-C1A	8.75	110.67	106.68
31	G	614	CLA	C4A-NA-C1A	8.74	110.67	106.68
31	r1	608	CLA	C4A-NA-C1A	8.73	110.66	106.68
31	g1	610	CLA	C4A-NA-C1A	8.72	110.66	106.68
31	R1	610	CLA	C4A-NA-C1A	8.72	110.66	106.68
33	C	515	BCR	C20-C19-C18	8.72	150.26	126.36
31	C1	501	CLA	C4A-NA-C1A	8.71	110.65	106.68
31	c1	513	CLA	C4A-NA-C1A	8.70	110.65	106.68
31	R	604	CLA	C4A-NA-C1A	8.69	110.64	106.68
31	n	614	CLA	C4A-NA-C1A	8.69	110.64	106.68
31	D1	402	CLA	C4A-NA-C1A	8.69	110.64	106.68
31	N	604	CLA	C4A-NA-C1A	8.69	110.64	106.68
31	C1	507	CLA	C4A-NA-C1A	8.68	110.64	106.68
31	c	512	CLA	C4A-NA-C1A	8.68	110.64	106.68
31	R	610	CLA	C4A-NA-C1A	8.68	110.64	106.68
31	B	616	CLA	C4A-NA-C1A	8.67	110.64	106.68
31	N	602	CLA	C4A-NA-C1A	8.67	110.64	106.68
31	G	611	CLA	C4A-NA-C1A	8.67	110.64	106.68
31	g1	612	CLA	C4A-NA-C1A	8.67	110.64	106.68
31	S	611	CLA	C4A-NA-C1A	8.67	110.63	106.68
31	C1	510	CLA	C4A-NA-C1A	8.67	110.63	106.68
31	Y	612	CLA	C4A-NA-C1A	8.67	110.63	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s	617	CLA	C4A-NA-C1A	8.66	110.63	106.68
31	b1	614	CLA	C4A-NA-C1A	8.66	110.63	106.68
31	r	611	CLA	C4A-NA-C1A	8.65	110.63	106.68
31	R1	609	CLA	C4A-NA-C1A	8.65	110.63	106.68
31	y1	602	CLA	C4A-NA-C1A	8.65	110.63	106.68
31	y	614	CLA	C4A-NA-C1A	8.64	110.62	106.68
31	g1	603	CLA	C4A-NA-C1A	8.64	110.62	106.68
31	y1	611	CLA	C4A-NA-C1A	8.64	110.62	106.68
31	G1	603	CLA	C4A-NA-C1A	8.63	110.62	106.68
31	y	610	CLA	C4A-NA-C1A	8.62	110.61	106.68
31	C	503	CLA	C4A-NA-C1A	8.61	110.61	106.68
31	S	614	CLA	C4A-NA-C1A	8.61	110.61	106.68
47	s1	601	CHL	C1B-CHB-C4A	8.61	126.86	121.32
31	c1	510	CLA	C4A-NA-C1A	8.60	110.60	106.68
31	n1	604	CLA	C4A-NA-C1A	8.60	110.60	106.68
33	b	618	BCR	C20-C19-C18	8.60	149.93	126.36
31	d1	403	CLA	C4A-NA-C1A	8.59	110.60	106.68
31	y1	612	CLA	C4A-NA-C1A	8.59	110.60	106.68
31	a1	410	CLA	C4A-NA-C1A	8.59	110.60	106.68
31	c1	506	CLA	C4A-NA-C1A	8.58	110.59	106.68
31	C	508	CLA	C4A-NA-C1A	8.58	110.59	106.68
31	S	610	CLA	C4A-NA-C1A	8.58	110.59	106.68
31	r	608	CLA	C4A-NA-C1A	8.57	110.59	106.68
31	b	614	CLA	C4A-NA-C1A	8.57	110.59	106.68
46	H1	101	RRX	C38-C26-C25	-8.57	115.14	124.48
31	b	616	CLA	C4A-NA-C1A	8.57	110.59	106.68
31	y	611	CLA	C4A-NA-C1A	8.57	110.59	106.68
31	Y	608	CLA	C4A-NA-C1A	8.56	110.58	106.68
31	c	513	CLA	C4A-NA-C1A	8.56	110.58	106.68
31	G1	611	CLA	C4A-NA-C1A	8.55	110.58	106.68
31	g1	604	CLA	C4A-NA-C1A	8.55	110.58	106.68
31	B	617	CLA	C4A-NA-C1A	8.54	110.58	106.68
31	c	510	CLA	C4A-NA-C1A	8.54	110.58	106.68
31	y1	604	CLA	C4A-NA-C1A	8.54	110.58	106.68
31	s	603	CLA	C4A-NA-C1A	8.54	110.57	106.68
31	c	511	CLA	C4A-NA-C1A	8.52	110.57	106.68
31	Y1	608	CLA	C4A-NA-C1A	8.52	110.57	106.68
31	A	407	CLA	C4A-NA-C1A	8.51	110.56	106.68
31	B1	607	CLA	C4A-NA-C1A	8.48	110.55	106.68
31	s	611	CLA	C4A-NA-C1A	8.47	110.55	106.68
33	C1	514	BCR	C20-C19-C18	8.47	149.59	126.36
31	Y1	611	CLA	C4A-NA-C1A	8.46	110.54	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	506	CLA	C4A-NA-C1A	8.46	110.54	106.68
31	C	507	CLA	C4A-NA-C1A	8.46	110.54	106.68
31	C	512	CLA	C4A-NA-C1A	8.44	110.53	106.68
47	n1	601	CHL	C1B-CHB-C4A	8.44	126.75	121.32
31	r1	610	CLA	C4A-NA-C1A	8.42	110.52	106.68
31	y	608	CLA	C4A-NA-C1A	8.42	110.52	106.68
31	R	612	CLA	C4A-NA-C1A	8.41	110.52	106.68
31	B	606	CLA	C4A-NA-C1A	8.41	110.52	106.68
31	S	603	CLA	C4A-NA-C1A	8.41	110.51	106.68
31	R	602	CLA	C4A-NA-C1A	8.39	110.51	106.68
31	Y	611	CLA	C4A-NA-C1A	8.37	110.50	106.68
31	b	611	CLA	C4A-NA-C1A	8.37	110.50	106.68
31	b1	611	CLA	C4A-NA-C1A	8.36	110.50	106.68
31	B	611	CLA	C4A-NA-C1A	8.36	110.49	106.68
47	G1	606	CHL	C1B-CHB-C4A	8.35	126.69	121.32
31	S	609	CLA	C4A-NA-C1A	8.35	110.49	106.68
31	R1	603	CLA	C4A-NA-C1A	8.34	110.48	106.68
31	b1	615	CLA	C4A-NA-C1A	8.34	110.48	106.68
33	B1	618	BCR	C20-C19-C18	8.34	149.22	126.36
31	d	403	CLA	C4A-NA-C1A	8.31	110.47	106.68
31	s	610	CLA	C4A-NA-C1A	8.30	110.47	106.68
31	B1	616	CLA	C4A-NA-C1A	8.29	110.46	106.68
31	n1	612	CLA	C4A-NA-C1A	8.29	110.46	106.68
31	d1	402	CLA	C4A-NA-C1A	8.29	110.46	106.68
31	b1	616	CLA	C4A-NA-C1A	8.27	110.45	106.68
31	B1	604	CLA	C4A-NA-C1A	8.24	110.44	106.68
31	R	609	CLA	C4A-NA-C1A	8.24	110.44	106.68
31	c1	505	CLA	C4A-NA-C1A	8.24	110.44	106.68
31	s1	611	CLA	C4A-NA-C1A	8.23	110.43	106.68
31	n	602	CLA	C4A-NA-C1A	8.23	110.43	106.68
31	D1	403	CLA	C4A-NA-C1A	8.23	110.43	106.68
47	r	607	CHL	C1B-CHB-C4A	8.22	126.61	121.32
33	B1	619	BCR	C20-C19-C18	8.21	148.88	126.36
31	c1	507	CLA	C4A-NA-C1A	8.20	110.42	106.68
33	c	516	BCR	C20-C19-C18	8.19	148.81	126.36
31	s	609	CLA	C4A-NA-C1A	8.19	110.41	106.68
31	S1	614	CLA	C4A-NA-C1A	8.17	110.41	106.68
31	r1	612	CLA	C4A-NA-C1A	8.17	110.41	106.68
31	a	407	CLA	C4A-NA-C1A	8.16	110.40	106.68
33	A	411	BCR	C20-C19-C18	8.16	148.74	126.36
31	y1	614	CLA	C4A-NA-C1A	8.16	110.40	106.68
31	Y	602	CLA	C4A-NA-C1A	8.15	110.40	106.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	r1	603	CLA	C4A-NA-C1A	8.15	110.40	106.68
31	N	610	CLA	C4A-NA-C1A	8.15	110.39	106.68
31	N1	611	CLA	C4A-NA-C1A	8.14	110.39	106.68
33	c	514	BCR	C20-C19-C18	8.14	148.67	126.36
31	B1	612	CLA	C4A-NA-C1A	8.13	110.39	106.68
47	n1	606	CHL	C1B-CHB-C4A	8.12	126.55	121.32
33	c1	514	BCR	C20-C19-C18	8.12	148.62	126.36
32	a1	409	PHO	C4D-CHA-CBD	-8.11	104.56	108.45
47	R1	606	CHL	C1B-CHB-C4A	8.08	126.52	121.32
47	y	607	CHL	C1B-CHB-C4A	8.08	126.52	121.32
47	N	607	CHL	C1B-CHB-C4A	8.05	126.50	121.32
47	N1	609	CHL	C1B-CHB-C4A	8.05	126.50	121.32
47	R	607	CHL	C1B-CHB-C4A	8.04	126.50	121.32
31	s1	602	CLA	C4A-NA-C1A	8.04	110.35	106.68
31	G1	604	CLA	C4A-NA-C1A	8.02	110.34	106.68
47	s1	607	CHL	C1B-CHB-C4A	8.02	126.48	121.32
31	r	612	CLA	C4A-NA-C1A	8.01	110.33	106.68
33	b1	619	BCR	C20-C19-C18	8.00	148.29	126.36
47	y1	605	CHL	C1B-CHB-C4A	7.98	126.46	121.32
31	B	607	CLA	C4A-NA-C1A	7.93	110.30	106.68
32	a	409	PHO	C4D-CHA-CBD	-7.92	104.66	108.45
47	n1	607	CHL	C1B-CHB-C4A	7.91	126.41	121.32
31	b	609	CLA	C4A-NA-C1A	7.86	110.26	106.68
31	A1	405	CLA	C4A-NA-C1A	7.85	110.26	106.68
47	n	607	CHL	C1B-CHB-C4A	7.84	126.37	121.32
31	B	604	CLA	C4A-NA-C1A	7.82	110.25	106.68
33	d1	404	BCR	C20-C19-C18	7.82	147.79	126.36
33	C1	516	BCR	C20-C19-C18	7.81	147.77	126.36
33	a1	411	BCR	C20-C19-C18	7.80	147.75	126.36
50	N	623	NEX	C8-C7-C6	-7.78	168.49	177.66
47	Y1	607	CHL	C1B-CHB-C4A	7.74	126.30	121.32
47	r1	606	CHL	C1B-CHB-C4A	7.73	126.30	121.32
47	n	608	CHL	C1B-CHB-C4A	7.73	126.29	121.32
42	C1	527	LMK	O2-C4-O3	-7.69	106.63	124.08
46	h1	101	RRX	C38-C26-C25	-7.69	116.10	124.48
33	b	619	BCR	C20-C19-C18	7.68	147.43	126.36
47	g	606	CHL	C1B-CHB-C4A	7.68	126.26	121.32
31	d	402	CLA	C4A-NA-C1A	7.67	110.18	106.68
31	Y1	614	CLA	C4A-NA-C1A	7.65	110.17	106.68
47	G	607	CHL	C1B-CHB-C4A	7.64	126.24	121.32
47	S1	601	CHL	C1B-CHB-C4A	7.62	126.22	121.32
33	C	514	BCR	C20-C19-C18	7.60	147.19	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	g1	607	CHL	C1B-CHB-C4A	7.58	126.20	121.32
47	N	606	CHL	C1B-CHB-C4A	7.56	126.19	121.32
47	Y1	606	CHL	C1B-CHB-C4A	7.56	126.19	121.32
47	G1	607	CHL	C1B-CHB-C4A	7.56	126.19	121.32
47	s	601	CHL	C1B-CHB-C4A	7.54	126.17	121.32
31	b1	609	CLA	C4A-NA-C1A	7.52	110.11	106.68
47	n1	608	CHL	C1B-CHB-C4A	7.50	126.15	121.32
47	n	601	CHL	C1B-CHB-C4A	7.47	126.12	121.32
50	g1	623	NEX	C8-C7-C6	-7.44	168.88	177.66
47	Y	606	CHL	C1B-CHB-C4A	7.43	126.10	121.32
47	r1	607	CHL	C1B-CHB-C4A	7.43	126.10	121.32
47	r	606	CHL	C1B-CHB-C4A	7.42	126.10	121.32
47	S	601	CHL	C1B-CHB-C4A	7.40	126.08	121.32
47	Y1	605	CHL	C1B-CHB-C4A	7.38	126.07	121.32
47	R	606	CHL	C1B-CHB-C4A	7.36	126.06	121.32
47	g1	606	CHL	C1B-CHB-C4A	7.35	126.05	121.32
33	a	411	BCR	C20-C19-C18	7.34	146.49	126.36
47	N	601	CHL	C1B-CHB-C4A	7.31	126.03	121.32
47	n	606	CHL	C1B-CHB-C4A	7.30	126.02	121.32
31	Y1	602	CLA	C4A-NA-C1A	7.28	110.00	106.68
47	y	606	CHL	C1B-CHB-C4A	7.27	126.00	121.32
47	G1	605	CHL	C1B-CHB-C4A	7.26	126.00	121.32
46	H1	101	RRX	C15-C14-C13	-7.25	117.11	127.28
48	r	620	LUT	C21-C26-C27	7.24	121.15	112.83
49	y1	622	XAT	C37-C21-C26	-7.21	90.57	110.05
47	N1	607	CHL	C1B-CHB-C4A	7.21	125.96	121.32
47	S	607	CHL	C1B-CHB-C4A	7.17	125.94	121.32
49	Y	622	XAT	C36-C21-C22	7.16	121.56	108.97
49	Y1	622	XAT	C36-C21-C22	7.16	121.55	108.97
32	A	409	PHO	C4D-CHA-CBD	-7.15	105.03	108.45
31	s	613	CLA	O2D-CGD-CBD	7.14	123.71	111.23
47	Y	601	CHL	C1B-CHB-C4A	7.12	125.90	121.32
49	Y	622	XAT	C37-C21-C26	-7.11	90.84	110.05
47	g	605	CHL	C1B-CHB-C4A	7.10	125.89	121.32
47	G	608	CHL	C1B-CHB-C4A	7.10	125.89	121.32
33	C1	517	BCR	C20-C19-C18	7.10	145.82	126.36
49	Y1	622	XAT	C37-C21-C26	-7.09	90.89	110.05
49	y	622	XAT	C37-C21-C26	-7.06	90.97	110.05
47	g1	601	CHL	C1B-CHB-C4A	7.04	125.85	121.32
33	C	517	BCR	C20-C19-C18	7.03	145.65	126.36
49	y	622	XAT	C36-C21-C22	7.03	121.32	108.97
33	c1	516	BCR	C20-C19-C18	7.02	145.60	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	c1	517	BCR	C20-C19-C18	7.01	145.59	126.36
47	Y	609	CHL	C1B-CHB-C4A	7.01	125.83	121.32
31	b1	609	CLA	O2D-CGD-CBD	7.00	123.47	111.23
47	g1	608	CHL	C1B-CHB-C4A	7.00	125.83	121.32
49	y1	622	XAT	C36-C21-C22	6.99	121.25	108.97
33	c	517	BCR	C20-C19-C18	6.97	145.47	126.36
47	g1	605	CHL	C1B-CHB-C4A	6.96	125.80	121.32
56	r1	626	ERG	C14-C13-C17	6.95	106.99	99.72
31	R1	602	CLA	O2D-CGD-CBD	6.95	123.38	111.23
47	g	608	CHL	C1B-CHB-C4A	6.92	125.77	121.32
32	a	408	PHO	C4D-CHA-CBD	-6.92	105.14	108.45
48	n	621	LUT	C21-C26-C27	6.90	120.76	112.83
47	Y	607	CHL	C1B-CHB-C4A	6.90	125.76	121.32
47	y	609	CHL	C1B-CHB-C4A	6.89	125.76	121.32
47	G	606	CHL	C1B-CHB-C4A	6.89	125.76	121.32
50	y1	623	NEX	C17-C1-C6	-6.89	104.31	110.47
38	B	625	DGA	CDB-CCB-CBB	-6.87	79.63	114.37
31	n	612	CLA	C4A-NA-C1A	6.86	109.81	106.68
50	Y1	623	NEX	C16-C1-C6	-6.83	104.36	110.47
47	N	608	CHL	C1B-CHB-C4A	6.83	125.71	121.32
38	C1	524	DGA	CDB-CCB-CBB	-6.81	79.96	114.37
56	r1	626	ERG	C12-C13-C14	6.80	117.45	107.19
48	R1	620	LUT	C21-C26-C27	6.79	120.64	112.83
42	c1	527	LMK	O2-C4-O3	-6.79	108.67	124.08
47	G	605	CHL	C1B-CHB-C4A	6.79	125.69	121.32
44	D1	405	PL9	C7-C3-C4	6.78	122.49	116.91
31	s1	603	CLA	O2D-CGD-CBD	6.73	123.00	111.23
31	S1	603	CLA	O2D-CGD-CBD	6.73	123.00	111.23
38	b1	625	DGA	CDB-CCB-CBB	-6.73	80.36	114.37
38	b	623	DGA	CDB-CCB-CBB	-6.71	80.43	114.37
47	S1	608	CHL	C1B-CHB-C4A	6.71	125.64	121.32
47	y1	609	CHL	C1B-CHB-C4A	6.71	125.64	121.32
47	S1	606	CHL	C1B-CHB-C4A	6.70	125.63	121.32
38	c	524	DGA	CDB-CCB-CBB	-6.69	80.54	114.37
38	C	524	DGA	CDB-CCB-CBB	-6.68	80.58	114.37
47	S	606	CHL	C1B-CHB-C4A	6.68	125.62	121.32
47	s1	606	CHL	C1B-CHB-C4A	6.68	125.62	121.32
50	R	622	NEX	C2-C1-C6	6.65	115.68	109.21
33	B	619	BCR	C20-C19-C18	6.60	144.46	126.36
31	b	609	CLA	O2D-CGD-CBD	6.60	122.76	111.23
47	N1	606	CHL	C1B-CHB-C4A	6.56	125.55	121.32
47	s	607	CHL	C1B-CHB-C4A	6.56	125.54	121.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	c1	524	DGA	CDB-CCB-CBB	-6.56	81.21	114.37
32	A1	409	PHO	C4D-CHA-CBD	-6.55	105.31	108.45
31	B1	609	CLA	O2D-CGD-CBD	6.54	122.67	111.23
38	B1	625	DGA	CDB-CCB-CBB	-6.52	81.41	114.37
48	g	621	LUT	C21-C26-C27	6.51	120.31	112.83
47	R1	607	CHL	C1B-CHB-C4A	6.50	125.51	121.32
49	r	622	XAT	C15-C14-C13	-6.50	118.16	127.28
48	s1	621	LUT	C21-C26-C27	6.48	120.28	112.83
31	B1	606	CLA	CMD-C2D-C1D	6.48	136.14	124.73
31	b	607	CLA	O2D-CGD-CBD	6.45	122.51	111.23
31	S	613	CLA	O2D-CGD-CBD	6.44	122.49	111.23
31	C	506	CLA	O2D-CGD-CBD	6.43	122.47	111.23
42	c	627	LMK	O2-C4-O3	-6.41	109.54	124.08
32	A1	408	PHO	C4D-CHA-CBD	-6.39	105.39	108.45
47	G1	601	CHL	C1B-CHB-C4A	6.38	125.43	121.32
31	b	607	CLA	CMD-C2D-C1D	6.38	135.96	124.73
31	N	611	CLA	O2D-CGD-CBD	6.37	122.37	111.23
48	s	620	LUT	C21-C26-C27	6.37	120.15	112.83
37	b	620	C7Z	C11-C10-C9	-6.37	118.35	127.28
31	Y	604	CLA	O2D-CGD-CBD	6.35	122.33	111.23
48	R	620	LUT	C21-C26-C27	6.33	120.10	112.83
31	r	608	CLA	CMD-C2D-C1D	6.33	135.88	124.73
31	C	501	CLA	CMD-C2D-C1D	6.33	135.87	124.73
49	N1	622	XAT	C31-C30-C29	-6.33	118.40	127.28
42	C	527	LMK	O2-C4-O3	-6.29	109.81	124.08
31	Y1	613	CLA	CMD-C2D-C1D	6.29	135.80	124.73
33	A1	411	BCR	C20-C19-C18	6.28	143.59	126.36
47	S	608	CHL	C1B-CHB-C4A	6.26	125.35	121.32
47	N	609	CHL	C1B-CHB-C4A	6.24	125.34	121.32
32	A	408	PHO	C4D-CHA-CBD	-6.24	105.46	108.45
31	y1	614	CLA	CMD-C2D-C1D	6.23	135.70	124.73
37	B	620	C7Z	C11-C10-C9	-6.22	118.55	127.28
31	y	602	CLA	O2D-CGD-CBD	6.21	122.09	111.23
31	R1	604	CLA	O2A-C1-C2	6.19	123.73	108.99
37	b1	620	C7Z	C15-C14-C13	-6.19	118.60	127.28
48	r1	620	LUT	C21-C26-C27	6.19	119.94	112.83
47	Y	605	CHL	C1B-CHB-C4A	6.16	125.29	121.32
31	s	605	CLA	O2D-CGD-CBD	6.12	121.94	111.23
31	Y1	608	CLA	CMD-C2D-C1D	6.12	135.51	124.73
47	n1	605	CHL	C1B-CHB-C4A	6.11	125.25	121.32
31	y	608	CLA	CMD-C2D-C1D	6.11	135.48	124.73
49	Y	622	XAT	C15-C14-C13	-6.09	118.74	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	s	606	CHL	C1B-CHB-C4A	6.09	125.24	121.32
47	g	607	CHL	C1B-CHB-C4A	6.08	125.24	121.32
31	C1	503	CLA	CMD-C2D-C1D	6.08	135.44	124.73
31	y1	608	CLA	CMD-C2D-C1D	6.07	135.42	124.73
47	g	601	CHL	C1B-CHB-C4A	6.07	125.23	121.32
47	G1	608	CHL	C1B-CHB-C4A	6.06	125.22	121.32
50	S	622	NEX	C8-C7-C6	-6.06	170.51	177.66
32	a1	408	PHO	C4D-CHA-CBD	-6.05	105.56	108.45
47	N	605	CHL	C1B-CHB-C4A	6.04	125.21	121.32
31	B	609	CLA	O2D-CGD-CBD	6.02	121.75	111.23
47	S1	607	CHL	C1B-CHB-C4A	6.00	125.18	121.32
48	N1	621	LUT	C21-C26-C27	6.00	119.72	112.83
47	y	601	CHL	C1B-CHB-C4A	6.00	125.18	121.32
31	c1	505	CLA	O2D-CGD-CBD	6.00	121.71	111.23
33	d	404	BCR	C20-C19-C18	5.99	142.80	126.36
31	S1	614	CLA	CMD-C2D-C1D	5.99	135.28	124.73
31	N	604	CLA	O2D-CGD-CBD	5.99	121.70	111.23
56	R1	626	ERG	C14-C13-C17	5.97	105.97	99.72
31	g1	614	CLA	O2A-C1-C2	5.97	123.20	108.99
31	s	611	CLA	O2D-CGD-CBD	5.96	121.65	111.23
31	A1	405	CLA	CMD-C2D-C1D	5.96	135.22	124.73
47	y	605	CHL	C1B-CHB-C4A	5.95	125.15	121.32
47	y1	606	CHL	C1B-CHB-C4A	5.95	125.15	121.32
31	S1	602	CLA	O2D-CGD-CBD	5.95	121.63	111.23
49	R	621	XAT	C15-C14-C13	-5.94	118.94	127.28
31	g	604	CLA	CMD-C2D-C1D	5.94	135.19	124.73
46	h1	101	RRX	C1-C6-C5	-5.94	114.52	122.64
31	y1	604	CLA	O2D-CGD-CBD	5.93	121.60	111.23
31	c	501	CLA	O2D-CGD-CBD	5.92	121.59	111.23
31	B1	608	CLA	CMD-C2D-C1D	5.92	135.15	124.73
31	R	612	CLA	CMD-C2D-C1D	5.91	135.14	124.73
31	b	605	CLA	O2D-CGD-CBD	5.91	121.56	111.23
48	S1	620	LUT	C21-C26-C27	5.91	119.62	112.83
31	r	613	CLA	O2D-CGD-CBD	5.91	121.56	111.23
31	b	613	CLA	O2D-CGD-CBD	5.91	121.56	111.23
31	N1	604	CLA	CMD-C2D-C1D	5.90	135.12	124.73
31	N1	610	CLA	CMD-C2D-C1D	5.89	135.10	124.73
31	C	501	CLA	O2D-CGD-CBD	5.88	121.52	111.23
31	c	510	CLA	CMD-C2D-C1D	5.88	135.07	124.73
31	g1	610	CLA	CMD-C2D-C1D	5.87	135.07	124.73
31	C	511	CLA	CMD-C2D-C1D	5.87	135.06	124.73
31	B	606	CLA	CMD-C2D-C1D	5.86	135.05	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	Y	602	CLA	O2D-CGD-CBD	5.86	121.47	111.23
31	R	613	CLA	O2D-CGD-CBD	5.86	121.47	111.23
31	R	604	CLA	O2A-C1-C2	5.86	122.93	108.99
31	N	610	CLA	O2D-CGD-CBD	5.85	121.46	111.23
48	G	620	LUT	C21-C26-C27	5.85	119.55	112.83
31	Y1	602	CLA	CMD-C2D-C1D	5.85	135.02	124.73
31	G	610	CLA	CMD-C2D-C1D	5.84	135.01	124.73
31	b1	603	CLA	O2D-CGD-CBD	5.84	121.44	111.23
31	s	604	CLA	CMD-C2D-C1D	5.84	135.01	124.73
56	R1	626	ERG	C12-C13-C14	5.84	116.00	107.19
31	c	503	CLA	CMD-C2D-C1D	5.83	135.00	124.73
31	r1	604	CLA	O2A-C1-C2	5.83	122.86	108.99
31	a	406	CLA	CMD-C2D-C1D	5.83	134.99	124.73
37	B1	620	C7Z	C38-C25-C26	-5.82	118.13	124.48
50	r1	622	NEX	C2-C1-C6	5.82	114.87	109.21
31	s	610	CLA	CMD-C2D-C1D	5.82	134.98	124.73
31	y	603	CLA	O2D-CGD-CBD	5.81	121.39	111.23
31	G1	611	CLA	CMD-C2D-C1D	5.81	134.96	124.73
31	A1	407	CLA	CMD-C2D-C1D	5.81	134.95	124.73
33	D	404	BCR	C20-C19-C18	5.80	142.28	126.36
31	R1	608	CLA	CMD-C2D-C1D	5.80	134.95	124.73
31	C	502	CLA	O2D-CGD-CBD	5.80	121.36	111.23
31	C1	509	CLA	CMD-C2D-C1D	5.79	134.93	124.73
48	G	621	LUT	C21-C26-C27	5.79	119.48	112.83
31	y	613	CLA	CMD-C2D-C1D	5.78	134.91	124.73
31	C	503	CLA	CMD-C2D-C1D	5.77	134.90	124.73
31	C	513	CLA	O2D-CGD-CBD	5.77	121.32	111.23
31	b	602	CLA	CMD-C2D-C1D	5.77	134.89	124.73
31	N1	603	CLA	CMD-C2D-C1D	5.77	134.89	124.73
31	c	509	CLA	CMD-C2D-C1D	5.77	134.88	124.73
48	R1	620	LUT	C35-C34-C33	-5.77	119.19	127.28
31	S1	609	CLA	CMD-C2D-C1D	5.76	134.87	124.73
31	B1	616	CLA	CMD-C2D-C1D	5.76	134.87	124.73
31	B	605	CLA	CMD-C2D-C1D	5.76	134.87	124.73
31	C1	501	CLA	CMD-C2D-C1D	5.76	134.87	124.73
31	N1	614	CLA	O2A-C1-C2	5.75	122.68	108.99
31	a1	407	CLA	O2D-CGD-CBD	5.75	121.27	111.23
31	b1	613	CLA	CMD-C2D-C1D	5.74	134.84	124.73
31	y1	613	CLA	CMD-C2D-C1D	5.74	134.84	124.73
31	C1	504	CLA	CMD-C2D-C1D	5.73	134.82	124.73
47	G	601	CHL	C1B-CHB-C4A	5.73	125.01	121.32
31	R	603	CLA	O2D-CGD-CBD	5.73	121.24	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a1	405	CLA	CMD-C2D-C1D	5.73	134.81	124.73
31	Y	603	CLA	O2D-CGD-CBD	5.73	121.24	111.23
31	C1	512	CLA	CMD-C2D-C1D	5.72	134.81	124.73
31	G	602	CLA	CMD-C2D-C1D	5.72	134.81	124.73
31	n1	603	CLA	O2D-CGD-CBD	5.72	121.23	111.23
31	y1	610	CLA	CMD-C2D-C1D	5.72	134.80	124.73
49	g	622	XAT	C15-C14-C13	-5.72	119.26	127.28
31	s1	612	CLA	O2D-CGD-CBD	5.72	121.22	111.23
31	d	403	CLA	O2D-CGD-CBD	5.72	121.22	111.23
46	h	101	RRX	C15-C14-C13	-5.71	119.26	127.28
48	R	620	LUT	C31-C30-C29	-5.71	119.27	127.28
49	N1	622	XAT	C15-C14-C13	-5.71	119.27	127.28
31	r1	608	CLA	CMD-C2D-C1D	5.71	134.78	124.73
31	A1	406	CLA	CMD-C2D-C1D	5.70	134.77	124.73
31	B	609	CLA	CMD-C2D-C1D	5.70	134.76	124.73
47	g	609	CHL	C1B-CHB-C4A	5.70	124.99	121.32
31	C1	505	CLA	CMD-C2D-C1D	5.70	134.76	124.73
31	S	605	CLA	O2D-CGD-CBD	5.69	121.18	111.23
31	c	513	CLA	O2D-CGD-CBD	5.69	121.18	111.23
31	g	612	CLA	O2D-CGD-CBD	5.69	121.17	111.23
31	c	507	CLA	CMD-C2D-C1D	5.68	134.73	124.73
31	r	603	CLA	CMD-C2D-C1D	5.68	134.72	124.73
31	B1	607	CLA	CMD-C2D-C1D	5.67	134.72	124.73
47	N1	605	CHL	C1B-CHB-C4A	5.67	124.97	121.32
31	c1	511	CLA	CMD-C2D-C1D	5.67	134.71	124.73
43	D1	401	BCT	O2-C-O1	5.67	134.18	119.68
31	c1	503	CLA	CMD-C2D-C1D	5.67	134.71	124.73
31	G	604	CLA	O2D-CGD-CBD	5.67	121.14	111.23
31	G	613	CLA	CMD-C2D-C1D	5.67	134.71	124.73
31	n1	614	CLA	CMD-C2D-C1D	5.67	134.71	124.73
46	H	101	RRX	C11-C10-C9	-5.67	119.33	127.28
31	B	613	CLA	CMD-C2D-C1D	5.66	134.70	124.73
31	n	602	CLA	O2D-CGD-CBD	5.66	121.13	111.23
31	s	612	CLA	CMD-C2D-C1D	5.66	134.70	124.73
31	s	614	CLA	CMD-C2D-C1D	5.66	134.70	124.73
31	B	615	CLA	CMD-C2D-C1D	5.66	134.69	124.73
31	G	611	CLA	O2D-CGD-CBD	5.66	121.12	111.23
49	n	622	XAT	C15-C14-C13	-5.66	119.34	127.28
49	n	622	XAT	C31-C30-C29	-5.65	119.35	127.28
31	n	602	CLA	CMD-C2D-C1D	5.65	134.68	124.73
31	n1	602	CLA	CMD-C2D-C1D	5.65	134.68	124.73
31	C	504	CLA	O2D-CGD-CBD	5.65	121.10	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	G	614	CLA	CMD-C2D-C1D	5.65	134.67	124.73
31	s1	612	CLA	CMD-C2D-C1D	5.65	134.67	124.73
31	C	506	CLA	CMD-C2D-C1D	5.65	134.67	124.73
31	B1	614	CLA	CMD-C2D-C1D	5.64	134.67	124.73
31	R	608	CLA	CMD-C2D-C1D	5.64	134.66	124.73
31	S1	604	CLA	O2D-CGD-CBD	5.64	121.09	111.23
31	G	602	CLA	O2D-CGD-CBD	5.64	121.08	111.23
31	G1	603	CLA	CMD-C2D-C1D	5.64	134.66	124.73
31	n	603	CLA	CMD-C2D-C1D	5.64	134.65	124.73
31	c1	510	CLA	CMD-C2D-C1D	5.64	134.65	124.73
31	N	604	CLA	CMD-C2D-C1D	5.63	134.65	124.73
48	y1	621	LUT	C21-C26-C27	5.63	119.30	112.83
31	B1	613	CLA	O2D-CGD-CBD	5.63	121.08	111.23
31	A	410	CLA	CMD-C2D-C1D	5.63	134.65	124.73
31	B	616	CLA	O2D-CGD-CBD	5.63	121.08	111.23
31	r	611	CLA	CMD-C2D-C1D	5.63	134.63	124.73
31	Y	608	CLA	CMD-C2D-C1D	5.62	134.63	124.73
31	s	617	CLA	CMD-C2D-C1D	5.62	134.63	124.73
31	y1	612	CLA	O2D-CGD-CBD	5.62	121.06	111.23
31	B	607	CLA	CMD-C2D-C1D	5.62	134.63	124.73
31	b1	604	CLA	CMD-C2D-C1D	5.62	134.63	124.73
31	g1	611	CLA	CMD-C2D-C1D	5.62	134.63	124.73
31	c	506	CLA	O2D-CGD-CBD	5.62	121.06	111.23
31	b	615	CLA	CMD-C2D-C1D	5.62	134.62	124.73
31	G1	610	CLA	CMD-C2D-C1D	5.62	134.62	124.73
31	c1	506	CLA	O2D-CGD-CBD	5.62	121.05	111.23
31	n	612	CLA	CMD-C2D-C1D	5.61	134.62	124.73
31	S	611	CLA	O2D-CGD-CBD	5.61	121.04	111.23
31	y	612	CLA	O2D-CGD-CBD	5.61	121.04	111.23
31	G	604	CLA	CMD-C2D-C1D	5.61	134.61	124.73
31	b	608	CLA	CMD-C2D-C1D	5.61	134.61	124.73
31	g	611	CLA	O2D-CGD-CBD	5.61	121.04	111.23
31	B	614	CLA	CMD-C2D-C1D	5.61	134.60	124.73
31	g	610	CLA	CMD-C2D-C1D	5.61	134.60	124.73
31	y1	603	CLA	O2D-CGD-CBD	5.61	121.03	111.23
31	Y1	614	CLA	O2D-CGD-CBD	5.60	121.03	111.23
47	n	605	CHL	C1B-CHB-C4A	5.60	124.92	121.32
31	c	501	CLA	CMD-C2D-C1D	5.60	134.59	124.73
43	D	401	BCT	O2-C-O1	5.60	134.00	119.68
31	N	613	CLA	CMD-C2D-C1D	5.60	134.58	124.73
31	R1	604	CLA	CMD-C2D-C1D	5.60	134.58	124.73
31	r1	612	CLA	CMD-C2D-C1D	5.60	134.58	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
37	B1	620	C7Z	C15-C14-C13	-5.59	119.43	127.28
31	C1	507	CLA	CMD-C2D-C1D	5.59	134.58	124.73
31	A	406	CLA	CMD-C2D-C1D	5.59	134.58	124.73
31	R1	612	CLA	CMD-C2D-C1D	5.58	134.56	124.73
48	n1	621	LUT	C21-C26-C27	5.58	119.24	112.83
31	N1	604	CLA	O2D-CGD-CBD	5.58	120.99	111.23
31	c1	511	CLA	O2D-CGD-CBD	5.58	120.99	111.23
31	R	611	CLA	CMD-C2D-C1D	5.58	134.56	124.73
48	y1	621	LUT	C35-C34-C33	-5.58	119.45	127.28
31	Y	614	CLA	CMD-C2D-C1D	5.58	134.55	124.73
31	y	611	CLA	O2D-CGD-CBD	5.58	120.98	111.23
31	G	610	CLA	O2D-CGD-CBD	5.58	120.98	111.23
31	c	506	CLA	CMD-C2D-C1D	5.58	134.55	124.73
31	a1	407	CLA	CMD-C2D-C1D	5.57	134.54	124.73
31	r1	604	CLA	CMD-C2D-C1D	5.57	134.54	124.73
31	B	608	CLA	CMD-C2D-C1D	5.57	134.54	124.73
31	b1	605	CLA	CMD-C2D-C1D	5.57	134.53	124.73
31	B	603	CLA	CMD-C2D-C1D	5.56	134.53	124.73
48	S1	620	LUT	C35-C34-C33	-5.56	119.48	127.28
31	C	509	CLA	CMD-C2D-C1D	5.56	134.52	124.73
48	n1	621	LUT	C7-C8-C9	-5.56	118.01	126.23
31	S	605	CLA	CMD-C2D-C1D	5.56	134.52	124.73
31	c1	509	CLA	CMD-C2D-C1D	5.56	134.52	124.73
31	c	507	CLA	O2D-CGD-CBD	5.56	120.95	111.23
31	R	610	CLA	CMD-C2D-C1D	5.56	134.52	124.73
31	a1	406	CLA	CMD-C2D-C1D	5.56	134.51	124.73
31	S1	603	CLA	CMD-C2D-C1D	5.55	134.51	124.73
31	s1	602	CLA	CMD-C2D-C1D	5.55	134.51	124.73
31	d1	403	CLA	CMD-C2D-C1D	5.55	134.51	124.73
48	S	620	LUT	C21-C26-C27	5.55	119.20	112.83
31	b1	608	CLA	CMD-C2D-C1D	5.55	134.50	124.73
33	D1	404	BCR	C20-C19-C18	5.55	141.58	126.36
31	g	612	CLA	CMD-C2D-C1D	5.55	134.50	124.73
31	g1	604	CLA	O2D-CGD-CBD	5.55	120.92	111.23
31	R	609	CLA	CMD-C2D-C1D	5.55	134.49	124.73
31	G1	614	CLA	O2A-C1-C2	5.54	122.19	108.99
31	s1	609	CLA	O2D-CGD-CBD	5.54	120.92	111.23
31	y	610	CLA	CMD-C2D-C1D	5.54	134.49	124.73
31	r	604	CLA	O2A-C1-C2	5.54	122.19	108.99
31	R	602	CLA	O2D-CGD-CBD	5.54	120.92	111.23
31	g1	612	CLA	CMD-C2D-C1D	5.54	134.49	124.73
31	b1	614	CLA	CMD-C2D-C1D	5.54	134.49	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	r	604	CLA	CMD-C2D-C1D	5.54	134.48	124.73
31	Y	610	CLA	CMD-C2D-C1D	5.54	134.48	124.73
31	b	614	CLA	CMD-C2D-C1D	5.54	134.48	124.73
31	b1	606	CLA	CMD-C2D-C1D	5.54	134.48	124.73
31	c1	513	CLA	O2D-CGD-CBD	5.53	120.90	111.23
31	G	611	CLA	CMD-C2D-C1D	5.53	134.47	124.73
31	b	606	CLA	CMD-C2D-C1D	5.53	134.47	124.73
31	G	603	CLA	CMD-C2D-C1D	5.53	134.47	124.73
31	G1	613	CLA	CMD-C2D-C1D	5.53	134.46	124.73
31	s1	604	CLA	CMD-C2D-C1D	5.52	134.46	124.73
31	C	510	CLA	CMD-C2D-C1D	5.52	134.46	124.73
31	b1	603	CLA	CMD-C2D-C1D	5.52	134.46	124.73
31	R	613	CLA	CMD-C2D-C1D	5.52	134.45	124.73
31	B1	602	CLA	CMD-C2D-C1D	5.52	134.45	124.73
31	a	410	CLA	O2D-CGD-CBD	5.52	120.89	111.23
31	G1	612	CLA	O2D-CGD-CBD	5.52	120.88	111.23
46	H	101	RRX	C7-C8-C9	-5.52	118.07	126.23
48	G1	621	LUT	C7-C8-C9	-5.52	118.07	126.23
31	n1	604	CLA	CMD-C2D-C1D	5.52	134.45	124.73
31	Y1	603	CLA	O2D-CGD-CBD	5.52	120.88	111.23
31	s1	605	CLA	CMD-C2D-C1D	5.51	134.44	124.73
43	d	401	BCT	O2-C-O1	5.51	133.78	119.68
31	B	610	CLA	O2D-CGD-CBD	5.51	120.86	111.23
31	A	405	CLA	CMD-C2D-C1D	5.51	134.43	124.73
31	Y	612	CLA	O2D-CGD-CBD	5.51	120.86	111.23
47	n1	609	CHL	C1B-CHB-C4A	5.51	124.87	121.32
49	r	622	XAT	C7-C8-C9	-5.51	116.99	125.53
48	g1	621	LUT	C21-C26-C27	5.50	119.15	112.83
31	g1	603	CLA	CMD-C2D-C1D	5.50	134.42	124.73
31	Y1	611	CLA	CMD-C2D-C1D	5.50	134.42	124.73
31	g	602	CLA	CMD-C2D-C1D	5.50	134.42	124.73
31	g	613	CLA	CMD-C2D-C1D	5.50	134.41	124.73
48	s1	621	LUT	C35-C34-C33	-5.50	119.57	127.28
31	n1	610	CLA	CMD-C2D-C1D	5.49	134.40	124.73
31	n1	614	CLA	O2A-C1-C2	5.49	122.06	108.99
31	Y	604	CLA	CMD-C2D-C1D	5.49	134.40	124.73
31	s1	617	CLA	CMD-C2D-C1D	5.49	134.40	124.73
31	S1	605	CLA	CMD-C2D-C1D	5.48	134.39	124.73
31	n1	603	CLA	CMD-C2D-C1D	5.48	134.39	124.73
31	S	613	CLA	CMD-C2D-C1D	5.48	134.38	124.73
31	D	402	CLA	CMD-C2D-C1D	5.48	134.38	124.73
31	c	511	CLA	CMD-C2D-C1D	5.48	134.38	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	g1	613	CLA	CMD-C2D-C1D	5.48	134.38	124.73
31	s	611	CLA	CMD-C2D-C1D	5.48	134.37	124.73
31	C1	511	CLA	CMD-C2D-C1D	5.48	134.37	124.73
31	C	507	CLA	CMD-C2D-C1D	5.48	134.37	124.73
46	h1	101	RRX	C24-C23-C22	5.47	134.33	126.23
31	N1	611	CLA	CMD-C2D-C1D	5.47	134.37	124.73
48	n	620	LUT	C21-C26-C27	5.47	119.12	112.83
31	C1	510	CLA	CMD-C2D-C1D	5.47	134.36	124.73
31	D1	403	CLA	CMD-C2D-C1D	5.47	134.36	124.73
31	Y	611	CLA	CMD-C2D-C1D	5.47	134.36	124.73
31	c	510	CLA	O2D-CGD-CBD	5.47	120.79	111.23
31	n	611	CLA	CMD-C2D-C1D	5.46	134.35	124.73
31	b	605	CLA	CMD-C2D-C1D	5.46	134.35	124.73
31	s1	611	CLA	CMD-C2D-C1D	5.46	134.34	124.73
31	A	407	CLA	CMD-C2D-C1D	5.46	134.34	124.73
47	G1	609	CHL	C1B-CHB-C4A	5.46	124.83	121.32
31	B	605	CLA	O2D-CGD-CBD	5.46	120.77	111.23
48	r	620	LUT	C31-C30-C29	-5.46	119.62	127.28
49	y	622	XAT	C31-C30-C29	-5.46	119.62	127.28
31	a	407	CLA	O2A-C1-C2	5.45	121.97	108.99
31	y1	602	CLA	O2D-CGD-CBD	5.45	120.75	111.23
31	c1	502	CLA	CMD-C2D-C1D	5.45	134.32	124.73
31	g	614	CLA	CMD-C2D-C1D	5.44	134.32	124.73
31	B1	604	CLA	CMD-C2D-C1D	5.44	134.31	124.73
31	b1	607	CLA	O2D-CGD-CBD	5.44	120.74	111.23
31	y1	603	CLA	CMD-C2D-C1D	5.44	134.31	124.73
31	G1	604	CLA	CMD-C2D-C1D	5.44	134.31	124.73
31	s1	602	CLA	O2D-CGD-CBD	5.44	120.74	111.23
31	S1	604	CLA	CMD-C2D-C1D	5.44	134.31	124.73
31	B	602	CLA	CMD-C2D-C1D	5.44	134.30	124.73
31	g	602	CLA	O2D-CGD-CBD	5.44	120.73	111.23
31	Y	603	CLA	CMD-C2D-C1D	5.43	134.30	124.73
48	g1	620	LUT	C21-C26-C27	5.43	119.07	112.83
31	g	611	CLA	CMD-C2D-C1D	5.43	134.29	124.73
31	s1	613	CLA	CMD-C2D-C1D	5.43	134.29	124.73
31	s1	603	CLA	CMD-C2D-C1D	5.43	134.29	124.73
31	s	609	CLA	CMD-C2D-C1D	5.43	134.29	124.73
31	y	614	CLA	CMD-C2D-C1D	5.43	134.28	124.73
31	A	407	CLA	O2A-C1-C2	5.43	121.90	108.99
31	r	612	CLA	CMD-C2D-C1D	5.42	134.28	124.73
31	D	403	CLA	CMD-C2D-C1D	5.42	134.28	124.73
31	b1	616	CLA	CMD-C2D-C1D	5.42	134.28	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	607	CLA	O2D-CGD-CBD	5.42	120.71	111.23
50	g1	623	NEX	C17-C1-C6	-5.42	105.62	110.47
48	n	620	LUT	C7-C8-C9	-5.42	118.22	126.23
31	r1	602	CLA	O2D-CGD-CBD	5.42	120.71	111.23
31	n	604	CLA	O2D-CGD-CBD	5.42	120.71	111.23
31	y	614	CLA	O2D-CGD-CBD	5.42	120.70	111.23
31	S	614	CLA	O2D-CGD-CBD	5.42	120.70	111.23
31	N	611	CLA	CMD-C2D-C1D	5.42	134.27	124.73
31	R	604	CLA	CMD-C2D-C1D	5.42	134.27	124.73
31	n	614	CLA	O2A-C1-C2	5.42	121.88	108.99
31	A	410	CLA	O2D-CGD-CBD	5.41	120.70	111.23
31	S1	609	CLA	O2D-CGD-CBD	5.41	120.70	111.23
31	y	610	CLA	O2D-CGD-CBD	5.41	120.69	111.23
49	Y	622	XAT	C31-C30-C29	-5.41	119.69	127.28
31	c1	507	CLA	CMD-C2D-C1D	5.41	134.26	124.73
50	R1	622	NEX	C17-C1-C6	-5.41	105.63	110.47
31	C	504	CLA	CMD-C2D-C1D	5.41	134.25	124.73
31	n	611	CLA	O2D-CGD-CBD	5.41	120.68	111.23
31	R	603	CLA	CMD-C2D-C1D	5.41	134.25	124.73
31	b	603	CLA	CMD-C2D-C1D	5.40	134.25	124.73
31	B1	605	CLA	CMD-C2D-C1D	5.40	134.24	124.73
31	R	604	CLA	O2D-CGD-CBD	5.40	120.67	111.23
31	N1	612	CLA	CMD-C2D-C1D	5.40	134.24	124.73
46	H1	101	RRX	C37-C22-C23	5.40	126.34	118.09
31	c1	512	CLA	O2D-CGD-CBD	5.40	120.66	111.23
31	b	609	CLA	CMD-C2D-C1D	5.40	134.23	124.73
49	R1	621	XAT	C31-C30-C29	-5.40	119.71	127.28
31	b1	606	CLA	O2D-CGD-CBD	5.39	120.65	111.23
31	D	403	CLA	O2D-CGD-CBD	5.39	120.65	111.23
31	N1	614	CLA	CMD-C2D-C1D	5.39	134.22	124.73
31	c1	503	CLA	O2D-CGD-CBD	5.39	120.65	111.23
31	r1	602	CLA	CMD-C2D-C1D	5.39	134.22	124.73
31	S	604	CLA	CMD-C2D-C1D	5.39	134.22	124.73
31	n	604	CLA	CMD-C2D-C1D	5.39	134.22	124.73
31	S	609	CLA	O2D-CGD-CBD	5.39	120.64	111.23
31	c	504	CLA	CMD-C2D-C1D	5.38	134.21	124.73
31	b1	615	CLA	CMD-C2D-C1D	5.38	134.21	124.73
31	Y	610	CLA	O2D-CGD-CBD	5.38	120.64	111.23
47	s	608	CHL	C1B-CHB-C4A	5.38	124.78	121.32
37	B	620	C7Z	C15-C14-C13	-5.38	119.73	127.28
31	Y1	614	CLA	CMD-C2D-C1D	5.38	134.20	124.73
31	Y1	612	CLA	O2D-CGD-CBD	5.38	120.63	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	n1	622	XAT	C15-C14-C13	-5.38	119.74	127.28
31	n1	612	CLA	CMD-C2D-C1D	5.38	134.19	124.73
46	H	101	RRX	C16-C17-C18	-5.37	119.74	127.28
44	d1	405	PL9	C7-C3-C4	5.37	121.33	116.91
31	G	604	CLA	O2A-C1-C2	5.37	121.78	108.99
47	N1	601	CHL	C1B-CHB-C4A	5.37	124.78	121.32
31	s	602	CLA	CMD-C2D-C1D	5.37	134.19	124.73
31	b1	602	CLA	CMD-C2D-C1D	5.37	134.18	124.73
31	g	614	CLA	O2A-C1-C2	5.37	121.77	108.99
31	b	612	CLA	O2D-CGD-CBD	5.37	120.61	111.23
31	B1	610	CLA	CMD-C2D-C1D	5.36	134.17	124.73
31	B1	615	CLA	CMD-C2D-C1D	5.36	134.17	124.73
31	n	614	CLA	O2D-CGD-CBD	5.36	120.60	111.23
31	r	613	CLA	CMD-C2D-C1D	5.36	134.16	124.73
31	y1	611	CLA	CMD-C2D-C1D	5.36	134.16	124.73
48	S1	621	LUT	C7-C8-C9	-5.36	118.31	126.23
31	R1	603	CLA	CMD-C2D-C1D	5.35	134.16	124.73
50	S1	623	NEX	C17-C1-C6	-5.35	105.68	110.47
31	b	611	CLA	CMD-C2D-C1D	5.35	134.16	124.73
31	C	510	CLA	O2D-CGD-CBD	5.35	120.58	111.23
31	N	603	CLA	O2D-CGD-CBD	5.35	120.58	111.23
31	c1	501	CLA	CMD-C2D-C1D	5.35	134.14	124.73
31	g1	612	CLA	O2D-CGD-CBD	5.35	120.58	111.23
48	y	620	LUT	C35-C34-C33	-5.34	119.79	127.28
31	D1	403	CLA	O2D-CGD-CBD	5.34	120.57	111.23
49	r1	621	XAT	C38-C25-C24	5.34	120.24	114.24
31	n	613	CLA	CMD-C2D-C1D	5.33	134.12	124.73
31	n	610	CLA	CMD-C2D-C1D	5.33	134.12	124.73
31	S	609	CLA	CMD-C2D-C1D	5.33	134.12	124.73
31	g1	604	CLA	CMD-C2D-C1D	5.33	134.11	124.73
31	R	610	CLA	O2D-CGD-CBD	5.33	120.55	111.23
31	r	602	CLA	CMD-C2D-C1D	5.33	134.11	124.73
31	b1	617	CLA	CMD-C2D-C1D	5.33	134.11	124.73
31	Y1	604	CLA	CMD-C2D-C1D	5.33	134.11	124.73
31	c1	504	CLA	CMD-C2D-C1D	5.33	134.11	124.73
31	N	602	CLA	CMD-C2D-C1D	5.32	134.10	124.73
31	y	611	CLA	CMD-C2D-C1D	5.32	134.10	124.73
31	s1	611	CLA	O2D-CGD-CBD	5.32	120.53	111.23
31	S	612	CLA	O2D-CGD-CBD	5.32	120.53	111.23
31	n1	602	CLA	O2D-CGD-CBD	5.31	120.52	111.23
31	B	604	CLA	CMD-C2D-C1D	5.31	134.08	124.73
31	r	602	CLA	O2D-CGD-CBD	5.31	120.51	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	y1	602	CLA	CMD-C2D-C1D	5.31	134.08	124.73
31	r	612	CLA	O2D-CGD-CBD	5.31	120.51	111.23
48	G	621	LUT	C31-C30-C29	-5.31	119.83	127.28
31	c1	501	CLA	O2D-CGD-CBD	5.31	120.51	111.23
46	H	101	RRX	C15-C14-C13	-5.31	119.83	127.28
31	S1	612	CLA	CMD-C2D-C1D	5.31	134.07	124.73
31	Y1	604	CLA	O2D-CGD-CBD	5.31	120.51	111.23
31	c	512	CLA	CMD-C2D-C1D	5.30	134.07	124.73
31	C1	506	CLA	CMD-C2D-C1D	5.30	134.06	124.73
31	B1	603	CLA	O2D-CGD-CBD	5.30	120.49	111.23
31	c1	513	CLA	CMD-C2D-C1D	5.30	134.06	124.73
31	C1	503	CLA	O2D-CGD-CBD	5.30	120.49	111.23
31	C1	513	CLA	CMD-C2D-C1D	5.30	134.05	124.73
31	B	615	CLA	O2D-CGD-CBD	5.29	120.48	111.23
31	n1	611	CLA	CMD-C2D-C1D	5.29	134.04	124.73
31	B	603	CLA	O2D-CGD-CBD	5.29	120.47	111.23
48	g	620	LUT	C21-C26-C27	5.29	118.90	112.83
31	G	603	CLA	O2D-CGD-CBD	5.29	120.47	111.23
31	n	611	CLA	O2A-C1-C2	5.28	121.57	108.99
31	b	616	CLA	CMD-C2D-C1D	5.28	134.03	124.73
31	B	616	CLA	CMD-C2D-C1D	5.28	134.03	124.73
31	b1	613	CLA	O2D-CGD-CBD	5.28	120.46	111.23
31	r	610	CLA	CMD-C2D-C1D	5.28	134.02	124.73
31	a1	410	CLA	O2D-CGD-CBD	5.28	120.46	111.23
31	R	611	CLA	O2D-CGD-CBD	5.28	120.46	111.23
31	S1	614	CLA	O2D-CGD-CBD	5.28	120.45	111.23
31	N	614	CLA	O2A-C1-C2	5.28	121.55	108.99
31	y1	612	CLA	CMD-C2D-C1D	5.28	134.02	124.73
31	s1	604	CLA	O2D-CGD-CBD	5.27	120.45	111.23
31	r	604	CLA	O2D-CGD-CBD	5.27	120.45	111.23
31	b1	605	CLA	O2D-CGD-CBD	5.27	120.45	111.23
31	N1	610	CLA	O2D-CGD-CBD	5.27	120.44	111.23
31	c	502	CLA	CMD-C2D-C1D	5.27	134.01	124.73
31	G	614	CLA	O2D-CGD-CBD	5.27	120.44	111.23
31	g	614	CLA	O2D-CGD-CBD	5.27	120.44	111.23
31	b	604	CLA	CMD-C2D-C1D	5.27	134.00	124.73
31	G	614	CLA	O2A-C1-C2	5.27	121.52	108.99
31	b	610	CLA	O2D-CGD-CBD	5.27	120.44	111.23
48	n1	621	LUT	C11-C10-C9	-5.27	119.89	127.28
31	N	614	CLA	CMD-C2D-C1D	5.26	134.00	124.73
31	a	407	CLA	CMD-C2D-C1D	5.26	133.99	124.73
31	B1	617	CLA	CMD-C2D-C1D	5.26	133.99	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B1	603	CLA	CMD-C2D-C1D	5.26	133.99	124.73
31	y1	604	CLA	CMD-C2D-C1D	5.26	133.99	124.73
31	C	502	CLA	CMD-C2D-C1D	5.26	133.99	124.73
31	B1	611	CLA	CMD-C2D-C1D	5.26	133.99	124.73
31	g1	614	CLA	CMD-C2D-C1D	5.25	133.97	124.73
31	Y	614	CLA	O2D-CGD-CBD	5.25	120.41	111.23
31	A1	410	CLA	CMD-C2D-C1D	5.25	133.97	124.73
31	G1	611	CLA	O2D-CGD-CBD	5.25	120.41	111.23
31	G	612	CLA	CMD-C2D-C1D	5.25	133.97	124.73
31	R1	602	CLA	CMD-C2D-C1D	5.25	133.97	124.73
31	b	611	CLA	O2D-CGD-CBD	5.25	120.40	111.23
31	b1	610	CLA	CMD-C2D-C1D	5.25	133.97	124.73
31	s1	605	CLA	O2D-CGD-CBD	5.24	120.40	111.23
43	d1	401	BCT	O2-C-O1	5.24	133.08	119.68
31	g1	602	CLA	O2D-CGD-CBD	5.24	120.39	111.23
31	s1	610	CLA	O2D-CGD-CBD	5.24	120.39	111.23
31	n1	611	CLA	O2A-C1-C2	5.24	121.45	108.99
31	a1	410	CLA	CMD-C2D-C1D	5.24	133.95	124.73
31	s	605	CLA	CMD-C2D-C1D	5.24	133.95	124.73
49	n1	622	XAT	C31-C30-C29	-5.23	119.94	127.28
46	h1	101	RRX	C24-C25-C26	-5.23	109.50	121.56
31	G	613	CLA	O2D-CGD-CBD	5.23	120.38	111.23
50	s	623	NEX	C2-C1-C6	5.23	114.30	109.21
31	a	407	CLA	O2D-CGD-CBD	5.23	120.37	111.23
31	b1	611	CLA	O2D-CGD-CBD	5.23	120.37	111.23
31	s1	610	CLA	CMD-C2D-C1D	5.23	133.93	124.73
31	C1	502	CLA	CMD-C2D-C1D	5.23	133.93	124.73
31	n1	604	CLA	O2D-CGD-CBD	5.22	120.36	111.23
31	S1	613	CLA	CMD-C2D-C1D	5.22	133.93	124.73
40	B1	623	DGD	O2G-C1B-C2B	5.22	122.78	111.48
33	C1	516	BCR	C33-C5-C6	-5.22	118.79	124.48
31	S1	610	CLA	O2D-CGD-CBD	5.22	120.35	111.23
31	c1	510	CLA	O2D-CGD-CBD	5.22	120.35	111.23
31	b	613	CLA	CMD-C2D-C1D	5.22	133.91	124.73
31	n	613	CLA	O2D-CGD-CBD	5.21	120.34	111.23
31	D1	402	CLA	CMD-C2D-C1D	5.21	133.90	124.73
31	N	603	CLA	CMD-C2D-C1D	5.21	133.90	124.73
31	R	602	CLA	CMD-C2D-C1D	5.21	133.90	124.73
31	S	602	CLA	CMD-C2D-C1D	5.20	133.89	124.73
31	y	604	CLA	CMD-C2D-C1D	5.20	133.89	124.73
31	s	603	CLA	CMD-C2D-C1D	5.20	133.88	124.73
31	C	512	CLA	O2D-CGD-CBD	5.20	120.32	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a1	407	CLA	O2A-C1-C2	5.20	121.36	108.99
49	Y1	622	XAT	C15-C14-C13	-5.20	119.99	127.28
31	n	614	CLA	CMD-C2D-C1D	5.20	133.88	124.73
31	c	503	CLA	O2D-CGD-CBD	5.20	120.31	111.23
31	b	616	CLA	O2D-CGD-CBD	5.19	120.31	111.23
31	S	610	CLA	CMD-C2D-C1D	5.19	133.87	124.73
31	C	511	CLA	O2D-CGD-CBD	5.19	120.31	111.23
31	Y1	612	CLA	CMD-C2D-C1D	5.19	133.87	124.73
31	b1	609	CLA	CMD-C2D-C1D	5.19	133.87	124.73
31	a	405	CLA	CMD-C2D-C1D	5.19	133.86	124.73
33	c1	514	BCR	C15-C14-C13	-5.19	120.00	127.28
31	C	509	CLA	O2D-CGD-CBD	5.19	120.30	111.23
31	Y1	610	CLA	O2D-CGD-CBD	5.19	120.30	111.23
31	C	513	CLA	CMD-C2D-C1D	5.19	133.86	124.73
31	B1	616	CLA	O2D-CGD-CBD	5.19	120.30	111.23
31	C1	513	CLA	O2D-CGD-CBD	5.19	120.30	111.23
31	R1	610	CLA	O2D-CGD-CBD	5.18	120.29	111.23
31	r	609	CLA	CMD-C2D-C1D	5.18	133.86	124.73
31	a	410	CLA	CMD-C2D-C1D	5.18	133.85	124.73
48	s	621	LUT	C21-C26-C27	5.18	118.78	112.83
31	c1	506	CLA	CMD-C2D-C1D	5.18	133.85	124.73
31	G1	604	CLA	O2D-CGD-CBD	5.18	120.28	111.23
31	Y1	608	CLA	O2D-CGD-CBD	5.18	120.28	111.23
31	n1	613	CLA	CMD-C2D-C1D	5.17	133.84	124.73
31	S1	612	CLA	O2D-CGD-CBD	5.17	120.28	111.23
31	B1	612	CLA	O2D-CGD-CBD	5.17	120.26	111.23
31	y	603	CLA	CMD-C2D-C1D	5.17	133.83	124.73
31	N	614	CLA	O2D-CGD-CBD	5.17	120.26	111.23
31	n	612	CLA	O2D-CGD-CBD	5.17	120.26	111.23
31	g1	603	CLA	O2D-CGD-CBD	5.17	120.26	111.23
31	d	402	CLA	CMD-C2D-C1D	5.16	133.82	124.73
31	y1	614	CLA	O2D-CGD-CBD	5.16	120.25	111.23
31	S	603	CLA	CMD-C2D-C1D	5.16	133.82	124.73
31	S	604	CLA	O2D-CGD-CBD	5.16	120.25	111.23
31	R1	604	CLA	O2D-CGD-CBD	5.16	120.25	111.23
31	n1	611	CLA	O2D-CGD-CBD	5.16	120.25	111.23
31	N	602	CLA	O2D-CGD-CBD	5.16	120.25	111.23
31	R1	612	CLA	O2D-CGD-CBD	5.16	120.25	111.23
31	g	603	CLA	CMD-C2D-C1D	5.16	133.81	124.73
31	N1	614	CLA	O2D-CGD-CBD	5.16	120.24	111.23
47	Y1	609	CHL	C1C-CHC-C4B	5.15	134.51	116.07
31	N1	611	CLA	O2A-C1-C2	5.15	121.26	108.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	N1	613	CLA	CMD-C2D-C1D	5.15	133.80	124.73
47	s1	608	CHL	C1B-CHB-C4A	5.15	124.64	121.32
31	B	612	CLA	O2D-CGD-CBD	5.15	120.24	111.23
31	N1	613	CLA	O2D-CGD-CBD	5.15	120.23	111.23
31	B1	617	CLA	O2D-CGD-CBD	5.15	120.23	111.23
31	b1	612	CLA	O2D-CGD-CBD	5.15	120.23	111.23
31	G1	604	CLA	O2A-C1-C2	5.14	121.23	108.99
31	C	507	CLA	O2D-CGD-CBD	5.14	120.22	111.23
31	b1	607	CLA	CMD-C2D-C1D	5.14	133.78	124.73
37	B	620	C7Z	C38-C25-C26	-5.14	118.88	124.48
31	C	508	CLA	CMD-C2D-C1D	5.14	133.78	124.73
31	S1	605	CLA	O2D-CGD-CBD	5.14	120.22	111.23
31	G1	614	CLA	CMD-C2D-C1D	5.14	133.78	124.73
31	r1	603	CLA	O2D-CGD-CBD	5.14	120.21	111.23
31	b	610	CLA	CMD-C2D-C1D	5.14	133.77	124.73
31	S	617	CLA	O2D-CGD-CBD	5.14	120.21	111.23
37	b	620	C7Z	C18-C5-C6	-5.14	118.88	124.48
31	r1	612	CLA	O2D-CGD-CBD	5.14	120.21	111.23
31	C1	509	CLA	O2D-CGD-CBD	5.13	120.20	111.23
31	s	614	CLA	O2D-CGD-CBD	5.13	120.19	111.23
44	D	405	PL9	C7-C3-C4	5.13	121.13	116.91
31	B	602	CLA	O2D-CGD-CBD	5.13	120.19	111.23
31	g1	602	CLA	CMD-C2D-C1D	5.12	133.75	124.73
31	B1	602	CLA	O2D-CGD-CBD	5.12	120.18	111.23
49	N	622	XAT	C15-C14-C13	-5.12	120.10	127.28
31	c	511	CLA	O2D-CGD-CBD	5.12	120.18	111.23
31	Y1	603	CLA	CMD-C2D-C1D	5.12	133.74	124.73
31	n1	612	CLA	O2D-CGD-CBD	5.12	120.18	111.23
31	y	613	CLA	O2D-CGD-CBD	5.12	120.17	111.23
31	s	612	CLA	O2D-CGD-CBD	5.11	120.17	111.23
48	Y1	621	LUT	C21-C26-C27	5.11	118.70	112.83
31	s	617	CLA	O2D-CGD-CBD	5.11	120.17	111.23
31	g1	611	CLA	O2D-CGD-CBD	5.11	120.17	111.23
31	S1	617	CLA	O2D-CGD-CBD	5.11	120.16	111.23
49	y1	622	XAT	C31-C30-C29	-5.11	120.12	127.28
31	B	604	CLA	O2D-CGD-CBD	5.11	120.16	111.23
31	Y	608	CLA	O2D-CGD-CBD	5.11	120.16	111.23
31	c	508	CLA	O2D-CGD-CBD	5.10	120.15	111.23
31	S1	611	CLA	CMD-C2D-C1D	5.10	133.71	124.73
49	g1	622	XAT	C15-C14-C13	-5.10	120.13	127.28
31	S	611	CLA	CMD-C2D-C1D	5.10	133.71	124.73
33	C1	517	BCR	C15-C14-C13	-5.10	120.13	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	Y1	611	CLA	O2D-CGD-CBD	5.10	120.14	111.23
31	c1	505	CLA	CMD-C2D-C1D	5.10	133.70	124.73
31	G	612	CLA	O2D-CGD-CBD	5.10	120.14	111.23
31	b	603	CLA	O2D-CGD-CBD	5.10	120.14	111.23
48	N	620	LUT	C35-C34-C33	-5.09	120.14	127.28
31	Y	613	CLA	CMD-C2D-C1D	5.09	133.70	124.73
31	r1	610	CLA	CMD-C2D-C1D	5.09	133.70	124.73
31	b	604	CLA	O2D-CGD-CBD	5.09	120.13	111.23
37	b	620	C7Z	C35-C34-C33	-5.09	120.14	127.28
31	C1	506	CLA	O2D-CGD-CBD	5.09	120.12	111.23
31	S1	611	CLA	O2D-CGD-CBD	5.09	120.12	111.23
48	Y1	620	LUT	C15-C14-C13	-5.09	120.14	127.28
31	b1	617	CLA	O2D-CGD-CBD	5.09	120.12	111.23
31	s	613	CLA	CMD-C2D-C1D	5.09	133.69	124.73
47	n	609	CHL	C1C-CHC-C4B	5.08	134.26	116.07
31	g	603	CLA	O2D-CGD-CBD	5.08	120.12	111.23
31	N1	602	CLA	O2D-CGD-CBD	5.08	120.11	111.23
31	S	617	CLA	CMD-C2D-C1D	5.08	133.68	124.73
31	N1	612	CLA	O2D-CGD-CBD	5.08	120.11	111.23
31	C1	501	CLA	O2D-CGD-CBD	5.08	120.11	111.23
48	s	620	LUT	C35-C34-C33	-5.08	120.16	127.28
31	Y1	610	CLA	CMD-C2D-C1D	5.08	133.67	124.73
31	c	504	CLA	O2D-CGD-CBD	5.08	120.11	111.23
31	n	603	CLA	O2D-CGD-CBD	5.08	120.11	111.23
31	R	612	CLA	O2D-CGD-CBD	5.07	120.10	111.23
31	c1	509	CLA	O2D-CGD-CBD	5.07	120.10	111.23
31	g	604	CLA	O2A-C1-C2	5.07	121.06	108.99
31	R1	609	CLA	CMD-C2D-C1D	5.07	133.65	124.73
48	r	620	LUT	C7-C8-C9	-5.07	118.74	126.23
31	S1	602	CLA	CMD-C2D-C1D	5.06	133.65	124.73
31	R1	603	CLA	O2D-CGD-CBD	5.06	120.08	111.23
50	Y1	623	NEX	C2-C1-C6	5.06	114.13	109.21
31	R1	610	CLA	CMD-C2D-C1D	5.06	133.63	124.73
31	c	508	CLA	CMD-C2D-C1D	5.05	133.63	124.73
31	s1	609	CLA	CMD-C2D-C1D	5.05	133.63	124.73
50	Y	623	NEX	C2-C1-C6	5.05	114.12	109.21
31	r1	604	CLA	O2D-CGD-CBD	5.05	120.06	111.23
41	N	624	LHG	O7-C7-C8	5.05	122.40	111.48
31	b	606	CLA	O2D-CGD-CBD	5.04	120.05	111.23
31	C1	502	CLA	O2D-CGD-CBD	5.04	120.05	111.23
49	N	622	XAT	C31-C30-C29	-5.04	120.21	127.28
57	y1	627	PTY	O7-C8-C11	5.04	120.08	111.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c1	502	CLA	O2D-CGD-CBD	5.04	120.04	111.23
31	b1	616	CLA	O2D-CGD-CBD	5.04	120.04	111.23
31	B1	606	CLA	O2D-CGD-CBD	5.04	120.03	111.23
31	y	612	CLA	CMD-C2D-C1D	5.04	133.60	124.73
31	S	603	CLA	O2D-CGD-CBD	5.03	120.03	111.23
31	A1	410	CLA	O2D-CGD-CBD	5.03	120.03	111.23
46	H1	101	RRX	C7-C8-C9	-5.03	118.79	126.23
31	b1	612	CLA	CMD-C2D-C1D	5.02	133.58	124.73
31	c	509	CLA	O2D-CGD-CBD	5.02	120.01	111.23
48	g	620	LUT	C35-C34-C33	-5.02	120.23	127.28
31	B1	609	CLA	CMD-C2D-C1D	5.02	133.57	124.73
31	d	403	CLA	CMD-C2D-C1D	5.02	133.57	124.73
31	C	505	CLA	CMD-C2D-C1D	5.02	133.57	124.73
31	r1	609	CLA	CMD-C2D-C1D	5.02	133.56	124.73
47	n	605	CHL	C1C-CHC-C4B	5.01	134.00	116.07
31	r	608	CLA	O2D-CGD-CBD	5.01	119.99	111.23
31	y1	613	CLA	O2D-CGD-CBD	5.01	119.99	111.23
31	S1	610	CLA	CMD-C2D-C1D	5.01	133.55	124.73
31	C	512	CLA	CMD-C2D-C1D	5.01	133.54	124.73
31	C	503	CLA	O2D-CGD-CBD	5.01	119.98	111.23
49	G	622	XAT	C15-C14-C13	-5.00	120.26	127.28
31	r1	603	CLA	CMD-C2D-C1D	5.00	133.54	124.73
49	y	622	XAT	C15-C14-C13	-5.00	120.26	127.28
31	Y1	613	CLA	O2D-CGD-CBD	5.00	119.97	111.23
50	s1	623	NEX	C38-C25-C24	5.00	119.86	114.24
31	r	611	CLA	O2D-CGD-CBD	5.00	119.97	111.23
31	N	612	CLA	O2D-CGD-CBD	5.00	119.97	111.23
31	b	614	CLA	O2D-CGD-CBD	5.00	119.96	111.23
31	B1	611	CLA	O2D-CGD-CBD	5.00	119.96	111.23
47	N1	608	CHL	C1B-CHB-C4A	4.99	124.54	121.32
31	g	604	CLA	O2D-CGD-CBD	4.99	119.96	111.23
31	b	602	CLA	O2D-CGD-CBD	4.99	119.96	111.23
31	G1	614	CLA	O2D-CGD-CBD	4.99	119.96	111.23
48	s	620	LUT	C11-C10-C9	-4.99	120.28	127.28
47	G	609	CHL	C1C-CHC-C4B	4.99	133.93	116.07
31	s	609	CLA	O2D-CGD-CBD	4.99	119.96	111.23
31	S	614	CLA	CMD-C2D-C1D	4.99	133.52	124.73
31	B	617	CLA	O2D-CGD-CBD	4.99	119.95	111.23
47	G1	609	CHL	C1C-CHC-C4B	4.99	133.92	116.07
49	y1	622	XAT	C15-C14-C13	-4.99	120.29	127.28
35	c	521	LMG	O7-C10-C11	4.99	122.27	111.48
31	s1	614	CLA	CMD-C2D-C1D	4.98	133.50	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	N1	611	CLA	O2D-CGD-CBD	4.98	119.94	111.23
31	S1	617	CLA	CMD-C2D-C1D	4.98	133.50	124.73
31	B1	608	CLA	O2D-CGD-CBD	4.98	119.94	111.23
31	b1	615	CLA	O2D-CGD-CBD	4.98	119.94	111.23
31	r1	610	CLA	O2D-CGD-CBD	4.98	119.94	111.23
31	d1	403	CLA	O2D-CGD-CBD	4.98	119.93	111.23
31	Y1	602	CLA	O2D-CGD-CBD	4.97	119.93	111.23
31	b1	610	CLA	O2D-CGD-CBD	4.97	119.93	111.23
48	R1	620	LUT	C26-C27-C28	-4.97	116.84	124.58
57	Y1	627	PTY	O7-C8-C11	4.97	119.95	111.09
31	s	603	CLA	O2D-CGD-CBD	4.97	119.92	111.23
48	r	620	LUT	C15-C14-C13	-4.97	120.31	127.28
31	d1	402	CLA	CMD-C2D-C1D	4.96	133.47	124.73
31	B	613	CLA	O2D-CGD-CBD	4.96	119.91	111.23
37	B1	620	C7Z	C18-C5-C6	-4.96	119.07	124.48
31	D	402	CLA	O2D-CGD-CBD	4.96	119.90	111.23
31	b1	602	CLA	O2D-CGD-CBD	4.95	119.89	111.23
48	n	620	LUT	C35-C34-C33	-4.95	120.33	127.28
49	R	621	XAT	C38-C25-C24	4.95	119.80	114.24
31	b	617	CLA	O2D-CGD-CBD	4.94	119.87	111.23
37	b	620	C7Z	C15-C14-C13	-4.94	120.35	127.28
50	g1	623	NEX	C2-C1-C6	4.94	114.01	109.21
47	S1	607	CHL	C1C-CHC-C4B	4.94	133.73	116.07
49	N	622	XAT	C38-C25-C24	4.93	119.78	114.24
48	G1	621	LUT	C35-C34-C33	-4.93	120.36	127.28
31	Y	613	CLA	O2D-CGD-CBD	4.93	119.85	111.23
31	G1	602	CLA	O2D-CGD-CBD	4.93	119.85	111.23
47	G	601	CHL	C1C-CHC-C4B	4.93	133.70	116.07
31	S	602	CLA	O2D-CGD-CBD	4.93	119.84	111.23
31	G1	613	CLA	O2D-CGD-CBD	4.93	119.84	111.23
47	N1	605	CHL	C1C-CHC-C4B	4.93	133.70	116.07
48	R	620	LUT	C11-C10-C9	-4.92	120.37	127.28
31	G1	610	CLA	O2D-CGD-CBD	4.92	119.83	111.23
31	n1	614	CLA	O2D-CGD-CBD	4.92	119.83	111.23
31	C1	512	CLA	O2D-CGD-CBD	4.92	119.83	111.23
31	B1	612	CLA	CMD-C2D-C1D	4.92	133.39	124.73
47	s1	608	CHL	C1C-CHC-C4B	4.91	133.65	116.07
50	r	623	NEX	C38-C25-C24	4.91	119.76	114.24
31	g1	614	CLA	O2D-CGD-CBD	4.91	119.81	111.23
31	c1	508	CLA	O2D-CGD-CBD	4.91	119.81	111.23
47	N1	601	CHL	C1C-CHC-C4B	4.90	133.61	116.07
48	S1	621	LUT	C21-C26-C27	4.89	118.45	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	g1	609	CHL	C1C-CHC-C4B	4.89	133.57	116.07
48	N1	620	LUT	C21-C26-C27	4.89	118.44	112.83
31	b1	611	CLA	CMD-C2D-C1D	4.88	133.33	124.73
37	b1	620	C7Z	C11-C10-C9	-4.88	120.43	127.28
47	y	605	CHL	C1C-CHC-C4B	4.88	133.53	116.07
31	b	608	CLA	O2D-CGD-CBD	4.88	119.76	111.23
50	n1	623	NEX	C17-C1-C6	-4.88	106.11	110.47
31	c1	507	CLA	O2D-CGD-CBD	4.87	119.75	111.23
31	C1	507	CLA	O2D-CGD-CBD	4.87	119.75	111.23
33	c	514	BCR	C15-C14-C13	-4.87	120.45	127.28
47	N1	608	CHL	C1C-CHC-C4B	4.87	133.48	116.07
47	n1	609	CHL	C1C-CHC-C4B	4.86	133.46	116.07
31	b	615	CLA	O2D-CGD-CBD	4.86	119.73	111.23
47	s	608	CHL	C1C-CHC-C4B	4.86	133.46	116.07
31	d1	402	CLA	O2D-CGD-CBD	4.86	119.72	111.23
47	y1	606	CHL	C1C-CHC-C4B	4.85	133.43	116.07
47	G1	608	CHL	C1C-CHC-C4B	4.85	133.42	116.07
48	r1	620	LUT	C15-C14-C13	-4.85	120.48	127.28
47	n1	605	CHL	C1C-CHC-C4B	4.85	133.42	116.07
47	N	605	CHL	C1C-CHC-C4B	4.85	133.41	116.07
31	R1	609	CLA	O2D-CGD-CBD	4.85	119.70	111.23
31	D1	402	CLA	O2D-CGD-CBD	4.85	119.70	111.23
37	b1	620	C7Z	C38-C25-C26	-4.85	119.20	124.48
31	N	612	CLA	CMD-C2D-C1D	4.84	133.25	124.73
48	S	621	LUT	C21-C26-C27	4.84	118.39	112.83
40	b1	623	DGD	O2G-C1B-C2B	4.84	121.95	111.48
31	b1	608	CLA	O2D-CGD-CBD	4.84	119.69	111.23
31	g	613	CLA	O2D-CGD-CBD	4.84	119.68	111.23
31	B1	607	CLA	O2D-CGD-CBD	4.83	119.68	111.23
31	Y	612	CLA	CMD-C2D-C1D	4.83	133.24	124.73
31	c	502	CLA	O2D-CGD-CBD	4.83	119.68	111.23
31	B1	605	CLA	O2D-CGD-CBD	4.83	119.68	111.23
31	B	610	CLA	CMD-C2D-C1D	4.83	133.24	124.73
50	g1	623	NEX	C38-C25-C24	4.83	119.67	114.24
31	R	608	CLA	O2D-CGD-CBD	4.83	119.67	111.23
31	c1	504	CLA	O2D-CGD-CBD	4.83	119.67	111.23
31	g	610	CLA	O2D-CGD-CBD	4.83	119.67	111.23
46	h1	101	RRX	C15-C16-C17	-4.83	113.64	123.52
47	g	601	CHL	C1C-CHC-C4B	4.83	133.34	116.07
31	G1	603	CLA	O2D-CGD-CBD	4.83	119.67	111.23
47	g1	609	CHL	C1B-CHB-C4A	4.82	124.43	121.32
31	c	505	CLA	CMD-C2D-C1D	4.82	133.22	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	n1	613	CLA	O2D-CGD-CBD	4.82	119.66	111.23
31	N	613	CLA	O2D-CGD-CBD	4.82	119.66	111.23
49	n	622	XAT	C7-C8-C9	-4.82	118.05	125.53
50	y	623	NEX	C31-C30-C29	4.82	134.03	127.28
47	s	606	CHL	C1C-CHC-C4B	4.81	133.29	116.07
35	b	622	LMG	O7-C10-C11	4.81	121.89	111.48
47	S	608	CHL	C1C-CHC-C4B	4.81	133.26	116.07
31	N1	602	CLA	CMD-C2D-C1D	4.80	133.19	124.73
46	H1	101	RRX	C24-C25-C26	-4.80	110.50	121.56
47	Y	605	CHL	C1C-CHC-C4B	4.80	133.25	116.07
31	N	611	CLA	O2A-C1-C2	4.80	120.42	108.99
44	d	405	PL9	C7-C3-C4	4.80	120.86	116.91
31	r	603	CLA	O2D-CGD-CBD	4.79	119.61	111.23
31	B	611	CLA	O2D-CGD-CBD	4.79	119.60	111.23
31	C1	511	CLA	O2D-CGD-CBD	4.79	119.60	111.23
48	y1	620	LUT	C21-C26-C27	4.79	118.33	112.83
49	y	622	XAT	C18-C5-C4	4.78	119.61	114.24
37	B	620	C7Z	C18-C5-C6	-4.78	119.27	124.48
31	s	604	CLA	O2D-CGD-CBD	4.77	119.58	111.23
31	S	610	CLA	O2D-CGD-CBD	4.77	119.58	111.23
31	B	611	CLA	CMD-C2D-C1D	4.77	133.13	124.73
50	n1	623	NEX	C31-C30-C29	4.77	133.97	127.28
47	G1	601	CHL	C1C-CHC-C4B	4.77	133.13	116.07
37	b	620	C7Z	C38-C25-C26	-4.77	119.28	124.48
47	y1	609	CHL	C1C-CHC-C4B	4.77	133.13	116.07
48	s1	620	LUT	C21-C26-C27	4.76	118.30	112.83
31	N1	603	CLA	O2D-CGD-CBD	4.76	119.56	111.23
47	g1	608	CHL	C1C-CHC-C4B	4.76	133.11	116.07
31	R	609	CLA	O2D-CGD-CBD	4.76	119.55	111.23
31	y	608	CLA	O2D-CGD-CBD	4.76	119.55	111.23
31	r	609	CLA	O2D-CGD-CBD	4.76	119.55	111.23
47	S	606	CHL	C1C-CHC-C4B	4.75	133.08	116.07
47	N	609	CHL	C1C-CHC-C4B	4.75	133.08	116.07
31	g1	610	CLA	O2D-CGD-CBD	4.75	119.54	111.23
47	y	609	CHL	C1C-CHC-C4B	4.75	133.07	116.07
47	G	605	CHL	C1C-CHC-C4B	4.75	133.07	116.07
48	s1	620	LUT	C7-C8-C9	-4.75	119.21	126.23
31	B	608	CLA	O2D-CGD-CBD	4.75	119.53	111.23
49	G1	622	XAT	C15-C14-C13	-4.75	120.62	127.28
31	C	505	CLA	O2D-CGD-CBD	4.75	119.53	111.23
50	R1	622	NEX	C38-C25-C24	4.75	119.57	114.24
33	D1	404	BCR	C19-C18-C17	4.74	126.47	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	Y	620	LUT	C15-C14-C13	-4.74	120.63	127.28
48	r1	620	LUT	C7-C8-C9	-4.74	119.23	126.23
47	g	609	CHL	C1C-CHC-C4B	4.73	133.01	116.07
31	r1	609	CLA	O2D-CGD-CBD	4.73	119.50	111.23
49	Y1	622	XAT	C31-C30-C29	-4.73	120.64	127.28
47	N1	609	CHL	C3D-C4D-CHA	4.73	115.73	108.54
48	Y	621	LUT	C21-C26-C27	4.73	118.26	112.83
37	b1	620	C7Z	C1-C6-C5	-4.73	116.17	122.64
31	n	610	CLA	O2D-CGD-CBD	4.73	119.50	111.23
31	b1	604	CLA	O2D-CGD-CBD	4.73	119.50	111.23
47	s	607	CHL	C1C-CHC-C4B	4.73	132.99	116.07
47	y	601	CHL	C1C-CHC-C4B	4.73	132.99	116.07
37	B1	620	C7Z	C11-C10-C9	-4.73	120.65	127.28
50	g	623	NEX	C38-C25-C24	4.73	119.55	114.24
47	g	607	CHL	C1C-CHC-C4B	4.73	132.98	116.07
31	d	402	CLA	O2D-CGD-CBD	4.72	119.49	111.23
31	B1	604	CLA	O2D-CGD-CBD	4.72	119.49	111.23
46	H1	101	RRX	C11-C10-C9	-4.72	120.66	127.28
31	C1	510	CLA	O2D-CGD-CBD	4.72	119.48	111.23
48	N	621	LUT	C21-C26-C27	4.72	118.25	112.83
47	s1	606	CHL	C1C-CHC-C4B	4.72	132.95	116.07
48	g	620	LUT	C7-C8-C9	-4.72	119.26	126.23
31	y1	610	CLA	O2D-CGD-CBD	4.71	119.47	111.23
31	B	606	CLA	O2D-CGD-CBD	4.71	119.46	111.23
31	y	604	CLA	O2D-CGD-CBD	4.71	119.46	111.23
31	B1	610	CLA	O2D-CGD-CBD	4.71	119.46	111.23
47	G	608	CHL	C1C-CHC-C4B	4.71	132.91	116.07
50	s	623	NEX	C38-C25-C24	4.71	119.53	114.24
47	g1	605	CHL	C1C-CHC-C4B	4.71	132.91	116.07
49	y1	622	XAT	C7-C8-C9	-4.70	118.23	125.53
31	c	502	CLA	C1-C2-C3	-4.70	118.49	126.20
47	g1	601	CHL	C1C-CHC-C4B	4.70	132.89	116.07
47	N1	606	CHL	C1C-CHC-C4B	4.70	132.89	116.07
50	r	623	NEX	C17-C1-C6	-4.70	106.27	110.47
31	y1	608	CLA	O2D-CGD-CBD	4.70	119.44	111.23
47	R1	607	CHL	C1C-CHC-C4B	4.69	132.86	116.07
50	Y1	623	NEX	C38-C25-C24	4.69	119.51	114.24
44	D1	405	PL9	C7-C3-C2	-4.69	117.86	123.39
48	S	621	LUT	C35-C34-C33	-4.69	120.70	127.28
47	N	601	CHL	C1C-CHC-C4B	4.69	132.85	116.07
31	b1	614	CLA	O2D-CGD-CBD	4.69	119.42	111.23
31	r	610	CLA	O2D-CGD-CBD	4.69	119.42	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	G	620	LUT	C7-C8-C9	-4.69	119.30	126.23
47	Y1	605	CHL	C1C-CHC-C4B	4.69	132.84	116.07
31	s1	617	CLA	O2D-CGD-CBD	4.68	119.42	111.23
31	s	602	CLA	O2D-CGD-CBD	4.68	119.41	111.23
31	S	612	CLA	CMD-C2D-C1D	4.68	132.97	124.73
47	Y	606	CHL	C1C-CHC-C4B	4.68	132.80	116.07
48	R	620	LUT	C15-C14-C13	-4.67	120.73	127.28
47	G1	605	CHL	C1C-CHC-C4B	4.67	132.78	116.07
31	A1	405	CLA	O2D-CGD-CBD	4.67	119.39	111.23
49	R	621	XAT	C7-C8-C9	-4.67	118.28	125.53
41	C1	525	LHG	O7-C7-C8	4.66	121.57	111.48
47	g	606	CHL	C1C-CHC-C4B	4.66	132.75	116.07
47	g	605	CHL	C1C-CHC-C4B	4.66	132.75	116.07
31	N	610	CLA	CMD-C2D-C1D	4.66	132.93	124.73
49	g	622	XAT	C31-C30-C29	-4.66	120.74	127.28
50	s1	623	NEX	C8-C7-C6	-4.66	172.16	177.66
31	C	508	CLA	O2D-CGD-CBD	4.66	119.37	111.23
47	S1	608	CHL	C1C-CHC-C4B	4.65	132.73	116.07
31	g1	613	CLA	O2D-CGD-CBD	4.65	119.36	111.23
49	N1	622	XAT	C18-C5-C4	4.65	119.47	114.24
49	N1	622	XAT	C38-C25-C24	4.65	119.46	114.24
31	c	505	CLA	O2D-CGD-CBD	4.65	119.36	111.23
48	r1	620	LUT	C11-C10-C9	-4.65	120.76	127.28
49	G	622	XAT	C18-C5-C4	4.65	119.46	114.24
47	g	608	CHL	C1C-CHC-C4B	4.64	132.69	116.07
46	H1	101	RRX	C24-C23-C22	4.64	133.11	126.23
49	Y1	622	XAT	C38-C25-C24	4.64	119.46	114.24
47	G1	607	CHL	C1C-CHC-C4B	4.64	132.68	116.07
56	r1	626	ERG	C18-C13-C12	-4.64	103.76	110.61
47	g1	606	CHL	C1C-CHC-C4B	4.64	132.67	116.07
31	R1	608	CLA	O2D-CGD-CBD	4.64	119.34	111.23
47	S	607	CHL	C1C-CHC-C4B	4.64	132.67	116.07
47	Y1	606	CHL	C1C-CHC-C4B	4.64	132.66	116.07
50	Y	623	NEX	C38-C25-C24	4.63	119.45	114.24
47	y	606	CHL	C1C-CHC-C4B	4.63	132.65	116.07
31	s1	613	CLA	O2D-CGD-CBD	4.63	119.33	111.23
46	H1	101	RRX	C15-C16-C17	-4.63	114.04	123.52
31	C1	508	CLA	CMD-C2D-C1D	4.63	132.88	124.73
47	r1	607	CHL	C1C-CHC-C4B	4.63	132.64	116.07
31	S1	613	CLA	O2D-CGD-CBD	4.63	119.32	111.23
47	Y	609	CHL	C1C-CHC-C4B	4.63	132.63	116.07
48	y	620	LUT	C21-C26-C27	4.63	118.15	112.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	r1	622	NEX	C38-C25-C24	4.63	119.44	114.24
49	Y1	622	XAT	C18-C5-C4	4.63	119.44	114.24
50	R	622	NEX	C38-C25-C24	4.63	119.44	114.24
49	y1	622	XAT	C18-C5-C4	4.62	119.43	114.24
41	g	624	LHG	O7-C7-C8	4.62	121.47	111.48
49	R1	621	XAT	C18-C5-C4	4.62	119.43	114.24
47	N	608	CHL	C1C-CHC-C4B	4.62	132.59	116.07
31	B	614	CLA	O2D-CGD-CBD	4.62	119.30	111.23
33	C	516	BCR	C33-C5-C6	-4.61	119.45	124.48
47	r	606	CHL	C1C-CHC-C4B	4.61	132.58	116.07
48	Y	620	LUT	C21-C26-C27	4.61	118.13	112.83
35	W1	201	LMG	O7-C10-C11	4.61	121.45	111.48
47	g1	607	CHL	C1C-CHC-C4B	4.61	132.56	116.07
31	A1	405	CLA	CAC-C3C-C2C	4.61	136.02	127.56
47	N	607	CHL	C1C-CHC-C4B	4.60	132.54	116.07
49	R1	621	XAT	C38-C25-C24	4.60	119.41	114.24
49	Y	622	XAT	C38-C25-C24	4.60	119.41	114.24
47	S1	601	CHL	C1C-CHC-C4B	4.60	132.52	116.07
48	y	620	LUT	C7-C8-C9	-4.60	119.44	126.23
31	b	612	CLA	CMD-C2D-C1D	4.59	132.82	124.73
31	Y	602	CLA	CMD-C2D-C1D	4.59	132.82	124.73
47	n	601	CHL	C1C-CHC-C4B	4.59	132.51	116.07
31	s	610	CLA	O2A-C1-C2	4.59	125.78	108.11
49	G1	622	XAT	C31-C30-C29	-4.59	120.84	127.28
47	y1	605	CHL	C1C-CHC-C4B	4.59	132.50	116.07
31	c1	508	CLA	CMD-C2D-C1D	4.59	132.81	124.73
50	N	623	NEX	C38-C25-C24	4.58	119.39	114.24
48	s	620	LUT	C15-C14-C13	-4.58	120.86	127.28
31	G1	612	CLA	CMD-C2D-C1D	4.58	132.79	124.73
31	n1	610	CLA	O2D-CGD-CBD	4.58	119.23	111.23
35	A1	413	LMG	O7-C10-C11	4.57	121.38	111.48
47	n1	607	CHL	C1C-CHC-C4B	4.57	132.43	116.07
37	B1	620	C7Z	C7-C8-C9	-4.57	119.47	126.23
48	N	620	LUT	C15-C14-C13	-4.57	120.87	127.28
48	n	620	LUT	C11-C10-C9	-4.57	120.87	127.28
46	h1	101	RRX	C7-C8-C9	4.57	132.99	126.23
47	n1	601	CHL	C1C-CHC-C4B	4.56	132.40	116.07
47	Y	601	CHL	C1C-CHC-C4B	4.56	132.40	116.07
49	r	622	XAT	C38-C25-C24	4.56	119.37	114.24
41	n	624	LHG	O7-C7-C8	4.56	121.35	111.48
31	s	610	CLA	O2D-CGD-CBD	4.56	119.20	111.23
47	S1	606	CHL	C1C-CHC-C4B	4.56	132.39	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	n1	622	XAT	C18-C5-C4	4.56	119.36	114.24
50	N1	623	NEX	C38-C25-C24	4.56	119.36	114.24
47	Y1	607	CHL	C1C-CHC-C4B	4.56	132.38	116.07
31	B1	615	CLA	O2D-CGD-CBD	4.56	119.20	111.23
31	A	407	CLA	O2D-CGD-CBD	4.56	119.20	111.23
31	y1	611	CLA	O2D-CGD-CBD	4.55	119.19	111.23
35	B1	622	LMG	O7-C10-C11	4.55	121.33	111.48
48	G1	621	LUT	C21-C26-C27	4.55	118.06	112.83
47	n	607	CHL	C1C-CHC-C4B	4.55	132.35	116.07
47	G	607	CHL	C1C-CHC-C4B	4.55	132.34	116.07
47	R	606	CHL	C1C-CHC-C4B	4.54	132.33	116.07
47	n	609	CHL	C1B-CHB-C4A	4.54	124.25	121.32
47	S	601	CHL	C1C-CHC-C4B	4.54	132.33	116.07
31	C1	508	CLA	O2D-CGD-CBD	4.54	119.17	111.23
50	y	623	NEX	C2-C1-C6	4.54	113.62	109.21
47	N1	607	CHL	C1C-CHC-C4B	4.54	132.31	116.07
31	C1	504	CLA	O2D-CGD-CBD	4.54	119.16	111.23
49	n	622	XAT	C38-C25-C24	4.53	119.33	114.24
48	N1	621	LUT	C35-C34-C33	-4.53	120.92	127.28
47	n1	608	CHL	C1C-CHC-C4B	4.53	132.29	116.07
50	n	623	NEX	C27-C28-C29	-4.53	118.51	125.53
47	n	606	CHL	C1C-CHC-C4B	4.52	132.26	116.07
33	d	404	BCR	C1-C6-C5	-4.52	116.45	122.64
48	G1	620	LUT	C21-C26-C27	4.52	118.03	112.83
50	S1	623	NEX	C38-C25-C24	4.52	119.32	114.24
47	Y	607	CHL	C1C-CHC-C4B	4.52	132.24	116.07
49	r1	621	XAT	C18-C5-C4	4.52	119.32	114.24
35	b1	622	LMG	O7-C10-C11	4.52	121.25	111.48
47	s1	607	CHL	C1C-CHC-C4B	4.52	132.23	116.07
47	n	608	CHL	C1C-CHC-C4B	4.51	132.22	116.07
31	G1	602	CLA	CMD-C2D-C1D	4.51	132.67	124.73
47	N1	609	CHL	C1C-CHC-C4B	4.51	132.20	116.07
47	R	607	CHL	C1C-CHC-C4B	4.51	132.19	116.07
47	G	606	CHL	C1C-CHC-C4B	4.51	132.19	116.07
49	N	622	XAT	C18-C5-C4	4.50	119.30	114.24
48	n1	621	LUT	C35-C34-C33	-4.50	120.96	127.28
48	s	620	LUT	C31-C30-C29	-4.50	120.97	127.28
37	b1	620	C7Z	C27-C28-C29	-4.50	119.58	126.23
47	N1	608	CHL	C3D-C4D-CHA	4.50	115.37	108.54
48	y	621	LUT	C21-C26-C27	4.50	117.99	112.83
49	g	622	XAT	C18-C5-C4	4.49	119.29	114.24
31	c	513	CLA	CMD-C2D-C1D	4.49	132.64	124.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A	405	CLA	O2D-CGD-CBD	4.49	119.08	111.23
49	g1	622	XAT	C31-C30-C29	-4.49	120.98	127.28
47	s	601	CHL	C1C-CHC-C4B	4.49	132.13	116.07
48	g	621	LUT	C11-C10-C9	-4.49	120.98	127.28
31	c	504	CLA	O2A-C1-C2	4.49	125.37	108.11
47	r1	606	CHL	C1C-CHC-C4B	4.48	132.12	116.07
50	y1	623	NEX	C2-C1-C6	4.48	113.57	109.21
31	B1	613	CLA	CMD-C2D-C1D	4.48	132.62	124.73
47	R1	606	CHL	C1C-CHC-C4B	4.48	132.09	116.07
50	S	622	NEX	C38-C25-C24	4.48	119.27	114.24
47	y	607	CHL	C1C-CHC-C4B	4.47	132.07	116.07
31	A1	406	CLA	O2D-CGD-CBD	4.47	119.05	111.23
47	s1	601	CHL	C1C-CHC-C4B	4.47	132.05	116.07
48	n	620	LUT	C31-C30-C29	-4.47	121.02	127.28
31	Y	611	CLA	O2D-CGD-CBD	4.46	119.03	111.23
37	B	620	C7Z	C35-C34-C33	-4.46	121.02	127.28
47	r	607	CHL	C1C-CHC-C4B	4.46	132.02	116.07
48	Y	621	LUT	C35-C34-C33	-4.46	121.03	127.28
31	a	405	CLA	O2D-CGD-CBD	4.46	119.02	111.23
44	d1	405	PL9	C7-C3-C2	-4.46	118.14	123.39
48	y	620	LUT	C11-C10-C9	-4.45	121.03	127.28
31	B	617	CLA	C1-C2-C3	-4.45	118.90	126.20
47	N	606	CHL	C1C-CHC-C4B	4.45	131.98	116.07
50	G	623	NEX	C38-C25-C24	4.44	119.23	114.24
31	g1	604	CLA	O2A-C1-C2	4.44	119.55	108.99
49	G	622	XAT	C31-C30-C29	-4.43	121.06	127.28
48	Y1	621	LUT	C7-C8-C9	-4.43	119.68	126.23
48	N	621	LUT	C7-C8-C9	-4.43	119.68	126.23
31	a	406	CLA	O2D-CGD-CBD	4.43	118.97	111.23
48	R	620	LUT	C31-C32-C33	-4.43	114.22	126.36
48	s1	620	LUT	C11-C10-C9	-4.43	121.07	127.28
47	n1	606	CHL	C1C-CHC-C4B	4.42	131.90	116.07
49	r1	621	XAT	C31-C30-C29	-4.42	121.08	127.28
47	R1	606	CHL	C3D-C4D-CHA	4.42	115.26	108.54
31	r1	609	CLA	C1-C2-C3	-4.42	118.95	126.20
47	n	608	CHL	C3D-C4D-CHA	4.42	115.26	108.54
47	g	608	CHL	C3D-C4D-CHA	4.42	115.26	108.54
41	d	408	LHG	O7-C7-C8	4.42	121.03	111.48
49	G	622	XAT	C38-C25-C24	4.41	119.19	114.24
41	D	409	LHG	O7-C7-C8	4.41	121.02	111.48
47	y1	607	CHL	C3D-C4D-CHA	4.41	115.24	108.54
41	N1	624	LHG	O7-C7-C8	4.41	121.01	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	S1	621	LUT	C35-C34-C33	-4.40	121.10	127.28
50	R	622	NEX	C17-C1-C6	-4.40	106.53	110.47
48	G	620	LUT	C11-C10-C9	-4.40	121.11	127.28
46	H	101	RRX	C30-C25-C26	-4.40	116.63	122.64
35	c1	521	LMG	O7-C10-C11	4.40	120.99	111.48
48	N	621	LUT	C11-C10-C9	-4.39	121.11	127.28
31	y	602	CLA	CMD-C2D-C1D	4.39	132.46	124.73
47	Y1	601	CHL	C1C-CHC-C4B	4.39	131.78	116.07
47	G1	606	CHL	C1C-CHC-C4B	4.39	131.78	116.07
31	B	605	CLA	O2A-C1-C2	4.39	125.00	108.11
37	B1	620	C7Z	C35-C34-C33	-4.39	121.12	127.28
37	B1	620	C7Z	C21-C26-C25	-4.39	116.64	122.64
33	C1	514	BCR	C15-C14-C13	-4.38	121.13	127.28
31	a1	405	CLA	O2D-CGD-CBD	4.38	118.89	111.23
49	g1	622	XAT	C18-C5-C4	4.37	119.15	114.24
41	S1	624	LHG	O7-C7-C8	4.37	120.94	111.48
41	d	410	LHG	O7-C7-C8	4.37	120.93	111.48
31	C1	505	CLA	O2D-CGD-CBD	4.37	118.87	111.23
41	g1	624	LHG	O7-C7-C8	4.37	120.93	111.48
32	A1	408	PHO	C2B-C1B-NB	-4.37	106.27	109.43
31	s1	614	CLA	O2D-CGD-CBD	4.36	118.86	111.23
48	s1	621	LUT	C7-C8-C9	-4.36	119.78	126.23
40	C	519	DGD	O2G-C1B-C2B	4.36	120.91	111.48
48	S1	620	LUT	C7-C8-C9	-4.35	119.80	126.23
48	y	621	LUT	C7-C8-C9	-4.35	119.80	126.23
33	c	516	BCR	C23-C24-C25	-4.35	115.39	127.00
41	S	624	LHG	O7-C7-C8	4.35	120.88	111.48
48	R1	620	LUT	C15-C14-C13	-4.34	121.19	127.28
48	g1	620	LUT	C35-C34-C33	-4.34	121.19	127.28
50	S1	623	NEX	C2-C1-C6	4.34	113.43	109.21
31	c1	512	CLA	CMD-C2D-C1D	4.34	132.37	124.73
48	G1	620	LUT	C35-C34-C33	-4.34	121.19	127.28
47	R	606	CHL	C3D-C4D-CHA	4.34	115.13	108.54
47	r1	607	CHL	C3D-C4D-CHA	4.34	115.13	108.54
47	n1	607	CHL	C3D-C4D-CHA	4.33	115.12	108.54
49	g	622	XAT	C38-C25-C24	4.33	119.10	114.24
48	g	621	LUT	C7-C8-C9	-4.33	119.83	126.23
46	h1	101	RRX	C30-C25-C26	-4.33	116.72	122.64
47	G	609	CHL	C1B-CHB-C4A	4.32	124.10	121.32
41	G	630	LHG	O7-C7-C8	4.32	120.83	111.48
35	a	413	LMG	O7-C10-C11	4.32	120.83	111.48
31	A	406	CLA	O2D-CGD-CBD	4.32	118.78	111.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	N	607	CHL	C3D-C4D-CHA	4.32	115.11	108.54
31	B	617	CLA	CMD-C2D-C1D	4.32	132.34	124.73
49	G1	622	XAT	C18-C5-C4	4.32	119.09	114.24
31	r1	608	CLA	O2D-CGD-CBD	4.32	118.78	111.23
40	C	523	DGD	O2G-C1B-C2B	4.32	120.82	111.48
47	s	607	CHL	C3D-C4D-CHA	4.31	115.10	108.54
47	y1	601	CHL	C1C-CHC-C4B	4.31	131.50	116.07
41	d1	410	LHG	O7-C7-C8	4.31	120.81	111.48
48	G1	620	LUT	C15-C14-C13	-4.31	121.23	127.28
47	s1	601	CHL	C3D-C4D-CHA	4.31	115.08	108.54
31	C	502	CLA	C1-C2-C3	-4.30	119.14	126.20
41	D1	409	LHG	O7-C7-C8	4.30	120.79	111.48
47	R1	607	CHL	C3D-C4D-CHA	4.29	115.06	108.54
48	S	620	LUT	C35-C34-C33	-4.29	121.26	127.28
52	i	101	3PH	O21-C21-C22	4.29	120.75	111.48
47	n	609	CHL	C3D-C4D-CHA	4.28	115.05	108.54
46	H1	101	RRX	C21-C20-C19	-4.28	110.80	123.20
47	r	606	CHL	C3D-C4D-CHA	4.28	115.05	108.54
48	n1	620	LUT	C21-C26-C27	4.28	117.74	112.83
41	D1	408	LHG	O7-C7-C8	4.28	120.73	111.48
48	G1	620	LUT	C7-C8-C9	-4.28	119.91	126.23
37	B1	620	C7Z	C1-C6-C5	-4.28	116.79	122.64
49	y1	622	XAT	C36-C21-C26	4.27	121.58	110.05
49	R	621	XAT	C18-C5-C4	4.27	119.04	114.24
47	G1	607	CHL	C3D-C4D-CHA	4.27	115.03	108.54
48	s	620	LUT	C18-C5-C6	-4.27	119.83	124.48
33	c	516	BCR	C33-C5-C6	-4.27	119.83	124.48
48	G1	621	LUT	C11-C10-C9	-4.27	121.30	127.28
47	n1	606	CHL	C3D-C4D-CHA	4.26	115.02	108.54
31	B	617	CLA	O2A-C1-C2	4.26	124.50	108.11
31	b1	603	CLA	O2A-C1-C2	4.26	124.49	108.11
40	c	520	DGD	O2G-C1B-C2B	4.26	120.69	111.48
31	g	603	CLA	C1-C2-C3	-4.25	119.23	126.20
31	A1	407	CLA	O2D-CGD-CBD	4.25	118.66	111.23
49	G1	622	XAT	C38-C25-C24	4.25	119.02	114.24
50	r	623	NEX	C2-C1-C6	4.25	113.34	109.21
47	g	607	CHL	C3D-C4D-CHA	4.25	115.00	108.54
35	w1	201	LMG	O7-C10-C11	4.25	120.67	111.48
31	b1	608	CLA	O2A-C1-C2	4.25	124.45	108.11
31	C	504	CLA	C1-C2-C3	-4.25	119.24	126.20
49	R1	621	XAT	C15-C14-C13	-4.24	121.33	127.28
49	Y	622	XAT	C18-C5-C4	4.24	119.01	114.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	N	610	CLA	CAA-C2A-C3A	-4.24	101.55	113.00
32	A1	409	PHO	CMB-C2B-C3B	4.24	133.15	124.68
33	c1	516	BCR	C33-C5-C6	-4.24	119.86	124.48
31	C1	504	CLA	O2A-C1-C2	4.24	124.41	108.11
31	a1	406	CLA	O2D-CGD-CBD	4.23	118.63	111.23
47	g1	607	CHL	C3D-C4D-CHA	4.23	114.98	108.54
48	n1	620	LUT	C11-C10-C9	-4.23	121.34	127.28
47	N1	607	CHL	C3D-C4D-CHA	4.23	114.97	108.54
50	G1	623	NEX	C38-C25-C24	4.23	118.99	114.24
52	b1	624	3PH	O21-C21-C22	4.23	120.63	111.48
48	g	621	LUT	C35-C34-C33	-4.23	121.35	127.28
47	Y	607	CHL	C3D-C4D-CHA	4.23	114.97	108.54
31	b1	603	CLA	C1-C2-C3	-4.23	119.27	126.20
47	n1	601	CHL	C3D-C4D-CHA	4.23	114.97	108.54
48	Y1	620	LUT	C7-C8-C9	-4.23	119.98	126.23
47	R	607	CHL	C3D-C4D-CHA	4.23	114.96	108.54
48	r1	620	LUT	C31-C30-C29	-4.23	121.35	127.28
49	n	622	XAT	C18-C5-C4	4.22	118.98	114.24
47	y1	607	CHL	C1C-CHC-C4B	4.22	131.16	116.07
49	n1	622	XAT	C38-C25-C24	4.21	118.97	114.24
31	C1	507	CLA	O2A-C1-C2	4.21	124.31	108.11
35	D	411	LMG	O7-C10-C11	4.21	120.58	111.48
48	g	621	LUT	C15-C14-C13	-4.20	121.38	127.28
48	S	621	LUT	C11-C10-C9	-4.20	121.38	127.28
47	s	608	CHL	C3D-C4D-CHA	4.20	114.93	108.54
48	R1	620	LUT	C18-C5-C6	-4.20	119.90	124.48
31	B	605	CLA	C1-C2-C3	-4.20	119.31	126.20
47	S	607	CHL	C3D-C4D-CHA	4.20	114.92	108.54
31	c	512	CLA	O2D-CGD-CBD	4.20	118.57	111.23
47	r	607	CHL	C3D-C4D-CHA	4.20	114.92	108.54
47	y	601	CHL	C3D-C4D-CHA	4.19	114.92	108.54
35	h	102	LMG	O7-C10-C11	4.19	120.55	111.48
37	b1	620	C7Z	C7-C8-C9	-4.19	120.03	126.23
47	S1	608	CHL	C3D-C4D-CHA	4.19	114.91	108.54
47	g	605	CHL	C3D-C4D-CHA	4.19	114.91	108.54
31	n1	613	CLA	CAA-C2A-C3A	-4.19	101.68	113.00
48	y	620	LUT	C18-C5-C6	-4.19	119.91	124.48
31	n	603	CLA	O2A-C1-C2	4.18	124.21	108.11
47	g1	601	CHL	C3D-C4D-CHA	4.18	114.90	108.54
41	n1	624	LHG	O7-C7-C8	4.18	120.53	111.48
47	n	607	CHL	C3D-C4D-CHA	4.18	114.89	108.54
47	y	607	CHL	C3D-C4D-CHA	4.18	114.89	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s	614	CLA	O2A-C1-C2	4.18	124.18	108.11
47	S	608	CHL	C3D-C4D-CHA	4.18	114.89	108.54
48	R1	620	LUT	C11-C10-C9	-4.17	121.42	127.28
48	s1	621	LUT	C31-C30-C29	-4.17	121.42	127.28
48	N1	621	LUT	C11-C10-C9	-4.17	121.43	127.28
47	n1	608	CHL	C3D-C4D-CHA	4.17	114.88	108.54
47	s1	608	CHL	C3D-C4D-CHA	4.17	114.88	108.54
47	N	601	CHL	C3D-C4D-CHA	4.17	114.87	108.54
47	s1	607	CHL	C3D-C4D-CHA	4.17	114.87	108.54
47	G1	601	CHL	C3D-C4D-CHA	4.16	114.87	108.54
49	Y1	622	XAT	C7-C8-C9	-4.16	119.07	125.53
47	G1	608	CHL	C3D-C4D-CHA	4.16	114.86	108.54
31	r1	609	CLA	O2A-C1-C2	4.16	124.12	108.11
37	B1	620	C7Z	C31-C30-C29	-4.15	121.45	127.28
31	y	604	CLA	O2A-C1-C2	4.15	124.09	108.11
49	N	622	XAT	C7-C8-C9	-4.15	119.09	125.53
50	N	623	NEX	C16-C1-C6	-4.15	106.76	110.47
48	s1	621	LUT	C18-C5-C6	-4.15	119.96	124.48
50	s1	623	NEX	C27-C28-C29	-4.14	119.11	125.53
47	Y1	609	CHL	C1B-CHB-C4A	4.14	123.98	121.32
47	G	605	CHL	C3D-C4D-CHA	4.14	114.83	108.54
48	g	620	LUT	C11-C10-C9	-4.14	121.47	127.28
31	b1	605	CLA	C2C-C1C-NC	4.14	114.33	109.98
47	Y	605	CHL	C3D-C4D-CHA	4.14	114.83	108.54
35	d1	411	LMG	O7-C10-C11	4.14	120.43	111.48
31	c1	513	CLA	C1-C2-C3	-4.13	119.42	126.20
49	G1	622	XAT	C7-C8-C9	-4.13	119.12	125.53
50	Y	623	NEX	C27-C28-C29	-4.13	119.12	125.53
48	N	621	LUT	C35-C34-C33	-4.13	121.49	127.28
41	s	624	LHG	O7-C7-C8	4.13	120.41	111.48
52	t1	101	3PH	O21-C21-C22	4.13	120.41	111.48
49	Y1	622	XAT	C36-C21-C26	4.13	121.19	110.05
46	H	101	RRX	C23-C24-C25	-4.13	115.98	127.00
47	G	606	CHL	C3D-C4D-CHA	4.12	114.81	108.54
33	D	404	BCR	C19-C18-C17	4.12	125.50	119.01
35	C1	523	LMG	O7-C10-C11	4.12	120.39	111.48
47	G	607	CHL	C3D-C4D-CHA	4.12	114.80	108.54
31	c	511	CLA	C1-C2-C3	-4.12	119.45	126.20
31	D1	402	CLA	O2A-C1-C2	4.12	123.95	108.11
47	g	609	CHL	C3D-C4D-CHA	4.11	114.79	108.54
47	y1	601	CHL	C3D-C4D-CHA	4.11	114.79	108.54
47	y	605	CHL	C3D-C4D-CHA	4.11	114.78	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	y	606	CHL	C3D-C4D-CHA	4.11	114.78	108.54
47	S1	601	CHL	C3D-C4D-CHA	4.11	114.78	108.54
50	n	623	NEX	C2-C1-C6	4.11	113.20	109.21
47	N	608	CHL	C3D-C4D-CHA	4.10	114.78	108.54
47	Y	606	CHL	C3D-C4D-CHA	4.10	114.78	108.54
48	y1	620	LUT	C7-C8-C9	-4.10	120.16	126.23
47	g1	608	CHL	C3D-C4D-CHA	4.10	114.78	108.54
47	N	606	CHL	C3D-C4D-CHA	4.10	114.78	108.54
47	n	606	CHL	C3D-C4D-CHA	4.10	114.78	108.54
38	c1	524	DGA	OG2-CB1-CB2	4.10	120.35	111.48
49	g1	622	XAT	C38-C25-C24	4.10	118.85	114.24
47	S1	606	CHL	C3D-C4D-CHA	4.10	114.77	108.54
47	n	601	CHL	C3D-C4D-CHA	4.10	114.77	108.54
47	Y1	609	CHL	C3D-C4D-CHA	4.10	114.77	108.54
49	y	622	XAT	C36-C21-C26	4.09	121.09	110.05
47	G	609	CHL	C3D-C4D-CHA	4.09	114.76	108.54
47	y1	609	CHL	C3D-C4D-CHA	4.09	114.76	108.54
50	s	623	NEX	C16-C1-C6	-4.09	106.81	110.47
41	D	408	LHG	O7-C7-C8	4.09	120.32	111.48
50	y1	623	NEX	C38-C25-C24	4.09	118.83	114.24
48	S	620	LUT	C7-C8-C9	-4.08	120.19	126.23
50	G1	623	NEX	C31-C30-C29	4.08	133.01	127.28
33	d	404	BCR	C4-C5-C6	-4.08	117.19	122.70
41	y	624	LHG	O7-C7-C8	4.08	120.31	111.48
31	S	604	CLA	C1-C2-C3	-4.07	119.53	126.20
48	Y1	621	LUT	C35-C34-C33	-4.07	121.57	127.28
33	b1	618	BCR	C15-C14-C13	-4.07	121.57	127.28
47	g1	605	CHL	C3D-C4D-CHA	4.07	114.72	108.54
35	C	521	LMG	O7-C10-C11	4.06	120.27	111.48
47	r1	606	CHL	C3D-C4D-CHA	4.06	114.72	108.54
31	c1	511	CLA	O2A-C1-C2	4.06	123.75	108.11
49	Y	622	XAT	C36-C21-C26	4.06	121.02	110.05
47	Y1	607	CHL	C3D-C4D-CHA	4.06	114.72	108.54
47	y1	605	CHL	C3D-C4D-CHA	4.06	114.71	108.54
50	G	623	NEX	C31-C30-C29	4.06	132.97	127.28
31	c	502	CLA	O2A-C1-C2	4.06	123.73	108.11
47	G1	606	CHL	C3D-C4D-CHA	4.06	114.71	108.54
41	D1	410	LHG	O7-C7-C8	4.06	120.26	111.48
47	s	606	CHL	C3D-C4D-CHA	4.06	114.71	108.54
48	y	621	LUT	C11-C10-C9	-4.06	121.59	127.28
31	S	605	CLA	O2A-C1-C2	4.06	123.71	108.11
40	c	523	DGD	O2G-C1B-C2B	4.05	120.25	111.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	N1	606	CHL	C3D-C4D-CHA	4.05	114.70	108.54
46	H1	101	RRX	C4-C5-C6	-4.05	117.23	122.70
47	Y1	605	CHL	C3D-C4D-CHA	4.05	114.70	108.54
31	B1	605	CLA	C1-C2-C3	-4.05	119.56	126.20
31	a	410	CLA	C1-C2-C3	-4.05	119.56	126.20
31	R1	609	CLA	C1-C2-C3	-4.04	119.57	126.20
31	C	504	CLA	O2A-C1-C2	4.04	123.66	108.11
31	B1	612	CLA	O2A-C1-C2	4.04	123.66	108.11
41	C	525	LHG	O7-C7-C8	4.04	120.22	111.48
47	Y1	601	CHL	C3D-C4D-CHA	4.04	114.68	108.54
54	I1	102	4RF	O21-C22-C24	4.04	120.22	111.48
31	c	513	CLA	O2A-C1-C2	4.04	123.65	108.11
48	R	620	LUT	C35-C34-C33	-4.04	121.62	127.28
31	n	602	CLA	O2A-C1-C2	4.04	123.64	108.11
47	G	608	CHL	C3D-C4D-CHA	4.04	114.67	108.54
47	s	601	CHL	C3D-C4D-CHA	4.04	114.67	108.54
47	N1	601	CHL	C3D-C4D-CHA	4.04	114.67	108.54
35	J	101	LMG	O7-C10-C11	4.04	120.21	111.48
47	Y1	606	CHL	C3D-C4D-CHA	4.03	114.67	108.54
31	d	402	CLA	O2A-C1-C2	4.03	123.62	108.11
47	G1	609	CHL	C3D-C4D-CHA	4.03	114.67	108.54
31	B	615	CLA	O2A-C1-C2	4.03	123.62	108.11
33	c1	516	BCR	C15-C14-C13	-4.03	121.62	127.28
47	g1	609	CHL	C3D-C4D-CHA	4.03	114.66	108.54
31	b	608	CLA	O2A-C1-C2	4.03	123.61	108.11
31	B	612	CLA	CMD-C2D-C1D	4.03	131.82	124.73
31	B1	614	CLA	O2D-CGD-CBD	4.03	118.27	111.23
31	c1	504	CLA	O2A-C1-C2	4.02	123.59	108.11
48	N	621	LUT	C15-C14-C13	-4.02	121.64	127.28
47	S	606	CHL	C3D-C4D-CHA	4.02	114.65	108.54
50	G	623	NEX	C2-C1-C6	4.02	113.12	109.21
47	N	605	CHL	C3D-C4D-CHA	4.02	114.65	108.54
40	C	520	DGD	O2G-C1B-C2B	4.02	120.17	111.48
31	A1	405	CLA	CAC-C3C-C4C	-4.02	119.56	124.79
57	y1	626	PTY	O7-C8-C11	4.02	120.17	111.48
47	S1	607	CHL	C3D-C4D-CHA	4.02	114.64	108.54
44	D	405	PL9	C7-C3-C2	-4.01	118.66	123.39
48	Y1	620	LUT	C21-C26-C27	4.01	117.44	112.83
56	R1	626	ERG	C1-C2-C3	4.01	115.79	110.48
48	Y	621	LUT	C7-C8-C9	-4.01	120.30	126.23
33	C1	517	BCR	C23-C22-C21	4.01	125.31	119.01
50	G	623	NEX	C27-C28-C29	-4.00	119.32	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	d	404	BCR	C19-C18-C17	4.00	125.31	119.01
31	g1	603	CLA	C1-C2-C3	-4.00	119.64	126.20
48	N1	621	LUT	C7-C8-C9	-4.00	120.31	126.23
48	G	620	LUT	C15-C14-C13	-4.00	121.67	127.28
47	n1	605	CHL	C3D-C4D-CHA	4.00	114.62	108.54
41	c1	525	LHG	O7-C7-C8	4.00	120.13	111.48
46	h	101	RRX	C11-C10-C9	-4.00	121.67	127.28
35	h1	102	LMG	O7-C10-C11	3.99	120.12	111.48
31	N1	604	CLA	O2A-C1-C2	3.99	123.47	108.11
33	d1	404	BCR	C1-C6-C5	-3.99	117.18	122.64
31	n	604	CLA	O2A-C1-C2	3.99	123.47	108.11
31	S1	617	CLA	C1-C2-C3	-3.99	120.31	126.76
31	b	617	CLA	CMD-C2D-C1D	3.99	131.75	124.73
50	y	623	NEX	C27-C28-C29	-3.99	119.34	125.53
31	S1	613	CLA	C1-C2-C3	-3.99	119.67	126.20
47	g	601	CHL	C3D-C4D-CHA	3.99	114.60	108.54
31	c1	513	CLA	O2A-C1-C2	3.99	123.45	108.11
47	G1	605	CHL	C3D-C4D-CHA	3.99	114.60	108.54
47	s1	606	CHL	C3D-C4D-CHA	3.99	114.60	108.54
31	A	406	CLA	C1-C2-C3	-3.98	119.67	126.20
38	b	623	DGA	OG2-CB1-CB2	3.98	120.10	111.48
31	B1	606	CLA	O2A-C1-C2	3.98	123.42	108.11
48	N	620	LUT	C7-C8-C9	-3.98	120.35	126.23
56	r1	626	ERG	C2-C1-C10	3.98	121.25	112.78
47	y	609	CHL	C3D-C4D-CHA	3.98	114.59	108.54
31	c1	501	CLA	O2A-C1-C2	3.98	123.41	108.11
50	g	623	NEX	C2-C1-C6	3.97	113.07	109.21
52	s	626	3PH	O21-C21-C22	3.97	120.08	111.48
31	b1	603	CLA	C1-O2A-CGA	3.97	126.27	116.65
31	y	608	CLA	O2A-C1-C2	3.97	123.40	108.11
31	S	617	CLA	C1-C2-C3	-3.97	120.34	126.76
50	n	623	NEX	C38-C25-C24	3.97	118.70	114.24
48	g1	620	LUT	C15-C14-C13	-3.97	121.71	127.28
31	Y1	610	CLA	C1-C2-C3	-3.97	119.70	126.20
31	s1	613	CLA	C1-C2-C3	-3.97	119.70	126.20
52	T1	101	3PH	O21-C21-C22	3.97	120.06	111.48
31	r1	603	CLA	O2A-C1-C2	3.97	123.37	108.11
31	r1	610	CLA	O2A-C1-C2	3.96	123.36	108.11
31	S1	604	CLA	O2A-C1-C2	3.96	123.36	108.11
31	G1	613	CLA	C1-C2-C3	-3.96	119.71	126.20
48	n	621	LUT	C7-C8-C9	-3.96	120.38	126.23
48	S1	620	LUT	C18-C5-C6	-3.96	120.17	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	n	605	CHL	C3D-C4D-CHA	3.95	114.55	108.54
49	r	622	XAT	C18-C5-C4	3.95	118.68	114.24
47	g1	606	CHL	C3D-C4D-CHA	3.95	114.55	108.54
31	B1	610	CLA	O2A-C1-C2	3.95	123.31	108.11
48	Y1	620	LUT	C35-C34-C33	-3.95	121.74	127.28
31	c	509	CLA	C2C-C1C-NC	3.95	114.13	109.98
40	c1	520	DGD	O2G-C1B-C2B	3.95	120.02	111.48
33	B	618	BCR	C23-C24-C25	-3.95	116.45	127.00
31	c	503	CLA	C1-C2-C3	-3.95	119.73	126.20
33	A	411	BCR	C33-C5-C6	-3.94	120.18	124.48
31	C1	508	CLA	O2A-C1-C2	3.94	123.27	108.11
52	S	626	3PH	O21-C21-C22	3.94	120.00	111.48
49	y1	622	XAT	C38-C25-C24	3.94	118.67	114.24
50	N	623	NEX	C27-C28-C29	-3.94	119.42	125.53
47	Y	601	CHL	C3D-C4D-CHA	3.94	114.52	108.54
31	g	610	CLA	C1-C2-C3	-3.93	119.75	126.20
31	n	610	CLA	O2A-C1-C2	3.93	123.25	108.11
35	B	622	LMG	O7-C10-C11	3.93	119.99	111.48
50	Y	623	NEX	C31-C30-C29	3.93	132.79	127.28
41	d1	409	LHG	O7-C7-C8	3.93	119.98	111.48
31	B1	612	CLA	C1-C2-C3	-3.93	119.76	126.20
31	c1	507	CLA	O2A-C1-C2	3.93	123.22	108.11
31	s1	605	CLA	O2A-C1-C2	3.93	123.21	108.11
50	y1	623	NEX	C31-C30-C29	3.92	132.78	127.28
47	N1	605	CHL	C3D-C4D-CHA	3.92	114.50	108.54
48	y1	620	LUT	C18-C5-C6	-3.92	120.20	124.48
46	H1	101	RRX	C1-C6-C5	-3.92	117.28	122.64
50	Y1	623	NEX	C27-C28-C29	-3.92	119.44	125.53
31	n	613	CLA	O2A-C1-C2	3.92	123.20	108.11
35	A	413	LMG	O7-C10-C11	3.92	119.96	111.48
47	N	609	CHL	C3D-C4D-CHA	3.92	114.50	108.54
31	a1	405	CLA	O2A-C1-C2	3.92	123.20	108.11
41	G1	624	LHG	O7-C7-C8	3.92	119.96	111.48
57	Y1	626	PTY	O7-C8-C11	3.92	119.96	111.48
31	B1	605	CLA	O2A-C1-C2	3.92	123.19	108.11
31	G1	603	CLA	O2A-C1-C2	3.92	123.18	108.11
31	B1	608	CLA	O2A-C1-C2	3.92	123.18	108.11
31	G1	613	CLA	O2A-C1-C2	3.91	123.17	108.11
31	N1	604	CLA	C1-C2-C3	-3.91	119.79	126.20
31	C	508	CLA	O2A-C1-C2	3.91	123.16	108.11
46	h1	101	RRX	C21-C20-C19	-3.91	111.88	123.20
47	S	601	CHL	C3D-C4D-CHA	3.91	114.48	108.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	c	524	DGA	OG2-CB1-CB2	3.91	119.93	111.48
47	y1	606	CHL	C3D-C4D-CHA	3.91	114.48	108.54
31	n1	602	CLA	C1-C2-C3	-3.90	119.80	126.20
56	R1	626	ERG	C18-C13-C12	-3.90	104.85	110.61
31	C	502	CLA	O2A-C1-C2	3.90	123.12	108.11
47	n1	609	CHL	C3D-C4D-CHA	3.90	114.46	108.54
31	b	610	CLA	O2A-C1-C2	3.90	123.10	108.11
31	G	613	CLA	CMA-C3A-C4A	3.90	122.25	111.77
48	y1	621	LUT	C7-C8-C9	-3.89	120.48	126.23
31	b1	605	CLA	O2A-C1-C2	3.89	123.08	108.11
31	y1	608	CLA	C1-C2-C3	-3.89	120.47	126.76
49	y	622	XAT	C38-C25-C24	3.89	118.61	114.24
31	b1	609	CLA	C1-C2-C3	-3.89	119.83	126.20
48	S1	621	LUT	C18-C5-C6	-3.89	120.24	124.48
31	s	613	CLA	C1-C2-C3	-3.89	119.83	126.20
31	g	610	CLA	O2A-C1-C2	3.89	123.06	108.11
31	c	508	CLA	C1-C2-C3	-3.88	119.83	126.20
31	S1	605	CLA	O2A-C1-C2	3.88	123.05	108.11
31	C1	505	CLA	O2A-C1-C2	3.88	123.05	108.11
46	h	101	RRX	C1-C6-C5	-3.88	117.33	122.64
31	N1	603	CLA	O2A-C1-C2	3.88	123.04	108.11
31	S1	604	CLA	C1-C2-C3	-3.88	119.84	126.20
31	B	603	CLA	C1-C2-C3	-3.88	119.84	126.20
31	a	405	CLA	O2A-C1-C2	3.88	123.03	108.11
31	c	512	CLA	O2A-C1-C2	3.88	123.02	108.11
31	y1	611	CLA	O2A-C1-C2	3.87	123.02	108.11
31	n1	602	CLA	O2A-C1-C2	3.87	123.02	108.11
31	N	604	CLA	O2A-C1-C2	3.87	123.02	108.11
31	c1	501	CLA	C1-C2-C3	-3.87	119.85	126.20
50	N	623	NEX	C2-C1-C6	3.87	112.97	109.21
52	B1	624	3PH	O21-C21-C22	3.87	119.86	111.48
42	c	627	LMK	O3-C4-C3	-3.87	110.01	122.95
47	g	606	CHL	C3D-C4D-CHA	3.87	114.42	108.54
41	Y1	624	LHG	O7-C7-C8	3.87	119.85	111.48
48	Y	621	LUT	C11-C10-C9	-3.87	121.85	127.28
50	N1	623	NEX	C27-C28-C29	-3.86	119.54	125.53
31	G1	610	CLA	O2A-C1-C2	3.86	122.96	108.11
47	Y	609	CHL	C3D-C4D-CHA	3.86	114.40	108.54
33	B	618	BCR	C15-C14-C13	-3.86	121.87	127.28
48	Y	620	LUT	C31-C30-C29	-3.86	121.87	127.28
35	a1	413	LMG	O7-C10-C11	3.86	119.82	111.48
48	N1	620	LUT	C35-C34-C33	-3.85	121.87	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	G	621	LUT	C15-C14-C13	-3.85	121.88	127.28
47	G	601	CHL	C3D-C4D-CHA	3.85	114.39	108.54
35	j	101	LMG	O7-C10-C11	3.85	119.80	111.48
31	C	509	CLA	C1-C2-C3	-3.85	119.90	126.20
31	N	613	CLA	O2A-C1-C2	3.85	122.91	108.11
48	N	620	LUT	C21-C26-C27	3.84	117.25	112.83
37	B1	620	C7Z	C27-C28-C29	-3.84	120.55	126.23
31	g1	603	CLA	O2A-C1-C2	3.84	122.90	108.11
35	C1	521	LMG	O7-C10-C11	3.84	119.79	111.48
38	B	625	DGA	OG2-CB1-CB2	3.84	119.79	111.48
31	G	602	CLA	O2A-C1-C2	3.84	122.87	108.11
49	R	621	XAT	C38-C25-C26	-3.84	115.99	122.30
38	C	524	DGA	OG2-CB1-CB2	3.84	119.78	111.48
31	B	615	CLA	CAA-C2A-C3A	-3.83	102.64	113.00
31	n	613	CLA	CMA-C3A-C4A	3.83	122.08	111.77
33	D	404	BCR	C23-C22-C21	3.83	125.04	119.01
50	n1	623	NEX	C38-C25-C24	3.83	118.55	114.24
31	R1	610	CLA	C1-C2-C3	-3.83	119.92	126.20
32	a1	408	PHO	C2B-C1B-NB	-3.83	106.66	109.43
31	r	609	CLA	O2A-C1-C2	3.83	122.83	108.11
31	B	611	CLA	O2A-C1-C2	3.82	122.82	108.11
31	b	615	CLA	CAA-C2A-C3A	-3.82	102.67	113.00
48	g1	621	LUT	C7-C8-C9	-3.82	120.58	126.23
31	s	614	CLA	C1-C2-C3	-3.82	119.94	126.20
31	A1	405	CLA	C1-C2-C3	-3.82	119.94	126.20
32	A	409	PHO	C2B-C1B-NB	-3.82	106.67	109.43
41	Y	624	LHG	O7-C7-C8	3.82	119.75	111.48
31	g1	602	CLA	O2A-C1-C2	3.82	122.81	108.11
31	D	402	CLA	O2A-C1-C2	3.82	122.80	108.11
54	i1	101	4RF	O21-C22-C24	3.82	119.74	111.48
31	y1	611	CLA	C1-C2-C3	-3.82	119.94	126.20
50	Y	623	NEX	C17-C1-C6	-3.82	107.06	110.47
31	R1	609	CLA	O2A-C1-C2	3.82	122.79	108.11
56	R1	626	ERG	C2-C1-C10	3.81	120.90	112.78
31	g	602	CLA	O2A-C1-C2	3.81	122.78	108.11
38	J1	101	DGA	OG2-CB1-CB2	3.81	119.72	111.48
48	y	621	LUT	C35-C34-C33	-3.81	121.94	127.28
50	g1	623	NEX	C27-C28-C29	-3.81	119.62	125.53
31	s	602	CLA	O2A-C1-C2	3.80	122.75	108.11
46	H	101	RRX	C1-C6-C5	-3.80	117.44	122.64
31	b	603	CLA	O2A-C1-C2	3.80	122.75	108.11
31	Y1	608	CLA	C1-C2-C3	-3.80	120.61	126.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	S1	603	CLA	O2A-C1-C2	3.80	122.74	108.11
31	b	617	CLA	C1-C2-C3	-3.80	119.97	126.20
31	C	513	CLA	O2A-C1-C2	3.80	122.73	108.11
33	c	515	BCR	C4-C5-C6	-3.80	117.57	122.70
31	s	609	CLA	CMA-C3A-C4A	3.80	121.97	111.77
31	C	508	CLA	C1-C2-C3	-3.80	119.98	126.20
31	B	615	CLA	CBA-CAA-C2A	3.80	125.08	113.79
31	s1	611	CLA	OBD-CAD-C3D	-3.79	119.55	128.42
31	r1	612	CLA	O2A-C1-C2	3.79	122.70	108.11
31	Y	613	CLA	C1-C2-C3	-3.79	119.98	126.20
50	n1	623	NEX	C27-C28-C29	-3.79	119.65	125.53
47	G	601	CHL	CHA-C1A-C2A	-3.79	124.41	133.31
31	b1	612	CLA	O2A-C1-C2	3.79	122.69	108.11
31	C1	512	CLA	C1-C2-C3	-3.79	119.99	126.20
48	G1	620	LUT	C31-C30-C29	-3.79	121.97	127.28
32	A	408	PHO	C2B-C1B-NB	-3.78	106.69	109.43
31	c	501	CLA	O2A-C1-C2	3.78	122.65	108.11
50	g1	623	NEX	C31-C30-C29	3.78	132.58	127.28
48	g1	621	LUT	C11-C10-C9	-3.78	121.98	127.28
31	B	606	CLA	O2A-C1-C2	3.77	122.64	108.11
31	s1	613	CLA	O2A-C1-C2	3.77	122.63	108.11
31	s	617	CLA	C1-C2-C3	-3.77	120.66	126.76
48	N	621	LUT	C26-C27-C28	-3.77	118.71	124.58
40	c	518	DGD	O2G-C1B-C2B	3.77	119.64	111.48
48	S	620	LUT	C15-C14-C13	-3.77	121.99	127.28
31	c	505	CLA	C1-C2-C3	-3.77	120.02	126.20
31	S1	602	CLA	O2A-C1-C2	3.77	122.61	108.11
35	d	411	LMG	O7-C10-C11	3.77	119.63	111.48
48	n	621	LUT	C11-C10-C9	-3.77	122.00	127.28
48	s1	621	LUT	C11-C10-C9	-3.76	122.00	127.28
31	c1	512	CLA	O2A-C1-C2	3.76	122.59	108.11
41	d1	408	LHG	O7-C7-C8	3.76	119.62	111.48
31	s	605	CLA	O2A-C1-C2	3.76	122.58	108.11
31	y	610	CLA	O2A-C1-C2	3.76	122.58	108.11
46	h1	101	RRX	C4-C5-C6	-3.76	117.62	122.70
31	b	615	CLA	O2A-C1-C2	3.76	122.58	108.11
41	c	625	LHG	O7-C7-C8	3.76	119.62	111.48
31	N1	613	CLA	O2A-C1-C2	3.76	122.58	108.11
33	b1	618	BCR	C27-C26-C25	-3.76	117.63	122.70
38	j1	101	DGA	OG2-CB1-CB2	3.76	119.61	111.48
40	c1	519	DGD	O2G-C1B-C2B	3.75	119.60	111.48
48	R	620	LUT	C26-C27-C28	-3.75	118.74	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	510	CLA	O2A-C1-C2	3.75	122.56	108.11
31	c1	511	CLA	C1-C2-C3	-3.75	120.05	126.20
38	C1	524	DGA	OG2-CB1-CB2	3.75	119.60	111.48
33	C	515	BCR	C33-C5-C6	-3.75	120.39	124.48
50	R1	622	NEX	C27-C28-C29	-3.75	119.71	125.53
31	G	610	CLA	O2A-C1-C2	3.75	122.55	108.11
31	r1	608	CLA	O2A-C1-C2	3.75	122.54	108.11
31	b	609	CLA	C1-C2-C3	-3.75	120.05	126.20
41	s1	624	LHG	O7-C7-C8	3.75	119.59	111.48
31	S	613	CLA	O2A-C1-C2	3.75	122.54	108.11
31	g1	611	CLA	O2A-C1-C2	3.75	122.54	108.11
54	k1	101	4RF	O21-C22-C24	3.75	119.59	111.48
31	G1	610	CLA	C1-C2-C3	-3.75	120.06	126.20
31	c	511	CLA	CMA-C3A-C4A	3.75	121.85	111.77
31	c	510	CLA	C1-C2-C3	-3.75	120.06	126.20
31	B1	604	CLA	O2A-C1-C2	3.74	122.52	108.11
33	C1	515	BCR	C33-C5-C6	-3.74	120.40	124.48
31	c	504	CLA	C1-C2-C3	-3.74	120.07	126.20
48	G	620	LUT	C35-C34-C33	-3.74	122.03	127.28
42	c1	527	LMK	O3-C4-C3	-3.74	110.45	122.95
48	s	621	LUT	C31-C30-C29	-3.74	122.04	127.28
31	C1	501	CLA	O2A-C1-C2	3.74	122.49	108.11
31	R	602	CLA	O2A-C1-C2	3.74	122.49	108.11
31	n1	604	CLA	O2A-C1-C2	3.74	122.48	108.11
56	R1	626	ERG	C9-C10-C5	3.74	115.61	109.66
31	A	410	CLA	O2A-C1-C2	3.73	122.48	108.11
31	b	617	CLA	O2A-C1-C2	3.73	122.47	108.11
46	h1	101	RRX	C37-C22-C23	3.73	123.79	118.09
40	c	519	DGD	O2G-C1B-C2B	3.73	119.55	111.48
48	s1	620	LUT	C18-C5-C6	-3.73	120.41	124.48
31	Y1	603	CLA	O2A-C1-C2	3.73	122.46	108.11
31	C1	510	CLA	C1-C2-C3	-3.73	120.09	126.20
50	G1	623	NEX	C2-C1-C6	3.73	112.83	109.21
31	Y1	610	CLA	O2A-C1-C2	3.73	122.45	108.11
33	B1	618	BCR	C1-C6-C5	-3.73	117.55	122.64
31	r1	602	CLA	C1-C2-C3	-3.73	120.09	126.20
37	b1	620	C7Z	C35-C34-C33	-3.72	122.05	127.28
48	S	621	LUT	C7-C8-C9	-3.72	120.73	126.23
33	c	515	BCR	C23-C24-C25	-3.72	117.06	127.00
50	s	623	NEX	C17-C1-C6	-3.71	107.15	110.47
48	Y	620	LUT	C15-C35-C34	-3.71	115.92	123.52
50	S	622	NEX	C27-C28-C29	-3.71	119.77	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	y	602	CLA	O2A-C1-C2	3.71	122.39	108.11
31	B	609	CLA	O2A-C1-C2	3.71	122.39	108.11
35	H1	102	LMG	O7-C10-C11	3.71	119.51	111.48
31	n	604	CLA	C1-C2-C3	-3.71	120.12	126.20
49	r	622	XAT	C26-C27-C28	-3.71	118.15	125.99
31	S	617	CLA	O2A-C1-C2	3.71	122.38	108.11
31	y1	610	CLA	O2A-C1-C2	3.71	122.38	108.11
31	d1	403	CLA	C1-C2-C3	-3.71	120.12	126.20
32	a1	409	PHO	CMB-C2B-C3B	3.70	132.09	124.68
37	B	620	C7Z	C1-C6-C5	-3.70	117.57	122.64
48	G1	621	LUT	C15-C14-C13	-3.70	122.08	127.28
31	S1	613	CLA	O2A-C1-C2	3.70	122.35	108.11
31	c1	505	CLA	C1-C2-C3	-3.70	120.13	126.20
37	B	620	C7Z	C31-C30-C29	-3.70	122.09	127.28
31	n	610	CLA	CAA-C2A-C3A	-3.70	103.00	113.00
31	C1	512	CLA	O2A-C1-C2	3.70	122.33	108.11
31	d	403	CLA	C1-C2-C3	-3.70	120.14	126.20
31	b1	616	CLA	O2A-C1-C2	3.69	122.33	108.11
31	Y	614	CLA	O2A-C1-C2	3.69	122.32	108.11
40	C1	520	DGD	O2G-C1B-C2B	3.69	119.47	111.48
31	Y	610	CLA	O2A-C1-C2	3.69	122.32	108.11
31	s1	609	CLA	O2A-C1-C2	3.69	122.31	108.11
31	R1	612	CLA	O2A-C1-C2	3.69	122.30	108.11
31	r	612	CLA	O2A-C1-C2	3.69	122.30	108.11
50	n	623	NEX	C8-C7-C6	-3.68	173.32	177.66
31	B	604	CLA	O2A-C1-C2	3.68	122.27	108.11
33	c1	517	BCR	C15-C14-C13	-3.68	122.12	127.28
31	G1	602	CLA	O2A-C1-C2	3.68	122.27	108.11
50	s1	623	NEX	C31-C30-C29	3.68	132.44	127.28
31	d1	403	CLA	O2A-C1-C2	3.68	122.26	108.11
47	n	605	CHL	CHA-C1A-C2A	-3.68	124.67	133.31
31	b	611	CLA	O2A-C1-C2	3.68	122.26	108.11
31	B	603	CLA	O2A-C1-C2	3.67	122.24	108.11
31	c	505	CLA	O2A-C1-C2	3.67	122.24	108.11
50	y	623	NEX	C38-C25-C24	3.67	118.37	114.24
33	d1	404	BCR	C4-C5-C6	-3.67	117.74	122.70
32	a1	409	PHO	C2B-C1B-NB	-3.67	106.78	109.43
31	s	613	CLA	O2A-C1-C2	3.67	122.23	108.11
31	b1	607	CLA	O2A-C1-C2	3.67	122.23	108.11
48	N1	621	LUT	C15-C14-C13	-3.67	122.13	127.28
31	R	610	CLA	O2A-C1-C2	3.67	122.22	108.11
31	b1	605	CLA	C1C-C2C-C3C	-3.66	103.13	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	D1	403	CLA	C1-C2-C3	-3.66	120.20	126.20
46	h	101	RRX	C4-C5-C6	-3.66	117.75	122.70
37	b	620	C7Z	C27-C28-C29	-3.66	120.82	126.23
31	D	403	CLA	O2A-C1-C2	3.66	122.20	108.11
31	s	605	CLA	C1-C2-C3	-3.66	120.84	126.76
31	r	609	CLA	C1-C2-C3	-3.66	120.20	126.20
47	S1	608	CHL	C4D-CHA-CBD	-3.66	105.28	108.97
31	Y	602	CLA	O2A-C1-C2	3.66	122.18	108.11
31	b	602	CLA	O2A-C1-C2	3.66	122.18	108.11
31	B1	616	CLA	C1-C2-C3	-3.66	120.21	126.20
41	l	101	LHG	O7-C7-C8	3.66	119.39	111.48
48	G1	621	LUT	C31-C30-C29	-3.65	122.15	127.28
31	B	616	CLA	C1-C2-C3	-3.65	120.21	126.20
48	R1	620	LUT	C7-C8-C9	-3.65	120.83	126.23
31	y1	612	CLA	O2A-C1-C2	3.65	122.16	108.11
40	c1	518	DGD	O2G-C1B-C2B	3.65	119.38	111.48
31	b	603	CLA	C1-C2-C3	-3.65	120.22	126.20
41	d	409	LHG	O7-C7-C8	3.65	119.37	111.48
31	B	610	CLA	C1-C2-C3	-3.65	120.22	126.20
31	b	612	CLA	O2A-C1-C2	3.64	122.13	108.11
48	s1	620	LUT	C15-C14-C13	-3.64	122.17	127.28
33	c1	515	BCR	C34-C9-C10	-3.64	116.92	122.82
31	c	506	CLA	O2A-C1-C2	3.64	122.12	108.11
31	g1	613	CLA	O2A-C1-C2	3.64	122.12	108.11
41	y1	624	LHG	O7-C7-C8	3.64	119.36	111.48
31	n1	613	CLA	O2A-C1-C2	3.64	122.11	108.11
31	Y1	602	CLA	O2A-C1-C2	3.64	122.10	108.11
48	y1	620	LUT	C35-C34-C33	-3.64	122.18	127.28
31	n1	603	CLA	O2A-C1-C2	3.63	122.09	108.11
31	S1	617	CLA	O2A-C1-C2	3.63	122.09	108.11
46	H	101	RRX	C24-C23-C22	3.63	131.61	126.23
31	s	610	CLA	C1-O2A-CGA	3.63	125.44	116.65
35	H	102	LMG	O7-C10-C11	3.63	119.34	111.48
31	N	610	CLA	CMA-C3A-C4A	3.63	121.53	111.77
31	c1	508	CLA	O2A-C1-C2	3.63	122.08	108.11
50	Y	623	NEX	C11-C10-C9	3.63	132.37	127.28
33	A1	411	BCR	C33-C5-C6	-3.63	120.52	124.48
50	S	622	NEX	C2-C1-C6	3.63	112.74	109.21
50	y1	623	NEX	C27-C28-C29	-3.63	119.90	125.53
33	c	515	BCR	C33-C5-C4	3.63	121.33	113.60
31	b1	617	CLA	O2A-C1-C2	3.63	122.06	108.11
31	R	609	CLA	O2A-C1-C2	3.63	122.06	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	y1	604	CLA	O2A-C1-C2	3.62	122.06	108.11
48	g	621	LUT	C18-C5-C6	-3.62	120.53	124.48
40	C1	518	DGD	O2G-C1B-C2B	3.62	119.32	111.48
48	S1	620	LUT	C35-C15-C14	-3.62	116.11	123.52
46	H1	101	RRX	C33-C5-C6	-3.62	120.53	124.48
31	y1	610	CLA	C1-C2-C3	-3.62	120.27	126.20
35	c1	523	LMG	O7-C10-C11	3.62	119.31	111.48
31	A	406	CLA	O2A-C1-C2	3.62	122.03	108.11
31	C	506	CLA	O2A-C1-C2	3.62	122.03	108.11
31	A	405	CLA	O2A-C1-C2	3.62	122.03	108.11
31	R	608	CLA	O2A-C1-C2	3.62	122.03	108.11
31	g	603	CLA	O2A-C1-C2	3.62	122.02	108.11
31	y	612	CLA	O2A-C1-C2	3.61	122.01	108.11
31	S1	610	CLA	O2A-C1-C2	3.61	122.01	108.11
44	d	405	PL9	C7-C3-C2	-3.61	119.13	123.39
47	N1	605	CHL	CHA-C1A-C2A	-3.61	124.83	133.31
31	B1	616	CLA	O2A-C1-C2	3.61	122.00	108.11
31	y1	602	CLA	C1-C2-C3	-3.61	120.28	126.20
31	G	613	CLA	C1-C2-C3	-3.61	120.28	126.20
31	S	602	CLA	O2A-C1-C2	3.61	121.98	108.11
31	S	610	CLA	O2A-C1-C2	3.61	121.98	108.11
31	r	610	CLA	O2A-C1-C2	3.60	121.98	108.11
31	n1	604	CLA	C1-C2-C3	-3.60	120.29	126.20
31	N	603	CLA	O2A-C1-C2	3.60	121.98	108.11
31	B	608	CLA	O2A-C1-C2	3.60	121.97	108.11
31	r	602	CLA	O2A-C1-C2	3.60	121.97	108.11
48	R	620	LUT	C7-C8-C9	-3.60	120.91	126.23
31	Y1	613	CLA	O2A-C1-C2	3.60	121.97	108.11
50	N1	623	NEX	C31-C30-C29	3.60	132.33	127.28
31	D1	403	CLA	O2A-C1-C2	3.60	121.96	108.11
33	b1	618	BCR	C33-C5-C6	-3.60	120.56	124.48
50	G	623	NEX	C17-C1-C6	-3.60	107.25	110.47
31	n	602	CLA	C1-C2-C3	-3.60	120.31	126.20
31	C	501	CLA	O2A-C1-C2	3.59	121.94	108.11
35	D1	411	LMG	O7-C10-C11	3.59	119.25	111.48
31	y1	602	CLA	O2A-C1-C2	3.59	121.93	108.11
42	C	527	LMK	O3-C4-C3	-3.59	110.95	122.95
48	N	620	LUT	C11-C10-C9	-3.59	122.25	127.28
47	g1	609	CHL	CHA-C1A-C2A	-3.58	124.89	133.31
31	b1	617	CLA	C2C-C1C-NC	3.58	113.75	109.98
50	S	622	NEX	C17-C1-C6	-3.58	107.27	110.47
48	S	621	LUT	C18-C5-C6	-3.58	120.57	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	Y	604	CLA	O2A-C1-C2	3.58	121.90	108.11
31	b1	609	CLA	O2D-CGD-O1D	-3.58	116.88	123.85
49	r1	621	XAT	C7-C8-C9	-3.58	119.97	125.53
38	b1	625	DGA	OG2-CB1-CB2	3.58	119.23	111.48
31	G1	602	CLA	C1-C2-C3	-3.58	120.33	126.20
31	R1	610	CLA	O2A-C1-C2	3.58	121.88	108.11
47	g	609	CHL	CHA-C1A-C2A	-3.58	124.91	133.31
31	y	602	CLA	C1-C2-C3	-3.58	120.33	126.20
31	a	410	CLA	O2A-C1-C2	3.58	121.87	108.11
47	Y1	609	CHL	CHA-C1A-C2A	-3.57	124.92	133.31
31	b1	611	CLA	O2A-C1-C2	3.57	121.86	108.11
31	B	611	CLA	C1-C2-C3	-3.57	120.34	126.20
31	d	403	CLA	O2A-C1-C2	3.57	121.85	108.11
48	y	621	LUT	C15-C14-C13	-3.57	122.27	127.28
47	N	609	CHL	CHA-C1A-C2A	-3.57	124.93	133.31
31	Y	608	CLA	O2A-C1-C2	3.57	121.84	108.11
31	G	613	CLA	O2A-C1-C2	3.57	121.84	108.11
31	G1	611	CLA	O2A-C1-C2	3.57	121.84	108.11
31	C	505	CLA	O2A-C1-C2	3.57	121.84	108.11
50	N1	623	NEX	C8-C7-C6	-3.57	173.45	177.66
31	s1	610	CLA	O2A-C1-C2	3.57	121.83	108.11
31	n1	610	CLA	CAA-C2A-C3A	-3.57	103.36	113.00
31	C	510	CLA	O2A-C1-C2	3.57	121.83	108.11
32	a	408	PHO	C2B-C1B-NB	-3.57	106.85	109.43
33	a	411	BCR	C23-C24-C25	-3.56	117.48	127.00
31	b1	615	CLA	O2A-C1-C2	3.56	121.82	108.11
50	G1	623	NEX	C39-C29-C30	-3.56	117.05	122.82
31	b1	604	CLA	O2A-C1-C2	3.56	121.80	108.11
47	g	608	CHL	C4D-CHA-CBD	-3.56	105.38	108.97
31	c	508	CLA	O2A-C1-C2	3.56	121.80	108.11
46	H	101	RRX	C4-C5-C6	-3.56	117.90	122.70
31	r1	610	CLA	C1-C2-C3	-3.56	120.37	126.20
31	g1	610	CLA	C1-C2-C3	-3.56	120.37	126.20
31	B1	609	CLA	O2A-C1-C2	3.56	121.79	108.11
50	R1	622	NEX	C1-C2-C3	3.55	121.39	113.59
31	R	610	CLA	CMA-C3A-C4A	3.55	121.32	111.77
47	y1	606	CHL	CHA-C1A-C2A	-3.55	124.97	133.31
31	s	613	CLA	O2D-CGD-O1D	-3.55	116.94	123.85
40	C1	519	DGD	O2G-C1B-C2B	3.55	119.16	111.48
49	G	622	XAT	C7-C8-C9	-3.55	120.03	125.53
49	g	622	XAT	C6-C7-C8	-3.55	118.50	125.99
48	S1	621	LUT	C35-C15-C14	-3.55	116.26	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	509	CLA	C1-C2-C3	-3.54	120.39	126.20
31	s1	610	CLA	C1-C2-C3	-3.54	120.39	126.20
48	N	620	LUT	C18-C5-C6	-3.54	120.62	124.48
47	Y1	609	CHL	C1A-CHA-C4D	3.54	124.89	118.98
33	B	619	BCR	C33-C5-C6	-3.54	120.62	124.48
33	c1	517	BCR	C33-C5-C6	-3.54	120.62	124.48
31	S1	611	CLA	C2C-C1C-NC	3.54	113.70	109.98
31	b1	616	CLA	C1-C2-C3	-3.54	120.39	126.20
31	b1	610	CLA	O2A-C1-C2	3.54	121.72	108.11
31	s	604	CLA	O2A-C1-C2	3.53	121.71	108.11
46	h1	101	RRX	C16-C17-C18	-3.53	122.32	127.28
48	N	620	LUT	C31-C30-C29	-3.53	122.32	127.28
31	b	614	CLA	O2A-C1-C2	3.53	121.71	108.11
56	r1	626	ERG	C1-C10-C5	3.53	114.83	108.74
47	n1	605	CHL	CHA-C1A-C2A	-3.53	125.02	133.31
31	d	402	CLA	C1-C2-C3	-3.53	120.42	126.20
47	Y	601	CHL	CHA-C1A-C2A	-3.53	125.03	133.31
31	y1	603	CLA	O2A-C1-C2	3.53	121.68	108.11
49	g	622	XAT	C38-C25-C26	-3.53	116.50	122.30
33	c	517	BCR	C15-C14-C13	-3.53	122.33	127.28
48	G1	620	LUT	C11-C10-C9	-3.53	122.33	127.28
48	y1	620	LUT	C15-C14-C13	-3.53	122.33	127.28
50	g	623	NEX	C16-C1-C6	-3.52	107.32	110.47
50	g	623	NEX	O24-C25-C38	-3.52	111.11	115.05
31	N	610	CLA	O2A-C1-C2	3.52	121.67	108.11
31	b1	602	CLA	O2A-C1-C2	3.52	121.67	108.11
31	C1	506	CLA	O2A-C1-C2	3.52	121.66	108.11
49	R1	621	XAT	C7-C8-C9	-3.52	120.07	125.53
31	B	616	CLA	O2A-C1-C2	3.52	121.65	108.11
47	n1	609	CHL	CHA-C1A-C2A	-3.52	125.05	133.31
47	y1	609	CHL	CHA-C1A-C2A	-3.52	125.05	133.31
31	s1	603	CLA	O2A-C1-C2	3.52	121.64	108.11
31	s1	611	CLA	O2A-C1-C2	3.52	121.64	108.11
31	c1	503	CLA	O2A-C1-C2	3.51	121.63	108.11
33	d	404	BCR	C36-C18-C17	-3.51	117.12	122.82
31	a1	406	CLA	O2A-C1-C2	3.51	121.62	108.11
31	s1	604	CLA	C1-C2-C3	-3.51	120.45	126.20
31	N	602	CLA	O2A-C1-C2	3.51	121.61	108.11
31	C	511	CLA	O2A-C1-C2	3.51	121.60	108.11
49	r	622	XAT	C38-C25-C26	-3.50	116.53	122.30
31	d1	402	CLA	O2A-C1-C2	3.50	121.59	108.11
31	Y1	612	CLA	O2A-C1-C2	3.50	121.59	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
38	B1	625	DGA	OG2-CB1-CB2	3.50	119.06	111.48
31	A1	405	CLA	O2A-C1-C2	3.50	121.58	108.11
31	c	503	CLA	O2A-C1-C2	3.50	121.58	108.11
31	S	603	CLA	O2A-C1-C2	3.50	121.58	108.11
31	y1	608	CLA	O2A-C1-C2	3.50	121.58	108.11
31	y	611	CLA	O2A-C1-C2	3.50	121.57	108.11
31	S	613	CLA	O2D-CGD-O1D	-3.50	117.04	123.85
49	r1	621	XAT	C15-C14-C13	-3.50	122.37	127.28
48	S	620	LUT	C18-C5-C6	-3.50	120.67	124.48
31	s	610	CLA	CAA-C2A-C3A	-3.50	103.55	113.00
47	s	606	CHL	CHA-C1A-C2A	-3.50	125.10	133.31
48	Y	621	LUT	C15-C14-C13	-3.50	122.37	127.28
31	C1	502	CLA	O2A-C1-C2	3.50	121.56	108.11
47	g	601	CHL	CHA-C1A-C2A	-3.50	125.10	133.31
40	C	518	DGD	O2G-C1B-C2B	3.50	119.04	111.48
31	R1	603	CLA	O2A-C1-C2	3.50	121.56	108.11
31	G	604	CLA	CMA-C3A-C4A	3.49	121.16	111.77
31	B1	617	CLA	O2A-C1-C2	3.49	121.55	108.11
49	r1	621	XAT	C26-C27-C28	-3.49	118.61	125.99
37	b1	620	C7Z	C18-C5-C6	-3.49	120.68	124.48
49	y	622	XAT	C7-C8-C9	-3.49	120.11	125.53
47	N	605	CHL	CHA-C1A-C2A	-3.49	125.11	133.31
41	D	410	LHG	O7-C7-C8	3.49	119.03	111.48
32	A	409	PHO	CMB-C2B-C3B	3.49	131.65	124.68
48	g1	620	LUT	C11-C10-C9	-3.49	122.39	127.28
31	d	402	CLA	C3B-C4B-NB	-3.48	107.42	110.53
31	g	613	CLA	O2A-C1-C2	3.48	121.50	108.11
40	C1	519	DGD	O1G-C1A-C2A	3.48	122.45	111.83
50	R	622	NEX	C8-C7-C6	-3.48	173.56	177.66
46	H	101	RRX	C38-C26-C25	-3.48	120.69	124.48
49	n	622	XAT	C38-C25-C26	-3.48	116.58	122.30
31	y	613	CLA	C1-C2-C3	-3.48	120.50	126.20
31	R	603	CLA	O2A-C1-C2	3.47	121.47	108.11
46	H	101	RRX	C33-C5-C4	3.47	121.00	113.60
47	N	607	CHL	C4D-CHA-CBD	-3.47	105.47	108.97
48	r	620	LUT	C11-C10-C9	-3.47	122.41	127.28
31	A	406	CLA	C1C-C2C-C3C	-3.47	103.33	106.98
48	r1	620	LUT	C18-C5-C6	-3.47	120.70	124.48
31	b	616	CLA	O2A-C1-C2	3.47	121.44	108.11
31	b1	603	CLA	O2A-CGA-CBA	3.46	122.39	111.83
31	C1	513	CLA	O2A-C1-C2	3.46	121.43	108.11
31	G1	603	CLA	C1-C2-C3	-3.46	120.53	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	S1	611	CLA	O2A-C1-C2	3.46	121.42	108.11
31	R	603	CLA	CMA-C3A-C4A	3.46	121.07	111.77
31	B1	611	CLA	O2A-C1-C2	3.46	121.41	108.11
31	A1	407	CLA	C1-C2-C3	-3.45	121.17	126.76
47	G1	605	CHL	CHA-C1A-C2A	-3.45	125.20	133.31
31	b	615	CLA	C2C-C1C-NC	3.45	113.61	109.98
31	g	602	CLA	C1C-C2C-C3C	-3.45	103.35	106.98
31	N1	610	CLA	O2A-C1-C2	3.45	121.39	108.11
31	B1	603	CLA	O2A-C1-C2	3.45	121.39	108.11
31	s	611	CLA	O2A-C1-C2	3.45	121.39	108.11
31	S	614	CLA	O2A-C1-C2	3.45	121.38	108.11
48	N	621	LUT	C18-C5-C6	-3.45	120.72	124.48
45	f	101	HEM	C3B-C2B-C1B	3.45	109.00	106.41
32	a	409	PHO	C2B-C1B-NB	-3.45	106.94	109.43
47	n	608	CHL	C4D-CHA-CBD	-3.45	105.49	108.97
31	R	610	CLA	C1-C2-C3	-3.45	120.55	126.20
48	n	621	LUT	C31-C30-C29	-3.45	122.45	127.28
47	s1	608	CHL	CHA-C1A-C2A	-3.45	125.22	133.31
46	H	101	RRX	C33-C5-C6	-3.44	120.72	124.48
31	G	613	CLA	CAC-C3C-C4C	3.44	129.27	124.79
33	d	404	BCR	C27-C26-C25	-3.44	118.05	122.70
48	s	621	LUT	C18-C5-C6	-3.44	120.73	124.48
31	B1	613	CLA	O2A-C1-C2	3.44	121.35	108.11
46	h1	101	RRX	C34-C9-C8	3.44	123.34	118.09
31	b1	606	CLA	O2A-C1-C2	3.44	121.34	108.11
31	A1	410	CLA	O2A-C1-C2	3.44	121.34	108.11
31	N1	602	CLA	O2A-C1-C2	3.44	121.34	108.11
31	Y1	611	CLA	O2A-C1-C2	3.44	121.34	108.11
31	c1	502	CLA	O2A-C1-C2	3.44	121.34	108.11
31	A1	406	CLA	O2A-C1-C2	3.44	121.34	108.11
33	c1	516	BCR	C19-C18-C17	3.44	124.42	119.01
33	B1	619	BCR	C33-C5-C4	3.44	120.92	113.60
31	s1	617	CLA	CMA-C3A-C4A	3.44	121.01	111.77
37	b1	620	C7Z	C18-C5-C4	3.44	120.74	114.42
48	s1	621	LUT	C26-C27-C28	-3.44	119.23	124.58
31	s	609	CLA	O2A-C1-C2	3.44	121.33	108.11
33	B	618	BCR	C33-C5-C6	-3.43	120.74	124.48
31	B1	607	CLA	O2A-C1-C2	3.43	121.32	108.11
31	Y	610	CLA	C1-C2-C3	-3.43	120.57	126.20
31	a	406	CLA	C1-C2-C3	-3.43	120.58	126.20
31	b	605	CLA	C1-C2-C3	-3.43	120.58	126.20
47	s	608	CHL	C1A-CHA-C4D	3.43	124.70	118.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	S	608	CHL	CHA-C1A-C2A	-3.43	125.26	133.31
31	g	613	CLA	CMA-C3A-C4A	3.43	120.99	111.77
33	c1	515	BCR	C33-C5-C6	-3.43	120.74	124.48
31	s	604	CLA	C1-C2-C3	-3.43	120.58	126.20
31	Y1	602	CLA	C1-C2-C3	-3.43	120.58	126.20
31	S	605	CLA	C1-C2-C3	-3.43	121.22	126.76
31	S	617	CLA	CMA-C3A-C4A	3.43	120.98	111.77
31	N	610	CLA	O2A-CGA-CBA	3.42	122.28	111.83
48	G	621	LUT	C27-C28-C29	-3.42	118.96	126.32
31	G	603	CLA	O2A-C1-C2	3.42	121.28	108.11
50	s1	623	NEX	C1-C2-C3	3.42	121.10	113.59
31	s1	604	CLA	O2A-C1-C2	3.42	121.27	108.11
47	S	606	CHL	CHA-C1A-C2A	-3.42	125.28	133.31
47	n	607	CHL	C1-O2A-CGA	3.42	124.93	116.65
31	N1	613	CLA	CMA-C3A-C4A	3.42	120.96	111.77
31	g1	610	CLA	O2A-C1-C2	3.42	121.26	108.11
50	R1	622	NEX	C8-C7-C6	-3.42	173.63	177.66
47	N1	607	CHL	C4D-CHA-CBD	-3.42	105.52	108.97
31	C1	509	CLA	C1C-C2C-C3C	-3.42	103.39	106.98
33	C	514	BCR	C15-C14-C13	-3.41	122.49	127.28
31	c	504	CLA	CMA-C3A-C4A	3.41	120.95	111.77
48	n1	620	LUT	C7-C8-C9	-3.41	121.19	126.23
47	Y	605	CHL	CHA-C1A-C2A	-3.41	125.29	133.31
50	G1	623	NEX	C27-C28-C29	-3.41	120.24	125.53
31	Y1	614	CLA	O2A-C1-C2	3.41	121.23	108.11
31	B	602	CLA	CMA-C3A-C4A	3.41	120.94	111.77
31	R1	612	CLA	C1-C2-C3	-3.41	120.61	126.20
46	h	101	RRX	C7-C8-C9	-3.41	121.19	126.23
31	G	603	CLA	C1C-C2C-C3C	-3.41	103.40	106.98
33	A1	411	BCR	C38-C26-C25	-3.41	120.77	124.48
31	R1	608	CLA	O2A-C1-C2	3.41	121.22	108.11
31	s1	603	CLA	C1-C2-C3	-3.40	120.62	126.20
33	B1	618	BCR	C33-C5-C6	-3.40	120.77	124.48
31	N	603	CLA	C1-C2-C3	-3.40	120.62	126.20
48	n	621	LUT	C18-C5-C6	-3.40	120.77	124.48
31	s1	602	CLA	O2A-C1-C2	3.40	121.19	108.11
48	s	621	LUT	C15-C14-C13	-3.40	122.51	127.28
47	n1	607	CHL	C4D-CHA-CBD	-3.40	105.54	108.97
48	Y	620	LUT	C18-C5-C6	-3.40	120.78	124.48
31	b	606	CLA	O2A-C1-C2	3.40	121.19	108.11
47	y1	607	CHL	C4D-CHA-CBD	-3.40	105.54	108.97
32	a1	408	PHO	O1D-CGD-CBD	3.40	129.88	124.72

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	614	CLA	O2A-C1-C2	3.39	121.17	108.11
31	b	609	CLA	O2A-C1-C2	3.39	121.17	108.11
31	c	507	CLA	O2A-C1-C2	3.39	121.16	108.11
54	K1	101	4RF	O21-C22-C24	3.39	118.82	111.48
31	G1	613	CLA	CMA-C3A-C4A	3.39	120.88	111.77
31	C	503	CLA	O2A-C1-C2	3.39	121.14	108.11
32	A1	409	PHO	C2B-C1B-NB	-3.39	106.98	109.43
31	y	608	CLA	C1-C2-C3	-3.38	121.29	126.76
31	B	604	CLA	C1-C2-C3	-3.38	120.65	126.20
31	n	603	CLA	C1-C2-C3	-3.38	120.65	126.20
31	C1	513	CLA	CAA-C2A-C3A	-3.38	103.86	113.00
31	a	406	CLA	O2A-C1-C2	3.38	121.12	108.11
31	c	509	CLA	O2A-C1-C2	3.38	121.11	108.11
33	b1	618	BCR	C1-C6-C5	-3.38	118.02	122.64
47	r1	607	CHL	CHA-C1A-C2A	-3.38	125.37	133.31
47	Y1	606	CHL	CHA-C1A-C2A	-3.38	125.37	133.31
56	R1	626	ERG	C7-C6-C5	-3.38	115.98	122.95
49	n1	622	XAT	C38-C25-C26	-3.38	116.74	122.30
47	G1	601	CHL	C1A-CHA-C4D	3.38	124.61	118.98
33	B1	619	BCR	C4-C5-C6	-3.38	118.14	122.70
31	n	611	CLA	CMA-C3A-C4A	3.37	120.84	111.77
31	N	604	CLA	C1-C2-C3	-3.37	120.67	126.20
31	b	615	CLA	C1-C2-C3	-3.37	120.67	126.20
31	b	611	CLA	C1-C2-C3	-3.37	120.67	126.20
31	S1	605	CLA	C1-C2-C3	-3.37	121.31	126.76
31	B	602	CLA	O2A-C1-C2	3.37	121.08	108.11
31	A1	406	CLA	CMA-C3A-C4A	3.37	120.83	111.77
31	B1	615	CLA	C1-C2-C3	-3.37	120.68	126.20
31	n1	613	CLA	CMA-C3A-C4A	3.37	120.83	111.77
31	c	504	CLA	O2A-CGA-CBA	3.37	122.11	111.83
31	n1	603	CLA	C1-C2-C3	-3.37	120.68	126.20
31	B	611	CLA	C3B-C4B-NB	-3.37	107.53	110.53
32	a	409	PHO	O1D-CGD-CBD	3.36	129.83	124.72
31	c1	508	CLA	C1-C2-C3	-3.36	120.69	126.20
31	G	603	CLA	CMA-C3A-C4A	3.36	120.81	111.77
50	S	622	NEX	C31-C30-C29	3.36	131.99	127.28
31	C1	505	CLA	C1-C2-C3	-3.36	120.69	126.20
31	a1	410	CLA	O2A-C1-C2	3.35	121.02	108.11
33	C1	517	BCR	C37-C22-C21	-3.35	117.38	122.82
31	c	511	CLA	O2A-C1-C2	3.35	121.00	108.11
37	b	620	C7Z	C8-C7-C6	-3.35	118.05	127.00
48	G1	621	LUT	C18-C5-C6	-3.35	120.83	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	Y1	607	CHL	C4D-CHA-CBD	-3.35	105.59	108.97
31	b1	605	CLA	O2A-CGA-CBA	3.35	122.04	111.83
47	g	605	CHL	CHA-C1A-C2A	-3.35	125.45	133.31
31	s1	609	CLA	C1-C2-C3	-3.34	120.72	126.20
31	c1	510	CLA	O2A-C1-C2	3.34	120.98	108.11
43	d1	401	BCT	O3-C-O1	-3.34	111.12	119.68
47	Y	607	CHL	C4D-CHA-CBD	-3.34	105.60	108.97
47	S1	607	CHL	CHA-C1A-C2A	-3.34	125.46	133.31
56	r1	626	ERG	C16-C17-C13	3.34	107.77	103.84
31	Y1	604	CLA	O2A-C1-C2	3.34	120.97	108.11
47	n1	608	CHL	C1-O2A-CGA	3.34	124.74	116.65
31	b	609	CLA	C1C-C2C-C3C	-3.34	103.47	106.98
31	S	609	CLA	O2A-C1-C2	3.34	120.96	108.11
31	C1	504	CLA	C1-C2-C3	-3.34	120.72	126.20
47	g1	605	CHL	CHA-C1A-C2A	-3.34	125.47	133.31
31	a	410	CLA	CMA-C3A-C4A	3.34	120.75	111.77
31	b1	602	CLA	C2C-C1C-NC	3.34	113.49	109.98
31	C	507	CLA	O2A-C1-C2	3.34	120.95	108.11
31	c	509	CLA	C1C-C2C-C3C	-3.34	103.47	106.98
33	B1	618	BCR	C15-C14-C13	-3.34	122.60	127.28
31	b	606	CLA	C2C-C1C-NC	3.34	113.49	109.98
33	a1	411	BCR	C33-C5-C6	-3.33	120.84	124.48
31	R	608	CLA	C1-C2-C3	-3.33	120.73	126.20
50	R1	622	NEX	C2-C1-C6	3.33	112.45	109.21
41	s	624	LHG	C5-O7-C7	-3.33	109.82	117.80
31	Y	612	CLA	O2A-C1-C2	3.33	120.92	108.11
47	y	609	CHL	CHA-C1A-C2A	-3.33	125.49	133.31
48	N1	621	LUT	C31-C30-C29	-3.33	122.61	127.28
31	B1	602	CLA	O2A-C1-C2	3.33	120.92	108.11
31	B1	603	CLA	C1-C2-C3	-3.33	120.74	126.20
31	B	607	CLA	CAA-C2A-C3A	-3.33	104.01	113.00
31	B1	606	CLA	C1-C2-C3	-3.33	120.75	126.20
47	G1	608	CHL	C1A-CHA-C4D	3.33	124.53	118.98
31	c	503	CLA	CMA-C3A-C4A	3.33	120.72	111.77
47	n	601	CHL	CHA-C1A-C2A	-3.33	125.50	133.31
47	s	607	CHL	CHA-C1A-C2A	-3.33	125.50	133.31
47	n	607	CHL	C1-C2-C3	-3.32	120.75	126.20
31	N1	603	CLA	C1-C2-C3	-3.32	120.75	126.20
46	h1	101	RRX	C33-C5-C6	-3.32	120.86	124.48
48	G1	621	LUT	C26-C27-C28	-3.32	119.41	124.58
47	G	606	CHL	CHA-C1A-C2A	-3.32	125.51	133.31
31	S1	614	CLA	O2A-C1-C2	3.32	120.89	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	S	613	CLA	CMA-C3A-C4A	3.32	120.69	111.77
50	g1	623	NEX	C38-C25-C26	-3.32	116.84	122.30
31	Y	613	CLA	O2A-C1-C2	3.32	120.88	108.11
31	b1	617	CLA	C1-C2-C3	-3.32	120.76	126.20
47	S	607	CHL	CHA-C1A-C2A	-3.31	125.52	133.31
31	Y	613	CLA	CMA-C3A-C4A	3.31	120.68	111.77
31	B	612	CLA	O2A-C1-C2	3.31	120.86	108.11
31	S	604	CLA	O2A-C1-C2	3.31	120.86	108.11
31	n1	610	CLA	O2A-C1-C2	3.31	120.85	108.11
50	S1	623	NEX	C27-C28-C29	-3.31	120.39	125.53
50	G	623	NEX	C1-C2-C3	3.31	120.85	113.59
47	G	605	CHL	CHA-C1A-C2A	-3.31	125.54	133.31
49	N1	622	XAT	C6-C7-C8	-3.31	119.00	125.99
31	B	610	CLA	O2A-C1-C2	3.31	120.83	108.11
49	G1	622	XAT	C38-C25-C26	-3.31	116.86	122.30
31	s1	605	CLA	C2C-C1C-NC	3.31	113.45	109.98
48	S1	620	LUT	C26-C27-C28	-3.31	119.44	124.58
50	G1	623	NEX	C17-C1-C6	-3.31	107.51	110.47
31	y	603	CLA	O2A-C1-C2	3.30	120.83	108.11
31	S	611	CLA	O2A-C1-C2	3.30	120.82	108.11
31	b1	609	CLA	O2A-C1-C2	3.30	120.82	108.11
31	b	605	CLA	C2C-C1C-NC	3.30	113.45	109.98
31	a1	406	CLA	C1-C2-C3	-3.30	120.79	126.20
47	G	608	CHL	CHA-C1A-C2A	-3.30	125.56	133.31
31	s1	617	CLA	O2A-C1-C2	3.30	120.81	108.11
47	Y	609	CHL	CHA-C1A-C2A	-3.30	125.56	133.31
46	H1	101	RRX	C23-C22-C21	-3.30	113.82	119.01
31	s1	613	CLA	CMA-C3A-C4A	3.30	120.64	111.77
50	g	623	NEX	C27-C28-C29	-3.30	120.41	125.53
31	s1	603	CLA	O2D-CGD-O1D	-3.30	117.43	123.85
31	a1	406	CLA	C1C-C2C-C3C	-3.30	103.51	106.98
47	N1	609	CHL	CHA-C1A-C2A	-3.30	125.56	133.31
31	y1	614	CLA	O2A-C1-C2	3.30	120.80	108.11
31	S1	609	CLA	O2A-C1-C2	3.30	120.79	108.11
31	b	606	CLA	C1C-C2C-C3C	-3.30	103.51	106.98
33	B1	618	BCR	C33-C5-C4	3.30	120.62	113.60
48	s	621	LUT	C7-C8-C9	-3.30	121.36	126.23
31	y1	612	CLA	C1-C2-C3	-3.29	120.80	126.20
31	Y1	611	CLA	C1-C2-C3	-3.29	120.80	126.20
31	Y	603	CLA	O2A-C1-C2	3.29	120.78	108.11
31	G	610	CLA	C1-C2-C3	-3.29	120.80	126.20
31	r	608	CLA	O2A-C1-C2	3.29	120.77	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	N1	620	LUT	C15-C14-C13	-3.29	122.66	127.28
48	y1	621	LUT	C22-C23-C24	-3.29	106.30	111.18
31	Y	611	CLA	O2A-C1-C2	3.29	120.77	108.11
47	S1	606	CHL	CHA-C1A-C2A	-3.29	125.58	133.31
48	y	620	LUT	C35-C15-C14	-3.29	116.79	123.52
48	g1	621	LUT	C15-C14-C13	-3.29	122.67	127.28
49	g1	622	XAT	C7-C8-C9	-3.29	120.43	125.53
31	c1	513	CLA	CAA-C2A-C3A	-3.29	104.12	113.00
47	s	608	CHL	CHA-C1A-C2A	-3.28	125.59	133.31
48	g	620	LUT	C15-C14-C13	-3.28	122.67	127.28
31	D	402	CLA	C1D-ND-C4D	-3.28	104.01	106.31
33	c1	516	BCR	C36-C18-C17	-3.28	117.50	122.82
37	b	620	C7Z	C31-C30-C29	-3.28	122.67	127.28
47	G1	609	CHL	CHA-C1A-C2A	-3.28	125.60	133.31
50	r1	622	NEX	C27-C28-C29	-3.28	120.44	125.53
47	N1	601	CHL	C1A-CHA-C4D	3.28	124.45	118.98
31	C	512	CLA	O2A-C1-C2	3.28	120.73	108.11
47	Y	605	CHL	C3C-C4C-NC	-3.28	106.63	114.65
31	b1	615	CLA	C1-C2-C3	-3.28	120.83	126.20
56	r1	626	ERG	C18-C13-C14	-3.28	104.91	110.35
31	y	602	CLA	C1D-ND-C4D	-3.28	104.01	106.31
48	G	621	LUT	C7-C8-C9	-3.28	121.39	126.23
33	c1	514	BCR	C38-C26-C25	-3.28	120.91	124.48
47	n1	607	CHL	CHA-C1A-C2A	-3.28	125.61	133.31
31	B	607	CLA	CMA-C3A-C4A	3.27	120.57	111.77
33	c	514	BCR	C33-C5-C6	-3.27	120.91	124.48
47	G1	607	CHL	C4D-CHA-CBD	-3.27	105.67	108.97
50	S1	623	NEX	C31-C30-C29	3.27	131.87	127.28
50	Y	623	NEX	C39-C29-C30	-3.27	117.51	122.82
47	N	608	CHL	CHA-C1A-C2A	-3.27	125.62	133.31
31	c1	502	CLA	C1-C2-C3	-3.27	120.83	126.20
47	y	605	CHL	CHA-C1A-C2A	-3.27	125.62	133.31
31	R	609	CLA	C1-C2-C3	-3.27	120.84	126.20
31	B	613	CLA	O2A-C1-C2	3.27	120.69	108.11
43	D	401	BCT	O3-C-O1	-3.27	111.31	119.68
47	y	601	CHL	CHA-C1A-C2A	-3.27	125.64	133.31
47	g	607	CHL	CHA-C1A-C2A	-3.27	125.64	133.31
31	s1	613	CLA	C2C-C1C-NC	3.27	113.41	109.98
48	y	621	LUT	C18-C5-C6	-3.27	120.92	124.48
33	a1	411	BCR	C23-C24-C25	-3.26	118.28	127.00
31	C1	510	CLA	O2A-C1-C2	3.26	120.67	108.11
31	G1	602	CLA	C1D-ND-C4D	-3.26	104.02	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
46	h	101	RRX	C15-C16-C17	-3.26	116.85	123.52
40	C	523	DGD	O1G-C1A-C2A	3.26	121.78	111.83
31	c1	504	CLA	C1-C2-C3	-3.26	120.86	126.20
31	b	615	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
31	b	605	CLA	O2A-C1-C2	3.26	120.65	108.11
47	s1	606	CHL	CHA-C1A-C2A	-3.26	125.65	133.31
50	y	623	NEX	C17-C1-C6	-3.26	107.56	110.47
47	N1	601	CHL	C3C-C4C-NC	-3.26	106.68	114.65
31	S1	603	CLA	O2D-CGD-O1D	-3.26	117.50	123.85
48	G	620	LUT	C18-C5-C6	-3.26	120.93	124.48
50	g1	623	NEX	C11-C10-C9	3.26	131.85	127.28
47	N	606	CHL	CHA-C1A-C2A	-3.26	125.66	133.31
31	Y	614	CLA	C1-C2-C3	-3.26	120.86	126.20
31	Y1	614	CLA	C1-C2-C3	-3.26	120.86	126.20
47	S	608	CHL	C1A-CHA-C4D	3.26	124.42	118.98
31	b1	612	CLA	C1-C2-C3	-3.26	120.86	126.20
31	N	613	CLA	O2A-CGA-CBA	3.25	121.76	111.83
33	B1	619	BCR	C33-C5-C6	-3.25	120.93	124.48
47	N1	605	CHL	C3C-C4C-NC	-3.25	106.70	114.65
48	Y1	621	LUT	C11-C10-C9	-3.25	122.72	127.28
31	b1	610	CLA	C2C-C1C-NC	3.25	113.40	109.98
31	B	609	CLA	C1-C2-C3	-3.25	120.87	126.20
49	g1	622	XAT	C38-C25-C26	-3.25	116.95	122.30
33	b1	619	BCR	C33-C5-C4	3.25	120.53	113.60
31	B1	614	CLA	O2A-C1-C2	3.25	120.61	108.11
50	y	623	NEX	C39-C29-C30	-3.25	117.55	122.82
47	G1	601	CHL	C3C-C4C-NC	-3.25	106.71	114.65
31	y	602	CLA	CMC-C2C-C1C	3.25	130.11	125.03
31	B	612	CLA	CMA-C3A-C4A	3.25	120.50	111.77
47	Y1	601	CHL	CHA-C1A-C2A	-3.25	125.69	133.31
47	s1	607	CHL	CHA-C1A-C2A	-3.24	125.69	133.31
31	r	610	CLA	CMA-C3A-C4A	3.24	120.49	111.77
50	r	623	NEX	C27-C28-C29	-3.24	120.50	125.53
31	Y1	608	CLA	O2A-C1-C2	3.24	120.59	108.11
35	d	411	LMG	O8-C28-C29	3.24	121.72	111.83
49	Y	622	XAT	C38-C25-C26	-3.24	116.97	122.30
31	c	513	CLA	C1-C2-C3	-3.24	120.89	126.20
37	B1	620	C7Z	C18-C5-C4	3.24	120.38	114.42
48	n1	620	LUT	C18-C5-C6	-3.24	120.95	124.48
33	C1	517	BCR	C23-C24-C25	-3.24	118.35	127.00
47	g	606	CHL	CHA-C1A-C2A	-3.24	125.70	133.31
31	B1	609	CLA	O2D-CGD-O1D	-3.24	117.55	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	G1	608	CHL	CHA-C1A-C2A	-3.24	125.70	133.31
31	r1	608	CLA	C1-C2-C3	-3.24	120.89	126.20
50	G1	623	NEX	C16-C1-C6	-3.24	107.58	110.47
31	Y	604	CLA	C1-C2-C3	-3.23	120.90	126.20
47	N1	605	CHL	C1A-CHA-C4D	3.23	124.38	118.98
31	R	602	CLA	C1-C2-C3	-3.23	120.90	126.20
31	r	602	CLA	C1-C2-C3	-3.23	120.90	126.20
31	y1	604	CLA	C1-C2-C3	-3.23	120.90	126.20
31	y1	613	CLA	O2A-C1-C2	3.23	120.54	108.11
47	N1	608	CHL	C1A-CHA-C4D	3.23	124.37	118.98
48	S1	621	LUT	C11-C10-C9	-3.23	122.75	127.28
31	Y1	603	CLA	C2C-C1C-NC	3.23	113.37	109.98
31	D	402	CLA	C1-C2-C3	-3.23	120.91	126.20
47	g	601	CHL	C1-O2A-CGA	3.23	124.47	116.65
47	S1	608	CHL	C1A-CHA-C4D	3.23	124.37	118.98
31	y	610	CLA	C1-C2-C3	-3.23	120.91	126.20
31	s1	617	CLA	C1-C2-C3	-3.23	121.54	126.76
48	G	621	LUT	C10-C11-C12	-3.23	113.85	123.20
31	b1	607	CLA	CMA-C3A-C4A	3.23	120.44	111.77
31	C	501	CLA	C1-C2-C3	-3.23	120.91	126.20
47	g	606	CHL	C1A-CHA-C4D	3.23	124.36	118.98
47	Y	609	CHL	C1-O2A-CGA	3.22	124.46	116.65
47	n	607	CHL	CHA-C1A-C2A	-3.22	125.73	133.31
46	h	101	RRX	C30-C25-C26	-3.22	118.23	122.64
31	b1	611	CLA	C1C-C2C-C3C	-3.22	103.59	106.98
33	D	404	BCR	C37-C22-C21	-3.22	117.59	122.82
48	s	620	LUT	C22-C23-C24	-3.22	106.40	111.18
47	N1	606	CHL	CHA-C1A-C2A	-3.22	125.74	133.31
47	y	601	CHL	C1A-CHA-C4D	3.22	124.36	118.98
31	R	612	CLA	O2A-C1-C2	3.22	120.51	108.11
33	D	404	BCR	C36-C18-C17	-3.22	117.60	122.82
31	C1	510	CLA	C2C-C1C-NC	3.22	113.36	109.98
48	S1	621	LUT	C26-C27-C28	-3.22	119.57	124.58
49	N	622	XAT	C38-C25-C26	-3.22	117.00	122.30
31	C1	511	CLA	O2A-C1-C2	3.22	120.49	108.11
31	N	612	CLA	CMA-C3A-C4A	3.22	120.42	111.77
31	s1	614	CLA	O2A-C1-C2	3.22	120.49	108.11
31	b	611	CLA	CMA-C3A-C4A	3.22	120.42	111.77
47	S1	607	CHL	C1A-CHA-C4D	3.22	124.35	118.98
49	G	622	XAT	C38-C25-C26	-3.22	117.01	122.30
31	n	610	CLA	O2D-CGD-O1D	-3.22	117.59	123.85
31	c1	505	CLA	O2A-C1-C2	3.21	120.48	108.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	602	CLA	CMA-C3A-C4A	3.21	120.41	111.77
31	S1	603	CLA	C1-C2-C3	-3.21	120.93	126.20
47	S	601	CHL	CHA-C1A-C2A	-3.21	125.76	133.31
50	n1	623	NEX	C39-C29-C30	-3.21	117.61	122.82
33	a	411	BCR	C33-C5-C6	-3.21	120.98	124.48
31	R1	602	CLA	O2A-C1-C2	3.21	120.47	108.11
40	c1	519	DGD	O1G-C1A-C2A	3.21	121.62	111.83
31	N1	602	CLA	C1-C2-C3	-3.21	120.94	126.20
31	c1	512	CLA	C1-C2-C3	-3.21	120.94	126.20
50	s1	623	NEX	C19-C9-C10	-3.21	117.62	122.82
31	N	602	CLA	C1-C2-C3	-3.21	120.94	126.20
47	g	606	CHL	C3C-C4C-NC	-3.21	106.81	114.65
48	G	621	LUT	C18-C5-C6	-3.20	120.99	124.48
31	y1	603	CLA	C1-C2-C3	-3.20	120.95	126.20
31	B1	609	CLA	C2C-C1C-NC	3.20	113.35	109.98
31	s	602	CLA	C1-C2-C3	-3.20	120.95	126.20
47	r	606	CHL	CHA-C1A-C2A	-3.20	125.79	133.31
47	n	601	CHL	C3C-C4C-NC	-3.20	106.82	114.65
47	N	605	CHL	C1A-CHA-C4D	3.20	124.33	118.98
48	g	620	LUT	C31-C30-C29	-3.20	122.79	127.28
47	n1	609	CHL	C1A-CHA-C4D	3.20	124.32	118.98
31	b	607	CLA	CMD-C2D-C3D	-3.20	120.35	127.69
46	h1	101	RRX	C33-C5-C4	3.20	120.42	113.60
47	n1	606	CHL	C4D-CHA-CBD	-3.20	105.74	108.97
31	Y1	613	CLA	C1C-C2C-C3C	-3.20	103.62	106.98
31	n1	613	CLA	C1-C2-C3	-3.20	120.96	126.20
47	y1	601	CHL	CHA-C1A-C2A	-3.20	125.80	133.31
47	g	601	CHL	C3C-C4C-NC	-3.20	106.83	114.65
50	G	623	NEX	C39-C29-C30	-3.20	117.64	122.82
31	C	510	CLA	C1-C2-C3	-3.20	120.96	126.20
47	Y1	605	CHL	CHA-C1A-C2A	-3.20	125.80	133.31
47	y1	605	CHL	CHA-C1A-C2A	-3.20	125.80	133.31
31	c	513	CLA	C3B-C4B-NB	-3.20	107.68	110.53
31	s	603	CLA	O2A-C1-C2	3.19	120.40	108.11
31	s	617	CLA	O2A-C1-C2	3.19	120.40	108.11
33	c	514	BCR	C31-C1-C6	-3.19	105.23	110.24
31	A1	410	CLA	CMA-C3A-C4A	3.19	120.36	111.77
48	y1	620	LUT	C11-C10-C9	-3.19	122.80	127.28
31	C	506	CLA	O2D-CGD-O1D	-3.19	117.63	123.85
31	S	602	CLA	C1-C2-C3	-3.19	120.97	126.20
31	B1	611	CLA	C2C-C1C-NC	3.19	113.33	109.98
47	s1	601	CHL	C4D-CHA-CBD	-3.19	105.75	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	Y1	607	CHL	C3C-C4C-NC	-3.19	106.85	114.65
47	n	609	CHL	CHA-C1A-C2A	-3.19	125.82	133.31
47	N1	608	CHL	C4D-CHA-CBD	-3.19	105.75	108.97
31	A1	407	CLA	O2A-C1-C2	3.19	120.38	108.11
31	g	603	CLA	CMA-C3A-C4A	3.19	120.35	111.77
47	G1	609	CHL	C1A-CHA-C4D	3.19	124.30	118.98
31	r1	608	CLA	C2C-C1C-NC	3.19	113.33	109.98
31	Y1	603	CLA	CMA-C3A-C4A	3.19	120.34	111.77
49	Y	622	XAT	C6-C7-C8	-3.19	119.25	125.99
31	A1	405	CLA	CBC-CAC-C3C	3.19	121.06	112.42
31	B1	615	CLA	O2A-C1-C2	3.19	120.38	108.11
49	N1	622	XAT	C7-C8-C9	-3.19	120.58	125.53
48	y	620	LUT	C26-C27-C28	-3.19	119.62	124.58
33	b1	619	BCR	C4-C5-C6	-3.19	118.40	122.70
49	R	621	XAT	C26-C27-C28	-3.18	119.26	125.99
31	s1	605	CLA	C1-C2-C3	-3.18	121.61	126.76
47	R1	607	CHL	C1A-CHA-C4D	3.18	124.29	118.98
47	n	608	CHL	CHA-C1A-C2A	-3.18	125.83	133.31
31	b	602	CLA	C1-C2-C3	-3.18	120.98	126.20
48	s	620	LUT	C7-C8-C9	-3.18	121.53	126.23
48	G1	620	LUT	C27-C28-C29	-3.18	119.48	126.32
48	G1	620	LUT	C18-C5-C6	-3.18	121.01	124.48
48	Y1	620	LUT	C18-C5-C6	-3.18	121.01	124.48
41	L	101	LHG	O7-C7-C8	3.18	118.36	111.48
31	y1	603	CLA	CMA-C3A-C4A	3.18	120.32	111.77
47	G	609	CHL	CHA-C1A-C2A	-3.18	125.84	133.31
31	B	615	CLA	C1-C2-C3	-3.18	120.99	126.20
31	A	407	CLA	C2C-C1C-NC	3.18	113.32	109.98
31	Y	602	CLA	O2D-CGD-O1D	-3.18	117.66	123.85
47	N	608	CHL	C1-O2A-CGA	3.18	124.34	116.65
31	S1	603	CLA	CMA-C3A-C4A	3.17	120.31	111.77
31	S1	611	CLA	C1C-C2C-C3C	-3.17	103.64	106.98
48	s1	620	LUT	C26-C27-C28	-3.17	119.64	124.58
31	g	603	CLA	C1C-C2C-C3C	-3.17	103.64	106.98
46	h	101	RRX	C33-C5-C4	3.17	120.36	113.60
31	c	505	CLA	CMA-C3A-C4A	3.17	120.29	111.77
31	c1	501	CLA	CMA-C3A-C4A	3.17	120.29	111.77
47	G	606	CHL	C3C-C4C-NC	-3.17	106.90	114.65
31	b	611	CLA	C3B-C4B-NB	-3.17	107.70	110.53
31	r1	602	CLA	O2A-C1-C2	3.17	120.30	108.11
47	N1	606	CHL	C3C-C4C-NC	-3.17	106.91	114.65
47	N	601	CHL	CHA-C1A-C2A	-3.17	125.87	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	G	612	CLA	C2C-C1C-NC	3.17	113.31	109.98
48	n	620	LUT	C31-C32-C33	-3.17	117.68	126.36
31	R1	604	CLA	CMA-C3A-C4A	3.17	120.28	111.77
47	R	606	CHL	CHA-C1A-C2A	-3.16	125.88	133.31
31	a	407	CLA	CMA-C3A-C4A	3.16	120.28	111.77
47	N1	607	CHL	C1A-CHA-C4D	3.16	124.26	118.98
47	n	605	CHL	C3C-C4C-NC	-3.16	106.92	114.65
47	r	607	CHL	C3C-C4C-NC	-3.16	106.92	114.65
47	n	606	CHL	C4D-CHA-CBD	-3.16	105.78	108.97
31	A	406	CLA	C2C-C1C-NC	3.16	113.30	109.98
31	C1	509	CLA	C2C-C1C-NC	3.16	113.30	109.98
31	C1	508	CLA	C1-C2-C3	-3.16	121.02	126.20
31	b1	602	CLA	C1-C2-C3	-3.16	121.02	126.20
31	G1	611	CLA	C1-C2-C3	-3.16	121.02	126.20
31	b	607	CLA	O2A-C1-C2	3.16	120.26	108.11
48	Y	620	LUT	C22-C23-C24	-3.16	106.50	111.18
47	n	607	CHL	C4D-CHA-CBD	-3.16	105.78	108.97
31	G	603	CLA	CBC-CAC-C3C	-3.16	103.86	112.42
48	Y	621	LUT	C26-C27-C28	-3.16	119.67	124.58
31	b1	614	CLA	O2A-C1-C2	3.16	120.25	108.11
37	b	620	C7Z	C1-C6-C5	-3.16	118.32	122.64
48	r1	620	LUT	C26-C27-C28	-3.16	119.67	124.58
47	n1	609	CHL	C3C-C4C-NC	-3.16	106.94	114.65
47	R1	607	CHL	C4D-CHA-CBD	-3.16	105.79	108.97
47	S1	608	CHL	C1-O2A-CGA	3.15	124.28	116.65
47	N1	601	CHL	CHA-C1A-C2A	-3.15	125.90	133.31
31	r	613	CLA	CMA-C3A-C4A	3.15	120.25	111.77
31	S1	613	CLA	C2C-C1C-NC	3.15	113.29	109.98
47	N	601	CHL	C3C-C4C-NC	-3.15	106.95	114.65
47	G1	606	CHL	C3C-C4C-NC	-3.15	106.95	114.65
31	B	613	CLA	C1-C2-C3	-3.15	121.04	126.20
31	B1	613	CLA	C1-C2-C3	-3.15	121.04	126.20
49	N1	622	XAT	C38-C25-C26	-3.15	117.12	122.30
31	n	612	CLA	C3B-C4B-NB	-3.15	107.72	110.53
31	y1	614	CLA	C1-C2-C3	-3.15	121.04	126.20
31	Y1	613	CLA	CMA-C3A-C4A	3.15	120.23	111.77
33	b1	618	BCR	C33-C5-C4	3.15	120.31	113.60
31	b	604	CLA	C2C-C1C-NC	3.15	113.29	109.98
31	c	501	CLA	C1-C2-C3	-3.15	121.04	126.20
31	A1	407	CLA	CMA-C3A-C4A	3.14	120.22	111.77
47	Y	607	CHL	C1-O2A-CGA	3.14	124.26	116.65
31	s1	603	CLA	CMA-C3A-C4A	3.14	120.22	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	605	CLA	C2C-C1C-NC	3.14	113.28	109.98
31	S1	613	CLA	CMA-C3A-C4A	3.14	120.22	111.77
47	R1	606	CHL	C4D-CHA-CBD	-3.14	105.80	108.97
47	G	601	CHL	C3C-C4C-NC	-3.14	106.97	114.65
31	y	613	CLA	O2A-C1-C2	3.14	120.20	108.11
31	B1	604	CLA	C1-C2-C3	-3.14	121.05	126.20
33	c	516	BCR	C37-C22-C23	3.14	122.88	118.09
31	S	610	CLA	C4B-CHC-C1C	3.14	133.63	126.25
47	G	607	CHL	C3C-C4C-NC	-3.14	106.98	114.65
31	D	403	CLA	C1-C2-C3	-3.14	121.06	126.20
54	I1	102	4RF	O40-C41-C43	3.14	121.40	111.83
47	S1	601	CHL	CHA-C1A-C2A	-3.14	125.94	133.31
31	c1	510	CLA	C1-C2-C3	-3.14	121.06	126.20
31	b1	603	CLA	CMA-C3A-C4A	3.14	120.20	111.77
35	a	413	LMG	O8-C28-C29	3.14	121.40	111.83
31	G1	611	CLA	C2C-C1C-NC	3.14	113.28	109.98
48	Y1	621	LUT	C18-C5-C6	-3.14	121.06	124.48
31	Y1	602	CLA	CMA-C3A-C4A	3.14	120.20	111.77
31	S1	602	CLA	CAA-C2A-C3A	-3.14	104.53	113.00
47	R1	607	CHL	CHA-C1A-C2A	-3.14	125.94	133.31
47	G	608	CHL	C3C-C4C-NC	-3.13	106.99	114.65
32	a	409	PHO	CMB-C2B-C3B	3.13	130.95	124.68
47	N	606	CHL	C3C-C4C-NC	-3.13	106.99	114.65
31	d	403	CLA	C2C-C1C-NC	3.13	113.27	109.98
31	g	603	CLA	C2C-C1C-NC	3.13	113.27	109.98
37	b1	620	C7Z	C31-C30-C29	-3.13	122.88	127.28
47	Y	606	CHL	CHA-C1A-C2A	-3.13	125.95	133.31
31	s1	604	CLA	C2C-C1C-NC	3.13	113.27	109.98
47	g	607	CHL	C1A-CHA-C4D	3.13	124.21	118.98
33	c	515	BCR	C1-C6-C5	-3.13	118.36	122.64
31	c	507	CLA	C2C-C1C-NC	3.13	113.27	109.98
31	s	614	CLA	C1C-C2C-C3C	-3.13	103.69	106.98
31	S	611	CLA	C2C-C1C-NC	3.13	113.27	109.98
31	c	507	CLA	C1C-C2C-C3C	-3.13	103.69	106.98
33	B	619	BCR	C33-C5-C4	3.13	120.26	113.60
31	s	610	CLA	CMA-C3A-C4A	3.13	120.18	111.77
31	s	613	CLA	C2C-C1C-NC	3.13	113.27	109.98
33	c	517	BCR	C3-C4-C5	-3.13	108.48	114.06
33	b1	619	BCR	C33-C5-C6	-3.13	121.07	124.48
31	C1	501	CLA	CMA-C3A-C4A	3.12	120.17	111.77
47	r1	606	CHL	CHA-C1A-C2A	-3.12	125.97	133.31
31	s	613	CLA	CMA-C3A-C4A	3.12	120.17	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	n1	601	CHL	C3C-C4C-NC	-3.12	107.01	114.65
31	y	602	CLA	C1C-C2C-C3C	-3.12	103.69	106.98
48	r	620	LUT	C27-C28-C29	-3.12	119.60	126.32
47	G1	609	CHL	C1-O2A-CGA	3.12	124.21	116.65
47	Y	609	CHL	C3C-C4C-NC	-3.12	107.02	114.65
48	S1	620	LUT	C11-C10-C9	-3.12	122.90	127.28
31	S1	611	CLA	C1-C2-C3	-3.12	121.08	126.20
47	y1	609	CHL	C3C-C4C-NC	-3.12	107.02	114.65
40	b1	623	DGD	O1G-C1A-C2A	3.12	121.35	111.83
49	g	622	XAT	O4-C5-C4	-3.12	110.57	113.49
48	y	621	LUT	C35-C15-C14	-3.12	117.14	123.52
47	g1	607	CHL	CHA-C1A-C2A	-3.12	125.98	133.31
56	R1	626	ERG	C13-C17-C20	-3.12	115.64	119.38
48	g1	620	LUT	C18-C5-C6	-3.12	121.08	124.48
47	g	606	CHL	C1-O2A-CGA	3.12	124.20	116.65
31	G	603	CLA	C2C-C1C-NC	3.12	113.25	109.98
47	N	607	CHL	C3C-C4C-NC	-3.12	107.04	114.65
40	c1	520	DGD	O6D-C5D-C6D	3.12	112.87	106.69
47	g	605	CHL	C3C-C4C-NC	-3.11	107.04	114.65
31	a1	410	CLA	C1-C2-C3	-3.11	121.09	126.20
31	A	410	CLA	C2C-C1C-NC	3.11	113.25	109.98
31	C	509	CLA	O2A-C1-C2	3.11	120.09	108.11
47	g1	601	CHL	CHA-C1A-C2A	-3.11	126.00	133.31
31	S1	617	CLA	CMA-C3A-C4A	3.11	120.14	111.77
31	C	503	CLA	CMA-C3A-C4A	3.11	120.13	111.77
47	g1	609	CHL	C1A-CHA-C4D	3.11	124.17	118.98
48	n1	621	LUT	C18-C5-C6	-3.11	121.09	124.48
31	B	609	CLA	C1C-C2C-C3C	-3.11	103.71	106.98
31	r1	603	CLA	C2C-C1C-NC	3.11	113.25	109.98
47	n1	607	CHL	C1-C2-C3	-3.11	121.10	126.20
47	S1	607	CHL	C3C-C4C-NC	-3.11	107.06	114.65
47	S	601	CHL	C3C-C4C-NC	-3.11	107.06	114.65
31	B1	610	CLA	C1-C2-C3	-3.11	121.11	126.20
47	g1	606	CHL	C3C-C4C-NC	-3.11	107.06	114.65
31	B	607	CLA	O2A-C1-C2	3.11	120.06	108.11
31	r	603	CLA	C2C-C1C-NC	3.11	113.24	109.98
31	y	613	CLA	C2C-C1C-NC	3.11	113.24	109.98
47	g1	607	CHL	C4D-CHA-CBD	-3.11	105.84	108.97
31	r	608	CLA	C1-C2-C3	-3.11	121.11	126.20
33	c	515	BCR	C33-C5-C6	-3.10	121.10	124.48
31	Y	612	CLA	C1-C2-C3	-3.10	121.11	126.20
31	b	615	CLA	C1C-C2C-C3C	-3.10	103.72	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	511	CLA	CMA-C3A-C4A	3.10	120.11	111.77
31	s	617	CLA	CMA-C3A-C4A	3.10	120.11	111.77
31	B1	616	CLA	C2C-C1C-NC	3.10	113.24	109.98
31	s	611	CLA	C1-C2-C3	-3.10	121.12	126.20
50	Y	623	NEX	C19-C9-C10	-3.10	117.80	122.82
47	s1	608	CHL	C3C-C4C-NC	-3.10	107.08	114.65
47	y1	605	CHL	C3C-C4C-NC	-3.10	107.08	114.65
31	S	614	CLA	C1-C2-C3	-3.10	121.12	126.20
47	N1	608	CHL	C3C-C4C-NC	-3.10	107.08	114.65
46	H	101	RRX	C38-C26-C27	3.10	120.12	114.42
31	r1	608	CLA	CMA-C3A-C4A	3.10	120.10	111.77
31	s1	605	CLA	CMA-C3A-C4A	3.10	120.10	111.77
31	a1	405	CLA	C1-C2-C3	-3.10	121.12	126.20
47	N	601	CHL	C1-O2A-CGA	3.10	124.14	116.65
47	Y1	605	CHL	C1A-CHA-C4D	3.10	124.15	118.98
33	c1	515	BCR	C31-C1-C6	-3.10	105.39	110.24
31	c1	502	CLA	C2C-C1C-NC	3.10	113.23	109.98
31	N	614	CLA	CMA-C3A-C4A	3.10	120.09	111.77
31	Y	611	CLA	C1-C2-C3	-3.09	121.13	126.20
31	b1	603	CLA	C2C-C1C-NC	3.09	113.23	109.98
47	n1	608	CHL	CHA-C1A-C2A	-3.09	126.04	133.31
47	G	605	CHL	C3C-C4C-NC	-3.09	107.09	114.65
32	a1	408	PHO	CMB-C2B-C3B	3.09	130.86	124.68
47	n1	608	CHL	C3C-C4C-NC	-3.09	107.10	114.65
48	n1	621	LUT	C15-C14-C13	-3.09	122.94	127.28
31	c1	509	CLA	CMA-C3A-C4A	3.09	120.07	111.77
46	H1	101	RRX	C36-C18-C19	3.09	122.80	118.09
47	S	606	CHL	C3C-C4C-NC	-3.09	107.11	114.65
31	g	610	CLA	CMA-C3A-C4A	3.09	120.07	111.77
31	b	608	CLA	C1-C2-C3	-3.08	121.14	126.20
47	y	605	CHL	C3C-C4C-NC	-3.08	107.11	114.65
31	b	605	CLA	CMA-C3A-C4A	3.08	120.06	111.77
31	A	410	CLA	C1-C2-C3	-3.08	121.15	126.20
47	r1	607	CHL	C3C-C4C-NC	-3.08	107.12	114.65
31	Y1	603	CLA	C1C-C2C-C3C	-3.08	103.74	106.98
48	g	620	LUT	C18-C5-C6	-3.08	121.12	124.48
31	R1	609	CLA	CMA-C3A-C4A	3.08	120.05	111.77
48	G	621	LUT	C11-C10-C9	-3.08	122.96	127.28
31	b1	613	CLA	CMA-C3A-C4A	3.08	120.05	111.77
31	b1	613	CLA	C2C-C1C-NC	3.08	113.22	109.98
47	g	608	CHL	C3C-C4C-NC	-3.08	107.13	114.65
31	B1	615	CLA	C2C-C1C-NC	3.08	113.22	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	R	621	XAT	C18-C5-C6	-3.08	117.24	122.30
31	Y	603	CLA	C1C-C2C-C3C	-3.08	103.74	106.98
47	N	609	CHL	C3C-C4C-NC	-3.08	107.13	114.65
31	B	609	CLA	C2C-C1C-NC	3.08	113.21	109.98
47	g1	605	CHL	C3C-C4C-NC	-3.08	107.13	114.65
31	y	611	CLA	C1-C2-C3	-3.08	121.16	126.20
31	y	602	CLA	C2D-C1D-ND	3.08	113.17	110.13
47	n	607	CHL	C3C-C4C-NC	-3.08	107.13	114.65
31	r	613	CLA	C2C-C1C-NC	3.08	113.21	109.98
47	s1	606	CHL	C3C-C4C-NC	-3.08	107.13	114.65
47	R	607	CHL	C3C-C4C-NC	-3.08	107.13	114.65
31	y	602	CLA	C3B-C4B-NB	-3.07	107.78	110.53
47	n	609	CHL	CMA-C3A-C4A	3.07	121.23	114.61
33	c	515	BCR	C8-C7-C6	-3.07	118.79	127.00
47	y	607	CHL	C3C-C4C-NC	-3.07	107.14	114.65
47	G1	608	CHL	C4D-CHA-CBD	-3.07	105.87	108.97
47	s1	607	CHL	C3C-C4C-NC	-3.07	107.14	114.65
47	Y	605	CHL	C1A-CHA-C4D	3.07	124.11	118.98
31	B1	606	CLA	C2C-C1C-NC	3.07	113.21	109.98
48	n	620	LUT	C27-C28-C29	-3.07	119.72	126.32
31	b1	613	CLA	CMB-C2B-C1B	3.07	130.09	125.42
47	n1	601	CHL	CHA-C1A-C2A	-3.07	126.10	133.31
47	s1	606	CHL	C1A-CHA-C4D	3.07	124.11	118.98
47	r	607	CHL	CHA-C1A-C2A	-3.07	126.10	133.31
31	s1	610	CLA	C2C-C1C-NC	3.07	113.21	109.98
31	B1	606	CLA	CMD-C2D-C3D	-3.07	120.65	127.69
33	B	619	BCR	C27-C26-C25	-3.07	118.56	122.70
31	Y1	613	CLA	C2C-C1C-NC	3.07	113.20	109.98
47	G	608	CHL	C1A-CHA-C4D	3.07	124.10	118.98
31	C1	510	CLA	C1C-C2C-C3C	-3.07	103.75	106.98
50	R	622	NEX	O24-C25-C38	-3.07	111.62	115.05
50	N1	623	NEX	C38-C25-C26	-3.07	117.26	122.30
31	s1	611	CLA	CMA-C3A-C4A	3.07	120.01	111.77
31	b1	613	CLA	O2A-C1-C2	3.06	119.90	108.11
50	s1	623	NEX	C39-C29-C30	-3.06	117.85	122.82
32	a1	409	PHO	C4D-ND-C1D	-3.06	105.20	108.87
31	c1	503	CLA	C1-C2-C3	-3.06	121.18	126.20
31	n1	614	CLA	CMA-C3A-C4A	3.06	120.01	111.77
31	s	614	CLA	C2C-C1C-NC	3.06	113.20	109.98
31	g	602	CLA	CMA-C3A-C4A	3.06	120.00	111.77
31	b1	609	CLA	C1C-C2C-C3C	-3.06	103.76	106.98
47	G1	607	CHL	CHA-C1A-C2A	-3.06	126.12	133.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	g1	608	CHL	C4D-CHA-CBD	-3.06	105.88	108.97
31	c	510	CLA	C1C-C2C-C3C	-3.06	103.76	106.98
31	R	609	CLA	C3B-C4B-NB	-3.06	107.80	110.53
32	a	408	PHO	O1D-CGD-CBD	3.06	129.36	124.72
31	c1	506	CLA	O2A-C1-C2	3.06	119.88	108.11
31	b	616	CLA	C2C-C1C-NC	3.06	113.20	109.98
31	c1	504	CLA	C2C-C1C-NC	3.06	113.20	109.98
35	a	413	LMG	C8-O7-C10	-3.06	110.47	117.80
47	N	608	CHL	C3C-C4C-NC	-3.06	107.17	114.65
47	Y1	606	CHL	C3C-C4C-NC	-3.06	107.17	114.65
31	b1	611	CLA	C1-C2-C3	-3.06	121.19	126.20
31	y	604	CLA	C2C-C1C-NC	3.06	113.19	109.98
31	r	610	CLA	C1-C2-C3	-3.06	121.19	126.20
31	B1	609	CLA	C1-C2-C3	-3.06	121.19	126.20
47	Y	607	CHL	C3C-C4C-NC	-3.06	107.17	114.65
47	Y	607	CHL	C1A-CHA-C4D	3.06	124.08	118.98
47	y	609	CHL	C3C-C4C-NC	-3.06	107.18	114.65
31	B	606	CLA	C1-C2-C3	-3.06	121.19	126.20
46	h1	101	RRX	C7-C6-C5	-3.06	114.52	121.56
47	N1	607	CHL	CHA-C1A-C2A	-3.06	126.13	133.31
33	d1	404	BCR	C33-C5-C4	3.06	120.11	113.60
50	y1	623	NEX	C1-C2-C3	3.05	120.29	113.59
31	B1	613	CLA	CMA-C3A-C4A	3.05	119.98	111.77
48	Y1	620	LUT	C11-C10-C9	-3.05	123.00	127.28
47	s	601	CHL	C3C-C4C-NC	-3.05	107.19	114.65
41	d1	409	LHG	O8-C23-C24	3.05	121.14	111.83
56	r1	626	ERG	C13-C17-C20	-3.05	115.72	119.38
31	a1	407	CLA	C2C-C1C-NC	3.05	113.19	109.98
31	s1	612	CLA	C2C-C1C-NC	3.05	113.19	109.98
47	y1	607	CHL	C3C-C4C-NC	-3.05	107.19	114.65
33	d	404	BCR	C33-C5-C4	3.05	120.10	113.60
49	Y1	622	XAT	C38-C25-C26	-3.05	117.28	122.30
31	C1	502	CLA	C1-C2-C3	-3.05	121.20	126.20
47	G1	601	CHL	C4D-CHA-CBD	-3.05	105.89	108.97
47	s	607	CHL	C3C-C4C-NC	-3.05	107.20	114.65
47	S1	606	CHL	C3C-C4C-NC	-3.05	107.20	114.65
47	g1	601	CHL	C4D-CHA-CBD	-3.05	105.89	108.97
33	b	619	BCR	C36-C18-C17	-3.05	117.88	122.82
31	S1	602	CLA	O2A-CGA-CBA	3.05	121.13	111.83
31	b	609	CLA	C2C-C1C-NC	3.05	113.18	109.98
31	r1	612	CLA	C1-C2-C3	-3.05	121.21	126.20
47	y1	605	CHL	C4D-CHA-CBD	-3.05	105.90	108.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s1	604	CLA	CMA-C3A-C4A	3.04	119.96	111.77
47	G	601	CHL	C1-O2A-CGA	3.04	124.02	116.65
50	y	623	NEX	C38-C25-C26	-3.04	117.29	122.30
31	S	603	CLA	C1-C2-C3	-3.04	121.21	126.20
48	Y1	621	LUT	C22-C23-C24	-3.04	106.67	111.18
47	G1	605	CHL	C3C-C4C-NC	-3.04	107.22	114.65
33	b	619	BCR	C19-C18-C17	3.04	123.79	119.01
48	n1	620	LUT	C15-C14-C13	-3.04	123.01	127.28
47	Y1	605	CHL	C3C-C4C-NC	-3.04	107.22	114.65
31	n	603	CLA	C1C-C2C-C3C	-3.04	103.78	106.98
47	N	607	CHL	C1-C2-C3	-3.04	121.22	126.20
31	n1	613	CLA	CBA-CAA-C2A	3.04	122.83	113.79
32	a	409	PHO	O2D-CGD-O1D	-3.04	117.93	123.85
31	b	604	CLA	O2A-C1-C2	3.04	119.80	108.11
31	B1	604	CLA	C3B-C4B-NB	-3.04	107.82	110.53
31	y	614	CLA	C2C-C1C-NC	3.04	113.17	109.98
49	n1	622	XAT	C6-C7-C8	-3.04	119.57	125.99
47	Y1	607	CHL	C1A-CHA-C4D	3.04	124.05	118.98
31	g1	612	CLA	C2C-C1C-NC	3.04	113.17	109.98
47	n	606	CHL	CHA-C1A-C2A	-3.04	126.18	133.31
31	b1	609	CLA	C2C-C1C-NC	3.04	113.17	109.98
33	B1	618	BCR	C4-C5-C6	-3.03	118.60	122.70
31	C	501	CLA	CMD-C2D-C3D	-3.03	120.73	127.69
48	S	621	LUT	C31-C30-C29	-3.03	123.02	127.28
38	j1	101	DGA	OG1-CA1-CA2	3.03	121.08	111.83
47	s	606	CHL	C3C-C4C-NC	-3.03	107.24	114.65
56	r1	626	ERG	C4-C5-C10	3.03	120.31	116.42
31	A1	410	CLA	C1-C2-C3	-3.03	121.23	126.20
47	G1	608	CHL	C3C-C4C-NC	-3.03	107.24	114.65
47	Y1	609	CHL	C3C-C4C-NC	-3.03	107.24	114.65
31	B	607	CLA	O2A-CGA-CBA	3.03	121.08	111.83
31	B	602	CLA	C1-C2-C3	-3.03	121.23	126.20
31	r1	609	CLA	CMA-C3A-C4A	3.03	119.92	111.77
31	C1	503	CLA	O2A-C1-C2	3.03	119.77	108.11
31	a	407	CLA	C2C-C1C-NC	3.03	113.17	109.98
47	n	605	CHL	C1A-CHA-C4D	3.03	124.04	118.98
31	Y	602	CLA	C1-C2-C3	-3.03	121.23	126.20
31	b	615	CLA	CBA-CAA-C2A	3.03	122.81	113.79
47	y	607	CHL	C4D-CHA-CBD	-3.03	105.91	108.97
47	s	601	CHL	CHA-C1A-C2A	-3.03	126.19	133.31
47	g1	601	CHL	C1A-CHA-C4D	3.03	124.04	118.98
31	A	405	CLA	C1-C2-C3	-3.03	121.23	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	502	CLA	O2D-CGD-O1D	-3.03	117.95	123.85
46	h	101	RRX	C33-C5-C6	-3.03	121.18	124.48
31	s	614	CLA	C1-O2A-CGA	3.03	123.98	116.65
31	B1	611	CLA	C1C-C2C-C3C	-3.03	103.80	106.98
47	s1	608	CHL	C1A-CHA-C4D	3.03	124.03	118.98
47	g1	608	CHL	CHA-C1A-C2A	-3.03	126.20	133.31
31	n	610	CLA	O2A-CGA-CBA	3.03	121.07	111.83
31	S	609	CLA	CMA-C3A-C4A	3.03	119.91	111.77
31	a	406	CLA	CMA-C3A-C4A	3.03	119.91	111.77
31	S1	603	CLA	C2C-C1C-NC	3.03	113.16	109.98
31	N	602	CLA	CMA-C3A-C4A	3.03	119.91	111.77
31	S1	614	CLA	C1-C2-C3	-3.03	121.24	126.20
47	N	608	CHL	C4D-CHA-CBD	-3.03	105.92	108.97
47	G	607	CHL	C4D-CHA-CBD	-3.03	105.92	108.97
47	r	606	CHL	C4D-CHA-CBD	-3.03	105.92	108.97
47	S1	601	CHL	C3C-C4C-NC	-3.02	107.26	114.65
47	y1	606	CHL	C1A-CHA-C4D	3.02	124.03	118.98
47	S	607	CHL	C3C-C4C-NC	-3.02	107.26	114.65
31	B1	602	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
31	b	613	CLA	O2A-C1-C2	3.02	119.74	108.11
47	y	606	CHL	C3C-C4C-NC	-3.02	107.26	114.65
31	S	612	CLA	C2C-C1C-NC	3.02	113.16	109.98
31	b1	603	CLA	O2D-CGD-O1D	-3.02	117.96	123.85
47	n1	609	CHL	C1-O2A-CGA	3.02	123.97	116.65
31	B1	609	CLA	C1C-C2C-C3C	-3.02	103.80	106.98
47	N	605	CHL	C3C-C4C-NC	-3.02	107.27	114.65
47	g1	601	CHL	C3C-C4C-NC	-3.02	107.27	114.65
31	g1	603	CLA	CMA-C3A-C4A	3.02	119.89	111.77
31	C	503	CLA	C3B-C4B-NB	-3.02	107.83	110.53
31	N	611	CLA	CMA-C3A-C4A	3.02	119.89	111.77
31	Y	603	CLA	C1-C2-C3	-3.02	121.25	126.20
50	g1	623	NEX	C16-C1-C6	-3.02	107.77	110.47
47	Y	606	CHL	C1-C2-C3	-3.02	121.25	126.20
31	b1	615	CLA	C2C-C1C-NC	3.02	113.15	109.98
50	N1	623	NEX	C17-C1-C6	-3.02	107.77	110.47
31	A	407	CLA	CMA-C3A-C4A	3.02	119.88	111.77
31	G	614	CLA	CMA-C3A-C4A	3.02	119.88	111.77
35	C1	521	LMG	O8-C28-C29	3.02	121.03	111.83
31	b	609	CLA	O2D-CGD-O1D	-3.02	117.98	123.85
31	S	605	CLA	O2A-CGA-CBA	3.02	121.03	111.83
31	C	510	CLA	C1C-C2C-C3C	-3.02	103.81	106.98
48	g1	620	LUT	C31-C30-C29	-3.01	123.05	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	n	623	NEX	C39-C29-C30	-3.01	117.93	122.82
47	R	607	CHL	CHA-C1A-C2A	-3.01	126.23	133.31
31	s1	614	CLA	C2C-C1C-NC	3.01	113.15	109.98
47	Y	606	CHL	C4D-CHA-CBD	-3.01	105.93	108.97
47	N	608	CHL	C1A-CHA-C4D	3.01	124.01	118.98
47	g	601	CHL	C1A-CHA-C4D	3.01	124.01	118.98
31	A	405	CLA	C6-C5-C3	-3.01	106.13	113.47
48	N1	620	LUT	C10-C11-C12	-3.01	114.47	123.20
31	c1	502	CLA	CMA-C3A-C4A	3.01	119.87	111.77
31	R	612	CLA	C4B-CHC-C1C	3.01	133.32	126.25
47	S	607	CHL	C1A-CHA-C4D	3.01	124.00	118.98
31	y	602	CLA	CAA-C2A-C3A	-3.01	104.87	113.00
31	g1	613	CLA	CMA-C3A-C4A	3.01	119.86	111.77
31	A	410	CLA	CMA-C3A-C4A	3.01	119.86	111.77
33	D	404	BCR	C27-C26-C25	-3.01	118.64	122.70
31	G1	611	CLA	CMA-C3A-C4A	3.01	119.86	111.77
41	D1	409	LHG	O8-C23-C24	3.01	121.00	111.83
31	R	604	CLA	C2C-C1C-NC	3.01	113.14	109.98
50	R1	622	NEX	O24-C25-C38	-3.01	111.69	115.05
31	s	614	CLA	O2A-CGA-CBA	3.01	121.00	111.83
47	G	607	CHL	CHA-C1A-C2A	-3.01	126.25	133.31
47	n1	606	CHL	C3C-C4C-NC	-3.00	107.31	114.65
31	S1	605	CLA	C2C-C1C-NC	3.00	113.14	109.98
47	n	606	CHL	C3C-C4C-NC	-3.00	107.31	114.65
47	y1	601	CHL	C3C-C4C-NC	-3.00	107.31	114.65
31	C	509	CLA	C2C-C1C-NC	3.00	113.14	109.98
31	B	617	CLA	O2A-CGA-CBA	3.00	120.99	111.83
31	C1	512	CLA	C2C-C1C-NC	3.00	113.14	109.98
47	G1	606	CHL	CHA-C1A-C2A	-3.00	126.26	133.31
31	R1	602	CLA	O2D-CGD-O1D	-3.00	118.00	123.85
47	n1	605	CHL	C3C-C4C-NC	-3.00	107.31	114.65
31	B	602	CLA	C2C-C1C-NC	3.00	113.13	109.98
31	B1	603	CLA	C2C-C1C-NC	3.00	113.13	109.98
31	A1	406	CLA	C1-C2-C3	-3.00	121.28	126.20
47	n	609	CHL	C1A-CHA-C4D	3.00	123.99	118.98
31	R1	608	CLA	CMA-C3A-C4A	3.00	119.83	111.77
31	s1	603	CLA	C2C-C1C-NC	3.00	113.13	109.98
31	n1	603	CLA	C2C-C1C-NC	3.00	113.13	109.98
47	S	606	CHL	C1A-CHA-C4D	3.00	123.98	118.98
47	R1	607	CHL	C3C-C4C-NC	-3.00	107.32	114.65
47	G	601	CHL	C1-C2-C3	-3.00	121.29	126.20
31	c1	510	CLA	C2C-C1C-NC	3.00	113.13	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	g1	606	CHL	CHA-C1A-C2A	-3.00	126.27	133.31
31	d	403	CLA	CMA-C3A-C4A	3.00	119.82	111.77
31	b1	612	CLA	CMA-C3A-C4A	3.00	119.82	111.77
31	R1	604	CLA	C2C-C1C-NC	3.00	113.13	109.98
47	y1	606	CHL	C3C-C4C-NC	-2.99	107.33	114.65
31	R1	603	CLA	C1-C2-C3	-2.99	121.29	126.20
31	a1	407	CLA	CMA-C3A-C4A	2.99	119.82	111.77
50	g	623	NEX	C17-C1-C6	-2.99	107.79	110.47
31	c	506	CLA	C2C-C1C-NC	2.99	113.13	109.98
47	Y	601	CHL	C3C-C4C-NC	-2.99	107.33	114.65
47	s	608	CHL	C4D-CHA-CBD	-2.99	105.95	108.97
31	B	614	CLA	C1-C2-C3	-2.99	121.29	126.20
31	d	403	CLA	O2D-CGD-O1D	-2.99	118.02	123.85
49	N1	622	XAT	O4-C6-C7	-2.99	108.31	116.88
31	R1	602	CLA	O1D-CGD-CBD	-2.99	118.62	124.52
31	y1	614	CLA	CMD-C2D-C3D	-2.99	120.83	127.69
47	N1	609	CHL	C3C-C4C-NC	-2.99	107.34	114.65
31	C	503	CLA	C1-C2-C3	-2.99	121.30	126.20
31	b	611	CLA	C4B-CHC-C1C	2.99	133.28	126.25
31	Y	608	CLA	CMA-C3A-C4A	2.99	119.81	111.77
48	n1	620	LUT	C35-C34-C33	-2.99	123.09	127.28
47	g	607	CHL	C4D-CHA-CBD	-2.99	105.95	108.97
31	c	509	CLA	O2A-CGA-CBA	2.99	120.95	111.83
33	C	515	BCR	C33-C5-C4	2.99	119.97	113.60
31	N	603	CLA	C1C-C2C-C3C	-2.99	103.84	106.98
47	S	608	CHL	C3C-C4C-NC	-2.99	107.35	114.65
31	y	614	CLA	C1C-C2C-C3C	-2.99	103.84	106.98
31	B	609	CLA	CMA-C3A-C4A	2.99	119.80	111.77
50	Y	623	NEX	C16-C1-C6	-2.98	107.80	110.47
31	g	614	CLA	CMA-C3A-C4A	2.98	119.79	111.77
31	c1	508	CLA	C1D-ND-C4D	-2.98	104.22	106.31
31	N	612	CLA	C2C-C1C-NC	2.98	113.11	109.98
47	Y	606	CHL	C1A-CHA-C4D	2.98	123.96	118.98
31	b	603	CLA	CMA-C3A-C4A	2.98	119.79	111.77
33	A1	411	BCR	C15-C14-C13	-2.98	123.09	127.28
48	S	621	LUT	C15-C14-C13	-2.98	123.09	127.28
31	N1	603	CLA	C1C-C2C-C3C	-2.98	103.84	106.98
48	R	620	LUT	C27-C28-C29	-2.98	119.91	126.32
47	N	609	CHL	C1A-CHA-C4D	2.98	123.96	118.98
31	Y1	613	CLA	CMD-C2D-C3D	-2.98	120.85	127.69
35	d1	411	LMG	O8-C28-C29	2.98	120.92	111.83
47	Y	606	CHL	C3C-C4C-NC	-2.98	107.36	114.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B1	605	CLA	O2A-CGA-CBA	2.98	120.92	111.83
47	S1	601	CHL	C4D-CHA-CBD	-2.98	105.96	108.97
48	s	621	LUT	C11-C10-C9	-2.98	123.10	127.28
33	b	619	BCR	C33-C5-C6	-2.98	121.23	124.48
49	y	622	XAT	O4-C5-C4	-2.98	110.70	113.49
31	y1	611	CLA	OBD-CAD-C3D	-2.98	121.45	128.42
33	a1	411	BCR	C15-C14-C13	-2.98	123.10	127.28
31	D	402	CLA	C3B-C4B-NB	-2.98	107.87	110.53
48	G1	621	LUT	C31-C32-C33	-2.98	118.19	126.36
31	s1	602	CLA	O2A-CGA-CBA	2.98	120.92	111.83
31	R	603	CLA	O1D-CGD-CBD	-2.98	118.64	124.52
31	N	610	CLA	C3B-C4B-NB	-2.98	107.87	110.53
31	A1	405	CLA	C3B-C4B-NB	-2.98	107.87	110.53
31	S1	605	CLA	C1-O2A-CGA	2.98	123.86	116.65
31	a1	406	CLA	CMA-C3A-C4A	2.98	119.77	111.77
33	b1	619	BCR	C1-C6-C5	-2.98	118.57	122.64
37	b1	620	C7Z	C11-C12-C13	-2.98	118.20	126.36
47	R	607	CHL	C4D-CHA-CBD	-2.98	105.97	108.97
31	C1	507	CLA	C1-O2A-CGA	2.98	123.86	116.65
48	g	621	LUT	C31-C30-C29	-2.98	123.10	127.28
31	C1	511	CLA	C2C-C1C-NC	2.98	113.11	109.98
48	n1	621	LUT	C22-C23-C24	-2.98	106.76	111.18
47	n	608	CHL	C3C-C4C-NC	-2.98	107.38	114.65
56	r1	626	ERG	C7-C6-C5	-2.98	116.81	122.95
47	r1	607	CHL	C4D-CHA-CBD	-2.97	105.97	108.97
31	s	603	CLA	C2C-C1C-NC	2.97	113.11	109.98
31	Y1	608	CLA	C2C-C1C-NC	2.97	113.11	109.98
31	C1	511	CLA	C1-C2-C3	-2.97	121.32	126.20
40	C	519	DGD	O1G-C1A-C2A	2.97	120.90	111.83
31	s	605	CLA	CMA-C3A-C4A	2.97	119.77	111.77
31	c	504	CLA	C1C-C2C-C3C	-2.97	103.85	106.98
40	C1	520	DGD	O1G-C1A-C2A	2.97	120.90	111.83
47	y	607	CHL	CHA-C1A-C2A	-2.97	126.33	133.31
49	r	622	XAT	C31-C30-C29	-2.97	123.11	127.28
48	G	621	LUT	C15-C35-C34	-2.97	117.44	123.52
31	R1	604	CLA	C1C-C2C-C3C	-2.97	103.86	106.98
31	d1	402	CLA	C3B-C4B-NB	-2.97	107.88	110.53
31	Y1	613	CLA	C1-C2-C3	-2.97	121.33	126.20
33	A	411	BCR	C23-C24-C25	-2.97	119.06	127.00
47	y	606	CHL	C1A-CHA-C4D	2.97	123.94	118.98
45	F	101	HEM	C3B-C2B-C1B	2.97	108.64	106.41
50	Y1	623	NEX	C38-C25-C26	-2.97	117.41	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	c1	517	BCR	C37-C22-C21	-2.97	118.00	122.82
31	N1	614	CLA	CMA-C3A-C4A	2.97	119.75	111.77
31	r	611	CLA	CMA-C3A-C4A	2.97	119.75	111.77
31	r	608	CLA	CMA-C3A-C4A	2.97	119.75	111.77
31	C	505	CLA	C3B-C4B-NB	-2.97	107.88	110.53
31	Y	608	CLA	C1-C2-C3	-2.97	121.96	126.76
31	c	502	CLA	CMA-C3A-C4A	2.97	119.75	111.77
31	g	611	CLA	OBD-CAD-C3D	-2.97	121.48	128.42
31	c1	506	CLA	O2D-CGD-O1D	-2.97	118.07	123.85
31	C1	506	CLA	C1-C2-C3	-2.97	121.34	126.20
31	B	615	CLA	C1-O2A-CGA	2.97	123.83	116.65
31	r1	604	CLA	C2C-C1C-NC	2.96	113.10	109.98
47	g	607	CHL	C3C-C4C-NC	-2.96	107.40	114.65
31	Y	602	CLA	C4B-CHC-C1C	2.96	133.22	126.25
31	b	616	CLA	C1-C2-C3	-2.96	121.34	126.20
31	c1	504	CLA	O2D-CGD-O1D	-2.96	118.08	123.85
31	A	407	CLA	C1C-C2C-C3C	-2.96	103.86	106.98
31	C	507	CLA	C1C-C2C-C3C	-2.96	103.86	106.98
48	g1	620	LUT	C7-C8-C9	-2.96	121.85	126.23
44	D1	405	PL9	C22-C23-C24	-2.96	120.84	127.62
31	B1	617	CLA	C1-C2-C3	-2.96	121.34	126.20
33	C1	516	BCR	C28-C27-C26	-2.96	108.77	114.06
35	D1	411	LMG	O8-C28-C29	2.96	120.87	111.83
31	D	403	CLA	CMA-C3A-C4A	2.96	119.73	111.77
33	C1	514	BCR	C33-C5-C6	-2.96	121.25	124.48
50	g	623	NEX	C31-C30-C29	2.96	131.43	127.28
31	r1	609	CLA	C2C-C1C-NC	2.96	113.09	109.98
47	n	601	CHL	C1-C2-C3	-2.96	121.35	126.20
31	r	608	CLA	CMD-C2D-C3D	-2.96	120.90	127.69
31	b	612	CLA	CMA-C3A-C4A	2.96	119.73	111.77
44	D1	405	PL9	C7-C8-C9	-2.96	121.73	126.83
31	Y1	603	CLA	C1-C2-C3	-2.96	121.35	126.20
31	C1	508	CLA	CMA-C3A-C4A	2.96	119.73	111.77
33	B1	619	BCR	C1-C6-C5	-2.96	118.59	122.64
31	b1	611	CLA	C2C-C1C-NC	2.96	113.09	109.98
47	n1	605	CHL	C1A-CHA-C4D	2.96	123.92	118.98
31	D1	403	CLA	O2A-CGA-CBA	2.96	120.86	111.83
31	c	511	CLA	C3B-C4B-NB	-2.96	107.89	110.53
31	S	603	CLA	C2C-C1C-NC	2.96	113.09	109.98
47	y	605	CHL	C1A-CHA-C4D	2.96	123.92	118.98
31	S1	604	CLA	C2C-C1C-NC	2.96	113.09	109.98
31	Y	611	CLA	CMA-C3A-C4A	2.96	119.72	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	n	613	CLA	CAC-C3C-C4C	2.96	128.64	124.79
31	c1	506	CLA	C1-C2-C3	-2.96	121.35	126.20
47	Y1	605	CHL	C4D-CHA-CBD	-2.96	105.99	108.97
31	N1	611	CLA	C2C-C1C-NC	2.95	113.08	109.98
31	n1	603	CLA	CMA-C3A-C4A	2.95	119.71	111.77
47	g	609	CHL	C3C-C4C-NC	-2.95	107.43	114.65
31	S1	614	CLA	C2C-C1C-NC	2.95	113.08	109.98
47	G	605	CHL	C1A-CHA-C4D	2.95	123.91	118.98
32	A1	409	PHO	O1D-CGD-CBD	2.95	129.20	124.72
31	B1	612	CLA	CMC-C2C-C1C	2.95	129.65	125.03
48	n	621	LUT	C22-C23-C24	-2.95	106.80	111.18
33	D1	404	BCR	C15-C14-C13	-2.95	123.14	127.28
47	n1	606	CHL	CHA-C1A-C2A	-2.95	126.38	133.31
31	C	506	CLA	C1-C2-C3	-2.95	121.36	126.20
47	Y1	609	CHL	C4D-CHA-CBD	-2.95	105.99	108.97
31	R1	612	CLA	C2C-C1C-NC	2.95	113.08	109.98
44	d1	405	PL9	C36-C34-C33	-2.95	114.55	121.17
31	C1	503	CLA	CMA-C3A-C4A	2.95	119.70	111.77
50	s	623	NEX	C27-C28-C29	-2.95	120.95	125.53
31	y	614	CLA	CMA-C3A-C4A	2.95	119.70	111.77
31	B	612	CLA	C1-C2-C3	-2.95	121.37	126.20
31	n	603	CLA	C2C-C1C-NC	2.95	113.08	109.98
47	g	608	CHL	C1A-CHA-C4D	2.95	123.90	118.98
31	C1	504	CLA	C1C-C2C-C3C	-2.95	103.88	106.98
31	s	605	CLA	C2C-C1C-NC	2.95	113.08	109.98
50	S	622	NEX	C39-C29-C30	-2.95	118.04	122.82
48	s1	620	LUT	C35-C34-C33	-2.95	123.15	127.28
47	n1	608	CHL	C4D-CHA-CBD	-2.95	106.00	108.97
31	D	402	CLA	C2D-C1D-ND	2.95	113.04	110.13
31	C1	502	CLA	CMA-C3A-C4A	2.95	119.69	111.77
41	L	101	LHG	O8-C23-C24	2.95	120.81	111.83
31	S1	609	CLA	CMA-C3A-C4A	2.94	119.69	111.77
49	r	622	XAT	C19-C9-C10	-2.94	118.05	122.82
31	G1	603	CLA	C2C-C1C-NC	2.94	113.08	109.98
50	N	623	NEX	C38-C25-C26	-2.94	117.46	122.30
38	J1	101	DGA	OG1-CA1-CA2	2.94	120.81	111.83
31	B1	603	CLA	CMA-C3A-C4A	2.94	119.68	111.77
31	y	612	CLA	C2C-C1C-NC	2.94	113.07	109.98
47	y	605	CHL	C4D-CHA-CBD	-2.94	106.00	108.97
31	b1	606	CLA	O2A-CGA-CBA	2.94	120.80	111.83
31	R	611	CLA	CMA-C3A-C4A	2.94	119.68	111.77
49	r	622	XAT	C27-C28-C29	2.94	130.09	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	s	606	CHL	C1A-CHA-C4D	2.94	123.89	118.98
31	G	604	CLA	C2C-C1C-NC	2.94	113.07	109.98
31	y1	611	CLA	C2C-C1C-NC	2.94	113.07	109.98
47	S	608	CHL	C4D-CHA-CBD	-2.94	106.00	108.97
50	Y	623	NEX	C38-C25-C26	-2.94	117.46	122.30
31	g	612	CLA	CMA-C3A-C4A	2.94	119.67	111.77
50	n	623	NEX	O24-C25-C38	-2.94	111.76	115.05
47	N1	607	CHL	C3C-C4C-NC	-2.94	107.47	114.65
47	g	605	CHL	C1A-CHA-C4D	2.94	123.88	118.98
31	B	604	CLA	CMA-C3A-C4A	2.94	119.67	111.77
31	B1	608	CLA	C2C-C1C-NC	2.94	113.07	109.98
31	b1	616	CLA	C2C-C1C-NC	2.94	113.07	109.98
50	y1	623	NEX	C39-C29-C30	-2.94	118.06	122.82
31	S	605	CLA	O2D-CGD-O1D	-2.94	118.13	123.85
31	c1	511	CLA	CAA-C2A-C1A	2.94	121.59	111.97
47	s1	601	CHL	CHA-C1A-C2A	-2.93	126.42	133.31
31	B1	608	CLA	CMA-C3A-C4A	2.93	119.66	111.77
48	S	620	LUT	C31-C30-C29	-2.93	123.16	127.28
31	S	614	CLA	C2C-C1C-NC	2.93	113.06	109.98
31	s1	611	CLA	C2C-C1C-NC	2.93	113.06	109.98
49	G	622	XAT	C26-C27-C28	-2.93	119.79	125.99
31	S	610	CLA	C1-C2-C3	-2.93	121.39	126.20
47	y	601	CHL	C1-O2A-CGA	2.93	123.75	116.65
48	R1	620	LUT	C18-C5-C4	2.93	119.81	114.42
31	B1	602	CLA	C2C-C1C-NC	2.93	113.06	109.98
31	y	602	CLA	O2D-CGD-O1D	-2.93	118.14	123.85
33	C1	515	BCR	C33-C5-C4	2.93	119.84	113.60
47	G	609	CHL	C1A-CHA-C4D	2.93	123.87	118.98
35	c1	521	LMG	O8-C28-C29	2.93	120.77	111.83
31	s1	617	CLA	C1C-C2C-C3C	-2.93	103.90	106.98
31	C1	504	CLA	CMA-C3A-C4A	2.93	119.64	111.77
48	g1	621	LUT	C35-C34-C33	-2.93	123.17	127.28
31	B	606	CLA	O2A-CGA-CBA	2.93	120.76	111.83
31	c	513	CLA	O2A-CGA-CBA	2.93	120.76	111.83
47	r1	606	CHL	C4D-CHA-CBD	-2.93	106.02	108.97
35	C1	523	LMG	O8-C28-C29	2.93	120.76	111.83
41	S1	624	LHG	C5-O7-C7	-2.93	110.79	117.80
31	C1	502	CLA	C2C-C1C-NC	2.93	113.06	109.98
31	c1	506	CLA	C2C-C1C-NC	2.93	113.06	109.98
31	N1	602	CLA	C1D-ND-C4D	-2.93	104.26	106.31
56	r1	626	ERG	C1-C2-C3	2.93	114.36	110.48
31	y1	602	CLA	O2A-CGA-CBA	2.93	120.76	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	y	611	CLA	C2C-C1C-NC	2.93	113.06	109.98
31	S	605	CLA	CMA-C3A-C4A	2.93	119.64	111.77
31	N1	602	CLA	CMA-C3A-C4A	2.93	119.64	111.77
31	g1	602	CLA	C1-C2-C3	-2.93	121.40	126.20
47	y1	609	CHL	C1-O2A-CGA	2.93	123.73	116.65
31	b	607	CLA	C2C-C1C-NC	2.92	113.05	109.98
31	S1	605	CLA	CMA-C3A-C4A	2.92	119.63	111.77
54	i1	101	4RF	O40-C41-C43	2.92	120.75	111.83
47	g1	601	CHL	CMA-C3A-C4A	2.92	120.91	114.61
47	G1	609	CHL	C4D-CHA-CBD	-2.92	106.02	108.97
44	D	405	PL9	C40-C39-C41	2.92	120.30	115.23
31	N1	613	CLA	C2C-C1C-NC	2.92	113.05	109.98
47	s	608	CHL	C1-O2A-CGA	2.92	123.72	116.65
47	N1	606	CHL	C1A-CHA-C4D	2.92	123.86	118.98
31	s1	602	CLA	CAA-C2A-C3A	-2.92	105.11	113.00
31	G	610	CLA	O1D-CGD-CBD	-2.92	118.76	124.52
31	Y1	612	CLA	C2C-C1C-NC	2.92	113.05	109.98
31	y	603	CLA	C4B-CHC-C1C	2.92	133.11	126.25
41	S	624	LHG	O8-C23-C24	2.92	120.74	111.83
31	S1	604	CLA	CMA-C3A-C4A	2.92	119.62	111.77
31	r	608	CLA	C2C-C1C-NC	2.92	113.05	109.98
31	G1	612	CLA	CMA-C3A-C4A	2.92	119.62	111.77
48	g1	621	LUT	C26-C27-C28	-2.92	120.04	124.58
50	s	623	NEX	C26-C27-C28	-2.92	119.82	125.99
47	Y1	607	CHL	CHA-C1A-C2A	-2.92	126.45	133.31
47	g1	608	CHL	C1A-CHA-C4D	2.92	123.85	118.98
31	b1	604	CLA	CMA-C3A-C4A	2.92	119.61	111.77
31	S1	605	CLA	O2A-CGA-CBA	2.92	120.73	111.83
31	C	507	CLA	C2C-C1C-NC	2.92	113.05	109.98
31	C1	512	CLA	C1C-C2C-C3C	-2.92	103.91	106.98
31	y	614	CLA	O2A-C1-C2	2.92	119.33	108.11
49	G1	622	XAT	C26-C27-C28	-2.92	119.83	125.99
31	G1	603	CLA	C3B-C4B-NB	-2.92	107.93	110.53
49	R1	621	XAT	C38-C25-C26	-2.92	117.50	122.30
47	S1	606	CHL	C1A-CHA-C4D	2.92	123.85	118.98
31	Y1	614	CLA	CMA-C3A-C4A	2.92	119.61	111.77
47	Y1	606	CHL	C1-O2A-CGA	2.92	123.71	116.65
47	Y1	601	CHL	C3C-C4C-NC	-2.92	107.53	114.65
47	r	607	CHL	C4D-CHA-CBD	-2.92	106.03	108.97
47	S	607	CHL	CMA-C3A-C4A	2.91	120.89	114.61
31	b	617	CLA	O2A-CGA-CBA	2.91	120.72	111.83
49	R	621	XAT	C27-C28-C29	2.91	130.05	125.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	C	520	DGD	O1G-C1A-C2A	2.91	120.72	111.83
31	b1	608	CLA	CMA-C3A-C4A	2.91	119.60	111.77
47	G	609	CHL	C3C-C4C-NC	-2.91	107.53	114.65
31	g1	611	CLA	CMA-C3A-C4A	2.91	119.60	111.77
31	C1	501	CLA	C4B-CHC-C1C	2.91	133.09	126.25
31	R	612	CLA	C2C-C1C-NC	2.91	113.04	109.98
31	A1	406	CLA	O2A-CGA-CBA	2.91	120.71	111.83
32	A	409	PHO	O1D-CGD-CBD	2.91	129.14	124.72
31	b	610	CLA	C1-C2-C3	-2.91	121.43	126.20
31	C1	503	CLA	C1-C2-C3	-2.91	121.43	126.20
47	S1	608	CHL	C1-C2-C3	-2.91	121.43	126.20
31	b	612	CLA	C1-C2-C3	-2.91	121.43	126.20
31	y1	613	CLA	CMA-C3A-C4A	2.91	119.59	111.77
31	N	611	CLA	O2D-CGD-O1D	-2.91	118.19	123.85
33	D1	404	BCR	C36-C18-C17	-2.91	118.11	122.82
47	g	606	CHL	C4D-CHA-CBD	-2.91	106.04	108.97
48	r1	620	LUT	C35-C34-C33	-2.91	123.20	127.28
33	A1	411	BCR	C33-C5-C4	2.91	119.79	113.60
31	N	603	CLA	C2C-C1C-NC	2.91	113.03	109.98
31	a	406	CLA	C2C-C1C-NC	2.91	113.03	109.98
31	R1	602	CLA	C1-C2-C3	-2.91	121.44	126.20
48	s1	621	LUT	C15-C14-C13	-2.91	123.20	127.28
49	r	622	XAT	C11-C10-C9	-2.91	123.20	127.28
31	G	611	CLA	CMA-C3A-C4A	2.90	119.58	111.77
31	r1	602	CLA	CMA-C3A-C4A	2.90	119.58	111.77
47	s	608	CHL	C3C-C4C-NC	-2.90	107.55	114.65
47	G1	607	CHL	C1A-CHA-C4D	2.90	123.83	118.98
32	a	408	PHO	O2D-CGD-O1D	-2.90	118.20	123.85
31	b1	607	CLA	CAA-C2A-C3A	-2.90	105.16	113.00
31	r1	603	CLA	C1-C2-C3	-2.90	121.44	126.20
31	n	610	CLA	C1C-C2C-C3C	-2.90	103.93	106.98
31	Y1	608	CLA	CMA-C3A-C4A	2.90	119.57	111.77
47	N1	601	CHL	C4D-CHA-CBD	-2.90	106.04	108.97
50	r	623	NEX	C38-C25-C26	-2.90	117.53	122.30
47	y	606	CHL	CHA-C1A-C2A	-2.90	126.50	133.31
31	c	512	CLA	C2C-C1C-NC	2.90	113.03	109.98
51	S	625	LPX	O3-P1-O4	2.90	125.93	112.44
47	n	609	CHL	CAA-C2A-C3A	-2.90	105.17	113.00
31	a	407	CLA	C1C-C2C-C3C	-2.90	103.93	106.98
48	g1	621	LUT	C18-C5-C6	-2.90	121.32	124.48
33	c	516	BCR	C19-C18-C17	2.90	123.57	119.01
31	N1	612	CLA	C2C-C1C-NC	2.90	113.03	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	r1	612	CLA	C2C-C1C-NC	2.90	113.03	109.98
31	S	602	CLA	CMA-C3A-C4A	2.90	119.56	111.77
31	b	609	CLA	C3B-C4B-NB	-2.90	107.94	110.53
50	Y1	623	NEX	C35-C34-C33	2.90	131.34	127.28
33	C	514	BCR	C23-C24-C25	-2.90	119.26	127.00
31	y	603	CLA	C2C-C1C-NC	2.90	113.03	109.98
31	y	604	CLA	C1-C2-C3	-2.90	121.45	126.20
47	N	606	CHL	C4D-CHA-CBD	-2.90	106.05	108.97
45	F	101	HEM	C3B-C4B-NB	-2.90	107.39	109.47
47	s	607	CHL	C4D-CHA-CBD	-2.90	106.05	108.97
32	a1	409	PHO	O1D-CGD-CBD	2.89	129.11	124.72
33	c1	517	BCR	C35-C13-C14	-2.89	118.13	122.82
31	B	617	CLA	C2C-C1C-NC	2.89	113.02	109.98
47	S	601	CHL	C4D-CHA-CBD	-2.89	106.05	108.97
48	g	620	LUT	C35-C15-C14	-2.89	117.60	123.52
47	S	606	CHL	C4D-CHA-CBD	-2.89	106.05	108.97
32	A	408	PHO	CMB-C2B-C3B	2.89	130.46	124.68
31	c1	505	CLA	C3B-C4B-NB	-2.89	107.95	110.53
31	b	614	CLA	C1-C2-C3	-2.89	121.46	126.20
47	n1	607	CHL	C3C-C4C-NC	-2.89	107.59	114.65
31	Y1	612	CLA	C1C-C2C-C3C	-2.89	103.94	106.98
31	B1	612	CLA	C3B-C4B-NB	-2.89	107.95	110.53
47	n1	605	CHL	C1-O2A-CGA	2.89	123.64	116.65
31	N	614	CLA	C2C-C1C-NC	2.89	113.02	109.98
51	s	625	LPX	O3-P1-O4	2.89	125.88	112.44
47	s	607	CHL	C1A-CHA-C4D	2.89	123.80	118.98
31	y	613	CLA	CMA-C3A-C4A	2.89	119.53	111.77
33	C	516	BCR	C31-C1-C6	-2.89	105.72	110.24
47	Y	609	CHL	C1A-CHA-C4D	2.89	123.80	118.98
48	Y	620	LUT	C10-C11-C12	-2.89	114.84	123.20
31	b1	602	CLA	C1C-C2C-C3C	-2.89	103.94	106.98
48	n	621	LUT	C26-C27-C28	-2.89	120.09	124.58
31	S1	617	CLA	C2C-C1C-NC	2.88	113.01	109.98
31	Y1	613	CLA	O2A-CGA-CBA	2.88	120.63	111.83
31	B	603	CLA	CAC-C3C-C4C	2.88	128.54	124.79
47	G	605	CHL	C4D-CHA-CBD	-2.88	106.06	108.97
49	g	622	XAT	O4-C6-C7	-2.88	108.62	116.88
48	y1	620	LUT	C27-C28-C29	-2.88	120.13	126.32
47	R1	606	CHL	CHA-C1A-C2A	-2.88	126.54	133.31
34	B	621	SQD	O7-S-C6	-2.88	102.45	106.76
31	g	614	CLA	C2C-C1C-NC	2.88	113.01	109.98
31	g1	603	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	c	501	CLA	O2D-CGD-O1D	-2.88	118.24	123.85
33	C1	516	BCR	C37-C22-C21	-2.88	118.15	122.82
41	y	624	LHG	C6-C5-C4	-2.88	105.07	111.78
50	g1	623	NEX	C39-C29-C30	-2.88	118.15	122.82
34	m1	101	SQD	O7-S-C6	-2.88	102.46	106.76
31	B	603	CLA	C2C-C1C-NC	2.88	113.01	109.98
31	S1	610	CLA	CMA-C3A-C4A	2.88	119.51	111.77
31	S1	609	CLA	CAA-C2A-C3A	-2.88	105.22	113.00
31	G1	602	CLA	CMC-C2C-C1C	2.88	129.53	125.03
31	b1	610	CLA	C1C-C2C-C3C	-2.88	103.95	106.98
31	C	511	CLA	O2A-CGA-CBA	2.88	120.61	111.83
32	a	408	PHO	CMB-C2B-C3B	2.88	130.43	124.68
31	B	603	CLA	C1C-C2C-C3C	-2.88	103.95	106.98
31	b1	608	CLA	O2D-CGD-O1D	-2.88	118.25	123.85
31	y1	613	CLA	C1-C2-C3	-2.88	121.49	126.20
49	g1	622	XAT	C26-C27-C28	-2.88	119.91	125.99
31	b1	611	CLA	C4B-CHC-C1C	2.87	133.01	126.25
47	s1	601	CHL	C3C-C4C-NC	-2.87	107.63	114.65
33	c	514	BCR	C38-C26-C25	-2.87	121.35	124.48
33	B	619	BCR	C19-C18-C17	2.87	123.53	119.01
31	g	602	CLA	O2A-CGA-CBA	2.87	120.59	111.83
31	Y	614	CLA	C2C-C1C-NC	2.87	113.00	109.98
31	B1	617	CLA	C2C-C1C-NC	2.87	113.00	109.98
31	y1	614	CLA	CMA-C3A-C4A	2.87	119.49	111.77
31	A	410	CLA	C1C-C2C-C3C	-2.87	103.96	106.98
31	S	604	CLA	C1C-C2C-C3C	-2.87	103.96	106.98
47	g1	607	CHL	C1A-CHA-C4D	2.87	123.77	118.98
31	y	610	CLA	O1D-CGD-CBD	-2.87	118.86	124.52
31	c	505	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
31	G1	602	CLA	O2D-CGD-O1D	-2.87	118.26	123.85
31	b1	614	CLA	C2C-C1C-NC	2.87	113.00	109.98
31	y1	603	CLA	C2C-C1C-NC	2.87	113.00	109.98
31	y1	612	CLA	C2C-C1C-NC	2.87	113.00	109.98
31	g	611	CLA	CMA-C3A-C4A	2.87	119.48	111.77
47	G	607	CHL	C1-O2A-CGA	2.87	123.59	116.65
41	C1	525	LHG	O8-C23-C24	2.87	120.58	111.83
31	r	612	CLA	C3B-C4B-NB	-2.87	107.97	110.53
31	s	617	CLA	C1C-C2C-C3C	-2.87	103.96	106.98
31	G1	603	CLA	C1C-C2C-C3C	-2.87	103.96	106.98
31	c1	512	CLA	C2C-C1C-NC	2.87	112.99	109.98
31	G1	602	CLA	CMA-C3A-C4A	2.87	119.48	111.77
31	Y	604	CLA	O2D-CGD-O1D	-2.87	118.27	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C1	511	CLA	CMA-C3A-C4A	2.87	119.47	111.77
32	A1	409	PHO	C2D-C1D-ND	-2.87	107.36	109.43
31	C	502	CLA	CMA-C3A-C4A	2.87	119.47	111.77
52	S1	626	3PH	O31-C31-C32	2.86	120.57	111.83
31	r	609	CLA	C2C-C1C-NC	2.86	112.99	109.98
31	Y	603	CLA	C3B-C4B-NB	-2.86	107.97	110.53
31	S	613	CLA	C1-C2-C3	-2.86	121.51	126.20
31	s1	612	CLA	C1C-C2C-C3C	-2.86	103.97	106.98
41	S	624	LHG	C5-O7-C7	-2.86	110.94	117.80
31	g1	613	CLA	C1-C2-C3	-2.86	121.51	126.20
49	R	621	XAT	C19-C9-C10	-2.86	118.18	122.82
31	S	613	CLA	C2C-C1C-NC	2.86	112.99	109.98
31	G1	604	CLA	CMA-C3A-C4A	2.86	119.47	111.77
31	C	509	CLA	C1C-C2C-C3C	-2.86	103.97	106.98
31	B1	605	CLA	C1C-C2C-C3C	-2.86	103.97	106.98
31	N	613	CLA	C1-C2-C3	-2.86	121.51	126.20
47	N	605	CHL	C1-O2A-CGA	2.86	123.58	116.65
31	y	613	CLA	C1C-C2C-C3C	-2.86	103.97	106.98
47	R	606	CHL	C3C-C4C-NC	-2.86	107.66	114.65
49	R1	621	XAT	O4-C5-C4	-2.86	110.81	113.49
35	w1	201	LMG	O8-C28-C29	2.86	120.56	111.83
47	N1	601	CHL	C1-C2-C3	-2.86	121.51	126.20
31	N1	602	CLA	C2D-C1D-ND	2.86	112.95	110.13
31	B	613	CLA	C2C-C1C-NC	2.86	112.98	109.98
48	y1	621	LUT	C15-C14-C13	-2.86	123.27	127.28
48	Y	621	LUT	C35-C15-C14	-2.86	117.67	123.52
52	b1	624	3PH	O31-C31-C32	2.86	120.55	111.83
48	n1	621	LUT	C35-C15-C14	-2.86	117.67	123.52
31	s1	609	CLA	C2C-C1C-NC	2.86	112.98	109.98
31	Y1	610	CLA	C1D-ND-C4D	-2.86	104.31	106.31
33	b	619	BCR	C33-C5-C4	2.86	119.69	113.60
51	s1	625	LPX	O3-P1-O4	2.86	125.73	112.44
32	A	409	PHO	O2D-CGD-O1D	-2.86	118.29	123.85
31	a	410	CLA	C2C-C1C-NC	2.86	112.98	109.98
31	C1	504	CLA	C2C-C1C-NC	2.86	112.98	109.98
34	a	412	SQD	O7-S-C6	-2.86	102.49	106.76
31	C1	501	CLA	C1-C2-C3	-2.85	121.52	126.20
31	C1	507	CLA	CMA-C3A-C4A	2.85	119.44	111.77
31	S1	612	CLA	CMA-C3A-C4A	2.85	119.44	111.77
31	B	610	CLA	C2C-C1C-NC	2.85	112.98	109.98
47	n	609	CHL	C4D-ND-C1D	2.85	107.39	105.22
31	y	610	CLA	CMA-C3A-C4A	2.85	119.44	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	y1	607	CHL	C1-O2A-CGA	2.85	123.56	116.65
31	C	513	CLA	O2A-CGA-CBA	2.85	120.53	111.83
47	n	601	CHL	C4D-CHA-CBD	-2.85	106.09	108.97
31	b1	608	CLA	C2C-C1C-NC	2.85	112.98	109.98
44	d	405	PL9	C7-C8-C9	-2.85	121.92	126.83
31	y	610	CLA	C4B-CHC-C1C	2.85	132.95	126.25
52	i	101	3PH	O31-C31-C32	2.85	120.53	111.83
47	n1	606	CHL	C1A-CHA-C4D	2.85	123.74	118.98
31	S1	610	CLA	C4B-CHC-C1C	2.85	132.95	126.25
31	s1	604	CLA	C1C-C2C-C3C	-2.85	103.98	106.98
31	R	613	CLA	O2D-CGD-O1D	-2.85	118.30	123.85
31	C	501	CLA	C3B-C4B-NB	-2.85	107.99	110.53
31	b	606	CLA	C1-C2-C3	-2.85	121.53	126.20
41	D	408	LHG	O8-C23-C24	2.85	120.52	111.83
31	B1	612	CLA	C1D-ND-C4D	-2.85	104.31	106.31
31	R	602	CLA	CMA-C3A-C4A	2.85	119.43	111.77
31	n	614	CLA	CMA-C3A-C4A	2.85	119.42	111.77
47	S1	608	CHL	C3C-C4C-NC	-2.85	107.69	114.65
41	L1	101	LHG	O8-C23-C24	2.85	120.52	111.83
31	N	611	CLA	C2C-C1C-NC	2.85	112.97	109.98
31	D	403	CLA	C3B-C4B-NB	-2.85	107.99	110.53
31	C1	511	CLA	C1C-C2C-C3C	-2.85	103.99	106.98
49	r1	621	XAT	C38-C25-C26	-2.85	117.62	122.30
34	B1	626	SQD	O7-S-C6	-2.85	102.51	106.76
47	n1	608	CHL	C1A-CHA-C4D	2.85	123.73	118.98
50	r1	622	NEX	C19-C9-C10	-2.84	118.21	122.82
31	C	506	CLA	C2C-C1C-NC	2.84	112.97	109.98
31	R	611	CLA	C2C-C1C-NC	2.84	112.97	109.98
47	S	607	CHL	C4D-CHA-CBD	-2.84	106.10	108.97
31	n	610	CLA	CMA-C3A-C4A	2.84	119.42	111.77
31	C	505	CLA	C1-O2A-CGA	2.84	123.53	116.65
50	s1	623	NEX	C38-C25-C26	-2.84	117.62	122.30
31	y1	603	CLA	C1C-C2C-C3C	-2.84	103.99	106.98
31	n	611	CLA	C2C-C1C-NC	2.84	112.97	109.98
31	S1	610	CLA	C2C-C1C-NC	2.84	112.97	109.98
47	R1	607	CHL	C1-O2A-CGA	2.84	123.53	116.65
31	C1	501	CLA	C1C-C2C-C3C	-2.84	103.99	106.98
31	g	611	CLA	C2C-C1C-NC	2.84	112.97	109.98
31	b1	615	CLA	C1C-C2C-C3C	-2.84	103.99	106.98
47	G1	607	CHL	C1-O2A-CGA	2.84	123.53	116.65
31	g1	611	CLA	C1-C2-C3	-2.84	121.54	126.20
52	t1	101	3PH	O31-C31-C32	2.84	120.50	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	y1	612	CLA	C1C-C2C-C3C	-2.84	103.99	106.98
35	c1	523	LMG	O8-C28-C29	2.84	120.49	111.83
48	n	620	LUT	C15-C14-C13	-2.84	123.30	127.28
31	A	406	CLA	CMA-C3A-C4A	2.84	119.40	111.77
33	b1	619	BCR	C15-C14-C13	-2.84	123.30	127.28
41	c	625	LHG	O8-C23-C24	2.84	120.49	111.83
47	N	607	CHL	C1A-CHA-C4D	2.84	123.72	118.98
31	Y1	611	CLA	C2C-C1C-NC	2.84	112.96	109.98
47	R	606	CHL	C4D-CHA-CBD	-2.84	106.11	108.97
47	Y	607	CHL	CHA-C1A-C2A	-2.84	126.65	133.31
44	d1	405	PL9	C22-C23-C24	-2.83	121.14	127.62
34	b1	621	SQD	O7-S-C6	-2.83	102.52	106.76
31	c	512	CLA	C1C-C2C-C3C	-2.83	104.00	106.98
31	B1	611	CLA	CMA-C3A-C4A	2.83	119.39	111.77
31	d1	403	CLA	C2C-C1C-NC	2.83	112.96	109.98
31	n1	603	CLA	C1C-C2C-C3C	-2.83	104.00	106.98
31	C1	512	CLA	CMA-C3A-C4A	2.83	119.39	111.77
47	n	606	CHL	C1-C2-C3	-2.83	121.56	126.20
31	R	603	CLA	C2C-C1C-NC	2.83	112.96	109.98
31	a1	407	CLA	C1C-C2C-C3C	-2.83	104.00	106.98
31	b1	602	CLA	CMA-C3A-C4A	2.83	119.39	111.77
31	C	505	CLA	O2A-CGA-CBA	2.83	120.47	111.83
31	r1	603	CLA	C1C-C2C-C3C	-2.83	104.00	106.98
31	b1	610	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
31	n	610	CLA	C1-C2-C3	-2.83	121.56	126.20
47	y	606	CHL	C4D-CHA-CBD	-2.83	106.11	108.97
47	y1	601	CHL	C1-C2-C3	-2.83	121.56	126.20
48	S	621	LUT	C35-C15-C14	-2.83	117.73	123.52
31	c1	505	CLA	C2C-C1C-NC	2.83	112.95	109.98
31	r	603	CLA	CMA-C3A-C4A	2.83	119.37	111.77
41	D	409	LHG	C5-O7-C7	-2.83	111.03	117.80
31	c	506	CLA	CMA-C3A-C4A	2.83	119.37	111.77
31	g1	614	CLA	O2D-CGD-O1D	-2.83	118.34	123.85
31	s1	602	CLA	C1-C2-C3	-2.83	121.56	126.20
31	Y1	614	CLA	C3B-C4B-NB	-2.83	108.01	110.53
40	c1	518	DGD	O1G-C1A-C2A	2.83	120.45	111.83
33	d1	404	BCR	C34-C9-C10	-2.83	118.24	122.82
47	G1	601	CHL	CHA-C1A-C2A	-2.83	126.67	133.31
31	n1	612	CLA	C2C-C1C-NC	2.82	112.95	109.98
31	Y1	604	CLA	C1-C2-C3	-2.82	121.57	126.20
50	G	623	NEX	C5-C6-C1	2.82	122.50	119.70
31	N	604	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	b	615	CLA	CAC-C3C-C4C	2.82	128.46	124.79
35	A1	413	LMG	C8-O7-C10	-2.82	111.04	117.80
31	c1	512	CLA	O2A-CGA-CBA	2.82	120.44	111.83
31	c1	513	CLA	C3B-C4B-NB	-2.82	108.01	110.53
31	b1	609	CLA	CHA-C4D-ND	2.82	138.37	132.55
31	C	510	CLA	C2C-C1C-NC	2.82	112.94	109.98
50	N	623	NEX	C40-C33-C34	-2.82	118.25	122.82
49	r1	621	XAT	O24-C26-C27	-2.82	108.80	116.88
47	n	609	CHL	C3C-C4C-NC	-2.82	107.76	114.65
31	C1	505	CLA	C2C-C1C-NC	2.82	112.94	109.98
32	A1	408	PHO	O1D-CGD-CBD	2.82	129.00	124.72
31	n1	612	CLA	C3B-C4B-NB	-2.82	108.02	110.53
31	S	605	CLA	C2C-C1C-NC	2.82	112.94	109.98
47	N1	608	CHL	CHA-C1A-C2A	-2.82	126.69	133.31
47	g1	607	CHL	C1-C2-C3	-2.82	121.58	126.20
33	D1	404	BCR	C38-C26-C25	-2.82	121.41	124.48
41	D1	409	LHG	C5-O7-C7	-2.82	111.06	117.80
31	C1	507	CLA	C2C-C1C-NC	2.82	112.94	109.98
31	b1	611	CLA	C3B-C4B-NB	-2.82	108.02	110.53
47	g1	606	CHL	C4D-CHA-CBD	-2.81	106.13	108.97
31	r	611	CLA	C2C-C1C-NC	2.81	112.94	109.98
31	s	605	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
31	s1	605	CLA	O2D-CGD-O1D	-2.81	118.37	123.85
41	d1	410	LHG	C5-O7-C7	-2.81	111.06	117.80
31	Y1	614	CLA	C2C-C1C-NC	2.81	112.94	109.98
47	g	609	CHL	C1-O2A-CGA	2.81	123.46	116.65
31	G1	611	CLA	C1C-C2C-C3C	-2.81	104.02	106.98
46	h	101	RRX	C21-C20-C19	-2.81	115.05	123.20
31	G	612	CLA	CMA-C3A-C4A	2.81	119.33	111.77
31	y1	604	CLA	C2C-C1C-NC	2.81	112.94	109.98
31	G1	603	CLA	CMA-C3A-C4A	2.81	119.33	111.77
33	C1	515	BCR	C1-C6-C5	-2.81	118.79	122.64
37	B	620	C7Z	C27-C28-C29	-2.81	122.08	126.23
31	B1	603	CLA	C1C-C2C-C3C	-2.81	104.02	106.98
31	B1	616	CLA	C4B-CHC-C1C	2.81	132.86	126.25
47	N	605	CHL	C4D-CHA-CBD	-2.81	106.13	108.97
31	B	616	CLA	C2C-C1C-NC	2.81	112.93	109.98
31	s	609	CLA	C1-C2-C3	-2.81	121.59	126.20
31	c	504	CLA	C2C-C1C-NC	2.81	112.93	109.98
33	A1	411	BCR	C23-C24-C25	-2.81	119.49	127.00
31	a1	407	CLA	O1D-CGD-CBD	-2.81	118.98	124.52
31	b	613	CLA	O2D-CGD-O1D	-2.81	118.38	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	y1	604	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
47	N1	609	CHL	C4D-CHA-CBD	-2.81	106.14	108.97
31	C1	505	CLA	C1C-C2C-C3C	-2.81	104.03	106.98
47	n1	607	CHL	C1-O2A-CGA	2.81	123.45	116.65
31	b	607	CLA	O2D-CGD-O1D	-2.81	118.38	123.85
33	c	516	BCR	C33-C5-C4	2.81	119.58	113.60
47	y	609	CHL	C4D-CHA-CBD	-2.81	106.14	108.97
41	c1	525	LHG	O8-C23-C24	2.81	120.39	111.83
31	Y1	604	CLA	C2C-C1C-NC	2.81	112.93	109.98
31	g1	614	CLA	C2C-C1C-NC	2.81	112.93	109.98
31	g1	612	CLA	C1C-C2C-C3C	-2.81	104.03	106.98
47	s1	607	CHL	C4D-CHA-CBD	-2.81	106.14	108.97
31	S	614	CLA	C1C-C2C-C3C	-2.81	104.03	106.98
47	S1	608	CHL	CHA-C1A-C2A	-2.81	126.72	133.31
47	N	609	CHL	C1-O2A-CGA	2.81	123.44	116.65
32	a1	409	PHO	O2D-CGD-O1D	-2.81	118.39	123.85
34	a1	412	SQD	O7-S-C6	-2.80	102.57	106.76
47	s1	607	CHL	C1A-CHA-C4D	2.80	123.66	118.98
41	d1	408	LHG	O8-C23-C24	2.80	120.39	111.83
31	B	602	CLA	C1C-C2C-C3C	-2.80	104.03	106.98
31	N	614	CLA	C1C-C2C-C3C	-2.80	104.03	106.98
57	y1	626	PTY	O4-C30-C31	2.80	120.38	111.83
48	N	620	LUT	C27-C28-C29	-2.80	120.29	126.32
32	A1	408	PHO	CMB-C2B-C3B	2.80	130.28	124.68
33	A	411	BCR	C38-C26-C25	-2.80	121.43	124.48
37	B	620	C7Z	C8-C7-C6	-2.80	119.51	127.00
31	c1	508	CLA	CMA-C3A-C4A	2.80	119.30	111.77
31	s	617	CLA	C2C-C1C-NC	2.80	112.92	109.98
31	n	603	CLA	O2D-CGD-O1D	-2.80	118.39	123.85
47	g1	608	CHL	C3C-C4C-NC	-2.80	107.80	114.65
31	c	504	CLA	C1-O2A-CGA	2.80	123.43	116.65
46	h1	101	RRX	C23-C22-C21	-2.80	114.60	119.01
31	S1	610	CLA	C1-C2-C3	-2.80	121.61	126.20
31	r1	608	CLA	C1C-C2C-C3C	-2.80	104.03	106.98
47	n1	605	CHL	C4D-CHA-CBD	-2.80	106.14	108.97
31	G	602	CLA	C1-C2-C3	-2.80	121.61	126.20
31	B1	614	CLA	C1-C2-C3	-2.80	121.61	126.20
32	A1	409	PHO	O2D-CGD-O1D	-2.80	118.40	123.85
47	N1	609	CHL	C4C-CHD-C1D	2.80	126.08	116.07
47	g	609	CHL	C1-C2-C3	-2.80	121.61	126.20
31	c1	504	CLA	C1C-C2C-C3C	-2.80	104.04	106.98
51	S1	625	LPX	O3-P1-O4	2.80	125.45	112.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	B1	622	LMG	O8-C28-C29	2.80	120.36	111.83
41	d1	410	LHG	O8-C23-C24	2.80	120.36	111.83
31	s	613	CLA	C1C-C2C-C3C	-2.80	104.04	106.98
31	S1	603	CLA	C1C-C2C-C3C	-2.80	104.04	106.98
31	B	615	CLA	O2D-CGD-O1D	-2.80	118.41	123.85
47	y	607	CHL	C1-O2A-CGA	2.80	123.42	116.65
31	S1	602	CLA	CMA-C3A-C4A	2.80	119.29	111.77
31	d	403	CLA	C1C-C2C-C3C	-2.80	104.04	106.98
31	y1	608	CLA	C1C-C2C-C3C	-2.80	104.04	106.98
31	B1	611	CLA	O2A-CGA-CBA	2.80	120.36	111.83
31	s	609	CLA	C3B-C4B-NB	-2.79	108.03	110.53
33	C	516	BCR	C23-C24-C25	-2.79	119.53	127.00
47	y1	609	CHL	C1-C2-C3	-2.79	121.62	126.20
31	B	614	CLA	C2C-C1C-NC	2.79	112.92	109.98
50	N1	623	NEX	C39-C29-C30	-2.79	118.29	122.82
35	A	413	LMG	O8-C28-C29	2.79	120.35	111.83
31	y1	614	CLA	C3B-C4B-NB	-2.79	108.04	110.53
50	y	623	NEX	C16-C1-C6	-2.79	107.97	110.47
31	S1	610	CLA	C1C-C2C-C3C	-2.79	104.04	106.98
50	R	622	NEX	C27-C28-C29	-2.79	121.20	125.53
31	c1	507	CLA	O2A-CGA-CBA	2.79	120.35	111.83
31	c	505	CLA	C3B-C4B-NB	-2.79	108.04	110.53
31	y	603	CLA	C3B-C4B-NB	-2.79	108.04	110.53
31	Y	603	CLA	CMA-C3A-C4A	2.79	119.28	111.77
48	r	620	LUT	C15-C35-C34	-2.79	117.81	123.52
41	n1	624	LHG	O8-C23-C24	2.79	120.35	111.83
32	A	408	PHO	O2D-CGD-O1D	-2.79	118.42	123.85
31	n1	604	CLA	C2C-C1C-NC	2.79	112.91	109.98
41	L1	101	LHG	C5-O7-C7	-2.79	111.12	117.80
31	G1	602	CLA	C4B-CHC-C1C	2.79	132.81	126.25
49	Y	622	XAT	O4-C6-C7	-2.79	108.89	116.88
31	b	605	CLA	O2D-CGD-O1D	-2.79	118.42	123.85
31	S	617	CLA	C2C-C1C-NC	2.79	112.91	109.98
31	b1	606	CLA	C2C-C1C-NC	2.79	112.91	109.98
31	C1	508	CLA	C1D-ND-C4D	-2.79	104.36	106.31
31	d	403	CLA	O2A-CGA-CBA	2.79	120.34	111.83
47	y1	605	CHL	C1A-CHA-C4D	2.79	123.64	118.98
31	C1	503	CLA	C2C-C1C-NC	2.79	112.91	109.98
47	y1	607	CHL	CHA-C1A-C2A	-2.79	126.76	133.31
34	M1	101	SQD	O7-S-C6	-2.79	102.59	106.76
31	B	607	CLA	C2C-C1C-NC	2.79	112.91	109.98
31	S	609	CLA	C1-C2-C3	-2.79	121.63	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s1	609	CLA	CMA-C3A-C4A	2.79	119.26	111.77
31	G1	614	CLA	C2C-C1C-NC	2.79	112.91	109.98
52	B1	624	3PH	O31-C31-C32	2.79	120.33	111.83
41	d	408	LHG	O8-C23-C24	2.79	120.33	111.83
31	R	604	CLA	C1C-C2C-C3C	-2.78	104.05	106.98
31	b	604	CLA	C1C-C2C-C3C	-2.78	104.05	106.98
31	B1	606	CLA	C1C-C2C-C3C	-2.78	104.05	106.98
31	Y	614	CLA	CMA-C3A-C4A	2.78	119.26	111.77
54	k1	101	4RF	O18-C16-C15	2.78	120.33	111.83
31	D1	402	CLA	C1-C2-C3	-2.78	121.64	126.20
31	c1	501	CLA	C2C-C1C-NC	2.78	112.91	109.98
47	G1	607	CHL	C1-C2-C3	-2.78	121.64	126.20
31	C1	506	CLA	CMA-C3A-C4A	2.78	119.25	111.77
31	n	604	CLA	OBD-CAD-C3D	-2.78	121.91	128.42
31	b	612	CLA	C3B-C4B-NB	-2.78	108.05	110.53
31	s1	611	CLA	C3B-C4B-NB	-2.78	108.05	110.53
31	G1	614	CLA	CMA-C3A-C4A	2.78	119.25	111.77
31	g1	603	CLA	C2C-C1C-NC	2.78	112.90	109.98
31	C1	507	CLA	C1C-C2C-C3C	-2.78	104.05	106.98
47	Y1	601	CHL	C4D-CHA-CBD	-2.78	106.16	108.97
31	c1	501	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
33	B1	619	BCR	C15-C14-C13	-2.78	123.38	127.28
31	B	614	CLA	C1C-C2C-C3C	-2.78	104.06	106.98
31	b	609	CLA	CMA-C3A-C4A	2.78	119.24	111.77
31	N1	604	CLA	CHA-C4D-ND	2.78	138.28	132.55
48	s1	621	LUT	C27-C28-C29	-2.78	120.35	126.32
50	R	622	NEX	C26-C27-C28	-2.78	120.12	125.99
31	B1	613	CLA	O2D-CGD-O1D	-2.78	118.44	123.85
31	c1	510	CLA	C1C-C2C-C3C	-2.78	104.06	106.98
33	C	516	BCR	C37-C22-C23	2.78	122.33	118.09
47	r	606	CHL	C1A-CHA-C4D	2.78	123.61	118.98
31	y	603	CLA	C1C-C2C-C3C	-2.78	104.06	106.98
33	C1	515	BCR	C23-C24-C25	-2.77	119.59	127.00
48	y	621	LUT	C26-C27-C28	-2.77	120.26	124.58
31	s	611	CLA	O2D-CGD-O1D	-2.77	118.45	123.85
31	B1	615	CLA	CMA-C3A-C4A	2.77	119.23	111.77
47	y	601	CHL	C3C-C4C-NC	-2.77	107.87	114.65
48	S	620	LUT	C22-C23-C24	-2.77	107.07	111.18
40	C	518	DGD	O1G-C1A-C2A	2.77	120.29	111.83
47	g	608	CHL	CHA-C1A-C2A	-2.77	126.80	133.31
31	B1	614	CLA	C2C-C1C-NC	2.77	112.89	109.98
31	S1	612	CLA	C2C-C1C-NC	2.77	112.89	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	a1	406	CLA	C2C-C1C-NC	2.77	112.89	109.98
31	c1	513	CLA	CBA-CAA-C2A	2.77	122.04	113.79
48	s1	620	LUT	C22-C23-C24	-2.77	107.07	111.18
31	B	612	CLA	CAA-C2A-C3A	-2.77	105.51	113.00
31	c	505	CLA	C2C-C1C-NC	2.77	112.89	109.98
31	R1	608	CLA	C2C-C1C-NC	2.77	112.89	109.98
31	Y1	610	CLA	C2D-C1D-ND	2.77	112.87	110.13
47	n	605	CHL	C1-O2A-CGA	2.77	123.36	116.65
47	G1	606	CHL	C4D-CHA-CBD	-2.77	106.17	108.97
33	c1	517	BCR	C33-C5-C4	2.77	119.50	113.60
31	c1	512	CLA	CMA-C3A-C4A	2.77	119.22	111.77
31	c1	509	CLA	C2C-C1C-NC	2.77	112.89	109.98
31	b1	606	CLA	C1C-C2C-C3C	-2.77	104.07	106.98
47	N1	609	CHL	C1-O2A-CGA	2.77	123.36	116.65
31	Y1	608	CLA	CHA-C4D-ND	2.77	138.26	132.55
34	b1	626	SQD	O7-S-C6	-2.77	102.62	106.76
31	G	612	CLA	C1C-C2C-C3C	-2.77	104.07	106.98
50	g1	623	NEX	C4-C3-C2	2.77	115.97	110.79
31	g1	614	CLA	CMA-C3A-C4A	2.77	119.21	111.77
31	y1	614	CLA	C2C-C1C-NC	2.77	112.89	109.98
31	S1	617	CLA	C1C-C2C-C3C	-2.77	104.07	106.98
47	n1	601	CHL	C4D-CHA-CBD	-2.77	106.18	108.97
47	y1	601	CHL	C4C-CHD-C1D	2.77	125.97	116.07
40	c	519	DGD	O1G-C1A-C2A	2.77	120.27	111.83
32	a1	409	PHO	C3D-CAD-CBD	-2.77	103.96	107.61
31	s	609	CLA	C2C-C1C-NC	2.77	112.89	109.98
31	C1	501	CLA	C2C-C1C-NC	2.77	112.89	109.98
31	D1	403	CLA	C2C-C1C-NC	2.77	112.89	109.98
31	S	611	CLA	C1C-C2C-C3C	-2.77	104.07	106.98
34	C	526	SQD	O7-S-C6	-2.77	102.62	106.76
47	S	601	CHL	C1A-CHA-C4D	2.77	123.60	118.98
31	a	410	CLA	O2D-CGD-O1D	-2.77	118.46	123.85
40	B1	623	DGD	O1G-C1A-C2A	2.77	120.27	111.83
50	y1	623	NEX	C38-C25-C26	-2.77	117.75	122.30
49	G	622	XAT	C6-C7-C8	-2.77	120.14	125.99
41	s1	624	LHG	O8-C23-C24	2.77	120.27	111.83
31	B1	609	CLA	CMA-C3A-C4A	2.77	119.21	111.77
48	Y	620	LUT	C27-C28-C29	-2.77	120.38	126.32
31	R	613	CLA	C2C-C1C-NC	2.76	112.89	109.98
34	A	412	SQD	O7-S-C6	-2.76	102.63	106.76
33	C1	514	BCR	C36-C18-C17	-2.76	118.34	122.82
33	C1	515	BCR	C15-C14-C13	-2.76	123.40	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	N	613	CLA	CMA-C3A-C4A	2.76	119.20	111.77
31	R1	610	CLA	CMA-C3A-C4A	2.76	119.20	111.77
31	b	608	CLA	C2C-C1C-NC	2.76	112.89	109.98
31	b	607	CLA	C1-C2-C3	-2.76	121.67	126.20
31	g1	604	CLA	C3B-C4B-NB	-2.76	108.06	110.53
31	c	510	CLA	CMD-C2D-C3D	-2.76	121.35	127.69
49	r1	621	XAT	C40-C33-C34	-2.76	118.34	122.82
31	g1	604	CLA	CMA-C3A-C4A	2.76	119.20	111.77
35	D	411	LMG	O8-C28-C29	2.76	120.26	111.83
31	S	605	CLA	CAA-C2A-C3A	-2.76	105.53	113.00
31	y	614	CLA	C1-C2-C3	-2.76	121.67	126.20
31	Y1	602	CLA	O2A-CGA-CBA	2.76	120.26	111.83
31	g1	614	CLA	O2A-CGA-CBA	2.76	120.26	111.83
50	Y	623	NEX	C4-C3-C2	2.76	115.96	110.79
47	G1	607	CHL	CMA-C3A-C4A	2.76	120.56	114.61
47	Y	605	CHL	C4D-CHA-CBD	-2.76	106.18	108.97
47	N	607	CHL	CHA-C1A-C2A	-2.76	126.83	133.31
48	r1	620	LUT	C18-C5-C4	2.76	119.50	114.42
31	N1	603	CLA	C2C-C1C-NC	2.76	112.88	109.98
31	n1	603	CLA	O2D-CGD-O1D	-2.76	118.48	123.85
31	g	612	CLA	C2C-C1C-NC	2.76	112.88	109.98
31	c1	503	CLA	C2C-C1C-NC	2.76	112.88	109.98
33	C	515	BCR	C23-C24-C25	-2.76	119.63	127.00
31	a1	410	CLA	O2A-CGA-CBA	2.76	120.24	111.83
31	Y1	608	CLA	C1C-C2C-C3C	-2.76	104.08	106.98
31	G1	612	CLA	C2C-C1C-NC	2.76	112.88	109.98
38	b	623	DGA	OG1-CA1-CA2	2.76	120.24	111.83
31	n	611	CLA	C3D-C2D-C1D	-2.76	102.07	105.83
47	g	609	CHL	C1A-CHA-C4D	2.76	123.58	118.98
31	C	508	CLA	C2C-C1C-NC	2.76	112.88	109.98
38	C	524	DGA	OG1-CA1-CA2	2.76	120.24	111.83
34	C1	526	SQD	O7-S-C6	-2.76	102.64	106.76
31	G1	602	CLA	C2D-C1D-ND	2.75	112.85	110.13
31	S	612	CLA	C1C-C2C-C3C	-2.75	104.08	106.98
31	S1	605	CLA	C1C-C2C-C3C	-2.75	104.08	106.98
48	s1	620	LUT	C18-C5-C4	2.75	119.48	114.42
31	y	608	CLA	CMA-C3A-C4A	2.75	119.17	111.77
33	d	404	BCR	C38-C26-C27	2.75	119.47	113.60
31	S1	614	CLA	C1C-C2C-C3C	-2.75	104.08	106.98
33	b	619	BCR	C30-C25-C26	-2.75	118.88	122.64
31	y	603	CLA	C1-C2-C3	-2.75	121.69	126.20
47	g1	609	CHL	C3C-C4C-NC	-2.75	107.92	114.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	c	516	BCR	C34-C9-C10	-2.75	118.36	122.82
31	b	607	CLA	O1D-CGD-CBD	-2.75	119.09	124.52
33	C1	516	BCR	C27-C26-C25	-2.75	118.99	122.70
31	s1	602	CLA	C1D-ND-C4D	-2.75	104.38	106.31
48	s	620	LUT	C18-C5-C4	2.75	119.48	114.42
31	d1	402	CLA	C2C-C1C-NC	2.75	112.87	109.98
48	N1	620	LUT	C7-C8-C9	-2.75	122.17	126.23
37	b1	620	C7Z	C28-C27-C26	-2.75	119.65	127.00
31	N1	613	CLA	C1C-C2C-C3C	-2.75	104.09	106.98
31	N1	610	CLA	C1-C2-C3	-2.75	121.69	126.20
41	d	410	LHG	O8-C23-C24	2.75	120.22	111.83
31	S	610	CLA	C2C-C1C-NC	2.75	112.87	109.98
50	g1	623	NEX	C19-C9-C10	-2.75	118.36	122.82
31	s1	604	CLA	O2A-CGA-CBA	2.75	120.22	111.83
31	R1	603	CLA	C3B-C4B-NB	-2.75	108.08	110.53
31	c	503	CLA	C2C-C1C-NC	2.75	112.87	109.98
31	R1	609	CLA	C2C-C1C-NC	2.75	112.87	109.98
47	S1	607	CHL	C4D-CHA-CBD	-2.75	106.20	108.97
47	R	607	CHL	C1A-CHA-C4D	2.75	123.57	118.98
31	r	610	CLA	OBD-CAD-C3D	-2.75	122.00	128.42
31	b	602	CLA	C2C-C1C-NC	2.75	112.87	109.98
33	C	517	BCR	C15-C14-C13	-2.75	123.43	127.28
41	n1	624	LHG	C5-O7-C7	-2.75	111.22	117.80
47	N	601	CHL	C4D-CHA-CBD	-2.75	106.20	108.97
31	b1	616	CLA	C1C-C2C-C3C	-2.75	104.09	106.98
31	s1	610	CLA	C1C-C2C-C3C	-2.75	104.09	106.98
47	y	606	CHL	C1-O2A-CGA	2.74	123.30	116.65
35	W1	201	LMG	O8-C28-C29	2.74	120.20	111.83
31	c1	507	CLA	C3B-C4B-NB	-2.74	108.08	110.53
31	B	611	CLA	CMA-C3A-C4A	2.74	119.15	111.77
31	N1	602	CLA	C1C-C2C-C3C	-2.74	104.09	106.98
31	n1	602	CLA	C1C-C2C-C3C	-2.74	104.09	106.98
31	A1	410	CLA	C2C-C1C-NC	2.74	112.86	109.98
31	B1	607	CLA	O2A-CGA-CBA	2.74	120.20	111.83
31	s	603	CLA	C1-C2-C3	-2.74	121.70	126.20
56	R1	626	ERG	C13-C14-C8	2.74	118.42	113.59
46	h	101	RRX	C8-C7-C6	-2.74	119.67	127.00
49	r	622	XAT	C18-C5-C6	-2.74	117.79	122.30
48	S	620	LUT	C38-C25-C24	-2.74	116.87	123.36
54	K1	101	4RF	O18-C16-C15	2.74	120.19	111.83
48	Y1	621	LUT	C15-C14-C13	-2.74	123.43	127.28
47	n1	601	CHL	C1-O2A-CGA	2.74	123.29	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	504	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
31	S	610	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
47	n1	609	CHL	CMA-C3A-C4A	2.74	120.52	114.61
31	Y	612	CLA	O2A-CGA-CBA	2.74	120.19	111.83
48	G	620	LUT	C31-C30-C29	-2.74	123.44	127.28
31	N	612	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
31	r	603	CLA	C1C-C2C-C3C	-2.74	104.10	106.98
31	R	608	CLA	C2C-C1C-NC	2.74	112.86	109.98
31	Y	612	CLA	C2C-C1C-NC	2.74	112.86	109.98
47	g1	606	CHL	C1A-CHA-C4D	2.74	123.55	118.98
31	S	604	CLA	C2C-C1C-NC	2.74	112.86	109.98
54	k1	101	4RF	O40-C41-C43	2.74	120.18	111.83
31	Y	610	CLA	O2A-CGA-CBA	2.74	120.18	111.83
47	Y1	606	CHL	C4D-CHA-CBD	-2.74	106.21	108.97
31	s	611	CLA	C2C-C1C-NC	2.74	112.86	109.98
31	n	611	CLA	C2D-C1D-ND	2.74	112.83	110.13
31	N	604	CLA	O2D-CGD-O1D	-2.74	118.52	123.85
35	C	521	LMG	O8-C28-C29	2.74	120.18	111.83
31	b	610	CLA	C2C-C1C-NC	2.74	112.86	109.98
31	s1	617	CLA	C2C-C1C-NC	2.74	112.86	109.98
31	n	603	CLA	CAA-C2A-C3A	-2.74	105.61	113.00
31	y	610	CLA	C2C-C1C-NC	2.74	112.86	109.98
31	y1	610	CLA	C2C-C1C-NC	2.74	112.86	109.98
47	g1	607	CHL	C1-O2A-CGA	2.74	123.27	116.65
48	n1	620	LUT	C31-C30-C29	-2.74	123.44	127.28
31	b1	608	CLA	C1-C2-C3	-2.73	121.72	126.20
31	Y	603	CLA	C2C-C1C-NC	2.73	112.85	109.98
31	g1	611	CLA	C2C-C1C-NC	2.73	112.85	109.98
31	g1	602	CLA	CMA-C3A-C4A	2.73	119.12	111.77
47	N	601	CHL	C1A-CHA-C4D	2.73	123.54	118.98
50	G1	623	NEX	C38-C25-C26	-2.73	117.80	122.30
31	C	501	CLA	CMA-C3A-C4A	2.73	119.12	111.77
31	C1	507	CLA	C1-C2-C3	-2.73	121.72	126.20
31	n	610	CLA	C2D-C1D-ND	2.73	112.83	110.13
31	s1	609	CLA	O2D-CGD-O1D	-2.73	118.53	123.85
31	b1	604	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
49	r	622	XAT	C20-C13-C14	-2.73	118.39	122.82
47	g	608	CHL	CMA-C3A-C4A	2.73	120.50	114.61
31	c1	501	CLA	C4B-CHC-C1C	2.73	132.67	126.25
31	N1	611	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
35	h	102	LMG	O8-C28-C29	2.73	120.16	111.83
31	a1	405	CLA	CMC-C2C-C1C	2.73	129.30	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	S	610	CLA	CAA-C2A-C3A	-2.73	105.62	113.00
31	n1	611	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
47	G	606	CHL	C1A-CHA-C4D	2.73	123.54	118.98
47	s	601	CHL	C1A-CHA-C4D	2.73	123.54	118.98
49	R1	621	XAT	C6-C7-C8	-2.73	120.22	125.99
40	c	518	DGD	O1G-C1A-C2A	2.73	120.16	111.83
31	N1	604	CLA	C2C-C1C-NC	2.73	112.85	109.98
31	n	613	CLA	C1-O2A-CGA	2.73	123.25	116.65
33	d1	404	BCR	C28-C27-C26	-2.73	109.19	114.06
31	N1	612	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
31	C1	512	CLA	O2A-CGA-CBA	2.73	120.15	111.83
48	y	621	LUT	C22-C23-C24	-2.73	107.13	111.18
31	c1	503	CLA	CAC-C3C-C4C	2.73	128.34	124.79
31	D1	402	CLA	C3B-C4B-NB	-2.73	108.10	110.53
48	N1	620	LUT	C18-C5-C6	-2.73	121.51	124.48
47	G	609	CHL	C4D-ND-C1D	2.73	107.29	105.22
35	J	101	LMG	O8-C28-C29	2.73	120.15	111.83
35	C	521	LMG	C8-O7-C10	-2.73	111.27	117.80
31	Y1	614	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
31	s1	605	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
31	s1	614	CLA	C1C-C2C-C3C	-2.73	104.11	106.98
31	b	609	CLA	CHA-C4D-ND	2.73	138.17	132.55
31	C	512	CLA	C1-C2-C3	-2.73	121.73	126.20
31	R	612	CLA	C1C-C2C-C3C	-2.72	104.11	106.98
31	s	611	CLA	C1C-C2C-C3C	-2.72	104.11	106.98
31	b1	613	CLA	C1C-C2C-C3C	-2.72	104.11	106.98
31	b1	614	CLA	C1C-C2C-C3C	-2.72	104.11	106.98
31	a1	410	CLA	C2C-C1C-NC	2.72	112.84	109.98
31	D1	403	CLA	C3B-C4B-NB	-2.72	108.10	110.53
31	G	604	CLA	C1C-C2C-C3C	-2.72	104.11	106.98
31	r	608	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
33	c	514	BCR	C40-C30-C25	-2.72	105.97	110.24
31	b	604	CLA	CMA-C3A-C4A	2.72	119.09	111.77
31	n1	603	CLA	CAA-C2A-C3A	-2.72	105.64	113.00
31	R	612	CLA	C3B-C4B-NB	-2.72	108.10	110.53
47	r	606	CHL	C3C-C4C-NC	-2.72	108.00	114.65
41	s	624	LHG	O8-C23-C24	2.72	120.13	111.83
31	Y	611	CLA	C2C-C1C-NC	2.72	112.84	109.98
31	b1	616	CLA	C3B-C4B-NB	-2.72	108.10	110.53
31	s1	617	CLA	O2A-CGA-CBA	2.72	120.13	111.83
52	T1	101	3PH	O31-C31-C32	2.72	120.13	111.83
50	S1	623	NEX	C1-C2-C3	2.72	119.56	113.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	Y1	622	XAT	C26-C27-C28	-2.72	120.24	125.99
47	Y1	606	CHL	C1A-CHA-C4D	2.72	123.52	118.98
31	a	410	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
31	A1	410	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
31	B	610	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
31	b1	613	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
47	S	608	CHL	CMA-C3A-C4A	2.72	120.47	114.61
32	A	409	PHO	C2D-C1D-ND	-2.72	107.47	109.43
40	c	523	DGD	O1G-C1A-C2A	2.72	120.12	111.83
31	S	611	CLA	CMA-C3A-C4A	2.72	119.08	111.77
31	A	410	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
32	A	408	PHO	O1D-CGD-CBD	2.72	128.84	124.72
31	b	607	CLA	CHA-C4D-ND	2.72	138.16	132.55
31	g	602	CLA	C1D-ND-C4D	-2.72	104.41	106.31
31	Y	614	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
31	D1	403	CLA	C1C-C2C-C3C	-2.72	104.12	106.98
31	G	603	CLA	C1-C2-C3	-2.72	121.75	126.20
33	B	619	BCR	C37-C22-C21	-2.72	118.42	122.82
31	B	608	CLA	CMA-C3A-C4A	2.72	119.07	111.77
31	r	610	CLA	C3B-C4B-NB	-2.72	108.11	110.53
31	B	612	CLA	O2D-CGD-O1D	-2.72	118.56	123.85
31	n1	610	CLA	C1-C2-C3	-2.71	121.75	126.20
31	G	610	CLA	O2A-CGA-CBA	2.71	120.11	111.83
31	s1	605	CLA	C1-O2A-CGA	2.71	123.22	116.65
31	c	508	CLA	CMA-C3A-C4A	2.71	119.07	111.77
31	B1	604	CLA	CMA-C3A-C4A	2.71	119.07	111.77
31	C1	503	CLA	CHA-C4D-ND	2.71	138.15	132.55
31	c	513	CLA	O2D-CGD-O1D	-2.71	118.56	123.85
35	j	101	LMG	O8-C28-C29	2.71	120.11	111.83
31	g	604	CLA	C2C-C1C-NC	2.71	112.83	109.98
31	s	604	CLA	C2C-C1C-NC	2.71	112.83	109.98
50	r	623	NEX	C26-C27-C28	-2.71	120.26	125.99
31	B	609	CLA	CHA-C4D-ND	2.71	138.15	132.55
31	y	612	CLA	C1-C2-C3	-2.71	121.75	126.20
31	c1	504	CLA	CMA-C3A-C4A	2.71	119.06	111.77
31	G1	610	CLA	O2A-CGA-CBA	2.71	120.10	111.83
31	a1	405	CLA	CAC-C3C-C4C	2.71	128.32	124.79
31	N	603	CLA	CMA-C3A-C4A	2.71	119.06	111.77
47	n1	601	CHL	C1A-CHA-C4D	2.71	123.50	118.98
31	r	610	CLA	CAA-C2A-C3A	-2.71	105.67	113.00
54	i1	101	4RF	O18-C16-C15	2.71	120.10	111.83
31	R	603	CLA	C1-C2-C3	-2.71	121.76	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	G1	612	CLA	C3B-C4B-NB	-2.71	108.11	110.53
31	b1	617	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
47	N1	606	CHL	C4D-CHA-CBD	-2.71	106.23	108.97
31	b	608	CLA	O2A-CGA-CBA	2.71	120.10	111.83
47	Y	601	CHL	C1-C2-C3	-2.71	121.76	126.20
31	n	611	CLA	O2D-CGD-O1D	-2.71	118.58	123.85
31	b	603	CLA	C3B-C4B-NB	-2.71	108.11	110.53
31	y	608	CLA	CMD-C2D-C3D	-2.71	121.48	127.69
31	d1	403	CLA	O2A-CGA-CBA	2.71	120.09	111.83
31	B1	602	CLA	C1C-C2C-C3C	-2.71	104.13	106.98
31	N1	614	CLA	C2C-C1C-NC	2.71	112.83	109.98
33	B	619	BCR	C23-C22-C21	2.71	123.27	119.01
48	N1	620	LUT	C22-C23-C24	-2.71	107.16	111.18
47	N1	605	CHL	C1-C2-C3	-2.71	121.76	126.20
47	g	605	CHL	C4D-CHA-CBD	-2.71	106.24	108.97
31	G	610	CLA	C1D-ND-C4D	-2.71	104.41	106.31
47	y1	601	CHL	C1-O2A-CGA	2.71	123.20	116.65
31	C1	508	CLA	C2D-C1D-ND	2.71	112.80	110.13
31	c1	510	CLA	O2A-CGA-CBA	2.71	120.08	111.83
49	Y	622	XAT	C7-C8-C9	-2.71	121.33	125.53
31	n1	604	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
31	C1	506	CLA	C2C-C1C-NC	2.70	112.82	109.98
50	S	622	NEX	C38-C25-C26	-2.70	117.85	122.30
47	Y1	606	CHL	CMA-C3A-C4A	2.70	120.43	114.61
31	Y	602	CLA	O2A-CGA-CBA	2.70	120.07	111.83
31	n1	611	CLA	C2C-C1C-NC	2.70	112.82	109.98
35	H1	102	LMG	O8-C28-C29	2.70	120.07	111.83
31	B	616	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
31	c	505	CLA	C1C-C2C-C3C	-2.70	104.14	106.98
31	B	603	CLA	CMC-C2C-C1C	2.70	129.25	125.03
31	d1	403	CLA	CMA-C3A-C4A	2.70	119.03	111.77
48	y1	621	LUT	C3-C4-C5	-2.70	105.46	112.18
35	A	413	LMG	C8-O7-C10	-2.70	111.33	117.80
41	y1	624	LHG	O8-C23-C24	2.70	120.07	111.83
47	y1	606	CHL	C1-O2A-CGA	2.70	123.19	116.65
31	S1	604	CLA	O2D-CGD-O1D	-2.70	118.59	123.85
47	s	606	CHL	C4D-CHA-CBD	-2.70	106.25	108.97
48	y1	620	LUT	C22-C23-C24	-2.70	107.18	111.18
48	Y	621	LUT	C18-C5-C6	-2.70	121.54	124.48
31	b	615	CLA	CHA-C4D-ND	2.70	138.12	132.55
31	B1	611	CLA	C4B-CHC-C1C	2.70	132.59	126.25
31	b	603	CLA	C2C-C1C-NC	2.70	112.81	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	g	613	CLA	C1-C2-C3	-2.70	121.78	126.20
34	A1	412	SQD	O7-S-C6	-2.70	102.73	106.76
31	D	403	CLA	C2C-C1C-NC	2.70	112.81	109.98
48	n1	621	LUT	C31-C30-C29	-2.70	123.50	127.28
47	s	601	CHL	C4D-CHA-CBD	-2.70	106.25	108.97
31	R1	603	CLA	C2C-C1C-NC	2.70	112.81	109.98
31	g1	604	CLA	C2C-C1C-NC	2.70	112.81	109.98
47	y	606	CHL	CMA-C3A-C4A	2.70	120.42	114.61
47	S	608	CHL	C1-O2A-CGA	2.69	123.17	116.65
31	R1	609	CLA	O2A-CGA-CBA	2.69	120.05	111.83
40	c1	520	DGD	O1G-C1A-C2A	2.69	120.05	111.83
31	c1	506	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
31	y1	614	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
31	Y	608	CLA	C3B-C4B-NB	-2.69	108.12	110.53
31	B1	615	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
50	N	623	NEX	C4-C3-C2	2.69	115.83	110.79
31	c1	506	CLA	CMA-C3A-C4A	2.69	119.01	111.77
31	S1	614	CLA	CMD-C2D-C3D	-2.69	121.51	127.69
31	s	612	CLA	CMA-C3A-C4A	2.69	119.01	111.77
31	B1	614	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
31	B1	616	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
31	b1	603	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
31	n	610	CLA	C1D-ND-C4D	-2.69	104.42	106.31
33	c1	515	BCR	C23-C24-C25	-2.69	119.81	127.00
31	S	609	CLA	C3B-C4B-NB	-2.69	108.13	110.53
31	C	501	CLA	CAA-C2A-C3A	-2.69	105.72	113.00
31	s	605	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
31	C	512	CLA	C2C-C1C-NC	2.69	112.81	109.98
47	n1	609	CHL	C4D-CHA-CBD	-2.69	106.25	108.97
47	G	606	CHL	CMA-C3A-C4A	2.69	120.41	114.61
42	C1	527	LMK	O3-C4-C3	-2.69	113.95	122.95
56	r1	626	ERG	C13-C14-C8	2.69	118.33	113.59
31	b	608	CLA	CMA-C3A-C4A	2.69	119.00	111.77
31	b1	605	CLA	CMA-C3A-C4A	2.69	119.00	111.77
48	g	620	LUT	C22-C23-C24	-2.69	107.19	111.18
31	r	612	CLA	O2A-CGA-CBA	2.69	120.04	111.83
49	N1	622	XAT	C18-C5-C6	-2.69	117.88	122.30
34	B1	621	SQD	O7-S-C6	-2.69	102.74	106.76
35	h1	102	LMG	O8-C28-C29	2.69	120.04	111.83
47	N	608	CHL	CMA-C3A-C4A	2.69	120.41	114.61
31	c	501	CLA	O2A-CGA-CBA	2.69	120.03	111.83
41	d	409	LHG	O8-C23-C24	2.69	120.03	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	n	609	CHL	C4D-CHA-CBD	-2.69	106.26	108.97
47	g	607	CHL	C1-O2A-CGA	2.69	123.16	116.65
31	B	609	CLA	O2D-CGD-O1D	-2.69	118.62	123.85
31	n1	602	CLA	C2C-C1C-NC	2.69	112.81	109.98
31	C	501	CLA	C1C-C2C-C3C	-2.69	104.15	106.98
38	c1	524	DGA	OG1-CA1-CA2	2.69	120.03	111.83
48	s	621	LUT	C35-C34-C33	-2.69	123.51	127.28
31	b1	614	CLA	C1-C2-C3	-2.69	121.80	126.20
49	G	622	XAT	O4-C6-C7	-2.69	109.18	116.88
48	Y1	620	LUT	C27-C28-C29	-2.69	120.55	126.32
47	S1	601	CHL	C1A-CHA-C4D	2.69	123.46	118.98
31	r	609	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
31	S1	611	CLA	CMA-C3A-C4A	2.68	118.99	111.77
31	s	613	CLA	CHA-C4D-ND	2.68	138.09	132.55
47	G1	607	CHL	C3C-C4C-NC	-2.68	108.09	114.65
47	r1	606	CHL	C1A-CHA-C4D	2.68	123.46	118.98
31	b1	607	CLA	O2A-CGA-CBA	2.68	120.02	111.83
47	n1	606	CHL	C1-O2A-CGA	2.68	123.15	116.65
31	C	501	CLA	CHA-C4D-ND	2.68	138.09	132.55
31	S	603	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
31	n	610	CLA	C2C-C1C-NC	2.68	112.80	109.98
31	S1	609	CLA	C2C-C1C-NC	2.68	112.80	109.98
31	y	602	CLA	CMA-C3A-C4A	2.68	118.98	111.77
31	B1	606	CLA	CHA-C4D-ND	2.68	138.08	132.55
31	B	615	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
31	y	608	CLA	C2C-C1C-NC	2.68	112.80	109.98
50	n1	623	NEX	C38-C25-C26	-2.68	117.89	122.30
31	Y1	602	CLA	C3B-C4B-NB	-2.68	108.14	110.53
31	G	614	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
31	n1	610	CLA	C2C-C1C-NC	2.68	112.80	109.98
31	N1	610	CLA	O1D-CGD-CBD	-2.68	119.23	124.52
31	s	611	CLA	C3B-C4B-NB	-2.68	108.14	110.53
31	g1	613	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
31	b	610	CLA	O2D-CGD-O1D	-2.68	118.63	123.85
31	S1	604	CLA	O2A-CGA-CBA	2.68	120.01	111.83
49	g1	622	XAT	O4-C6-C7	-2.68	109.20	116.88
33	b	619	BCR	C4-C5-C6	-2.68	119.08	122.70
31	y1	611	CLA	C1C-C2C-C3C	-2.68	104.16	106.98
53	Y1	625	SPH	C3-C4-C5	-2.68	119.14	124.69
47	s1	606	CHL	C4D-CHA-CBD	-2.68	106.27	108.97
47	R1	606	CHL	C3C-C4C-NC	-2.68	108.10	114.65
31	r	602	CLA	C2C-C1C-NC	2.68	112.80	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	R	612	CLA	O2A-CGA-CBA	2.68	120.00	111.83
57	Y1	626	PTY	O4-C30-C31	2.68	120.00	111.83
48	S1	620	LUT	C31-C30-C29	-2.68	123.52	127.28
31	y	608	CLA	C3B-C4B-NB	-2.68	108.14	110.53
47	y	607	CHL	C1A-CHA-C4D	2.68	123.45	118.98
31	g	614	CLA	C1C-C2C-C3C	-2.68	104.17	106.98
34	c	626	SQD	O7-S-C6	-2.68	102.76	106.76
31	C	513	CLA	C2C-C1C-NC	2.68	112.79	109.98
50	s1	623	NEX	C31-C32-C33	2.68	133.70	126.36
31	g	612	CLA	O2D-CGD-O1D	-2.68	118.64	123.85
31	S1	613	CLA	C1C-C2C-C3C	-2.68	104.17	106.98
31	a	410	CLA	CAA-C2A-C3A	-2.67	105.77	113.00
31	b1	605	CLA	CBC-CAC-C3C	-2.67	105.17	112.42
52	s	626	3PH	O31-C31-C32	2.67	119.99	111.83
48	y	621	LUT	C38-C25-C24	-2.67	117.03	123.36
35	B	622	LMG	O8-C28-C29	2.67	119.98	111.83
47	G1	608	CHL	CMA-C3A-C4A	2.67	120.37	114.61
44	D	405	PL9	C22-C23-C24	-2.67	121.51	127.62
31	s1	613	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
31	c	505	CLA	CHA-C4D-ND	2.67	138.06	132.55
48	s	621	LUT	C15-C35-C34	-2.67	118.05	123.52
38	C1	524	DGA	OG1-CA1-CA2	2.67	119.98	111.83
31	N1	610	CLA	CHD-C1D-ND	-2.67	121.05	124.80
49	y	622	XAT	C18-C5-C6	-2.67	117.91	122.30
33	C	516	BCR	C34-C9-C10	-2.67	118.49	122.82
31	C	504	CLA	C1D-ND-C4D	-2.67	104.44	106.31
31	b1	610	CLA	CHA-C4D-ND	2.67	138.06	132.55
44	d1	405	PL9	C20-C19-C21	2.67	119.86	115.23
48	y	621	LUT	C31-C30-C29	-2.67	123.53	127.28
32	a	409	PHO	C2D-C1D-ND	-2.67	107.50	109.43
31	c1	501	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
31	B1	607	CLA	C1-C2-C3	-2.67	121.83	126.20
41	D	409	LHG	O8-C23-C24	2.67	119.97	111.83
31	D1	402	CLA	C1D-ND-C4D	-2.67	104.44	106.31
31	Y	612	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
31	Y	608	CLA	C2C-C1C-NC	2.67	112.78	109.98
31	C1	511	CLA	O2A-CGA-CBA	2.67	119.97	111.83
31	B	604	CLA	CHA-C4D-ND	2.67	138.05	132.55
31	b	606	CLA	O2A-CGA-CBA	2.67	119.97	111.83
31	B1	610	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
31	y	611	CLA	CMA-C3A-C4A	2.67	118.94	111.77
47	r1	607	CHL	CMA-C3A-C4A	2.67	120.36	114.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s	604	CLA	C1C-C2C-C3C	-2.67	104.17	106.98
31	g1	613	CLA	C2C-C1C-NC	2.67	112.78	109.98
31	y1	602	CLA	CMA-C3A-C4A	2.67	118.94	111.77
33	b	618	BCR	C23-C24-C25	-2.67	119.88	127.00
31	d1	403	CLA	C1C-C2C-C3C	-2.67	104.18	106.98
31	y1	608	CLA	C2C-C1C-NC	2.67	112.78	109.98
31	C	509	CLA	O2D-CGD-O1D	-2.67	118.66	123.85
31	b	609	CLA	O1D-CGD-CBD	-2.67	119.26	124.52
31	y	608	CLA	C1C-C2C-C3C	-2.67	104.18	106.98
31	R1	608	CLA	C1C-C2C-C3C	-2.67	104.18	106.98
31	r	613	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
47	G1	609	CHL	C3C-C4C-NC	-2.66	108.14	114.65
31	b1	611	CLA	O2D-CGD-O1D	-2.66	118.66	123.85
47	n	601	CHL	C1A-CHA-C4D	2.66	123.43	118.98
47	G1	606	CHL	C1A-CHA-C4D	2.66	123.43	118.98
31	B	612	CLA	C3B-C4B-NB	-2.66	108.15	110.53
31	c	501	CLA	C3B-C4B-NB	-2.66	108.15	110.53
31	g	603	CLA	C4B-CHC-C1C	2.66	132.51	126.25
31	B1	609	CLA	CHA-C4D-ND	2.66	138.04	132.55
31	n1	613	CLA	C1-O2A-CGA	2.66	123.10	116.65
31	s	612	CLA	C2C-C1C-NC	2.66	112.78	109.98
31	n1	613	CLA	C2C-C1C-NC	2.66	112.78	109.98
48	G	621	LUT	C26-C27-C28	-2.66	120.44	124.58
47	n	606	CHL	C1A-CHA-C4D	2.66	123.42	118.98
49	g	622	XAT	C26-C27-C28	-2.66	120.36	125.99
31	b	603	CLA	C1C-C2C-C3C	-2.66	104.18	106.98
31	G	614	CLA	CAA-C2A-C3A	-2.66	105.81	113.00
47	g	601	CHL	C4D-CHA-CBD	-2.66	106.28	108.97
50	y1	623	NEX	C8-C7-C6	-2.66	174.52	177.66
31	A1	410	CLA	CAA-C2A-C3A	-2.66	105.81	113.00
49	n1	622	XAT	C7-C8-C9	-2.66	121.40	125.53
48	N1	621	LUT	C18-C5-C6	-2.66	121.58	124.48
31	b1	617	CLA	CMA-C3A-C4A	2.66	118.92	111.77
31	g1	610	CLA	CMA-C3A-C4A	2.66	118.92	111.77
31	C1	505	CLA	CHA-C4D-ND	2.66	138.04	132.55
33	C1	516	BCR	C23-C22-C21	2.66	123.19	119.01
35	A1	413	LMG	O8-C28-C29	2.66	119.95	111.83
31	y	610	CLA	CAA-C2A-C3A	-2.66	105.81	113.00
47	G	608	CHL	C4D-CHA-CBD	-2.66	106.29	108.97
34	c1	526	SQD	O7-S-C6	-2.66	102.79	106.76
46	H1	101	RRX	C33-C5-C4	2.66	119.27	113.60
31	y	603	CLA	CMA-C3A-C4A	2.66	118.92	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	602	CLA	C1C-C2C-C3C	-2.66	104.19	106.98
31	s1	603	CLA	C1C-C2C-C3C	-2.66	104.19	106.98
31	g	612	CLA	C3B-C4B-NB	-2.66	108.16	110.53
31	b1	612	CLA	CAC-C3C-C4C	2.66	128.25	124.79
31	R	609	CLA	O2A-CGA-CBA	2.66	119.94	111.83
31	Y	610	CLA	O1D-CGD-CBD	-2.66	119.28	124.52
31	B1	612	CLA	CMA-C3A-C4A	2.66	118.91	111.77
31	Y1	604	CLA	C1C-C2C-C3C	-2.66	104.19	106.98
31	C	511	CLA	C2C-C1C-NC	2.66	112.77	109.98
31	B1	605	CLA	C2C-C1C-NC	2.66	112.77	109.98
31	G1	613	CLA	C2C-C1C-NC	2.66	112.77	109.98
31	r	609	CLA	O2A-CGA-CBA	2.66	119.93	111.83
47	Y1	601	CHL	C1-C2-C3	-2.66	121.85	126.20
31	S	605	CLA	C1C-C2C-C3C	-2.66	104.19	106.98
56	R1	626	ERG	C1-C10-C5	2.65	113.32	108.74
31	G	602	CLA	CMA-C3A-C4A	2.65	118.91	111.77
49	n1	622	XAT	O4-C6-C7	-2.65	109.27	116.88
31	G1	612	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
33	B	619	BCR	C4-C5-C6	-2.65	119.12	122.70
31	Y1	608	CLA	CMD-C2D-C3D	-2.65	121.60	127.69
31	r	613	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
31	r1	603	CLA	C3B-C4B-NB	-2.65	108.16	110.53
47	n	606	CHL	CMA-C3A-C4A	2.65	120.33	114.61
48	g	620	LUT	C26-C27-C28	-2.65	120.45	124.58
47	N	606	CHL	C1-O2A-CGA	2.65	123.07	116.65
31	C	504	CLA	C2C-C1C-NC	2.65	112.77	109.98
49	R1	621	XAT	C18-C5-C6	-2.65	117.94	122.30
31	B1	608	CLA	CMD-C2D-C3D	-2.65	121.61	127.69
34	b	621	SQD	O7-S-C6	-2.65	102.80	106.76
48	s1	621	LUT	C35-C15-C14	-2.65	118.09	123.52
33	b1	618	BCR	C31-C1-C6	-2.65	106.09	110.24
31	g	602	CLA	CHD-C1D-ND	-2.65	121.07	124.80
31	C1	501	CLA	CMD-C2D-C3D	-2.65	121.61	127.69
31	y	610	CLA	O2A-CGA-CBA	2.65	119.92	111.83
41	D1	410	LHG	O8-C23-C24	2.65	119.92	111.83
31	b	614	CLA	C2C-C1C-NC	2.65	112.77	109.98
47	N	606	CHL	C1A-CHA-C4D	2.65	123.40	118.98
47	G	607	CHL	C1A-CHA-C4D	2.65	123.40	118.98
31	Y	613	CLA	O2A-CGA-CBA	2.65	119.92	111.83
31	y	612	CLA	C1C-C2C-C3C	-2.65	104.19	106.98
31	b	613	CLA	CHA-C4D-ND	2.65	138.02	132.55
31	R	610	CLA	C2C-C1C-NC	2.65	112.77	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s	605	CLA	O2A-CGA-CBA	2.65	119.91	111.83
48	r1	620	LUT	C15-C35-C34	-2.65	118.10	123.52
31	y	604	CLA	CMA-C3A-C4A	2.65	118.89	111.77
47	n	606	CHL	C1C-C2C-CMC	2.65	131.57	126.80
31	B1	608	CLA	C1C-C2C-C3C	-2.65	104.20	106.98
31	S1	604	CLA	C1C-C2C-C3C	-2.65	104.20	106.98
50	r1	622	NEX	C38-C25-C26	-2.65	117.95	122.30
31	c1	507	CLA	C1-C2-C3	-2.65	121.86	126.20
31	b1	612	CLA	O2A-CGA-CBA	2.65	119.90	111.83
31	C	501	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
31	C	511	CLA	C1C-C2C-C3C	-2.65	104.20	106.98
31	D1	403	CLA	O2D-CGD-O1D	-2.65	118.70	123.85
31	N	610	CLA	CAA-CBA-CGA	2.65	120.72	113.21
47	S1	606	CHL	C4D-CHA-CBD	-2.65	106.30	108.97
31	d1	402	CLA	O2A-CGA-CBA	2.65	119.90	111.83
31	R	613	CLA	C1C-C2C-C3C	-2.65	104.20	106.98
31	G1	604	CLA	C2C-C1C-NC	2.64	112.76	109.98
31	R	611	CLA	C3B-C4B-NB	-2.64	108.17	110.53
31	C1	501	CLA	C3B-C4B-NB	-2.64	108.17	110.53
33	b1	618	BCR	C4-C5-C6	-2.64	119.13	122.70
31	C1	503	CLA	CMD-C2D-C3D	-2.64	121.63	127.69
33	a	411	BCR	C33-C5-C4	2.64	119.23	113.60
31	S	609	CLA	CAA-C2A-C3A	-2.64	105.86	113.00
49	y	622	XAT	O24-C25-C38	-2.64	112.09	115.05
31	a	406	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
31	g1	614	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
47	s1	607	CHL	CMA-C3A-C4A	2.64	120.31	114.61
31	G	610	CLA	CAA-C2A-C3A	-2.64	105.86	113.00
31	G	611	CLA	C3B-C4B-NB	-2.64	108.17	110.53
31	C	503	CLA	O2A-CGA-CBA	2.64	119.89	111.83
31	n	613	CLA	O2A-CGA-CBA	2.64	119.89	111.83
47	N1	605	CHL	C4D-CHA-CBD	-2.64	106.30	108.97
31	g1	611	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
31	R1	609	CLA	CAA-C2A-C3A	-2.64	105.86	113.00
47	G1	601	CHL	C1-C2-C3	-2.64	121.87	126.20
31	Y1	602	CLA	CHD-C1D-ND	-2.64	121.08	124.80
31	b1	608	CLA	CHA-C4D-ND	2.64	138.00	132.55
31	c1	505	CLA	CHA-C4D-ND	2.64	138.00	132.55
31	r	603	CLA	O2A-C1-C2	2.64	118.27	108.11
31	B1	610	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
31	R1	603	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
31	y1	614	CLA	CHD-C1D-ND	-2.64	121.09	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s	609	CLA	C4B-CHC-C1C	2.64	132.46	126.25
47	N1	609	CHL	CMA-C3A-C4A	2.64	120.30	114.61
31	Y	604	CLA	C1C-C2C-C3C	-2.64	104.20	106.98
31	Y1	604	CLA	CMA-C3A-C4A	2.64	118.87	111.77
31	s1	605	CLA	O2A-CGA-CBA	2.64	119.89	111.83
31	c	504	CLA	C1D-ND-C4D	-2.64	104.46	106.31
47	y1	609	CHL	C1A-CHA-C4D	2.64	123.39	118.98
31	C	513	CLA	CMA-C3A-C4A	2.64	118.87	111.77
31	r1	602	CLA	O2A-CGA-CBA	2.64	119.88	111.83
31	b	614	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
31	r	608	CLA	CHA-C4D-ND	2.64	137.99	132.55
31	Y	603	CLA	CAA-C2A-C3A	-2.64	105.87	113.00
31	g1	612	CLA	CMA-C3A-C4A	2.64	118.86	111.77
47	g1	607	CHL	C3C-C4C-NC	-2.64	108.20	114.65
31	b	617	CLA	C2C-C1C-NC	2.64	112.75	109.98
31	a	405	CLA	C2D-C1D-ND	2.64	112.74	110.13
31	C	504	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
41	D	410	LHG	O8-C23-C24	2.64	119.88	111.83
41	N1	624	LHG	C5-O7-C7	-2.64	111.48	117.80
31	N	610	CLA	O2D-CGD-O1D	-2.64	118.71	123.85
31	a1	410	CLA	CMA-C3A-C4A	2.64	118.86	111.77
50	y	623	NEX	C1-C2-C3	2.64	119.38	113.59
31	C1	509	CLA	CMA-C3A-C4A	2.64	118.86	111.77
31	g1	603	CLA	C3B-C4B-NB	-2.64	108.18	110.53
31	b	612	CLA	C1D-ND-C4D	-2.64	104.46	106.31
31	B	607	CLA	CHA-C4D-ND	2.64	137.99	132.55
31	B1	613	CLA	C2C-C1C-NC	2.64	112.75	109.98
44	d1	405	PL9	C40-C39-C41	2.64	119.80	115.23
48	s	620	LUT	C8-C7-C6	-2.64	119.96	127.00
52	s1	626	3PH	O31-C31-C32	2.64	119.87	111.83
31	B	617	CLA	C3B-C4B-NB	-2.64	108.18	110.53
31	B	605	CLA	C1C-C2C-C3C	-2.64	104.21	106.98
31	g	611	CLA	C1C-C2C-C3C	-2.64	104.21	106.98
31	n	603	CLA	CMA-C3A-C4A	2.64	118.86	111.77
31	c	503	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
31	d	402	CLA	C4B-CHC-C1C	2.63	132.44	126.25
31	C	513	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
31	S1	602	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
44	D1	405	PL9	C20-C19-C21	2.63	119.80	115.23
31	c1	505	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
47	Y	609	CHL	C1-C2-C3	-2.63	121.88	126.20
41	G	630	LHG	O8-C23-C24	2.63	119.86	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	y1	605	CHL	CMA-C3A-C4A	2.63	120.28	114.61
31	B	610	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
31	c	501	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
31	R1	609	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
31	s	617	CLA	C3B-C4B-NB	-2.63	108.18	110.53
31	G	604	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
31	N1	602	CLA	O2A-CGA-CBA	2.63	119.86	111.83
50	S1	623	NEX	C38-C25-C26	-2.63	117.97	122.30
47	Y1	605	CHL	CMA-C3A-C4A	2.63	120.28	114.61
31	C1	501	CLA	O2A-CGA-CBA	2.63	119.86	111.83
31	y	603	CLA	O2D-CGD-O1D	-2.63	118.72	123.85
31	R1	612	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
47	n	607	CHL	C1A-CHA-C4D	2.63	123.37	118.98
31	b	615	CLA	CMA-C3A-C4A	2.63	118.85	111.77
31	b	617	CLA	CMA-C3A-C4A	2.63	118.85	111.77
31	r	604	CLA	C2C-C1C-NC	2.63	112.75	109.98
31	R	611	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
31	C1	509	CLA	O2A-C1-C2	2.63	118.23	108.11
45	F	101	HEM	C1B-NB-C4B	2.63	108.32	105.21
31	g	613	CLA	C1D-ND-C4D	-2.63	104.47	106.31
31	B1	607	CLA	C2C-C1C-NC	2.63	112.75	109.98
48	s	620	LUT	C38-C25-C24	-2.63	117.14	123.36
31	b1	613	CLA	CMD-C2D-C3D	-2.63	121.66	127.69
31	N	602	CLA	O2A-CGA-CBA	2.63	119.85	111.83
31	N1	614	CLA	C1C-C2C-C3C	-2.63	104.21	106.98
31	S	610	CLA	CHA-C4D-ND	2.63	137.97	132.55
47	N1	608	CHL	CMA-C3A-C4A	2.63	120.28	114.61
33	C	517	BCR	C28-C27-C26	-2.63	109.37	114.06
31	g1	610	CLA	C2C-C1C-NC	2.63	112.74	109.98
38	c	524	DGA	OG1-CA1-CA2	2.63	119.85	111.83
31	S	613	CLA	CHA-C4D-ND	2.63	137.97	132.55
31	A	410	CLA	CAA-C2A-C3A	-2.63	105.90	113.00
31	G1	614	CLA	O2D-CGD-O1D	-2.63	118.73	123.85
31	s	613	CLA	O1D-CGD-CBD	-2.63	119.34	124.52
31	b	616	CLA	C1C-C2C-C3C	-2.63	104.22	106.98
33	B	619	BCR	C36-C18-C17	-2.63	118.56	122.82
31	S	610	CLA	C3B-C4B-NB	-2.63	108.19	110.53
31	S	611	CLA	O2A-CGA-CBA	2.63	119.84	111.83
31	Y	603	CLA	O2D-CGD-O1D	-2.63	118.74	123.85
31	r1	603	CLA	O2A-CGA-CBA	2.63	119.84	111.83
31	b	614	CLA	C1C-C2C-C3C	-2.63	104.22	106.98
31	B	604	CLA	O2A-CGA-CBA	2.63	119.84	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	G1	610	CLA	CMA-C3A-C4A	2.63	118.83	111.77
33	C1	517	BCR	C38-C26-C25	-2.63	121.62	124.48
31	c1	513	CLA	O2D-CGD-O1D	-2.63	118.74	123.85
31	Y1	602	CLA	C4B-CHC-C1C	2.63	132.42	126.25
31	B	604	CLA	C2C-C1C-NC	2.62	112.74	109.98
48	s1	621	LUT	C1-C6-C5	-2.62	119.05	122.64
31	B	615	CLA	CHA-C4D-ND	2.62	137.96	132.55
31	y1	608	CLA	CMA-C3A-C4A	2.62	118.83	111.77
33	a	411	BCR	C35-C13-C12	2.62	122.10	118.09
31	n	611	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
31	y	604	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
31	r1	604	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
46	H1	101	RRX	C30-C25-C26	-2.62	119.05	122.64
31	b1	609	CLA	C3B-C4B-NB	-2.62	108.19	110.53
31	G	611	CLA	O2D-CGD-O1D	-2.62	118.74	123.85
47	Y	601	CHL	CMA-C3A-C4A	2.62	120.26	114.61
47	G1	601	CHL	C1-O2A-CGA	2.62	123.00	116.65
31	s1	610	CLA	CMA-C3A-C4A	2.62	118.82	111.77
31	B	605	CLA	CHA-C4D-ND	2.62	137.96	132.55
47	s1	608	CHL	C4D-CHA-CBD	-2.62	106.32	108.97
49	y	622	XAT	C38-C25-C26	-2.62	117.99	122.30
31	y	604	CLA	O2A-CGA-CBA	2.62	119.83	111.83
31	g1	613	CLA	O2A-CGA-CBA	2.62	119.83	111.83
31	a1	410	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
47	G1	605	CHL	CMA-C3A-C4A	2.62	120.26	114.61
47	y	609	CHL	C1A-CHA-C4D	2.62	123.36	118.98
31	s	603	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
31	n1	614	CLA	C2C-C1C-NC	2.62	112.73	109.98
31	r1	602	CLA	C4B-CHC-C1C	2.62	132.41	126.25
31	c	510	CLA	CHA-C4D-ND	2.62	137.95	132.55
47	r1	607	CHL	C1A-CHA-C4D	2.62	123.35	118.98
31	N1	613	CLA	C1-C2-C3	-2.62	121.91	126.20
31	C	512	CLA	C1C-C2C-C3C	-2.62	104.22	106.98
31	s1	609	CLA	C1C-C2C-C3C	-2.62	104.23	106.98
31	R	602	CLA	C2C-C1C-NC	2.62	112.73	109.98
31	y1	608	CLA	CMD-C2D-C3D	-2.62	121.69	127.69
31	n	611	CLA	C3B-C4B-NB	-2.62	108.19	110.53
47	N	609	CHL	C4D-CHA-CBD	-2.62	106.33	108.97
31	c	501	CLA	C2C-C1C-NC	2.62	112.73	109.98
31	y1	611	CLA	CHA-C4D-ND	2.62	137.95	132.55
48	g1	621	LUT	C15-C35-C34	-2.62	118.16	123.52
31	G	610	CLA	C2D-C1D-ND	2.62	112.72	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s1	603	CLA	CHA-C4D-ND	2.62	137.95	132.55
31	Y	608	CLA	O2D-CGD-O1D	-2.62	118.75	123.85
31	B	613	CLA	CHA-C4D-ND	2.62	137.95	132.55
31	N1	603	CLA	CHA-C4D-ND	2.62	137.95	132.55
32	A1	408	PHO	O2D-CGD-O1D	-2.62	118.76	123.85
31	C	504	CLA	CHD-C1D-ND	-2.62	121.12	124.80
31	s1	602	CLA	C1C-C2C-C3C	-2.62	104.23	106.98
31	r	602	CLA	O2D-CGD-O1D	-2.62	118.76	123.85
50	R1	622	NEX	C39-C29-C30	-2.62	118.58	122.82
31	R1	602	CLA	CMA-C3A-C4A	2.61	118.80	111.77
31	c1	501	CLA	O2A-CGA-CBA	2.61	119.81	111.83
31	r	611	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
31	N	610	CLA	C4B-CHC-C1C	2.61	132.39	126.25
31	y	608	CLA	C1-O2A-CGA	2.61	122.98	116.65
31	N	611	CLA	CHA-C4D-ND	2.61	137.94	132.55
31	A1	405	CLA	CHA-C4D-ND	2.61	137.94	132.55
47	g1	605	CHL	C4D-CHA-CBD	-2.61	106.33	108.97
31	y1	610	CLA	O2A-CGA-CBA	2.61	119.80	111.83
31	g	612	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
31	y1	613	CLA	C2C-C1C-NC	2.61	112.72	109.98
32	A1	408	PHO	C3B-C4B-NB	-2.61	105.76	107.46
47	r1	607	CHL	C4C-CHD-C1D	2.61	125.41	116.07
31	S	612	CLA	CMA-C3A-C4A	2.61	118.79	111.77
31	N1	614	CLA	C1D-ND-C4D	-2.61	104.48	106.31
31	b	608	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
48	s1	621	LUT	C18-C5-C4	2.61	119.22	114.42
45	f	101	HEM	C1B-NB-C4B	2.61	108.30	105.21
47	n	608	CHL	CMA-C3A-C4A	2.61	120.23	114.61
31	n	612	CLA	C4D-CHA-C1A	2.61	124.36	121.24
31	N	611	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
31	G1	613	CLA	C1C-C2C-C3C	-2.61	104.23	106.98
31	B1	602	CLA	C1-C2-C3	-2.61	121.92	126.20
47	r1	606	CHL	C3C-C4C-NC	-2.61	108.27	114.65
50	r1	622	NEX	C16-C1-C6	-2.61	108.14	110.47
31	r	611	CLA	C3B-C4B-NB	-2.61	108.20	110.53
31	r1	608	CLA	C4B-CHC-C1C	2.61	132.38	126.25
31	G	611	CLA	C2C-C1C-NC	2.61	112.72	109.98
47	G1	605	CHL	C1A-CHA-C4D	2.61	123.33	118.98
40	c	520	DGD	O1G-C1A-C2A	2.61	119.79	111.83
31	B	613	CLA	CMD-C2D-C3D	-2.61	121.71	127.69
31	c1	507	CLA	CHA-C4D-ND	2.61	137.93	132.55
50	G1	623	NEX	C4-C3-C2	2.61	115.67	110.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c1	512	CLA	O2D-CGD-O1D	-2.61	118.77	123.85
49	r	622	XAT	C8-C9-C10	2.61	123.11	119.01
48	S1	621	LUT	C15-C14-C13	-2.61	123.62	127.28
31	Y1	610	CLA	O2A-CGA-CBA	2.61	119.78	111.83
50	n	623	NEX	C31-C30-C29	2.61	130.93	127.28
31	C	513	CLA	C1C-C2C-C3C	-2.61	104.24	106.98
31	C1	506	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
31	c1	511	CLA	O2D-CGD-O1D	-2.61	118.78	123.85
47	n	606	CHL	C1-O2A-CGA	2.61	122.96	116.65
31	s1	611	CLA	C1-C2-C3	-2.61	121.93	126.20
31	d	403	CLA	C3B-C4B-NB	-2.61	108.20	110.53
31	s	611	CLA	CMA-C3A-C4A	2.61	118.78	111.77
31	R	608	CLA	C1C-C2C-C3C	-2.61	104.24	106.98
31	C1	513	CLA	CMA-C3A-C4A	2.60	118.77	111.77
31	r1	604	CLA	CMA-C3A-C4A	2.60	118.77	111.77
31	A1	407	CLA	CHD-C1D-ND	-2.60	121.14	124.80
41	N1	624	LHG	O8-C23-C24	2.60	119.78	111.83
49	R	621	XAT	C31-C30-C29	-2.60	123.63	127.28
31	d	402	CLA	C1D-ND-C4D	-2.60	104.48	106.31
31	B1	602	CLA	CHA-C4D-ND	2.60	137.92	132.55
31	n	614	CLA	O2D-CGD-O1D	-2.60	118.78	123.85
31	Y1	603	CLA	C4B-CHC-C1C	2.60	132.37	126.25
31	n1	611	CLA	C3B-C4B-NB	-2.60	108.21	110.53
31	Y1	602	CLA	C1C-C2C-C3C	-2.60	104.24	106.98
31	s1	605	CLA	CHA-C4D-ND	2.60	137.92	132.55
31	C	502	CLA	C2C-C1C-NC	2.60	112.72	109.98
56	R1	626	ERG	C2-C3-C4	2.60	113.95	110.29
31	c	509	CLA	CHA-C4D-ND	2.60	137.92	132.55
31	c	512	CLA	CHA-C4D-ND	2.60	137.92	132.55
31	c1	504	CLA	C1-O2A-CGA	2.60	122.95	116.65
31	C1	513	CLA	C1D-ND-C4D	-2.60	104.49	106.31
50	N	623	NEX	C17-C1-C6	-2.60	108.14	110.47
31	D	403	CLA	C1C-C2C-C3C	-2.60	104.24	106.98
31	c1	501	CLA	C3B-C4B-NB	-2.60	108.21	110.53
31	r1	610	CLA	C3B-C4B-NB	-2.60	108.21	110.53
31	g	613	CLA	O2A-CGA-CBA	2.60	119.77	111.83
33	c	517	BCR	C33-C5-C6	-2.60	121.64	124.48
31	B1	607	CLA	CHA-C4D-ND	2.60	137.92	132.55
31	c1	511	CLA	CBA-CAA-C2A	2.60	121.53	113.79
31	B	613	CLA	C1C-C2C-C3C	-2.60	104.24	106.98
31	y	611	CLA	C1C-C2C-C3C	-2.60	104.24	106.98
31	g1	610	CLA	C4B-CHC-C1C	2.60	132.36	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s	604	CLA	O2A-CGA-CBA	2.60	119.77	111.83
31	Y	612	CLA	C3B-C4B-NB	-2.60	108.21	110.53
31	D	402	CLA	C4B-CHC-C1C	2.60	132.36	126.25
31	R	612	CLA	CHA-C4D-ND	2.60	137.91	132.55
31	g	611	CLA	CHA-C4D-ND	2.60	137.91	132.55
31	c1	507	CLA	CMA-C3A-C4A	2.60	118.76	111.77
31	y	611	CLA	O2D-CGD-O1D	-2.60	118.79	123.85
31	R	602	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
31	S	610	CLA	O2A-CGA-CBA	2.60	119.76	111.83
31	N	602	CLA	CAA-C2A-C3A	-2.60	105.97	113.00
33	c	514	BCR	C33-C5-C4	2.60	119.14	113.60
31	R	608	CLA	C3B-C4B-NB	-2.60	108.21	110.53
31	Y1	603	CLA	OBD-CAD-C3D	-2.60	122.34	128.42
31	G1	614	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
31	C	503	CLA	C4B-CHC-C1C	2.60	132.36	126.25
31	g	604	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
31	G1	610	CLA	C1D-ND-C4D	-2.60	104.49	106.31
31	N	611	CLA	C3B-C4B-NB	-2.60	108.21	110.53
31	n	614	CLA	C3B-C4B-NB	-2.60	108.21	110.53
48	G1	621	LUT	C22-C23-C24	-2.60	107.33	111.18
31	B	608	CLA	C2C-C1C-NC	2.60	112.71	109.98
31	G	614	CLA	C2C-C1C-NC	2.60	112.71	109.98
47	s1	601	CHL	C1A-CHA-C4D	2.60	123.31	118.98
31	S1	605	CLA	O2D-CGD-O1D	-2.60	118.80	123.85
31	y1	603	CLA	O2D-CGD-O1D	-2.60	118.80	123.85
47	N	609	CHL	C1-C2-C3	-2.60	121.94	126.20
31	R	609	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
31	A1	406	CLA	C1C-C2C-C3C	-2.60	104.25	106.98
47	y	601	CHL	C4D-CHA-CBD	-2.60	106.35	108.97
41	C	525	LHG	O8-C23-C24	2.60	119.75	111.83
31	S	603	CLA	C3B-C4B-NB	-2.60	108.21	110.53
31	G1	614	CLA	C3B-C4B-NB	-2.60	108.21	110.53
31	S	614	CLA	O2D-CGD-O1D	-2.60	118.80	123.85
31	B1	610	CLA	O2A-CGA-CBA	2.59	119.75	111.83
54	K1	101	4RF	O40-C41-C43	2.59	119.75	111.83
47	n	607	CHL	CMA-C3A-C4A	2.59	120.20	114.61
31	Y	604	CLA	O1D-CGD-CBD	-2.59	119.40	124.52
31	B1	606	CLA	C1-O2A-CGA	2.59	122.93	116.65
31	B	606	CLA	C1C-C2C-C3C	-2.59	104.25	106.98
31	R	611	CLA	C1C-C2C-C3C	-2.59	104.25	106.98
33	c1	515	BCR	C1-C6-C7	2.59	122.69	115.65
31	S1	611	CLA	CHA-C4D-ND	2.59	137.90	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c1	503	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
31	Y1	610	CLA	O1D-CGD-CBD	-2.59	119.40	124.52
49	Y1	622	XAT	O4-C5-C18	-2.59	112.15	115.05
31	c	501	CLA	CAA-C2A-C3A	-2.59	105.99	113.00
31	G1	611	CLA	CMD-C2D-C3D	-2.59	121.74	127.69
47	y1	606	CHL	C1-C2-C3	-2.59	121.95	126.20
31	g	603	CLA	C2D-C1D-ND	2.59	112.69	110.13
31	r	612	CLA	C2C-C1C-NC	2.59	112.70	109.98
31	Y1	608	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
31	n1	610	CLA	O2A-CGA-CBA	2.59	119.74	111.83
49	g1	622	XAT	O24-C26-C27	-2.59	109.45	116.88
31	g	604	CLA	CMD-C2D-C3D	-2.59	121.75	127.69
50	s1	623	NEX	C2-C1-C6	2.59	111.73	109.21
31	n1	611	CLA	O2D-CGD-O1D	-2.59	118.80	123.85
31	Y	612	CLA	CMA-C3A-C4A	2.59	118.74	111.77
47	Y1	609	CHL	C1-C2-C3	-2.59	121.95	126.20
31	c1	505	CLA	O1D-CGD-CBD	-2.59	119.41	124.52
31	S	617	CLA	C1C-C2C-C3C	-2.59	104.25	106.98
47	y1	601	CHL	CMA-C3A-C4A	2.59	120.19	114.61
47	y1	601	CHL	C4D-CHA-CBD	-2.59	106.36	108.97
31	a	405	CLA	CHD-C1D-ND	-2.59	121.16	124.80
31	b	615	CLA	C1-O2A-CGA	2.59	122.92	116.65
31	s	611	CLA	O2A-CGA-CBA	2.59	119.73	111.83
49	n	622	XAT	C18-C5-C6	-2.59	118.04	122.30
49	Y1	622	XAT	O4-C6-C7	-2.59	109.46	116.88
33	b	619	BCR	C37-C22-C21	-2.59	118.62	122.82
31	B1	610	CLA	C4B-CHC-C1C	2.59	132.34	126.25
31	R	603	CLA	CHA-C4D-ND	2.59	137.89	132.55
31	G1	603	CLA	CHA-C4D-ND	2.59	137.89	132.55
31	C	510	CLA	O2A-CGA-CBA	2.59	119.73	111.83
31	s1	602	CLA	C4B-CHC-C1C	2.59	132.34	126.25
49	r1	621	XAT	C18-C5-C6	-2.59	118.04	122.30
31	B1	608	CLA	CHA-C4D-ND	2.59	137.89	132.55
31	D1	402	CLA	C2D-C1D-ND	2.59	112.69	110.13
33	b	618	BCR	C33-C5-C6	-2.59	121.66	124.48
31	c	501	CLA	CMD-C2D-C3D	-2.59	121.75	127.69
31	g	613	CLA	C2C-C1C-NC	2.59	112.70	109.98
31	S	611	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
48	N1	620	LUT	C38-C25-C24	-2.59	117.24	123.36
31	y	612	CLA	O2A-CGA-CBA	2.59	119.72	111.83
31	C	507	CLA	C1-C2-C3	-2.59	121.96	126.20
31	B	608	CLA	O2D-CGD-O1D	-2.59	118.81	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
54	I1	102	4RF	O18-C16-C15	2.59	119.72	111.83
31	g1	611	CLA	O2D-CGD-O1D	-2.59	118.81	123.85
31	R	610	CLA	C1C-C2C-C3C	-2.59	104.26	106.98
31	y	614	CLA	C4B-CHC-C1C	2.59	132.33	126.25
48	y1	621	LUT	C11-C10-C9	-2.59	123.65	127.28
31	R	608	CLA	CMA-C3A-C4A	2.59	118.72	111.77
31	s	610	CLA	CMD-C2D-C3D	-2.59	121.76	127.69
49	r	622	XAT	O4-C5-C4	-2.59	111.07	113.49
31	R1	612	CLA	O2D-CGD-O1D	-2.59	118.82	123.85
31	B1	604	CLA	O2A-CGA-CBA	2.59	119.72	111.83
50	S1	623	NEX	C39-C29-C30	-2.59	118.63	122.82
31	C	501	CLA	O2A-CGA-CBA	2.58	119.72	111.83
31	R	613	CLA	CMA-C3A-C4A	2.58	118.72	111.77
31	B	616	CLA	C1C-C2C-C3C	-2.58	104.26	106.98
31	c	511	CLA	O2A-CGA-CBA	2.58	119.71	111.83
31	G	613	CLA	C2C-C1C-NC	2.58	112.70	109.98
33	c1	516	BCR	C23-C24-C25	-2.58	120.10	127.00
31	b	611	CLA	C1C-C2C-C3C	-2.58	104.26	106.98
31	y1	602	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
31	r	610	CLA	O2A-CGA-CBA	2.58	119.71	111.83
31	y	614	CLA	O2D-CGD-O1D	-2.58	118.82	123.85
31	C	508	CLA	CMA-C3A-C4A	2.58	118.71	111.77
31	y1	608	CLA	CHA-C4D-ND	2.58	137.88	132.55
37	B1	620	C7Z	C1-C6-C7	2.58	122.65	115.65
31	G1	610	CLA	O1D-CGD-CBD	-2.58	119.42	124.52
31	N1	611	CLA	C3B-C4B-NB	-2.58	108.22	110.53
31	n1	614	CLA	C3B-C4B-NB	-2.58	108.22	110.53
31	R1	608	CLA	C1-C2-C3	-2.58	121.97	126.20
31	D	403	CLA	O2A-CGA-CBA	2.58	119.71	111.83
50	g	623	NEX	C39-C29-C30	-2.58	118.63	122.82
31	A1	405	CLA	CMD-C2D-C3D	-2.58	121.77	127.69
31	S	611	CLA	CHA-C4D-ND	2.58	137.87	132.55
47	g1	608	CHL	CMA-C3A-C4A	2.58	120.17	114.61
31	C	511	CLA	CHD-C1D-ND	-2.58	121.17	124.80
31	g	604	CLA	CMA-C3A-C4A	2.58	118.71	111.77
31	G	610	CLA	C3B-C4B-NB	-2.58	108.23	110.53
31	b1	615	CLA	CHA-C4D-ND	2.58	137.87	132.55
31	d1	402	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
31	y1	604	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
31	B	605	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
31	B	613	CLA	CMA-C3A-C4A	2.58	118.70	111.77
31	B	615	CLA	CMD-C2D-C3D	-2.58	121.78	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	n1	602	CLA	O2A-CGA-CBA	2.58	119.70	111.83
47	Y	601	CHL	C4D-CHA-CBD	-2.58	106.37	108.97
31	G1	604	CLA	C3B-C4B-NB	-2.58	108.23	110.53
31	S1	609	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
31	c1	510	CLA	CHA-C4D-ND	2.58	137.87	132.55
31	c	507	CLA	O2D-CGD-O1D	-2.58	118.83	123.85
31	n1	612	CLA	C1C-C2C-C3C	-2.58	104.27	106.98
31	r	603	CLA	CHA-C4D-ND	2.58	137.86	132.55
31	B1	610	CLA	C2C-C1C-NC	2.57	112.69	109.98
50	y	623	NEX	C4-C3-C2	2.57	115.61	110.79
33	c1	514	BCR	C33-C5-C6	-2.57	121.67	124.48
31	S	604	CLA	O2A-CGA-CBA	2.57	119.68	111.83
31	b	602	CLA	C3B-C4B-NB	-2.57	108.23	110.53
31	r1	609	CLA	CAA-C2A-C3A	-2.57	106.04	113.00
31	s	604	CLA	CHD-C1D-ND	-2.57	121.18	124.80
31	N	611	CLA	O1D-CGD-CBD	-2.57	119.44	124.52
31	y	610	CLA	C1C-C2C-C3C	-2.57	104.27	106.98
55	R1	625	LMT	C3'-C4'-C5'	-2.57	105.22	110.93
47	y1	606	CHL	CMA-C3A-C4A	2.57	120.16	114.61
31	n	612	CLA	CHA-C1A-NA	-2.57	120.56	126.39
56	R1	626	ERG	C19-C10-C1	-2.57	105.52	109.43
31	y1	612	CLA	O2A-CGA-CBA	2.57	119.68	111.83
31	Y	604	CLA	C2C-C1C-NC	2.57	112.68	109.98
31	G	613	CLA	CMC-C2C-C1C	2.57	129.05	125.03
47	Y	601	CHL	C1A-CHA-C4D	2.57	123.27	118.98
31	y	612	CLA	O2D-CGD-O1D	-2.57	118.84	123.85
31	B	606	CLA	CMD-C2D-C3D	-2.57	121.79	127.69
31	b1	617	CLA	CHA-C4D-ND	2.57	137.86	132.55
33	C1	516	BCR	C15-C14-C13	-2.57	123.67	127.28
31	G1	610	CLA	CHD-C1D-ND	-2.57	121.18	124.80
31	s1	611	CLA	C1C-C2C-C3C	-2.57	104.28	106.98
31	r1	603	CLA	C4B-CHC-C1C	2.57	132.29	126.25
31	C1	505	CLA	O2A-CGA-CBA	2.57	119.67	111.83
31	r1	612	CLA	C1C-C2C-C3C	-2.57	104.28	106.98
47	y	609	CHL	C1-O2A-CGA	2.57	122.87	116.65
41	S1	624	LHG	O8-C23-C24	2.57	119.67	111.83
47	r	607	CHL	C1A-CHA-C4D	2.57	123.27	118.98
31	D1	403	CLA	C6-C5-C3	-2.57	107.21	113.47
33	C1	516	BCR	C36-C18-C17	-2.57	118.65	122.82
31	S1	603	CLA	CHA-C4D-ND	2.57	137.85	132.55
31	C1	505	CLA	CMD-C2D-C3D	-2.57	121.80	127.69
31	N1	612	CLA	CMA-C3A-C4A	2.57	118.68	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	Y1	613	CLA	CHD-C1D-ND	-2.57	121.19	124.80
31	G	602	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
31	C1	502	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
31	N	614	CLA	C3B-C4B-NB	-2.57	108.24	110.53
31	C	511	CLA	C1-C2-C3	-2.57	121.99	126.20
31	A	410	CLA	O2A-CGA-CBA	2.57	119.67	111.83
31	B1	615	CLA	CHA-C4D-ND	2.57	137.85	132.55
31	y1	612	CLA	CHA-C4D-ND	2.57	137.85	132.55
31	y	613	CLA	O2D-CGD-O1D	-2.57	118.85	123.85
31	R	613	CLA	C3B-C4B-NB	-2.57	108.24	110.53
31	g1	610	CLA	C1C-C2C-C3C	-2.57	104.28	106.98
47	y1	606	CHL	C4D-CHA-CBD	-2.57	106.38	108.97
31	S	605	CLA	C4B-CHC-C1C	2.57	132.28	126.25
31	C1	508	CLA	C4B-CHC-C1C	2.57	132.28	126.25
31	B	609	CLA	CMD-C2D-C3D	-2.57	121.80	127.69
31	c	506	CLA	C4B-CHC-C1C	2.57	132.28	126.25
31	b1	604	CLA	O2A-CGA-CBA	2.57	119.66	111.83
31	y1	603	CLA	CAA-C2A-C3A	-2.57	106.07	113.00
33	D	404	BCR	C38-C26-C27	2.57	119.07	113.60
48	N1	621	LUT	C22-C23-C24	-2.57	107.37	111.18
47	s	607	CHL	CMA-C3A-C4A	2.57	120.14	114.61
31	c1	513	CLA	CMA-C3A-C4A	2.57	118.67	111.77
31	n1	612	CLA	CMA-C3A-C4A	2.57	118.67	111.77
31	b1	606	CLA	CHA-C4D-ND	2.56	137.84	132.55
31	C1	506	CLA	C1C-C2C-C3C	-2.56	104.28	106.98
31	g1	604	CLA	O2D-CGD-O1D	-2.56	118.86	123.85
31	n	602	CLA	O2A-CGA-CBA	2.56	119.65	111.83
31	c	512	CLA	O2A-CGA-CBA	2.56	119.65	111.83
31	B	604	CLA	C1C-C2C-C3C	-2.56	104.28	106.98
31	a1	410	CLA	C1C-C2C-C3C	-2.56	104.28	106.98
41	Y1	624	LHG	O8-C23-C24	2.56	119.65	111.83
31	B	606	CLA	CHD-C1D-ND	-2.56	121.20	124.80
31	c1	509	CLA	C1-C2-C3	-2.56	122.00	126.20
50	y	623	NEX	C11-C10-C9	2.56	130.87	127.28
47	s	608	CHL	CMA-C3A-C4A	2.56	120.13	114.61
31	Y1	610	CLA	CAA-C2A-C3A	-2.56	106.08	113.00
31	B	615	CLA	C2C-C1C-NC	2.56	112.67	109.98
31	R	609	CLA	CHA-C4D-ND	2.56	137.83	132.55
48	g1	621	LUT	C22-C23-C24	-2.56	107.38	111.18
48	g1	620	LUT	C27-C28-C29	-2.56	120.82	126.32
31	r1	612	CLA	C3B-C4B-NB	-2.56	108.25	110.53
46	H1	101	RRX	C19-C18-C17	-2.56	114.98	119.01

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	r	604	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
47	n1	605	CHL	C1-C2-C3	-2.56	122.00	126.20
46	h	101	RRX	C24-C23-C22	-2.56	122.45	126.23
31	N	604	CLA	C1C-C2C-C3C	-2.56	104.29	106.98
31	C1	502	CLA	C3B-C4B-NB	-2.56	108.25	110.53
31	s	604	CLA	CMD-C2D-C3D	-2.56	121.82	127.69
31	g	602	CLA	C2C-C1C-NC	2.56	112.67	109.98
31	g	610	CLA	O2A-CGA-CBA	2.56	119.64	111.83
38	B1	625	DGA	OG1-CA1-CA2	2.56	119.64	111.83
50	g	623	NEX	C4-C3-C2	2.56	115.57	110.79
31	b1	604	CLA	CMC-C2C-C1C	2.56	129.03	125.03
48	y	620	LUT	C39-C29-C28	2.56	122.00	118.09
31	n	602	CLA	CMA-C3A-C4A	2.56	118.65	111.77
40	C1	518	DGD	O1G-C1A-C2A	2.56	119.63	111.83
31	c	506	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
31	Y	613	CLA	C2C-C1C-NC	2.56	112.67	109.98
31	B1	611	CLA	O2D-CGD-O1D	-2.56	118.87	123.85
31	a	407	CLA	CAA-C2A-C3A	-2.56	106.09	113.00
31	C1	501	CLA	CAA-C2A-C3A	-2.56	106.09	113.00
31	C1	510	CLA	CHA-C4D-ND	2.56	137.82	132.55
31	N1	613	CLA	CHA-C4D-ND	2.56	137.82	132.55
47	G	606	CHL	C1-O2A-CGA	2.56	122.84	116.65
31	G	603	CLA	C4B-CHC-C1C	2.56	132.26	126.25
37	B	620	C7Z	C21-C26-C25	-2.56	119.14	122.64
50	s	623	NEX	C1-C2-C3	2.56	119.20	113.59
47	S	601	CHL	CMA-C3A-C4A	2.55	120.12	114.61
31	y	614	CLA	O2A-CGA-CBA	2.55	119.62	111.83
31	g	604	CLA	OBD-CAD-C3D	-2.55	122.44	128.42
31	Y1	612	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
31	b1	615	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
31	y	612	CLA	CHA-C4D-ND	2.55	137.82	132.55
31	B	611	CLA	C2D-C1D-ND	2.55	112.65	110.13
31	n	613	CLA	CMC-C2C-C1C	2.55	129.03	125.03
31	S	617	CLA	O2A-CGA-CBA	2.55	119.62	111.83
31	s	609	CLA	C1C-C2C-C3C	-2.55	104.29	106.98
31	b1	616	CLA	C4B-CHC-C1C	2.55	132.25	126.25
31	S1	614	CLA	O2A-CGA-CBA	2.55	119.62	111.83
31	S1	603	CLA	O1D-CGD-CBD	-2.55	119.48	124.52
31	c1	505	CLA	O2D-CGD-O1D	-2.55	118.88	123.85
45	f1	101	HEM	C4D-ND-C1D	2.55	108.23	105.21
31	r1	612	CLA	CHA-C4D-ND	2.55	137.81	132.55
48	R1	620	LUT	C35-C15-C14	-2.55	118.30	123.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	S1	603	CLA	C3B-C4B-NB	-2.55	108.25	110.53
31	C	505	CLA	C2C-C1C-NC	2.55	112.66	109.98
47	N1	601	CHL	C1-O2A-CGA	2.55	122.83	116.65
31	G	614	CLA	C4B-CHC-C1C	2.55	132.25	126.25
50	R1	622	NEX	C38-C25-C26	-2.55	118.10	122.30
33	b1	618	BCR	C23-C24-C25	-2.55	120.18	127.00
31	c1	512	CLA	C1C-C2C-C3C	-2.55	104.30	106.98
31	A	410	CLA	CHA-C4D-ND	2.55	137.81	132.55
31	Y	611	CLA	C3B-C4B-NB	-2.55	108.25	110.53
33	c	515	BCR	C29-C30-C25	-2.55	106.73	110.44
44	d	405	PL9	C22-C23-C24	-2.55	121.79	127.62
31	c	510	CLA	O2A-CGA-CBA	2.55	119.61	111.83
44	D1	405	PL9	C8-C7-C3	2.55	118.62	112.03
31	n	604	CLA	CHA-C4D-ND	2.55	137.81	132.55
47	N	607	CHL	C1-O2A-CGA	2.55	122.82	116.65
31	G	603	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
31	d1	403	CLA	CMA-C3A-C2A	2.55	123.84	113.98
31	s	617	CLA	CHD-C1D-ND	-2.55	121.22	124.80
31	c1	512	CLA	C1-O2A-CGA	2.55	122.82	116.65
31	A1	405	CLA	CHD-C1D-ND	-2.55	121.22	124.80
31	s	614	CLA	CHA-C4D-ND	2.55	137.81	132.55
31	y1	602	CLA	C3B-C4B-NB	-2.55	108.25	110.53
50	y	623	NEX	C28-C29-C30	2.55	123.02	119.01
31	R	603	CLA	C3B-C4B-NB	-2.55	108.26	110.53
31	g	610	CLA	CHD-C1D-ND	-2.55	121.22	124.80
49	Y1	622	XAT	C6-C7-C8	-2.55	120.61	125.99
31	c	513	CLA	CMA-C3A-C4A	2.55	118.62	111.77
31	c	511	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
31	c	501	CLA	CHA-C4D-ND	2.55	137.80	132.55
31	g	604	CLA	CHA-C4D-ND	2.55	137.80	132.55
31	C1	506	CLA	C3B-C4B-NB	-2.55	108.26	110.53
31	n	614	CLA	C2C-C1C-NC	2.55	112.66	109.98
31	s1	614	CLA	C1-C2-C3	-2.55	122.03	126.20
31	R	612	CLA	CMD-C2D-C3D	-2.55	121.85	127.69
31	C1	505	CLA	O2D-CGD-O1D	-2.55	118.89	123.85
31	s	605	CLA	CHA-C4D-ND	2.55	137.80	132.55
47	R1	607	CHL	CMA-C3A-C4A	2.55	120.09	114.61
31	g1	602	CLA	C3B-C4B-NB	-2.55	108.26	110.53
31	C	507	CLA	CHA-C4D-ND	2.55	137.80	132.55
31	d	402	CLA	CMC-C2C-C1C	2.54	129.01	125.03
31	A	405	CLA	CHA-C4D-ND	2.54	137.80	132.55
48	s1	620	LUT	C39-C29-C28	2.54	121.97	118.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	602	CLA	C4B-CHC-C1C	2.54	132.23	126.25
31	N	602	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
31	c	507	CLA	CHA-C4D-ND	2.54	137.80	132.55
31	r	611	CLA	CHA-C4D-ND	2.54	137.80	132.55
31	G1	604	CLA	CHA-C4D-ND	2.54	137.80	132.55
31	B	604	CLA	CMD-C2D-C3D	-2.54	121.86	127.69
31	Y1	603	CLA	C3B-C4B-NB	-2.54	108.26	110.53
31	N1	604	CLA	O2A-CGA-CBA	2.54	119.59	111.83
31	R1	604	CLA	O2D-CGD-O1D	-2.54	118.90	123.85
31	Y	613	CLA	C1C-C2C-C3C	-2.54	104.31	106.98
31	G1	604	CLA	C1C-C2C-C3C	-2.54	104.31	106.98
31	c	511	CLA	C4B-CHC-C1C	2.54	132.22	126.25
31	B	602	CLA	CHA-C4D-ND	2.54	137.79	132.55
31	C1	505	CLA	C1-O2A-CGA	2.54	122.80	116.65
31	G1	611	CLA	CHA-C4D-ND	2.54	137.79	132.55
31	G	613	CLA	O1D-CGD-CBD	-2.54	119.51	124.52
47	r	606	CHL	CMA-C3A-C4A	2.54	120.08	114.61
31	b1	606	CLA	C1-O2A-CGA	2.54	122.80	116.65
31	s1	614	CLA	O2A-CGA-CBA	2.54	119.58	111.83
31	g	603	CLA	C1D-ND-C4D	-2.54	104.53	106.31
31	b1	612	CLA	C1D-ND-C4D	-2.54	104.53	106.31
31	R	604	CLA	CHA-C4D-ND	2.54	137.79	132.55
31	s1	614	CLA	CHA-C4D-ND	2.54	137.79	132.55
31	g1	612	CLA	C3B-C4B-NB	-2.54	108.26	110.53
41	l	101	LHG	O8-C23-C24	2.54	119.58	111.83
31	c	510	CLA	C2C-C1C-NC	2.54	112.65	109.98
31	Y	612	CLA	C4B-CHC-C1C	2.54	132.22	126.25
31	r1	610	CLA	C4B-CHC-C1C	2.54	132.22	126.25
50	R	622	NEX	C16-C1-C6	-2.54	108.20	110.47
48	R	620	LUT	C18-C5-C6	-2.54	121.71	124.48
31	R1	603	CLA	CHA-C4D-ND	2.54	137.79	132.55
31	C	506	CLA	CMA-C3A-C4A	2.54	118.59	111.77
31	n	604	CLA	C4B-CHC-C1C	2.54	132.22	126.25
31	Y1	614	CLA	C4B-CHC-C1C	2.54	132.22	126.25
31	n	610	CLA	CHD-C1D-ND	-2.54	121.23	124.80
31	n	602	CLA	C1C-C2C-C3C	-2.54	104.31	106.98
47	y1	607	CHL	C4C-CHD-C1D	2.54	125.15	116.07
47	g1	605	CHL	CMA-C3A-C4A	2.54	120.08	114.61
31	c1	508	CLA	C2D-C1D-ND	2.54	112.64	110.13
31	A	405	CLA	CMD-C2D-C3D	-2.54	121.87	127.69
31	C	511	CLA	CHA-C4D-ND	2.54	137.78	132.55
31	n	602	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	r	604	CLA	O2D-CGD-O1D	-2.54	118.91	123.85
31	r	612	CLA	CHA-C4D-ND	2.54	137.78	132.55
31	c	512	CLA	C1-C2-C3	-2.54	122.04	126.20
31	B	608	CLA	C1C-C2C-C3C	-2.54	104.31	106.98
31	n	614	CLA	C1C-C2C-C3C	-2.54	104.31	106.98
31	R	609	CLA	C2C-C1C-NC	2.54	112.64	109.98
31	y	614	CLA	C3B-C4B-NB	-2.54	108.27	110.53
31	a1	405	CLA	CHA-C4D-ND	2.53	137.78	132.55
31	a	406	CLA	CMD-C2D-C3D	-2.53	121.88	127.69
31	S	609	CLA	C4B-CHC-C1C	2.53	132.21	126.25
31	n1	604	CLA	CHA-C4D-ND	2.53	137.78	132.55
33	c1	514	BCR	C40-C30-C25	-2.53	106.27	110.24
31	b1	604	CLA	C1D-ND-C4D	-2.53	104.53	106.31
31	c1	513	CLA	CHA-C4D-ND	2.53	137.78	132.55
31	C	505	CLA	C1C-C2C-C3C	-2.53	104.32	106.98
31	N1	612	CLA	C3B-C4B-NB	-2.53	108.27	110.53
31	b	607	CLA	O2A-CGA-CBA	2.53	119.56	111.83
35	c	521	LMG	O8-C28-C29	2.53	119.56	111.83
47	R1	607	CHL	C1C-C2C-CMC	2.53	131.37	126.80
31	B1	605	CLA	C2D-C1D-ND	2.53	112.63	110.13
47	s	608	CHL	C1-C2-C3	-2.53	122.05	126.20
41	y	624	LHG	O8-C23-C24	2.53	119.55	111.83
31	Y1	613	CLA	CHA-C4D-ND	2.53	137.77	132.55
31	D1	402	CLA	O2A-CGA-CBA	2.53	119.55	111.83
31	y1	612	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
31	A1	405	CLA	CMC-C2C-C3C	2.53	132.99	126.15
32	A	408	PHO	C3B-C4B-NB	-2.53	105.81	107.46
31	b1	610	CLA	C1-C2-C3	-2.53	122.05	126.20
31	d1	403	CLA	C4B-CHC-C1C	2.53	132.20	126.25
31	c	510	CLA	C1D-ND-C4D	-2.53	104.54	106.31
31	s1	617	CLA	C1D-ND-C4D	-2.53	104.54	106.31
31	y	608	CLA	CHA-C4D-ND	2.53	137.77	132.55
31	Y	604	CLA	C3B-C4B-NB	-2.53	108.27	110.53
31	B	607	CLA	O2D-CGD-O1D	-2.53	118.92	123.85
31	S	603	CLA	CHA-C4D-ND	2.53	137.77	132.55
31	Y1	614	CLA	CHA-C4D-ND	2.53	137.77	132.55
33	D1	404	BCR	C34-C9-C10	-2.53	118.72	122.82
50	n	623	NEX	C17-C1-C6	-2.53	108.21	110.47
31	c1	506	CLA	CHA-C4D-ND	2.53	137.77	132.55
32	a1	408	PHO	O2D-CGD-O1D	-2.53	118.93	123.85
31	b	604	CLA	CHA-C4D-ND	2.53	137.76	132.55
49	G	622	XAT	C18-C5-C6	-2.53	118.14	122.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C1	503	CLA	C1C-C2C-C3C	-2.53	104.32	106.98
31	s1	611	CLA	CHA-C4D-ND	2.53	137.76	132.55
33	c	516	BCR	C23-C22-C21	-2.53	115.03	119.01
31	b	608	CLA	CHA-C4D-ND	2.53	137.76	132.55
32	a	408	PHO	C1-C2-C3	-2.53	122.06	126.20
31	Y1	611	CLA	C1C-C2C-C3C	-2.53	104.32	106.98
31	G1	611	CLA	O2D-CGD-O1D	-2.53	118.93	123.85
31	N	603	CLA	CAA-C2A-C3A	-2.53	106.17	113.00
31	r	611	CLA	CAA-C2A-C3A	-2.53	106.17	113.00
31	b	612	CLA	C2D-C1D-ND	2.53	112.63	110.13
31	g1	614	CLA	CHA-C4D-ND	2.53	137.76	132.55
31	b	613	CLA	CMD-C2D-C3D	-2.53	121.90	127.69
31	C	505	CLA	CHA-C4D-ND	2.52	137.76	132.55
31	B	608	CLA	C1-C2-C3	-2.52	122.06	126.20
33	B	618	BCR	C37-C22-C23	2.52	121.94	118.09
31	C	501	CLA	C1D-ND-C4D	-2.52	104.54	106.31
31	a	405	CLA	C1D-ND-C4D	-2.52	104.54	106.31
31	s	610	CLA	C2C-C1C-NC	2.52	112.63	109.98
31	d	403	CLA	C4B-CHC-C1C	2.52	132.18	126.25
31	s	603	CLA	CMA-C3A-C4A	2.52	118.56	111.77
31	g	613	CLA	CHA-C4D-ND	2.52	137.75	132.55
31	N1	611	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
31	y	614	CLA	CHA-C4D-ND	2.52	137.75	132.55
31	A	407	CLA	CAA-C2A-C3A	-2.52	106.18	113.00
31	G1	612	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
31	B	613	CLA	O2A-CGA-CBA	2.52	119.53	111.83
31	g1	604	CLA	C1C-C2C-C3C	-2.52	104.33	106.98
31	R	608	CLA	CHA-C4D-ND	2.52	137.75	132.55
31	n	611	CLA	CHA-C4D-ND	2.52	137.75	132.55
41	D1	410	LHG	C5-O7-C7	-2.52	111.76	117.80
31	b1	605	CLA	C1-C2-C3	-2.52	122.07	126.20
31	b	614	CLA	CHA-C4D-ND	2.52	137.75	132.55
31	B1	607	CLA	CMD-C2D-C3D	-2.52	121.91	127.69
31	R	610	CLA	O1D-CGD-CBD	-2.52	119.55	124.52
31	C1	510	CLA	CHD-C1D-ND	-2.52	121.25	124.80
49	r	622	XAT	O24-C26-C27	-2.52	109.66	116.88
31	n	610	CLA	C4B-CHC-C1C	2.52	132.17	126.25
31	R1	602	CLA	O2A-CGA-CBA	2.52	119.52	111.83
44	d1	405	PL9	C7-C8-C9	-2.52	122.49	126.83
31	r1	608	CLA	CHA-C4D-ND	2.52	137.75	132.55
41	Y	624	LHG	O8-C23-C24	2.52	119.52	111.83
31	b	616	CLA	O2D-CGD-O1D	-2.52	118.94	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	S1	611	CLA	O2D-CGD-O1D	-2.52	118.94	123.85
31	R1	612	CLA	C3B-C4B-NB	-2.52	108.28	110.53
47	r	607	CHL	C4C-CHD-C1D	2.52	125.08	116.07
31	b1	613	CLA	CHA-C4D-ND	2.52	137.75	132.55
31	B	607	CLA	C1C-C2C-C3C	-2.52	104.33	106.98
31	C	510	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
31	C1	507	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
33	C1	514	BCR	C23-C24-C25	-2.52	120.27	127.00
31	S	611	CLA	C3B-C4B-NB	-2.52	108.28	110.53
47	r1	606	CHL	C4C-CHD-C1D	2.52	125.08	116.07
31	g	614	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
31	Y	614	CLA	CHA-C4D-ND	2.52	137.74	132.55
48	N	621	LUT	C35-C15-C14	-2.52	118.37	123.52
31	Y	612	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
31	g	603	CLA	O2D-CGD-O1D	-2.52	118.95	123.85
31	c	508	CLA	C4B-CHC-C1C	2.52	132.17	126.25
31	r	610	CLA	CHA-C4D-ND	2.52	137.74	132.55
31	a	405	CLA	C2C-C1C-NC	2.52	112.62	109.98
31	A1	407	CLA	C2C-C1C-NC	2.52	112.62	109.98
31	a	406	CLA	CHA-C4D-ND	2.52	137.74	132.55
31	A	410	CLA	C3B-C4B-NB	-2.52	108.28	110.53
31	s	612	CLA	C1C-C2C-C3C	-2.52	104.33	106.98
31	C1	513	CLA	CBA-CAA-C2A	2.52	121.28	113.79
31	S1	610	CLA	O2A-CGA-CBA	2.52	119.50	111.83
31	c1	511	CLA	O2A-CGA-CBA	2.52	119.50	111.83
31	a1	410	CLA	CHA-C4D-ND	2.52	137.74	132.55
33	A	411	BCR	C35-C13-C12	2.52	121.93	118.09
48	y1	621	LUT	C35-C15-C14	-2.51	118.37	123.52
31	Y	608	CLA	C1C-C2C-C3C	-2.51	104.33	106.98
31	G	604	CLA	CHA-C4D-ND	2.51	137.74	132.55
31	r1	603	CLA	CHA-C4D-ND	2.51	137.74	132.55
31	b1	604	CLA	C2C-C1C-NC	2.51	112.62	109.98
46	h	101	RRX	C23-C24-C25	-2.51	120.28	127.00
47	g1	607	CHL	CMA-C3A-C4A	2.51	120.03	114.61
31	r	612	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
31	n1	603	CLA	CHA-C4D-ND	2.51	137.74	132.55
31	c	509	CLA	CMD-C2D-C3D	-2.51	121.92	127.69
40	b1	623	DGD	O5D-C1E-C2E	2.51	112.09	108.27
31	C	509	CLA	O2A-CGA-CBA	2.51	119.50	111.83
31	r1	612	CLA	CHA-C1A-NA	-2.51	120.70	126.39
31	C1	501	CLA	CHA-C4D-ND	2.51	137.73	132.55
44	d	405	PL9	C40-C39-C41	2.51	119.59	115.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
35	b	622	LMG	O8-C28-C29	2.51	119.50	111.83
31	s1	603	CLA	O1D-CGD-CBD	-2.51	119.56	124.52
57	y1	627	PTY	C6-O7-C8	-2.51	113.41	117.85
31	S	611	CLA	C1-C2-C3	-2.51	122.08	126.20
31	s1	611	CLA	O2A-CGA-CBA	2.51	119.49	111.83
31	G1	610	CLA	C4B-CHC-C1C	2.51	132.15	126.25
31	S1	602	CLA	C3B-C4B-NB	-2.51	108.29	110.53
48	n	620	LUT	C35-C15-C14	-2.51	118.38	123.52
31	B	616	CLA	CHA-C4D-ND	2.51	137.73	132.55
31	B1	604	CLA	CHA-C4D-ND	2.51	137.73	132.55
41	g1	624	LHG	O8-C23-C24	2.51	119.49	111.83
31	S1	609	CLA	O2D-CGD-O1D	-2.51	118.96	123.85
31	b	612	CLA	CAA-C2A-C3A	-2.51	106.22	113.00
31	n1	610	CLA	C4B-CHC-C1C	2.51	132.15	126.25
47	Y1	601	CHL	C4C-CHD-C1D	2.51	125.05	116.07
31	b	602	CLA	CHA-C4D-ND	2.51	137.73	132.55
48	N	620	LUT	C31-C32-C33	-2.51	119.48	126.36
31	a1	406	CLA	CHD-C1D-ND	-2.51	121.27	124.80
31	r	608	CLA	C3B-C4B-NB	-2.51	108.29	110.53
31	b	606	CLA	CHA-C4D-ND	2.51	137.73	132.55
31	R1	612	CLA	CHA-C4D-ND	2.51	137.73	132.55
33	c1	517	BCR	C36-C18-C17	-2.51	118.75	122.82
37	B	620	C7Z	C28-C27-C26	-2.51	120.30	127.00
31	Y1	602	CLA	C2C-C1C-NC	2.51	112.62	109.98
31	b	615	CLA	CMD-C2D-C3D	-2.51	121.94	127.69
31	C	506	CLA	C1C-C2C-C3C	-2.51	104.34	106.98
31	n	613	CLA	C3B-C4B-NB	-2.51	108.29	110.53
31	S1	609	CLA	C3B-C4B-NB	-2.51	108.29	110.53
31	b	613	CLA	C2C-C1C-NC	2.51	112.62	109.98
31	B	614	CLA	CHA-C4D-ND	2.51	137.72	132.55
31	S1	605	CLA	CHA-C4D-ND	2.51	137.72	132.55
47	g	601	CHL	CMA-C3A-C4A	2.51	120.01	114.61
31	C	501	CLA	C2C-C1C-NC	2.51	112.61	109.98
31	N	604	CLA	CHA-C4D-ND	2.51	137.72	132.55
31	B1	605	CLA	CMA-C3A-C4A	2.51	118.51	111.77
31	G	610	CLA	CHD-C1D-ND	-2.51	121.28	124.80
33	C	515	BCR	C35-C13-C12	2.51	121.92	118.09
31	B	602	CLA	O2D-CGD-O1D	-2.51	118.97	123.85
31	b1	604	CLA	CHD-C1D-ND	-2.51	121.28	124.80
31	Y1	611	CLA	CHA-C4D-ND	2.51	137.72	132.55
31	C1	504	CLA	CMD-C2D-C3D	-2.51	121.94	127.69
31	c	503	CLA	C3B-C4B-NB	-2.50	108.29	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	Y1	612	CLA	C3B-C4B-NB	-2.50	108.29	110.53
31	s1	602	CLA	C3B-C4B-NB	-2.50	108.29	110.53
48	s	620	LUT	C11-C12-C13	-2.50	119.50	126.36
31	s1	613	CLA	CHA-C4D-ND	2.50	137.72	132.55
31	r	602	CLA	C1C-C2C-C3C	-2.50	104.35	106.98
47	Y	609	CHL	C4D-CHA-CBD	-2.50	106.44	108.97
50	N	623	NEX	C39-C29-C30	-2.50	118.76	122.82
31	S	609	CLA	CHA-C4D-ND	2.50	137.72	132.55
31	y1	614	CLA	CHA-C4D-ND	2.50	137.72	132.55
31	s	604	CLA	CMA-C3A-C4A	2.50	118.50	111.77
48	r1	620	LUT	C8-C7-C6	-2.50	120.31	127.00
31	g	614	CLA	O2A-CGA-CBA	2.50	119.47	111.83
49	R1	621	XAT	C26-C27-C28	-2.50	120.70	125.99
31	n1	603	CLA	C3B-C4B-NB	-2.50	108.30	110.53
31	Y1	602	CLA	CMD-C2D-C3D	-2.50	121.95	127.69
31	r1	602	CLA	C6-C5-C3	-2.50	107.37	113.47
48	n	620	LUT	C3-C4-C5	-2.50	105.95	112.18
31	g	613	CLA	C1-O2A-CGA	2.50	122.71	116.65
50	Y1	623	NEX	C39-C29-C30	-2.50	118.76	122.82
31	B	606	CLA	C2C-C1C-NC	2.50	112.61	109.98
31	N1	610	CLA	CHA-C4D-ND	2.50	137.71	132.55
31	C	507	CLA	CHA-C1A-NA	-2.50	120.73	126.39
31	b	602	CLA	CMD-C2D-C3D	-2.50	121.95	127.69
31	N1	612	CLA	CHA-C4D-ND	2.50	137.71	132.55
31	Y1	608	CLA	C3B-C4B-NB	-2.50	108.30	110.53
31	c	501	CLA	C1D-ND-C4D	-2.50	104.56	106.31
31	N1	603	CLA	CMD-C2D-C3D	-2.50	121.95	127.69
48	Y1	620	LUT	C38-C25-C24	-2.50	117.44	123.36
31	y	604	CLA	CHA-C4D-ND	2.50	137.71	132.55
31	c	504	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
31	b1	605	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
31	r1	602	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
31	S1	609	CLA	CHD-C1D-ND	-2.50	121.28	124.80
31	y1	608	CLA	CHD-C1D-ND	-2.50	121.28	124.80
31	C1	506	CLA	C2D-C1D-ND	2.50	112.60	110.13
33	C1	517	BCR	C3-C4-C5	-2.50	109.60	114.06
47	s1	608	CHL	CMA-C3A-C4A	2.50	120.00	114.61
31	C1	509	CLA	CHD-C1D-ND	-2.50	121.28	124.80
31	b1	606	CLA	CMD-C2D-C3D	-2.50	121.96	127.69
31	g1	612	CLA	CHA-C4D-ND	2.50	137.71	132.55
31	r	611	CLA	CMD-C2D-C3D	-2.50	121.96	127.69
31	s1	602	CLA	CHD-C1D-ND	-2.50	121.28	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	b	618	BCR	C33-C5-C4	2.50	118.92	113.60
47	G1	605	CHL	C4D-CHA-CBD	-2.50	106.45	108.97
47	Y1	601	CHL	C1A-CHA-C4D	2.50	123.15	118.98
31	R1	604	CLA	CHA-C4D-ND	2.50	137.71	132.55
31	y	602	CLA	C4B-CHC-C1C	2.50	132.12	126.25
31	c	506	CLA	C1C-C2C-C3C	-2.50	104.35	106.98
31	c1	507	CLA	O2D-CGD-O1D	-2.50	118.98	123.85
33	B	619	BCR	C30-C25-C26	-2.50	119.22	122.64
31	N	613	CLA	CHA-C4D-ND	2.50	137.70	132.55
31	Y1	603	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
49	R	621	XAT	C11-C10-C9	-2.50	123.78	127.28
31	d1	402	CLA	CMA-C3A-C4A	2.50	118.49	111.77
31	b1	608	CLA	O2A-CGA-CBA	2.50	119.45	111.83
31	a	405	CLA	CMA-C3A-C4A	2.50	118.48	111.77
31	N1	603	CLA	C3B-C4B-NB	-2.50	108.30	110.53
49	G1	622	XAT	C19-C9-C10	-2.50	118.77	122.82
31	N1	611	CLA	CHA-C4D-ND	2.50	137.70	132.55
31	r	612	CLA	C1-C2-C3	-2.50	122.11	126.20
31	b1	607	CLA	O2D-CGD-O1D	-2.50	118.99	123.85
40	c1	519	DGD	O1G-C1A-O1A	-2.50	117.39	123.63
31	B1	611	CLA	C1D-ND-C4D	-2.50	104.56	106.31
31	R1	604	CLA	CMD-C2D-C3D	-2.50	121.97	127.69
31	r	608	CLA	C4B-CHC-C1C	2.50	132.12	126.25
47	R1	606	CHL	C4C-CHD-C1D	2.50	125.00	116.07
31	b1	602	CLA	CHA-C4D-ND	2.50	137.70	132.55
47	S	606	CHL	CMA-C3A-C4A	2.50	119.99	114.61
48	S	620	LUT	C11-C10-C9	-2.49	123.78	127.28
32	A1	409	PHO	C1-C2-C3	-2.49	122.11	126.20
31	b1	614	CLA	CHA-C4D-ND	2.49	137.69	132.55
31	c	502	CLA	C1D-ND-C4D	-2.49	104.56	106.31
31	n	613	CLA	C1D-ND-C4D	-2.49	104.56	106.31
47	y	605	CHL	CMA-C3A-C4A	2.49	119.98	114.61
31	R	603	CLA	C1C-C2C-C3C	-2.49	104.36	106.98
31	N	612	CLA	CHA-C4D-ND	2.49	137.69	132.55
33	C	514	BCR	C33-C5-C6	-2.49	121.76	124.48
37	B1	620	C7Z	C21-C26-C27	2.49	122.41	115.65
31	Y	604	CLA	CHA-C4D-ND	2.49	137.69	132.55
31	C1	509	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
48	n1	620	LUT	C10-C11-C12	-2.49	115.98	123.20
31	R1	608	CLA	CMD-C2D-C3D	-2.49	121.97	127.69
47	R	606	CHL	C4C-CHD-C1D	2.49	124.99	116.07
31	R1	610	CLA	C1D-ND-C4D	-2.49	104.56	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s	614	CLA	CMD-C2D-C3D	-2.49	121.97	127.69
31	n	602	CLA	O1D-CGD-CBD	-2.49	119.60	124.52
31	A1	406	CLA	C4B-CHC-C1C	2.49	132.11	126.25
48	Y	620	LUT	C7-C8-C9	-2.49	122.55	126.23
31	c1	511	CLA	CHA-C4D-ND	2.49	137.69	132.55
31	c1	503	CLA	O2A-CGA-CBA	2.49	119.43	111.83
31	y	613	CLA	CMD-C2D-C3D	-2.49	121.97	127.69
31	g1	610	CLA	CMD-C2D-C3D	-2.49	121.97	127.69
31	b1	608	CLA	C1C-C2C-C3C	-2.49	104.36	106.98
31	B1	614	CLA	CHA-C4D-ND	2.49	137.69	132.55
31	N1	613	CLA	O2A-CGA-CBA	2.49	119.43	111.83
33	c1	515	BCR	C8-C9-C10	2.49	122.93	119.01
50	Y1	623	NEX	C31-C30-C29	2.49	130.77	127.28
31	C1	505	CLA	C3B-C4B-NB	-2.49	108.31	110.53
31	b	605	CLA	CHA-C4D-ND	2.49	137.69	132.55
31	g1	602	CLA	O2A-CGA-CBA	2.49	119.43	111.83
31	S1	610	CLA	CHA-C4D-ND	2.49	137.69	132.55
31	S	614	CLA	O2A-CGA-CBA	2.49	119.43	111.83
31	c	509	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
47	Y	606	CHL	C1-O2A-CGA	2.49	122.68	116.65
47	N1	607	CHL	C1-O2A-CGA	2.49	122.68	116.65
31	n1	603	CLA	C4B-CHC-C1C	2.49	132.10	126.25
31	y	611	CLA	CHA-C4D-ND	2.49	137.69	132.55
31	C1	502	CLA	CMB-C2B-C1B	2.49	129.21	125.42
31	C	506	CLA	CHD-C1D-ND	-2.49	121.30	124.80
31	S1	612	CLA	C1C-C2C-C3C	-2.49	104.36	106.98
33	d	404	BCR	C23-C24-C25	-2.49	120.35	127.00
31	n1	614	CLA	C4B-CHC-C1C	2.49	132.10	126.25
47	g1	609	CHL	C4D-CHA-CBD	-2.49	106.46	108.97
50	n	623	NEX	C4-C3-C2	2.49	115.44	110.79
31	S1	617	CLA	O2A-CGA-CBA	2.49	119.42	111.83
31	b1	602	CLA	C4B-CHC-C1C	2.49	132.10	126.25
31	N	612	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
31	c1	502	CLA	O2D-CGD-O1D	-2.49	119.00	123.85
31	N1	611	CLA	O2A-CGA-CBA	2.49	119.42	111.83
47	N	607	CHL	CMA-C3A-C4A	2.49	119.97	114.61
31	c	504	CLA	C2D-C1D-ND	2.49	112.59	110.13
31	n	602	CLA	CAA-C2A-C3A	-2.49	106.28	113.00
31	S1	604	CLA	CHA-C4D-ND	2.49	137.68	132.55
31	b	611	CLA	CMC-C2C-C1C	2.49	128.92	125.03
31	s1	611	CLA	CHA-C1A-NA	-2.49	120.76	126.39
31	b	617	CLA	O2D-CGD-O1D	-2.49	119.01	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	g1	612	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
31	s	602	CLA	C1D-ND-C4D	-2.49	104.57	106.31
38	b1	625	DGA	OG1-CA1-CA2	2.49	119.42	111.83
31	B	608	CLA	CHA-C4D-ND	2.49	137.68	132.55
31	C1	509	CLA	CHA-C4D-ND	2.49	137.68	132.55
31	g	612	CLA	CHA-C4D-ND	2.49	137.68	132.55
31	B	605	CLA	CMD-C2D-C3D	-2.49	121.99	127.69
31	y	604	CLA	C1-O2A-CGA	2.49	122.67	116.65
47	N	601	CHL	CMA-C3A-C4A	2.49	119.97	114.61
49	y1	622	XAT	O24-C25-C38	-2.49	112.27	115.05
31	s	612	CLA	C3B-C4B-NB	-2.49	108.31	110.53
31	S	612	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
31	Y1	604	CLA	O2D-CGD-O1D	-2.49	119.01	123.85
31	s	605	CLA	C1-O2A-CGA	2.49	122.67	116.65
31	s1	617	CLA	CHD-C1D-ND	-2.49	121.31	124.80
31	B	610	CLA	CHA-C4D-ND	2.48	137.68	132.55
31	B1	605	CLA	CHA-C4D-ND	2.48	137.68	132.55
31	C	503	CLA	C2C-C1C-NC	2.48	112.59	109.98
44	d1	405	PL9	O2-C1-C6	2.48	124.43	120.48
31	r	602	CLA	CMA-C3A-C4A	2.48	118.45	111.77
31	B	612	CLA	C2D-C1D-ND	2.48	112.58	110.13
31	N	603	CLA	O2D-CGD-O1D	-2.48	119.01	123.85
33	b1	618	BCR	C38-C26-C27	2.48	118.89	113.60
31	R1	612	CLA	C4B-CHC-C1C	2.48	132.09	126.25
31	S	604	CLA	CMA-C3A-C4A	2.48	118.45	111.77
31	C1	507	CLA	CMD-C2D-C3D	-2.48	121.99	127.69
44	d1	405	PL9	C27-C28-C29	-2.48	121.94	127.62
31	C1	506	CLA	CHA-C4D-ND	2.48	137.67	132.55
31	c1	502	CLA	CHA-C4D-ND	2.48	137.67	132.55
41	d	410	LHG	C5-O7-C7	-2.48	111.85	117.80
31	Y	603	CLA	CHA-C4D-ND	2.48	137.67	132.55
31	n1	614	CLA	CAA-C2A-C3A	-2.48	106.29	113.00
41	N	624	LHG	O8-C23-C24	2.48	119.41	111.83
31	r1	609	CLA	O2A-CGA-CBA	2.48	119.41	111.83
31	B1	612	CLA	C4B-CHC-C1C	2.48	132.09	126.25
31	s1	612	CLA	O1D-CGD-CBD	-2.48	119.62	124.52
31	C	509	CLA	CBC-CAC-C3C	-2.48	105.69	112.42
31	S	613	CLA	C1C-C2C-C3C	-2.48	104.37	106.98
41	s1	624	LHG	C5-O7-C7	-2.48	111.86	117.80
31	d1	402	CLA	C4B-CHC-C1C	2.48	132.08	126.25
31	b1	616	CLA	CHA-C4D-ND	2.48	137.67	132.55
31	n1	613	CLA	C1C-C2C-C3C	-2.48	104.37	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	S1	609	CLA	C1D-ND-C4D	-2.48	104.57	106.31
33	B	619	BCR	C1-C6-C5	-2.48	119.25	122.64
31	S1	617	CLA	C3B-C4B-NB	-2.48	108.31	110.53
31	R	602	CLA	C4B-CHC-C1C	2.48	132.08	126.25
48	S1	621	LUT	C18-C5-C4	2.48	118.98	114.42
31	Y1	614	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
31	s1	613	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
31	C	511	CLA	CMD-C2D-C3D	-2.48	122.00	127.69
31	Y	608	CLA	CHA-C4D-ND	2.48	137.67	132.55
31	n1	613	CLA	CHA-C4D-ND	2.48	137.67	132.55
31	G	612	CLA	O2D-CGD-O1D	-2.48	119.02	123.85
31	s	612	CLA	C4B-CHC-C1C	2.48	132.08	126.25
31	S1	612	CLA	CHA-C4D-ND	2.48	137.66	132.55
47	G	605	CHL	CMA-C3A-C4A	2.48	119.95	114.61
31	b	610	CLA	O2A-CGA-CBA	2.48	119.39	111.83
31	B	609	CLA	O1D-CGD-CBD	-2.48	119.63	124.52
31	B1	617	CLA	CHA-C4D-ND	2.48	137.66	132.55
31	B	604	CLA	C4B-CHC-C1C	2.48	132.07	126.25
31	a	405	CLA	C6-C5-C3	-2.48	107.43	113.47
31	c	505	CLA	O2A-CGA-CBA	2.48	119.39	111.83
31	B1	608	CLA	O2A-CGA-CBA	2.48	119.39	111.83
31	S1	614	CLA	CHA-C4D-ND	2.48	137.66	132.55
31	c1	509	CLA	O2A-C1-C2	2.48	117.64	108.11
31	B1	605	CLA	O2D-CGD-O1D	-2.48	119.03	123.85
31	G	612	CLA	CHA-C4D-ND	2.48	137.66	132.55
31	G1	612	CLA	CHA-C4D-ND	2.48	137.66	132.55
31	B	603	CLA	CMA-C3A-C4A	2.48	118.43	111.77
31	B1	611	CLA	C3B-C4B-NB	-2.48	108.32	110.53
31	y1	613	CLA	CHA-C4D-ND	2.48	137.66	132.55
31	B	605	CLA	C1-O2A-CGA	2.48	122.65	116.65
31	n	602	CLA	C4B-CHC-C1C	2.48	132.07	126.25
31	n	612	CLA	C4B-CHC-C1C	2.48	132.07	126.25
56	R1	626	ERG	C18-C13-C14	-2.48	106.24	110.35
31	C	510	CLA	CHA-C4D-ND	2.48	137.66	132.55
35	b1	622	LMG	O8-C28-C29	2.48	119.39	111.83
31	c	503	CLA	CHD-C1D-ND	-2.48	121.32	124.80
47	g1	605	CHL	C1A-CHA-C4D	2.48	123.11	118.98
41	G1	624	LHG	O8-C23-C24	2.48	119.38	111.83
31	a	407	CLA	CHA-C4D-ND	2.48	137.66	132.55
47	g1	606	CHL	C1-O2A-CGA	2.48	122.64	116.65
31	B	603	CLA	CHA-C4D-ND	2.48	137.66	132.55
31	D	403	CLA	O2D-CGD-O1D	-2.47	119.03	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	g	602	CLA	O2D-CGD-O1D	-2.47	119.03	123.85
31	Y1	610	CLA	CMA-C3A-C4A	2.47	118.42	111.77
31	N1	602	CLA	CMC-C2C-C1C	2.47	128.90	125.03
33	c	517	BCR	C36-C18-C17	-2.47	118.81	122.82
31	r	604	CLA	CHA-C4D-ND	2.47	137.65	132.55
47	R	607	CHL	C1-O2A-CGA	2.47	122.64	116.65
31	b1	609	CLA	O1D-CGD-CBD	-2.47	119.64	124.52
31	D1	403	CLA	CHA-C4D-ND	2.47	137.65	132.55
37	b1	620	C7Z	C38-C25-C24	2.47	118.97	114.42
49	Y	622	XAT	C26-C27-C28	-2.47	120.77	125.99
31	c	508	CLA	C2C-C1C-NC	2.47	112.58	109.98
31	c	503	CLA	CMD-C2D-C3D	-2.47	122.02	127.69
31	b	603	CLA	CAA-C2A-C3A	-2.47	106.32	113.00
31	S	610	CLA	CMA-C3A-C4A	2.47	118.42	111.77
31	n	611	CLA	C4B-CHC-C1C	2.47	132.06	126.25
52	S	626	3PH	O31-C31-C32	2.47	119.37	111.83
31	Y	610	CLA	CHA-C4D-ND	2.47	137.65	132.55
31	B1	610	CLA	CHA-C4D-ND	2.47	137.65	132.55
33	B	619	BCR	C28-C27-C26	-2.47	109.65	114.06
31	S	609	CLA	C2C-C1C-NC	2.47	112.58	109.98
31	Y	608	CLA	O2A-CGA-CBA	2.47	119.37	111.83
31	G	613	CLA	O2A-CGA-CBA	2.47	119.37	111.83
31	G	612	CLA	C4B-CHC-C1C	2.47	132.06	126.25
31	r1	603	CLA	O2D-CGD-O1D	-2.47	119.04	123.85
37	B1	620	C7Z	C28-C27-C26	-2.47	120.40	127.00
31	S1	602	CLA	O1D-CGD-CBD	-2.47	119.64	124.52
31	G1	614	CLA	CHA-C4D-ND	2.47	137.65	132.55
31	C1	501	CLA	C1D-ND-C4D	-2.47	104.58	106.31
31	n1	602	CLA	C4B-CHC-C1C	2.47	132.06	126.25
31	g	614	CLA	CHA-C4D-ND	2.47	137.64	132.55
33	B	619	BCR	C35-C13-C12	2.47	121.86	118.09
31	n	603	CLA	CHA-C4D-ND	2.47	137.64	132.55
47	G1	609	CHL	CMA-C3A-C4A	2.47	119.93	114.61
31	S1	609	CLA	CHA-C4D-ND	2.47	137.64	132.55
31	B	607	CLA	CMD-C2D-C3D	-2.47	122.03	127.69
31	g	612	CLA	C4B-CHC-C1C	2.47	132.05	126.25
31	b	610	CLA	CHA-C4D-ND	2.47	137.64	132.55
31	c	504	CLA	CAA-C2A-C3A	-2.47	106.33	113.00
31	B	616	CLA	CHA-C1A-NA	-2.47	120.80	126.39
31	c	506	CLA	C1-C2-C3	-2.47	122.15	126.20
31	g1	610	CLA	O2A-CGA-CBA	2.47	119.36	111.83
31	y	613	CLA	CHA-C4D-ND	2.47	137.64	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	G1	605	CHL	C1-O2A-CGA	2.47	123.68	116.67
47	N	609	CHL	CMA-C3A-C4A	2.47	119.93	114.61
49	N	622	XAT	O4-C5-C18	-2.47	112.29	115.05
31	b1	613	CLA	C3B-C4B-NB	-2.47	108.33	110.53
31	g1	614	CLA	C3B-C4B-NB	-2.47	108.33	110.53
31	s	612	CLA	CHA-C4D-ND	2.47	137.64	132.55
35	C1	521	LMG	C8-O7-C10	-2.47	111.89	117.80
31	R	611	CLA	CHA-C4D-ND	2.47	137.64	132.55
41	d	408	LHG	C6-C5-C4	-2.47	106.04	111.78
31	C1	504	CLA	CHA-C4D-ND	2.47	137.64	132.55
31	s1	602	CLA	O2D-CGD-O1D	-2.46	119.05	123.85
31	R	613	CLA	CHA-C4D-ND	2.46	137.63	132.55
31	Y	613	CLA	CHA-C4D-ND	2.46	137.63	132.55
31	G1	603	CLA	C4B-CHC-C1C	2.46	132.04	126.25
31	C1	510	CLA	CMD-C2D-C3D	-2.46	122.04	127.69
31	c1	503	CLA	CHD-C1D-ND	-2.46	121.33	124.80
31	N	614	CLA	O2D-CGD-O1D	-2.46	119.05	123.85
31	N1	612	CLA	C4B-CHC-C1C	2.46	132.04	126.25
40	C	518	DGD	O6D-C5D-C6D	2.46	111.58	106.69
31	B1	616	CLA	CHA-C4D-ND	2.46	137.63	132.55
31	S1	605	CLA	C3B-C4B-NB	-2.46	108.33	110.53
31	R	602	CLA	O2A-CGA-CBA	2.46	119.34	111.83
31	s	611	CLA	CHA-C4D-ND	2.46	137.63	132.55
33	C1	514	BCR	C38-C26-C25	-2.46	121.80	124.48
31	B	611	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
31	R1	602	CLA	CHA-C4D-ND	2.46	137.63	132.55
31	s1	610	CLA	CHA-C4D-ND	2.46	137.63	132.55
31	c	510	CLA	C3B-C4B-NB	-2.46	108.33	110.53
31	R1	603	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
31	n	612	CLA	CHD-C1D-ND	-2.46	121.34	124.80
31	C	503	CLA	CHA-C4D-ND	2.46	137.63	132.55
31	A1	407	CLA	C1C-C2C-C3C	-2.46	104.39	106.98
31	r1	609	CLA	C1C-C2C-C3C	-2.46	104.39	106.98
31	C1	509	CLA	CMD-C2D-C3D	-2.46	122.04	127.69
31	s1	603	CLA	C4B-CHC-C1C	2.46	132.03	126.25
31	n1	612	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
31	a	410	CLA	CHA-C4D-ND	2.46	137.63	132.55
31	R	610	CLA	CHD-C1D-ND	-2.46	121.34	124.80
31	C	505	CLA	C1-C2-C3	-2.46	122.17	126.20
31	g1	611	CLA	CAA-C2A-C3A	-2.46	106.35	113.00
31	G	602	CLA	CHA-C4D-ND	2.46	137.63	132.55
31	c	502	CLA	CHA-C4D-ND	2.46	137.63	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	d1	402	CLA	CHA-C4D-ND	2.46	137.63	132.55
31	b	606	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
47	n1	607	CHL	CMA-C3A-C4A	2.46	119.91	114.61
49	n1	622	XAT	C18-C5-C6	-2.46	118.25	122.30
31	C1	503	CLA	O2A-CGA-CBA	2.46	119.33	111.83
31	b1	611	CLA	C2D-C1D-ND	2.46	112.56	110.13
31	a	410	CLA	C3B-C4B-NB	-2.46	108.33	110.53
31	B	611	CLA	C1D-ND-C4D	-2.46	104.59	106.31
31	Y	603	CLA	C1D-ND-C4D	-2.46	104.59	106.31
31	B1	611	CLA	C1-C2-C3	-2.46	122.17	126.20
31	R	612	CLA	O2D-CGD-O1D	-2.46	119.06	123.85
31	N	603	CLA	C3B-C4B-NB	-2.46	108.34	110.53
48	y	620	LUT	C38-C25-C24	-2.46	117.54	123.36
31	s1	602	CLA	CMA-C3A-C4A	2.46	118.38	111.77
47	r1	606	CHL	CMA-C3A-C4A	2.46	119.91	114.61
31	d	402	CLA	CHA-C4D-ND	2.46	137.62	132.55
31	b1	605	CLA	CHA-C4D-ND	2.46	137.62	132.55
47	y	601	CHL	C1-C2-C3	-2.46	122.17	126.20
31	N	612	CLA	C4B-CHC-C1C	2.46	132.03	126.25
31	d1	403	CLA	CHA-C4D-ND	2.46	137.62	132.55
31	g1	611	CLA	CHA-C4D-ND	2.46	137.62	132.55
31	R	608	CLA	CMD-C2D-C3D	-2.46	122.06	127.69
31	y1	610	CLA	CMD-C2D-C3D	-2.46	122.06	127.69
50	G	623	NEX	C38-C25-C26	-2.46	118.26	122.30
31	c1	507	CLA	C4B-CHC-C1C	2.46	132.02	126.25
33	C1	515	BCR	C34-C9-C10	-2.46	118.84	122.82
31	Y1	603	CLA	CHA-C4D-ND	2.46	137.62	132.55
31	b	609	CLA	CMD-C2D-C3D	-2.46	122.06	127.69
31	b	602	CLA	C4B-CHC-C1C	2.46	132.02	126.25
31	Y	614	CLA	C4B-CHC-C1C	2.45	132.02	126.25
33	c1	516	BCR	C37-C22-C21	-2.45	118.84	122.82
31	C1	503	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
31	g1	602	CLA	CHA-C4D-ND	2.45	137.61	132.55
31	b1	609	CLA	CHA-C1A-NA	-2.45	120.83	126.39
48	s1	620	LUT	C35-C15-C14	-2.45	118.50	123.52
31	S	605	CLA	C3B-C4B-NB	-2.45	108.34	110.53
31	A1	406	CLA	C1D-ND-C4D	-2.45	104.59	106.31
49	y1	622	XAT	C38-C25-C26	-2.45	118.26	122.30
47	G	606	CHL	C4D-CHA-CBD	-2.45	106.49	108.97
49	y	622	XAT	C6-C7-C8	-2.45	120.81	125.99
31	C1	507	CLA	CHA-C4D-ND	2.45	137.61	132.55
31	r	610	CLA	C4B-CHC-C1C	2.45	132.02	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	g1	612	CLA	C4B-CHC-C1C	2.45	132.02	126.25
31	S	602	CLA	C3B-C4B-NB	-2.45	108.34	110.53
31	y	603	CLA	CHA-C4D-ND	2.45	137.61	132.55
31	s1	611	CLA	O2D-CGD-O1D	-2.45	119.07	123.85
31	C	508	CLA	C4B-CHC-C1C	2.45	132.01	126.25
48	s	620	LUT	C27-C28-C29	-2.45	121.05	126.32
31	g	613	CLA	C2D-C1D-ND	2.45	112.55	110.13
31	g	602	CLA	C3B-C4B-NB	-2.45	108.34	110.53
31	S	609	CLA	C1C-C2C-C3C	-2.45	104.40	106.98
31	R1	608	CLA	CHA-C4D-ND	2.45	137.61	132.55
31	y	611	CLA	CAA-C2A-C3A	-2.45	106.37	113.00
47	N1	605	CHL	C1-O2A-CGA	2.45	122.59	116.65
35	H	102	LMG	O8-C28-C29	2.45	119.31	111.83
31	N1	614	CLA	CHD-C1D-ND	-2.45	121.35	124.80
31	Y1	602	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
31	S	617	CLA	CHA-C4D-ND	2.45	137.61	132.55
31	r1	608	CLA	CMD-C2D-C3D	-2.45	122.07	127.69
31	C1	504	CLA	CHD-C1D-ND	-2.45	121.35	124.80
31	b	608	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
33	c	517	BCR	C2-C1-C6	2.45	114.00	110.44
31	s	609	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
31	Y1	611	CLA	O2D-CGD-O1D	-2.45	119.08	123.85
31	G1	611	CLA	CAA-C2A-C3A	-2.45	106.38	113.00
47	g	605	CHL	CMA-C3A-C4A	2.45	119.89	114.61
31	G1	603	CLA	CMD-C2D-C3D	-2.45	122.07	127.69
31	n	613	CLA	C4B-CHC-C1C	2.45	132.01	126.25
31	r	604	CLA	CHD-C1D-ND	-2.45	121.36	124.80
47	y1	607	CHL	C1-C2-C3	-2.45	122.18	126.20
31	b1	611	CLA	O2A-CGA-CBA	2.45	119.30	111.83
31	y1	613	CLA	CMD-C2D-C3D	-2.45	122.07	127.69
47	n	608	CHL	C4C-CHD-C1D	2.45	124.83	116.07
31	B	608	CLA	O2A-CGA-CBA	2.45	119.30	111.83
46	H1	101	RRX	C11-C12-C13	-2.45	119.65	126.36
31	y1	604	CLA	CMA-C3A-C4A	2.45	118.35	111.77
31	n1	610	CLA	C1C-C2C-C3C	-2.45	104.41	106.98
31	C	504	CLA	C2D-C1D-ND	2.45	112.55	110.13
31	Y	612	CLA	C2D-C1D-ND	2.45	112.55	110.13
31	B1	612	CLA	C2D-C1D-ND	2.45	112.55	110.13
31	S	605	CLA	CHA-C4D-ND	2.45	137.60	132.55
31	a1	405	CLA	OBD-CAD-C3D	-2.45	122.69	128.42
31	c	507	CLA	C1-C2-C3	-2.45	122.19	126.20
31	A	407	CLA	CHA-C4D-ND	2.45	137.60	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	S	612	CLA	CHA-C4D-ND	2.45	137.60	132.55
31	g1	613	CLA	C3B-C4B-NB	-2.45	108.35	110.53
47	G1	606	CHL	C4C-CHD-C1D	2.45	124.82	116.07
48	g1	620	LUT	C22-C23-C24	-2.45	107.55	111.18
31	R1	610	CLA	C2D-C1D-ND	2.45	112.55	110.13
31	s	613	CLA	C1-O2A-CGA	2.45	122.57	116.65
31	b1	605	CLA	CMB-C2B-C1B	2.45	129.14	125.42
31	s	605	CLA	O1D-CGD-CBD	-2.45	119.69	124.52
31	D1	403	CLA	CMA-C3A-C4A	2.45	118.34	111.77
31	c1	510	CLA	C4B-CHC-C1C	2.44	132.00	126.25
31	g	602	CLA	C2D-C1D-ND	2.44	112.55	110.13
31	B1	606	CLA	O2A-CGA-CBA	2.44	119.29	111.83
31	r	602	CLA	C4B-CHC-C1C	2.44	131.99	126.25
31	c	502	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
31	r	612	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
31	C	513	CLA	C1-C2-C3	-2.44	122.19	126.20
47	y1	609	CHL	C4D-CHA-CBD	-2.44	106.50	108.97
31	B1	606	CLA	O1D-CGD-CBD	-2.44	119.70	124.52
47	y	609	CHL	CMA-C3A-C4A	2.44	119.87	114.61
31	S1	614	CLA	CHD-C1D-ND	-2.44	121.36	124.80
31	c1	513	CLA	CHA-C1A-NA	-2.44	120.86	126.39
31	g1	611	CLA	CMD-C2D-C3D	-2.44	122.09	127.69
31	B	605	CLA	CMA-C3A-C4A	2.44	118.34	111.77
31	A1	405	CLA	C2C-C1C-NC	2.44	112.55	109.98
33	b	619	BCR	C27-C26-C25	-2.44	119.40	122.70
31	B	602	CLA	O2A-CGA-CBA	2.44	119.28	111.83
31	s	605	CLA	C3B-C4B-NB	-2.44	108.35	110.53
50	s	623	NEX	C38-C25-C26	-2.44	118.28	122.30
31	B1	608	CLA	O2D-CGD-O1D	-2.44	119.09	123.85
31	c1	503	CLA	C4B-CHC-C1C	2.44	131.99	126.25
31	Y1	612	CLA	C1-C2-C3	-2.44	122.20	126.20
31	S	617	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
48	S	620	LUT	C35-C15-C14	-2.44	118.52	123.52
31	G1	611	CLA	CHD-C1D-ND	-2.44	121.37	124.80
31	B	609	CLA	C3B-C4B-NB	-2.44	108.35	110.53
31	d	403	CLA	CHA-C4D-ND	2.44	137.59	132.55
31	r1	610	CLA	C2C-C1C-NC	2.44	112.55	109.98
49	Y1	622	XAT	C19-C9-C10	-2.44	118.86	122.82
33	C1	514	BCR	C33-C5-C4	2.44	118.80	113.60
33	c1	514	BCR	C33-C5-C4	2.44	118.80	113.60
31	b1	615	CLA	C3B-C4B-NB	-2.44	108.35	110.53
31	c1	511	CLA	CMD-C2D-C3D	-2.44	122.09	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	r1	610	CLA	C1C-C2C-C3C	-2.44	104.41	106.98
31	C	505	CLA	C4B-CHC-C1C	2.44	131.98	126.25
31	y1	614	CLA	C4B-CHC-C1C	2.44	131.98	126.25
31	g	604	CLA	O2A-CGA-CBA	2.44	119.27	111.83
31	R1	603	CLA	O2A-CGA-CBA	2.44	119.27	111.83
31	g	613	CLA	C1C-C2C-C3C	-2.44	104.42	106.98
31	c	503	CLA	CHA-C4D-ND	2.44	137.58	132.55
31	C1	513	CLA	CHA-C4D-ND	2.44	137.58	132.55
47	s	606	CHL	CMA-C3A-C4A	2.44	119.86	114.61
31	S	605	CLA	C1-O2A-CGA	2.44	122.55	116.65
31	C1	512	CLA	CHA-C4D-ND	2.44	137.58	132.55
31	y1	602	CLA	CHA-C4D-ND	2.44	137.58	132.55
31	s	612	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
31	s	603	CLA	CHA-C4D-ND	2.44	137.58	132.55
31	g	611	CLA	O2D-CGD-O1D	-2.44	119.10	123.85
31	R1	612	CLA	CMA-C3A-C4A	2.44	118.32	111.77
31	G	603	CLA	CHD-C1D-ND	-2.44	121.37	124.80
47	g1	606	CHL	CMA-C3A-C4A	2.44	119.86	114.61
31	A1	405	CLA	CHA-C1A-NA	-2.44	120.87	126.39
31	B1	616	CLA	CMD-C2D-C3D	-2.44	122.10	127.69
31	n	604	CLA	O2A-CGA-CBA	2.44	119.26	111.83
47	Y1	609	CHL	CMA-C3A-C4A	2.44	119.86	114.61
31	N1	603	CLA	CMA-C3A-C4A	2.44	118.32	111.77
33	b	618	BCR	C4-C5-C6	-2.44	119.41	122.70
31	g	602	CLA	CHA-C4D-ND	2.44	137.57	132.55
48	n	621	LUT	C15-C14-C13	-2.44	123.86	127.28
49	y	622	XAT	C40-C33-C34	-2.44	118.87	122.82
31	Y	602	CLA	C1C-C2C-C3C	-2.43	104.42	106.98
31	n1	612	CLA	C4B-CHC-C1C	2.43	131.97	126.25
35	a1	413	LMG	O8-C28-C29	2.43	119.26	111.83
31	b	611	CLA	C2C-C1C-NC	2.43	112.54	109.98
31	B	602	CLA	C3B-C4B-NB	-2.43	108.36	110.53
31	G	613	CLA	CHA-C4D-ND	2.43	137.57	132.55
31	N1	602	CLA	CAA-C2A-C3A	-2.43	106.42	113.00
49	Y1	622	XAT	O4-C5-C4	-2.43	111.21	113.49
31	g	614	CLA	C4B-CHC-C1C	2.43	131.97	126.25
31	s	611	CLA	C4B-CHC-C1C	2.43	131.97	126.25
50	n	623	NEX	C16-C1-C6	-2.43	108.29	110.47
31	C	512	CLA	CHA-C4D-ND	2.43	137.57	132.55
31	G1	613	CLA	CHA-C4D-ND	2.43	137.57	132.55
31	S1	602	CLA	C1-C2-C3	-2.43	122.21	126.20
31	b	617	CLA	C1-O2A-CGA	2.43	122.54	116.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	506	CLA	CHA-C4D-ND	2.43	137.57	132.55
31	Y	603	CLA	OBD-CAD-C3D	-2.43	122.73	128.42
31	Y	614	CLA	C3B-C4B-NB	-2.43	108.36	110.53
31	s	610	CLA	C3B-C4B-NB	-2.43	108.36	110.53
31	B	614	CLA	C1D-ND-C4D	-2.43	104.61	106.31
31	a1	406	CLA	C1D-ND-C4D	-2.43	104.61	106.31
31	N1	604	CLA	C3D-C2D-C1D	-2.43	102.51	105.83
31	S1	617	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
31	c	502	CLA	CMC-C2C-C1C	2.43	128.84	125.03
31	s	614	CLA	O2D-CGD-O1D	-2.43	119.11	123.85
31	a1	407	CLA	CHA-C1A-NA	-2.43	120.88	126.39
31	r1	604	CLA	CHA-C4D-ND	2.43	137.57	132.55
31	a1	407	CLA	C2A-C1A-CHA	2.43	128.09	123.87
31	C	510	CLA	C1D-ND-C4D	-2.43	104.61	106.31
31	G	610	CLA	C3D-C2D-C1D	-2.43	102.51	105.83
31	S	614	CLA	CHA-C4D-ND	2.43	137.56	132.55
31	C1	511	CLA	CHA-C4D-ND	2.43	137.56	132.55
31	c1	503	CLA	C1C-C2C-C3C	-2.43	104.42	106.98
31	s1	604	CLA	CHA-C4D-ND	2.43	137.56	132.55
35	c	521	LMG	O7-C10-O9	-2.43	118.02	123.70
31	c1	511	CLA	C4B-CHC-C1C	2.43	131.96	126.25
33	c	517	BCR	C34-C9-C10	-2.43	118.88	122.82
31	y1	602	CLA	C1D-ND-C4D	-2.43	104.61	106.31
31	b	611	CLA	C2D-C1D-ND	2.43	112.53	110.13
31	b1	612	CLA	C2D-C1D-ND	2.43	112.53	110.13
31	C1	507	CLA	CHD-C1D-ND	-2.43	121.38	124.80
47	s1	607	CHL	C4C-CHD-C1D	2.43	124.76	116.07
31	a	410	CLA	O2A-CGA-CBA	2.43	119.24	111.83
41	g	624	LHG	O8-C23-C24	2.43	119.24	111.83
31	c	510	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
31	R	610	CLA	CAA-C2A-C3A	-2.43	106.43	113.00
31	B	606	CLA	CHA-C4D-ND	2.43	137.56	132.55
49	Y	622	XAT	C18-C5-C6	-2.43	118.30	122.30
31	B	612	CLA	C4B-CHC-C1C	2.43	131.96	126.25
31	S1	603	CLA	C4B-CHC-C1C	2.43	131.96	126.25
48	Y1	621	LUT	C38-C25-C24	-2.43	117.61	123.36
31	n	602	CLA	CMD-C2D-C3D	-2.43	122.12	127.69
31	d1	403	CLA	CHA-C1A-NA	-2.43	120.89	126.39
31	C	510	CLA	C4B-CHC-C1C	2.43	131.96	126.25
31	B1	613	CLA	C3B-C4B-NB	-2.43	108.36	110.53
41	g1	624	LHG	C6-C5-C4	-2.43	106.12	111.78
31	A1	410	CLA	CHA-C4D-ND	2.43	137.56	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	603	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
31	r	610	CLA	O2D-CGD-O1D	-2.43	119.12	123.85
31	a	405	CLA	CAA-C2A-C3A	-2.43	106.44	113.00
31	C	501	CLA	C4B-CHC-C1C	2.43	131.96	126.25
38	B	625	DGA	OG1-CA1-CA2	2.43	119.24	111.83
31	r	609	CLA	C3B-C4B-NB	-2.43	108.36	110.53
31	r	609	CLA	CHA-C4D-ND	2.43	137.56	132.55
31	r	613	CLA	CHA-C4D-ND	2.43	137.56	132.55
31	C	502	CLA	CHA-C4D-ND	2.43	137.56	132.55
49	y	622	XAT	O4-C6-C7	-2.43	109.92	116.88
31	b	610	CLA	C1C-C2C-C3C	-2.43	104.43	106.98
31	n	610	CLA	C3D-C2D-C1D	-2.43	102.52	105.83
31	b	606	CLA	CMD-C2D-C3D	-2.43	122.12	127.69
31	C1	513	CLA	O2D-CGD-O1D	-2.43	119.13	123.85
31	b	616	CLA	CHA-C4D-ND	2.43	137.55	132.55
40	B1	623	DGD	C3G-C2G-C1G	-2.43	106.13	111.78
31	b	611	CLA	C1D-ND-C4D	-2.43	104.61	106.31
31	n	602	CLA	C1D-ND-C4D	-2.43	104.61	106.31
56	R1	626	ERG	C4-C5-C10	2.43	119.53	116.42
33	c1	517	BCR	C1-C6-C5	-2.43	119.32	122.64
31	N	610	CLA	CHA-C4D-ND	2.43	137.55	132.55
31	s	617	CLA	CHA-C4D-ND	2.43	137.55	132.55
33	B1	618	BCR	C30-C25-C26	-2.42	119.32	122.64
31	r	602	CLA	CHA-C4D-ND	2.42	137.55	132.55
47	R	607	CHL	C4C-CHD-C1D	2.42	124.74	116.07
31	g	610	CLA	O2D-CGD-O1D	-2.42	119.13	123.85
31	g	603	CLA	C3B-C4B-NB	-2.42	108.37	110.53
31	c	511	CLA	CAA-CBA-CGA	-2.42	106.33	113.21
31	R	609	CLA	CHA-C1A-NA	-2.42	120.90	126.39
31	Y1	604	CLA	CHA-C4D-ND	2.42	137.55	132.55
33	a1	411	BCR	C33-C5-C4	2.42	118.76	113.60
31	G	610	CLA	C4B-CHC-C1C	2.42	131.94	126.25
31	S	612	CLA	C4B-CHC-C1C	2.42	131.94	126.25
31	b1	605	CLA	CMC-C2C-C3C	2.42	132.70	126.15
31	A	405	CLA	CAA-C2A-C3A	-2.42	106.45	113.00
31	S	613	CLA	C4B-CHC-C1C	2.42	131.94	126.25
48	n	620	LUT	C18-C5-C6	-2.42	121.84	124.48
31	r	608	CLA	CHD-C1D-ND	-2.42	121.39	124.80
31	r	603	CLA	C3B-C4B-NB	-2.42	108.37	110.53
31	Y	611	CLA	C1C-C2C-C3C	-2.42	104.43	106.98
31	a	405	CLA	C1C-C2C-C3C	-2.42	104.43	106.98
31	r	603	CLA	CMD-C2D-C3D	-2.42	122.14	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	R	610	CLA	C4B-CHC-C1C	2.42	131.94	126.25
31	D1	403	CLA	C4B-CHC-C1C	2.42	131.94	126.25
41	c	625	LHG	C5-O7-C7	-2.42	112.00	117.80
31	b	603	CLA	O2A-CGA-CBA	2.42	119.22	111.83
31	n1	614	CLA	CHA-C4D-ND	2.42	137.54	132.55
31	S	613	CLA	C2D-C1D-ND	2.42	112.52	110.13
31	B	606	CLA	C3B-C4B-NB	-2.42	108.37	110.53
31	s1	603	CLA	C3B-C4B-NB	-2.42	108.37	110.53
31	B1	612	CLA	O2A-CGA-CBA	2.42	119.22	111.83
31	D1	402	CLA	CHD-C1D-ND	-2.42	121.40	124.80
31	r1	609	CLA	CHA-C4D-ND	2.42	137.54	132.55
31	r	612	CLA	C4B-CHC-C1C	2.42	131.94	126.25
31	g1	603	CLA	C4B-CHC-C1C	2.42	131.94	126.25
31	s	611	CLA	CHA-C1A-NA	-2.42	120.91	126.39
47	r	606	CHL	C4C-CHD-C1D	2.42	124.73	116.07
31	s	610	CLA	CHD-C1D-ND	-2.42	121.40	124.80
31	C1	512	CLA	CHD-C1D-ND	-2.42	121.40	124.80
31	b	605	CLA	CMD-C2D-C3D	-2.42	122.14	127.69
31	G1	613	CLA	C3B-C4B-NB	-2.42	108.37	110.53
31	s1	612	CLA	CHA-C4D-ND	2.42	137.54	132.55
33	c1	514	BCR	C23-C24-C25	-2.42	120.53	127.00
31	B1	615	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
31	g1	613	CLA	CHA-C4D-ND	2.42	137.54	132.55
31	s1	605	CLA	C4B-CHC-C1C	2.42	131.93	126.25
31	B1	612	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
31	c	512	CLA	C1-O2A-CGA	2.42	122.50	116.65
31	c1	508	CLA	C4B-CHC-C1C	2.42	131.93	126.25
31	A	406	CLA	CHA-C4D-ND	2.42	137.54	132.55
31	c1	512	CLA	CHA-C4D-ND	2.42	137.54	132.55
31	g1	610	CLA	CHA-C4D-ND	2.42	137.54	132.55
31	B1	615	CLA	C4B-CHC-C1C	2.42	131.93	126.25
37	b1	620	C7Z	C8-C7-C6	-2.42	120.54	127.00
31	S	613	CLA	O2A-CGA-CBA	2.42	119.21	111.83
31	a	407	CLA	C3B-C4B-NB	-2.42	108.37	110.53
31	R	602	CLA	O2D-CGD-O1D	-2.42	119.14	123.85
31	C	509	CLA	CHA-C4D-ND	2.42	137.54	132.55
31	N	603	CLA	CHA-C4D-ND	2.42	137.54	132.55
31	Y1	612	CLA	CHA-C4D-ND	2.42	137.54	132.55
31	c	509	CLA	CHA-C1A-NA	-2.42	120.92	126.39
31	s	603	CLA	C4B-CHC-C1C	2.42	131.93	126.25
31	S1	611	CLA	C4B-CHC-C1C	2.42	131.93	126.25
31	R	602	CLA	CHA-C4D-ND	2.42	137.53	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	611	CLA	CHA-C4D-ND	2.42	137.53	132.55
31	S1	613	CLA	CHA-C4D-ND	2.42	137.53	132.55
47	s1	606	CHL	CMA-C3A-C4A	2.42	119.82	114.61
31	S1	602	CLA	C1C-C2C-C3C	-2.42	104.44	106.98
31	s	610	CLA	O2A-CGA-CBA	2.42	119.20	111.83
31	y	610	CLA	CHA-C4D-ND	2.42	137.53	132.55
48	G	621	LUT	C20-C13-C12	2.42	121.78	118.09
31	D1	402	CLA	C4B-CHC-C1C	2.42	131.93	126.25
49	g1	622	XAT	C6-C7-C8	-2.42	120.89	125.99
31	c1	501	CLA	CAA-C2A-C3A	-2.42	106.47	113.00
47	S1	607	CHL	CMA-C3A-C4A	2.42	119.81	114.61
31	c	507	CLA	CHA-C1A-NA	-2.42	120.92	126.39
46	H	101	RRX	C30-C25-C24	2.42	122.20	115.65
31	n	604	CLA	O2D-CGD-O1D	-2.42	119.15	123.85
31	N1	604	CLA	O2D-CGD-O1D	-2.42	119.15	123.85
31	G1	613	CLA	O2D-CGD-O1D	-2.42	119.15	123.85
31	R1	610	CLA	C4B-CHC-C1C	2.41	131.93	126.25
50	S1	623	NEX	C26-C27-C28	-2.41	120.89	125.99
31	y1	603	CLA	C1D-ND-C4D	-2.41	104.62	106.31
31	y	602	CLA	O2A-CGA-CBA	2.41	119.20	111.83
31	Y1	613	CLA	C1-O2A-CGA	2.41	122.49	116.65
31	r1	602	CLA	CHA-C4D-ND	2.41	137.53	132.55
31	B	606	CLA	C4B-CHC-C1C	2.41	131.92	126.25
31	B1	613	CLA	CHA-C4D-ND	2.41	137.53	132.55
31	c1	503	CLA	CHA-C4D-ND	2.41	137.53	132.55
31	S1	609	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
31	S	604	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
31	y1	613	CLA	O2A-CGA-CBA	2.41	119.19	111.83
31	S1	602	CLA	C2D-C1D-ND	2.41	112.51	110.13
31	S	613	CLA	C1-O2A-CGA	2.41	122.49	116.65
48	y	620	LUT	C22-C23-C24	-2.41	107.60	111.18
31	c	507	CLA	CMD-C2D-C3D	-2.41	122.16	127.69
31	G	611	CLA	CHA-C4D-ND	2.41	137.53	132.55
31	c1	501	CLA	CHA-C4D-ND	2.41	137.53	132.55
47	Y1	606	CHL	C1C-C2C-CMC	2.41	131.15	126.80
31	s1	612	CLA	O2D-CGD-O1D	-2.41	119.15	123.85
47	N1	606	CHL	C1-C2-C3	-2.41	122.25	126.20
48	R1	620	LUT	C1-C6-C7	2.41	122.19	115.65
33	c	516	BCR	C8-C9-C10	2.41	122.80	119.01
31	Y1	612	CLA	O2A-CGA-CBA	2.41	119.19	111.83
31	S1	611	CLA	O2A-CGA-CBA	2.41	119.19	111.83
31	C1	512	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	Y1	610	CLA	C4B-CHC-C1C	2.41	131.92	126.25
31	g1	602	CLA	C4B-CHC-C1C	2.41	131.92	126.25
31	b	604	CLA	O2A-CGA-CBA	2.41	119.19	111.83
49	n1	622	XAT	O24-C25-C24	2.41	115.75	113.49
31	G	602	CLA	C1C-C2C-C3C	-2.41	104.44	106.98
31	b1	605	CLA	C3D-C2D-C1D	-2.41	102.54	105.83
31	N	611	CLA	C4B-CHC-C1C	2.41	131.91	126.25
47	Y1	609	CHL	C1-O2A-CGA	2.41	122.48	116.65
31	B	611	CLA	C2C-C1C-NC	2.41	112.51	109.98
31	y	602	CLA	O1D-CGD-CBD	-2.41	119.77	124.52
31	b1	607	CLA	C2C-C1C-NC	2.41	112.51	109.98
31	d1	402	CLA	C2D-C1D-ND	2.41	112.51	110.13
31	N	613	CLA	CMD-C2D-C3D	-2.41	122.17	127.69
31	a1	405	CLA	CMD-C2D-C3D	-2.41	122.17	127.69
31	N	613	CLA	C3B-C4B-NB	-2.41	108.38	110.53
31	S	613	CLA	C3B-C4B-NB	-2.41	108.38	110.53
31	s	604	CLA	CHA-C4D-ND	2.41	137.52	132.55
48	Y1	621	LUT	C35-C15-C14	-2.41	118.59	123.52
47	n1	608	CHL	CMA-C3A-C4A	2.41	119.80	114.61
31	r1	604	CLA	CHD-C1D-ND	-2.41	121.41	124.80
31	c1	509	CLA	C4B-CHC-C1C	2.41	131.91	126.25
33	c	514	BCR	C8-C9-C10	2.41	122.80	119.01
31	g1	603	CLA	CHA-C4D-ND	2.41	137.52	132.55
31	s1	602	CLA	CHA-C4D-ND	2.41	137.52	132.55
49	g1	622	XAT	C18-C5-C6	-2.41	118.34	122.30
50	G1	623	NEX	C11-C10-C9	2.41	130.65	127.28
31	G1	610	CLA	CAA-C2A-C3A	-2.41	106.49	113.00
33	C	515	BCR	C3-C4-C5	-2.41	109.76	114.06
31	y1	610	CLA	CHA-C4D-ND	2.41	137.51	132.55
56	R1	626	ERG	C20-C22-C23	-2.41	118.53	125.81
31	N1	610	CLA	CMD-C2D-C3D	-2.41	122.17	127.69
31	b1	607	CLA	CHD-C1D-ND	-2.41	121.42	124.80
33	d	404	BCR	C37-C22-C21	-2.41	118.92	122.82
33	C1	517	BCR	C36-C18-C17	-2.41	118.92	122.82
31	s	610	CLA	CHA-C4D-ND	2.41	137.51	132.55
31	S1	617	CLA	CHA-C4D-ND	2.41	137.51	132.55
48	G	621	LUT	C35-C34-C33	-2.41	123.90	127.28
31	N	604	CLA	O1D-CGD-CBD	-2.41	119.77	124.52
31	b	613	CLA	C4B-CHC-C1C	2.41	131.90	126.25
31	Y1	602	CLA	CHA-C4D-ND	2.41	137.51	132.55
31	g1	604	CLA	CHA-C4D-ND	2.41	137.51	132.55
31	n1	614	CLA	C1C-C2C-C3C	-2.41	104.45	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	G	607	CHL	C4C-CHD-C1D	2.41	124.67	116.07
31	D	402	CLA	CHD-C1D-ND	-2.40	121.42	124.80
47	r	607	CHL	C1-O2A-CGA	2.40	122.47	116.65
31	c1	510	CLA	CMD-C2D-C3D	-2.40	122.17	127.69
31	Y1	604	CLA	C4B-CHC-C1C	2.40	131.90	126.25
48	y1	621	LUT	C18-C5-C6	-2.40	121.86	124.48
31	S1	610	CLA	OBD-CAD-C3D	-2.40	122.80	128.42
48	Y	621	LUT	C31-C30-C29	-2.40	123.91	127.28
31	B1	602	CLA	C4B-CHC-C1C	2.40	131.90	126.25
31	S1	610	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
31	R1	608	CLA	CHD-C1D-ND	-2.40	121.42	124.80
31	g	610	CLA	CHA-C4D-ND	2.40	137.51	132.55
31	s1	609	CLA	CHA-C4D-ND	2.40	137.51	132.55
31	c	506	CLA	CHD-C1D-ND	-2.40	121.42	124.80
31	B1	609	CLA	O1D-CGD-CBD	-2.40	119.78	124.52
31	N	613	CLA	C2C-C1C-NC	2.40	112.51	109.98
31	r1	602	CLA	C1D-ND-C4D	-2.40	104.63	106.31
31	r	613	CLA	O1D-CGD-CBD	-2.40	119.78	124.52
31	g	603	CLA	CHA-C4D-ND	2.40	137.51	132.55
31	c1	504	CLA	CHA-C4D-ND	2.40	137.51	132.55
31	C	507	CLA	O2D-CGD-O1D	-2.40	119.17	123.85
31	C	508	CLA	CHA-C4D-ND	2.40	137.50	132.55
46	H	101	RRX	C11-C12-C13	-2.40	119.78	126.36
31	y1	603	CLA	C4B-CHC-C1C	2.40	131.90	126.25
31	C	503	CLA	CHD-C1D-ND	-2.40	121.42	124.80
48	Y	621	LUT	C31-C32-C33	-2.40	119.78	126.36
31	G1	610	CLA	C2C-C1C-NC	2.40	112.50	109.98
31	S	602	CLA	CHA-C4D-ND	2.40	137.50	132.55
46	H	101	RRX	C15-C16-C17	-2.40	118.61	123.52
49	N	622	XAT	C18-C5-C6	-2.40	118.35	122.30
31	b1	616	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
31	G	614	CLA	CHD-C1D-ND	-2.40	121.42	124.80
31	g1	610	CLA	CHD-C1D-ND	-2.40	121.42	124.80
31	C	501	CLA	O1D-CGD-CBD	-2.40	119.78	124.52
33	b1	618	BCR	C30-C25-C26	-2.40	119.36	122.64
31	y	613	CLA	CHD-C1D-ND	-2.40	121.43	124.80
31	G1	612	CLA	C4B-CHC-C1C	2.40	131.89	126.25
31	b	616	CLA	CHA-C1A-NA	-2.40	120.96	126.39
31	N	614	CLA	CHA-C4D-ND	2.40	137.50	132.55
31	s	610	CLA	C1C-C2C-C3C	-2.40	104.46	106.98
31	G	610	CLA	CHA-C4D-ND	2.40	137.50	132.55
31	n1	602	CLA	CHA-C4D-ND	2.40	137.50	132.55

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	d1	403	CLA	CHD-C1D-ND	-2.40	121.43	124.80
31	g1	611	CLA	CHD-C1D-ND	-2.40	121.43	124.80
31	B	608	CLA	C4B-CHC-C1C	2.40	131.89	126.25
31	G	612	CLA	C3B-C4B-NB	-2.40	108.39	110.53
31	N1	613	CLA	C1-O2A-CGA	2.40	122.46	116.65
31	c	511	CLA	CHA-C4D-ND	2.40	137.50	132.55
47	r	607	CHL	CMA-C3A-C4A	2.40	119.78	114.61
31	b1	606	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
31	b	604	CLA	C1-C2-C3	-2.40	122.27	126.20
31	r	611	CLA	C4B-CHC-C1C	2.40	131.88	126.25
31	g1	603	CLA	CHD-C1D-ND	-2.40	121.43	124.80
31	Y	614	CLA	CMD-C2D-C3D	-2.40	122.19	127.69
31	G1	602	CLA	C1C-C2C-C3C	-2.40	104.46	106.98
31	R	609	CLA	C4B-CHC-C1C	2.40	131.88	126.25
31	b	612	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
31	g	610	CLA	CMD-C2D-C3D	-2.40	122.19	127.69
31	g1	602	CLA	CMC-C2C-C1C	2.40	128.78	125.03
31	c	502	CLA	C2C-C1C-NC	2.40	112.50	109.98
31	n	602	CLA	C2C-C1C-NC	2.40	112.50	109.98
31	C1	504	CLA	O2D-CGD-O1D	-2.40	119.18	123.85
31	G	611	CLA	C4B-CHC-C1C	2.40	131.88	126.25
47	n	601	CHL	C4C-CHD-C1D	2.40	124.64	116.07
31	B	602	CLA	CHA-C1A-NA	-2.40	120.97	126.39
31	G	614	CLA	CMD-C2D-C3D	-2.40	122.20	127.69
31	y1	603	CLA	CHD-C1D-ND	-2.40	121.43	124.80
31	A1	410	CLA	O2A-CGA-CBA	2.39	119.14	111.83
31	C	512	CLA	O2A-CGA-CBA	2.39	119.14	111.83
31	n1	611	CLA	CHA-C4D-ND	2.39	137.49	132.55
31	B	616	CLA	C3B-C4B-NB	-2.39	108.39	110.53
47	s1	601	CHL	C4C-CHD-C1D	2.39	124.63	116.07
31	C1	513	CLA	C4B-CHC-C1C	2.39	131.88	126.25
31	A	407	CLA	C1-O2A-CGA	2.39	122.44	116.65
31	n1	604	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
31	b	612	CLA	C4B-CHC-C1C	2.39	131.88	126.25
31	s	617	CLA	C1D-ND-C4D	-2.39	104.63	106.31
31	n1	610	CLA	CHA-C4D-ND	2.39	137.49	132.55
31	G1	614	CLA	O2A-CGA-CBA	2.39	119.13	111.83
31	B1	608	CLA	C3B-C4B-NB	-2.39	108.39	110.53
31	N1	614	CLA	O2D-CGD-O1D	-2.39	119.19	123.85
31	R1	604	CLA	C1-O2A-CGA	2.39	122.44	116.65
31	A	410	CLA	C4B-CHC-C1C	2.39	131.87	126.25
31	r1	604	CLA	O2D-CGD-O1D	-2.39	119.19	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	n1	601	CHL	C4C-CHD-C1D	2.39	124.63	116.07
31	b	604	CLA	C3B-C4B-NB	-2.39	108.39	110.53
31	y	603	CLA	C2D-C1D-ND	2.39	112.49	110.13
31	y	610	CLA	CHD-C1D-ND	-2.39	121.44	124.80
31	y	612	CLA	C4B-CHC-C1C	2.39	131.87	126.25
31	S1	609	CLA	C4B-CHC-C1C	2.39	131.87	126.25
31	S	603	CLA	CHA-C1A-NA	-2.39	120.98	126.39
31	n1	613	CLA	C3B-C4B-NB	-2.39	108.40	110.53
31	Y1	604	CLA	C1D-ND-C4D	-2.39	104.64	106.31
31	b1	611	CLA	CHA-C4D-ND	2.39	137.48	132.55
31	N	602	CLA	C4B-CHC-C1C	2.39	131.87	126.25
31	A1	406	CLA	CHD-C1D-ND	-2.39	121.44	124.80
41	Y	624	LHG	C6-C5-C4	-2.39	106.21	111.78
31	N	602	CLA	C1D-ND-C4D	-2.39	104.64	106.31
31	n	603	CLA	CHD-C1D-ND	-2.39	121.44	124.80
31	B1	603	CLA	CHA-C4D-ND	2.39	137.48	132.55
31	y1	604	CLA	CHA-C4D-ND	2.39	137.48	132.55
48	y	620	LUT	C30-C31-C32	-2.39	116.28	123.20
31	D	403	CLA	CHA-C4D-ND	2.39	137.48	132.55
31	D	403	CLA	CHD-C1D-ND	-2.39	121.44	124.80
31	A1	410	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
31	g1	603	CLA	O2D-CGD-O1D	-2.39	119.20	123.85
31	y1	602	CLA	C4B-CHC-C1C	2.39	131.86	126.25
31	r	603	CLA	C1-C2-C3	-2.39	122.28	126.20
31	n	614	CLA	C4B-CHC-C1C	2.39	131.86	126.25
50	N	623	NEX	C31-C30-C29	2.39	130.63	127.28
31	y	603	CLA	C1D-ND-C4D	-2.39	104.64	106.31
48	s	621	LUT	C22-C23-C24	-2.39	107.64	111.18
31	a1	407	CLA	O2A-CGA-CBA	2.39	119.11	111.83
31	g1	611	CLA	C4B-CHC-C1C	2.39	131.86	126.25
50	g	623	NEX	C19-C9-C10	-2.39	118.95	122.82
56	R1	626	ERG	C1-C10-C9	-2.39	103.75	108.39
33	c1	517	BCR	C35-C13-C12	2.39	121.73	118.09
31	c	508	CLA	CHA-C4D-ND	2.39	137.47	132.55
31	R	611	CLA	C4B-CHC-C1C	2.39	131.86	126.25
31	S1	612	CLA	C4B-CHC-C1C	2.39	131.86	126.25
31	n1	610	CLA	CHD-C1D-ND	-2.39	121.44	124.80
31	B1	615	CLA	CMD-C2D-C3D	-2.39	122.22	127.69
31	Y	613	CLA	C4B-CHC-C1C	2.39	131.86	126.25
47	S1	606	CHL	C4C-CHD-C1D	2.39	124.61	116.07
31	s1	612	CLA	CHD-C1D-ND	-2.39	121.44	124.80
31	C	505	CLA	OBD-CAD-C3D	-2.39	122.84	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	Y	611	CLA	CHA-C1A-NA	-2.39	120.99	126.39
31	n1	611	CLA	C2D-C1D-ND	2.39	112.49	110.13
31	R	604	CLA	CMD-C2D-C3D	-2.39	122.22	127.69
55	r1	625	LMT	C1'-O5'-C5'	-2.39	109.06	113.72
33	c1	515	BCR	C33-C5-C4	2.38	118.68	113.60
47	G	606	CHL	C4C-CHD-C1D	2.38	124.60	116.07
31	y1	611	CLA	C3B-C4B-NB	-2.38	108.40	110.53
31	C1	504	CLA	C4B-CHC-C1C	2.38	131.85	126.25
31	n	603	CLA	CMD-C2D-C3D	-2.38	122.22	127.69
31	n	602	CLA	CHA-C4D-ND	2.38	137.47	132.55
31	b1	604	CLA	CHA-C4D-ND	2.38	137.47	132.55
47	Y1	607	CHL	C1-C2-C3	-2.38	122.29	126.20
47	r1	607	CHL	C1-O2A-CGA	2.38	122.42	116.65
47	Y	605	CHL	CMA-C3A-C4A	2.38	119.75	114.61
31	c1	511	CLA	C2C-C1C-NC	2.38	112.49	109.98
31	N	612	CLA	C3B-C4B-NB	-2.38	108.40	110.53
31	Y	604	CLA	CHD-C1D-ND	-2.38	121.45	124.80
31	y	614	CLA	CAA-CBA-CGA	-2.38	106.44	113.21
31	R	613	CLA	C4B-CHC-C1C	2.38	131.85	126.25
31	c1	506	CLA	O2A-CGA-CBA	2.38	119.10	111.83
31	r1	604	CLA	C4B-CHC-C1C	2.38	131.85	126.25
31	r	610	CLA	C1D-ND-C4D	-2.38	104.64	106.31
31	N	603	CLA	CBC-CAC-C3C	-2.38	105.96	112.42
31	B1	606	CLA	CHD-C1D-ND	-2.38	121.45	124.80
31	S1	602	CLA	CHA-C4D-ND	2.38	137.47	132.55
31	B1	602	CLA	C3B-C4B-NB	-2.38	108.40	110.53
31	s1	610	CLA	C3B-C4B-NB	-2.38	108.40	110.53
31	y1	608	CLA	C3B-C4B-NB	-2.38	108.40	110.53
31	B1	611	CLA	C2D-C1D-ND	2.38	112.48	110.13
31	b1	605	CLA	C2D-C1D-ND	2.38	112.48	110.13
31	c	513	CLA	CHA-C4D-ND	2.38	137.46	132.55
31	y	608	CLA	CHD-C1D-ND	-2.38	121.45	124.80
31	A1	407	CLA	CAA-CBA-CGA	-2.38	106.44	113.21
31	b1	615	CLA	CMA-C3A-C4A	2.38	118.17	111.77
48	S	621	LUT	C8-C7-C6	-2.38	120.64	127.00
31	Y1	614	CLA	CMD-C2D-C3D	-2.38	122.23	127.69
47	n1	607	CHL	C4C-CHD-C1D	2.38	124.59	116.07
31	C	509	CLA	C4B-CHC-C1C	2.38	131.85	126.25
31	Y	613	CLA	O2D-CGD-O1D	-2.38	119.21	123.85
31	B1	608	CLA	CHD-C1D-ND	-2.38	121.45	124.80
31	r	610	CLA	C2C-C1C-NC	2.38	112.48	109.98
31	y1	604	CLA	O2A-CGA-CBA	2.38	119.09	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	y1	612	CLA	CMA-C3A-C4A	2.38	118.17	111.77
31	N	610	CLA	O1D-CGD-CBD	-2.38	119.83	124.52
31	b	608	CLA	C3B-C4B-NB	-2.38	108.41	110.53
31	R1	608	CLA	C3B-C4B-NB	-2.38	108.41	110.53
31	r	611	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
33	D1	404	BCR	C33-C5-C6	-2.38	121.89	124.48
31	N	614	CLA	O2A-CGA-CBA	2.38	119.09	111.83
31	R	610	CLA	C1D-ND-C4D	-2.38	104.64	106.31
31	c	504	CLA	CHD-C1D-ND	-2.38	121.45	124.80
33	c1	517	BCR	C1-C6-C7	2.38	122.10	115.65
47	g	609	CHL	C4C-CHD-C1D	2.38	124.58	116.07
31	n	614	CLA	CHA-C4D-ND	2.38	137.46	132.55
31	N1	602	CLA	C4B-CHC-C1C	2.38	131.84	126.25
31	c	502	CLA	C2D-C1D-ND	2.38	112.48	110.13
31	c	511	CLA	C1D-ND-C4D	-2.38	104.64	106.31
49	G1	622	XAT	O4-C5-C4	-2.38	111.26	113.49
31	C1	513	CLA	C1-O2A-CGA	2.38	122.41	116.65
31	S	617	CLA	C4B-CHC-C1C	2.38	131.84	126.25
31	Y1	611	CLA	CMD-C2D-C3D	-2.38	122.24	127.69
44	D	405	PL9	C20-C19-C21	2.38	119.35	115.23
47	n	605	CHL	C4D-CHA-CBD	-2.38	106.57	108.97
31	G	603	CLA	C1D-ND-C4D	-2.38	104.64	106.31
48	y	620	LUT	C15-C14-C13	-2.38	123.95	127.28
31	s	614	CLA	CHD-C1D-ND	-2.38	121.46	124.80
31	b1	610	CLA	O2A-CGA-CBA	2.38	119.08	111.83
31	C1	506	CLA	CAA-C2A-C3A	-2.38	106.58	113.00
31	A1	406	CLA	C2C-C1C-NC	2.38	112.48	109.98
31	s1	612	CLA	C4B-CHC-C1C	2.38	131.83	126.25
47	g1	606	CHL	C4C-CHD-C1D	2.38	124.57	116.07
31	A1	410	CLA	CMC-C2C-C1C	2.38	128.75	125.03
31	A	406	CLA	CHD-C1D-ND	-2.38	121.46	124.80
31	c1	510	CLA	O2D-CGD-O1D	-2.38	119.22	123.85
31	b1	603	CLA	CHA-C4D-ND	2.37	137.45	132.55
31	N1	603	CLA	C4B-CHC-C1C	2.37	131.83	126.25
47	y1	607	CHL	C1A-CHA-C4D	2.37	122.94	118.98
31	g	610	CLA	C1D-ND-C4D	-2.37	104.65	106.31
31	b1	611	CLA	C1D-ND-C4D	-2.37	104.65	106.31
47	y1	609	CHL	CMA-C3A-C4A	2.37	119.73	114.61
47	Y	601	CHL	C1-O2A-CGA	2.37	122.40	116.65
31	c	506	CLA	CHA-C4D-ND	2.37	137.45	132.55
47	s1	601	CHL	CMA-C3A-C4A	2.37	119.73	114.61
48	s	621	LUT	C1-C6-C7	2.37	122.09	115.65

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
40	C	519	DGD	C2G-O2G-C1B	-2.37	112.11	117.80
31	Y1	612	CLA	C4B-CHC-C1C	2.37	131.83	126.25
31	y1	614	CLA	CAA-C2A-C3A	-2.37	106.59	113.00
47	n	601	CHL	C1-O2A-CGA	2.37	122.39	116.65
31	B	617	CLA	CHA-C4D-ND	2.37	137.44	132.55
31	G	611	CLA	C1D-ND-C4D	-2.37	104.65	106.31
47	G	601	CHL	CMA-C3A-C4A	2.37	119.72	114.61
31	S1	614	CLA	O2D-CGD-O1D	-2.37	119.23	123.85
31	G1	614	CLA	C4B-CHC-C1C	2.37	131.83	126.25
49	N	622	XAT	C6-C7-C8	-2.37	120.98	125.99
37	b1	620	C7Z	C15-C35-C34	-2.37	118.66	123.52
31	c	506	CLA	O2A-CGA-CBA	2.37	119.07	111.83
47	n1	605	CHL	CMA-C3A-C4A	2.37	119.72	114.61
50	n1	623	NEX	C31-C32-C33	2.37	132.87	126.36
33	a1	411	BCR	C38-C26-C25	-2.37	121.90	124.48
31	n	613	CLA	C2C-C1C-NC	2.37	112.47	109.98
31	r1	602	CLA	C2C-C1C-NC	2.37	112.47	109.98
31	g	611	CLA	C4B-CHC-C1C	2.37	131.82	126.25
31	G	603	CLA	C3B-C4B-NB	-2.37	108.41	110.53
31	s1	605	CLA	CHA-C1A-NA	-2.37	121.02	126.39
31	d1	403	CLA	CMD-C2D-C3D	-2.37	122.25	127.69
31	C1	507	CLA	CAC-C3C-C4C	2.37	127.88	124.79
47	Y1	601	CHL	C1-O2A-CGA	2.37	122.39	116.65
31	A1	410	CLA	C4B-CHC-C1C	2.37	131.82	126.25
31	s	610	CLA	C4B-CHC-C1C	2.37	131.82	126.25
31	S1	605	CLA	CMD-C2D-C3D	-2.37	122.25	127.69
31	b	613	CLA	O2A-CGA-CBA	2.37	119.06	111.83
45	f	101	HEM	C3D-C4D-ND	-2.37	107.57	110.17
35	d	411	LMG	O1-C1-C2	2.37	111.87	108.27
31	Y	608	CLA	CMD-C2D-C3D	-2.37	122.26	127.69
33	C	517	BCR	C23-C24-C25	-2.37	120.67	127.00
31	c1	513	CLA	C2C-C1C-NC	2.37	112.47	109.98
31	s	612	CLA	CHD-C1D-ND	-2.37	121.47	124.80
31	g1	604	CLA	C4B-CHC-C1C	2.37	131.82	126.25
31	N	602	CLA	CHA-C4D-ND	2.37	137.44	132.55
31	s	609	CLA	CHA-C4D-ND	2.37	137.44	132.55
31	C1	512	CLA	C3B-C4B-NB	-2.37	108.42	110.53
31	c1	508	CLA	C3B-C4B-NB	-2.37	108.42	110.53
48	S1	621	LUT	C31-C30-C29	-2.37	123.96	127.28
31	n	603	CLA	O2A-CGA-CBA	2.37	119.06	111.83
31	N	613	CLA	C1C-C2C-C3C	-2.37	104.49	106.98
31	A1	407	CLA	C4B-CHC-C1C	2.37	131.81	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c1	504	CLA	C4B-CHC-C1C	2.37	131.81	126.25
31	G1	604	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
31	C	503	CLA	C1D-ND-C4D	-2.37	104.65	106.31
31	c1	507	CLA	CAA-C2A-C3A	-2.37	106.60	113.00
31	C1	502	CLA	CHA-C4D-ND	2.37	137.43	132.55
31	g	613	CLA	C3B-C4B-NB	-2.37	108.42	110.53
31	R1	610	CLA	O2A-CGA-CBA	2.37	119.05	111.83
31	G	614	CLA	O2D-CGD-O1D	-2.37	119.24	123.85
31	A1	407	CLA	CHA-C4D-ND	2.37	137.43	132.55
31	N1	611	CLA	CHA-C1A-NA	-2.37	121.03	126.39
47	g1	606	CHL	CAA-C2A-C3A	-2.37	106.60	113.00
31	g1	614	CLA	C1-O2A-CGA	2.37	122.38	116.65
31	s1	612	CLA	C2D-C1D-ND	2.37	112.47	110.13
31	r	602	CLA	O2A-CGA-CBA	2.37	119.05	111.83
47	y	607	CHL	C4C-CHD-C1D	2.37	124.53	116.07
31	r1	610	CLA	C1D-ND-C4D	-2.37	104.65	106.31
31	b1	604	CLA	C3B-C4B-NB	-2.37	108.42	110.53
47	n	609	CHL	C1-C2-C3	-2.37	122.32	126.20
31	c	501	CLA	C4B-CHC-C1C	2.37	131.81	126.25
31	c	510	CLA	C4B-CHC-C1C	2.37	131.81	126.25
31	B1	617	CLA	C4B-CHC-C1C	2.37	131.81	126.25
48	N	620	LUT	C26-C27-C28	-2.37	120.90	124.58
31	N	612	CLA	CAA-C2A-C3A	-2.37	106.61	113.00
31	N1	614	CLA	C4B-CHC-C1C	2.37	131.81	126.25
31	B1	611	CLA	CHA-C4D-ND	2.36	137.43	132.55
48	n1	620	LUT	C35-C15-C14	-2.36	118.68	123.52
31	b	614	CLA	C1D-ND-C4D	-2.36	104.65	106.31
31	n1	602	CLA	CHD-C1D-ND	-2.36	121.47	124.80
31	g1	613	CLA	C4B-CHC-C1C	2.36	131.81	126.25
31	N1	614	CLA	C2D-C1D-ND	2.36	112.47	110.13
31	G	602	CLA	CMD-C2D-C3D	-2.36	122.27	127.69
31	g	611	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
31	G	602	CLA	C2C-C1C-NC	2.36	112.47	109.98
48	R1	620	LUT	C8-C7-C6	-2.36	120.68	127.00
31	g	604	CLA	CHD-C1D-ND	-2.36	121.48	124.80
31	n	603	CLA	C4B-CHC-C1C	2.36	131.81	126.25
31	G	604	CLA	CMD-C2D-C3D	-2.36	122.27	127.69
31	A1	405	CLA	C6-C5-C3	-2.36	107.71	113.47
50	y	623	NEX	C31-C32-C33	2.36	132.84	126.36
48	G	620	LUT	C27-C28-C29	-2.36	121.24	126.32
48	s	621	LUT	C10-C11-C12	-2.36	116.35	123.20
31	y	613	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	G	604	CLA	O2A-CGA-CBA	2.36	119.04	111.83
31	R1	603	CLA	CHA-C1A-NA	-2.36	121.04	126.39
31	N1	602	CLA	C3B-C4B-NB	-2.36	108.42	110.53
31	y1	603	CLA	C3B-C4B-NB	-2.36	108.42	110.53
31	B	612	CLA	CHA-C4D-ND	2.36	137.42	132.55
31	G	614	CLA	CHA-C4D-ND	2.36	137.42	132.55
50	R1	622	NEX	C31-C30-C29	2.36	130.59	127.28
31	b	607	CLA	CMA-C3A-C4A	2.36	118.12	111.77
49	R1	621	XAT	O4-C6-C7	-2.36	110.11	116.88
31	N1	604	CLA	O1D-CGD-CBD	-2.36	119.86	124.52
31	A1	406	CLA	CHA-C4D-ND	2.36	137.42	132.55
48	s	620	LUT	C35-C15-C14	-2.36	118.69	123.52
31	a	406	CLA	C4B-CHC-C1C	2.36	131.80	126.25
31	G	603	CLA	CHA-C4D-ND	2.36	137.42	132.55
31	r1	609	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
31	R1	602	CLA	C4B-CHC-C1C	2.36	131.80	126.25
31	R	610	CLA	O2A-CGA-CBA	2.36	119.03	111.83
31	b	602	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
31	b	607	CLA	CAC-C3C-C4C	2.36	127.86	124.79
31	b	604	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
31	n1	612	CLA	CHA-C4D-ND	2.36	137.42	132.55
53	y	625	SPH	C3-C4-C5	-2.36	119.80	124.69
31	R	608	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
31	S	609	CLA	O2D-CGD-O1D	-2.36	119.25	123.85
41	Y1	624	LHG	C6-C5-C4	-2.36	106.28	111.78
31	S	602	CLA	C2C-C1C-NC	2.36	112.46	109.98
31	N1	604	CLA	CHA-C1A-NA	-2.36	121.05	126.39
32	a1	408	PHO	C3B-C4B-NB	-2.36	105.93	107.46
31	y1	603	CLA	CHA-C4D-ND	2.36	137.41	132.55
47	S	601	CHL	C1C-C2C-CMC	2.36	131.05	126.80
34	a	412	SQD	O3-C3-C2	-2.36	104.82	110.38
47	Y1	601	CHL	CMA-C3A-C4A	2.36	119.69	114.61
31	s1	602	CLA	C2D-C1D-ND	2.36	112.46	110.13
49	r1	621	XAT	C6-C7-C8	-2.36	121.01	125.99
48	r1	620	LUT	C27-C28-C29	-2.36	121.25	126.32
31	N1	613	CLA	C3B-C4B-NB	-2.36	108.43	110.53
31	c1	504	CLA	C3B-C4B-NB	-2.36	108.43	110.53
31	R	609	CLA	CHD-C1D-ND	-2.36	121.49	124.80
31	N1	611	CLA	CHD-C1D-ND	-2.36	121.49	124.80
31	a	407	CLA	C4B-CHC-C1C	2.36	131.79	126.25
31	g	604	CLA	C4B-CHC-C1C	2.36	131.79	126.25
47	N1	607	CHL	C1-C2-C3	-2.36	122.34	126.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	D	403	CLA	C1D-ND-C4D	-2.36	104.66	106.31
47	N1	607	CHL	CMA-C3A-C4A	2.36	119.69	114.61
31	c1	509	CLA	CHA-C4D-ND	2.36	137.41	132.55
31	s1	617	CLA	CAA-C2A-C3A	-2.36	106.63	113.00
48	N	621	LUT	C22-C23-C24	-2.36	107.69	111.18
33	C	515	BCR	C38-C26-C25	-2.36	121.91	124.48
31	B1	603	CLA	CHD-C1D-ND	-2.36	121.49	124.80
41	D1	408	LHG	O8-C23-C24	2.36	119.02	111.83
31	C1	511	CLA	CMD-C2D-C3D	-2.36	122.29	127.69
37	b	620	C7Z	C7-C8-C9	-2.36	122.75	126.23
47	S1	608	CHL	CMA-C3A-C4A	2.35	119.69	114.61
47	N1	606	CHL	C1-O2A-CGA	2.35	122.35	116.65
31	Y1	604	CLA	O2A-CGA-CBA	2.35	119.02	111.83
31	C	503	CLA	CMD-C2D-C3D	-2.35	122.29	127.69
31	c1	503	CLA	C3B-C4B-NB	-2.35	108.43	110.53
31	b	606	CLA	CHD-C1D-ND	-2.35	121.49	124.80
31	y1	610	CLA	CHD-C1D-ND	-2.35	121.49	124.80
47	s	601	CHL	CMA-C3A-C4A	2.35	119.68	114.61
50	r1	622	NEX	C1-C2-C3	2.35	118.76	113.59
31	a	407	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
31	n	602	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
31	N	604	CLA	CHD-C1D-ND	-2.35	121.49	124.80
49	g	622	XAT	O24-C25-C24	2.35	115.70	113.49
31	C	507	CLA	C4B-CHC-C1C	2.35	131.78	126.25
31	Y	602	CLA	CAA-C2A-C3A	-2.35	106.64	113.00
31	S1	612	CLA	C1D-ND-C4D	-2.35	104.66	106.31
31	n	613	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
31	n1	602	CLA	CMD-C2D-C3D	-2.35	122.29	127.69
33	c	514	BCR	C34-C9-C10	-2.35	119.00	122.82
31	y	613	CLA	C4B-CHC-C1C	2.35	131.78	126.25
31	c	510	CLA	CAA-C2A-C3A	-2.35	106.64	113.00
31	d1	402	CLA	O2D-CGD-O1D	-2.35	119.27	123.85
31	B1	606	CLA	C3B-C4B-NB	-2.35	108.43	110.53
31	Y	603	CLA	CHD-C1D-ND	-2.35	121.49	124.80
32	a	409	PHO	C1-C2-C3	-2.35	122.34	126.20
31	Y	611	CLA	CHA-C4D-ND	2.35	137.40	132.55
31	C1	513	CLA	C2D-C1D-ND	2.35	112.45	110.13
31	d1	402	CLA	C1-C2-C3	-2.35	122.34	126.20
31	R1	612	CLA	CHD-C1D-ND	-2.35	121.49	124.80
31	Y1	604	CLA	CHD-C1D-ND	-2.35	121.49	124.80
31	R	609	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
31	N	602	CLA	C3B-C4B-NB	-2.35	108.43	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	S	604	CLA	CHA-C4D-ND	2.35	137.40	132.55
31	b1	617	CLA	C1-O2A-CGA	2.35	122.34	116.65
31	b1	615	CLA	CHA-C1A-NA	-2.35	121.07	126.39
37	B1	620	C7Z	C23-C24-C25	2.35	118.03	112.18
33	c1	514	BCR	C4-C5-C6	-2.35	119.53	122.70
31	s1	610	CLA	O1D-CGD-CBD	-2.35	119.88	124.52
31	y	603	CLA	O1D-CGD-CBD	-2.35	119.88	124.52
31	b	610	CLA	C1-O2A-CGA	2.35	122.34	116.65
31	c1	511	CLA	C1C-C2C-C3C	-2.35	104.51	106.98
31	b	603	CLA	CHD-C1D-ND	-2.35	121.50	124.80
31	S1	602	CLA	C1D-ND-C4D	-2.35	104.66	106.31
31	s	604	CLA	C4B-CHC-C1C	2.35	131.77	126.25
31	N	604	CLA	O2A-CGA-CBA	2.35	119.00	111.83
31	Y1	603	CLA	O2A-CGA-CBA	2.35	119.00	111.83
31	S	605	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
31	r1	610	CLA	CHA-C4D-ND	2.35	137.40	132.55
31	S	603	CLA	O2A-CGA-CBA	2.35	119.00	111.83
31	c1	503	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
31	n1	613	CLA	CHA-C1A-NA	-2.35	121.07	126.39
31	B	603	CLA	O2A-CGA-CBA	2.35	119.00	111.83
50	S1	623	NEX	C19-C9-C10	-2.35	119.01	122.82
31	r	604	CLA	CMA-C3A-C4A	2.35	118.09	111.77
31	r	612	CLA	CHA-C1A-NA	-2.35	121.07	126.39
31	b	611	CLA	O2D-CGD-O1D	-2.35	119.28	123.85
31	B	603	CLA	CHD-C1D-ND	-2.35	121.50	124.80
32	A	409	PHO	C1-C2-C3	-2.35	122.35	126.20
31	A	406	CLA	CMD-C2D-C3D	-2.35	122.30	127.69
31	a	410	CLA	C4B-CHC-C1C	2.35	131.77	126.25
31	b	603	CLA	C4B-CHC-C1C	2.35	131.77	126.25
31	a1	407	CLA	C4B-CHC-C1C	2.35	131.77	126.25
31	b1	604	CLA	C2D-C1D-ND	2.35	112.45	110.13
31	B	610	CLA	C3B-C4B-NB	-2.35	108.43	110.53
31	B	605	CLA	O2A-CGA-CBA	2.35	118.99	111.83
31	g	614	CLA	C1-O2A-CGA	2.35	122.33	116.65
31	G1	613	CLA	CHD-C1D-ND	-2.35	121.50	124.80
31	y1	604	CLA	C4B-CHC-C1C	2.35	131.77	126.25
50	r	623	NEX	C39-C29-C30	-2.35	119.01	122.82
33	c	514	BCR	C30-C25-C26	-2.35	119.43	122.64
31	s1	611	CLA	C4B-CHC-C1C	2.35	131.77	126.25
31	C	506	CLA	O1D-CGD-CBD	-2.35	119.89	124.52
31	b	603	CLA	CHA-C4D-ND	2.35	137.39	132.55
31	c1	506	CLA	C3B-C4B-NB	-2.35	108.44	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B1	603	CLA	O2A-CGA-CBA	2.35	118.99	111.83
33	c	515	BCR	C1-C6-C7	2.35	122.01	115.65
31	r	610	CLA	C2D-C1D-ND	2.35	112.45	110.13
31	s1	617	CLA	C2D-C1D-ND	2.35	112.45	110.13
31	C	510	CLA	CMD-C2D-C3D	-2.35	122.31	127.69
31	B	607	CLA	C3B-C4B-NB	-2.35	108.44	110.53
31	C	506	CLA	C4B-CHC-C1C	2.35	131.76	126.25
31	R	612	CLA	C1-C2-C3	-2.35	122.35	126.20
31	S1	603	CLA	CHA-C1A-NA	-2.35	121.08	126.39
31	G	613	CLA	CHD-C1D-ND	-2.35	121.50	124.80
31	C	513	CLA	C4B-CHC-C1C	2.35	131.76	126.25
31	r1	610	CLA	CMA-C3A-C4A	2.34	118.08	111.77
31	R	604	CLA	O2D-CGD-O1D	-2.34	119.28	123.85
31	n1	602	CLA	O2D-CGD-O1D	-2.34	119.28	123.85
47	n	607	CHL	C4C-CHD-C1D	2.34	124.46	116.07
31	C1	506	CLA	CHD-C1D-ND	-2.34	121.50	124.80
33	B1	619	BCR	C8-C7-C6	-2.34	120.73	127.00
31	s	611	CLA	CHD-C1D-ND	-2.34	121.50	124.80
47	y1	609	CHL	C4C-CHD-C1D	2.34	124.45	116.07
31	r1	612	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
31	c1	502	CLA	C1C-C2C-C3C	-2.34	104.52	106.98
47	g1	605	CHL	C4C-CHD-C1D	2.34	124.45	116.07
50	N1	623	NEX	C31-C32-C33	2.34	132.79	126.36
31	B	614	CLA	C4B-CHC-C1C	2.34	131.76	126.25
48	S	621	LUT	C22-C23-C24	-2.34	107.70	111.18
47	Y	601	CHL	C4C-CHD-C1D	2.34	124.45	116.07
44	d	405	PL9	O1-C4-C3	-2.34	118.26	120.73
33	c1	516	BCR	C33-C5-C4	2.34	118.59	113.60
31	c	513	CLA	C4B-CHC-C1C	2.34	131.76	126.25
31	S	604	CLA	CHD-C1D-ND	-2.34	121.51	124.80
31	c1	504	CLA	CHD-C1D-ND	-2.34	121.51	124.80
31	C	504	CLA	C4B-CHC-C1C	2.34	131.75	126.25
31	n	604	CLA	C2C-C1C-NC	2.34	112.44	109.98
31	C1	510	CLA	CAA-C2A-C3A	-2.34	106.67	113.00
31	A1	406	CLA	CMD-C2D-C3D	-2.34	122.32	127.69
31	R	604	CLA	O2A-CGA-CBA	2.34	118.97	111.83
31	s	611	CLA	O1D-CGD-CBD	-2.34	119.90	124.52
31	c1	511	CLA	C3B-C4B-NB	-2.34	108.44	110.53
31	g1	602	CLA	O2D-CGD-O1D	-2.34	119.29	123.85
31	C	509	CLA	CHD-C1D-ND	-2.34	121.51	124.80
31	D	403	CLA	C4B-CHC-C1C	2.34	131.75	126.25
31	c	502	CLA	C1C-C2C-C3C	-2.34	104.52	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	S1	621	LUT	C38-C25-C24	-2.34	117.82	123.36
31	y	608	CLA	C4B-CHC-C1C	2.34	131.75	126.25
47	N	607	CHL	C4C-CHD-C1D	2.34	124.44	116.07
31	c1	501	CLA	CHD-C1D-ND	-2.34	121.51	124.80
31	r	604	CLA	C1D-ND-C4D	-2.34	104.67	106.31
31	g1	602	CLA	C1D-ND-C4D	-2.34	104.67	106.31
31	G1	610	CLA	C2D-C1D-ND	2.34	112.44	110.13
48	s1	620	LUT	C1-C6-C5	-2.34	119.44	122.64
31	g1	614	CLA	C4B-CHC-C1C	2.34	131.75	126.25
31	b1	603	CLA	CHD-C1D-ND	-2.34	121.51	124.80
49	r1	621	XAT	O4-C6-C7	-2.34	110.17	116.88
41	D1	408	LHG	C5-O7-C7	-2.34	112.20	117.80
49	n	622	XAT	C19-C9-C10	-2.34	119.03	122.82
31	Y	603	CLA	C2D-C1D-ND	2.34	112.44	110.13
48	N1	621	LUT	C35-C15-C14	-2.34	118.73	123.52
31	n	602	CLA	C3B-C4B-NB	-2.34	108.44	110.53
31	y1	612	CLA	C3B-C4B-NB	-2.34	108.44	110.53
31	R	610	CLA	CHA-C4D-ND	2.34	137.37	132.55
31	b	617	CLA	CHA-C4D-ND	2.34	137.37	132.55
31	s	617	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
31	B1	604	CLA	C4B-CHC-C1C	2.34	131.75	126.25
31	a1	405	CLA	C1-O2A-CGA	2.34	122.31	116.65
31	G1	613	CLA	O2A-CGA-CBA	2.34	118.96	111.83
31	N1	604	CLA	C3B-C4B-NB	-2.34	108.44	110.53
31	g	602	CLA	CHA-C1A-NA	-2.34	121.10	126.39
47	N	606	CHL	C4C-CHD-C1D	2.34	124.43	116.07
48	Y	620	LUT	C38-C25-C24	-2.34	117.83	123.36
31	Y	614	CLA	O2D-CGD-O1D	-2.34	119.30	123.85
31	N1	614	CLA	CHA-C4D-ND	2.34	137.37	132.55
31	c	507	CLA	C1-O2A-CGA	2.34	122.31	116.65
48	n	621	LUT	C1-C6-C5	-2.34	119.44	122.64
31	S1	617	CLA	C2D-C1D-ND	2.34	112.44	110.13
31	r	609	CLA	CMA-C3A-C4A	2.34	118.05	111.77
31	s	612	CLA	CMD-C2D-C3D	-2.34	122.33	127.69
37	B1	620	C7Z	C11-C12-C13	-2.34	119.96	126.36
31	c	513	CLA	C2C-C1C-NC	2.34	112.44	109.98
33	c	517	BCR	C35-C13-C12	2.34	121.66	118.09
50	Y	623	NEX	C31-C32-C33	2.34	132.77	126.36
31	s	602	CLA	CMA-C3A-C4A	2.34	118.05	111.77
31	c	506	CLA	CHA-C1A-NA	-2.34	121.10	126.39
31	y1	613	CLA	C1C-C2C-C3C	-2.34	104.52	106.98
31	c	507	CLA	O2A-CGA-CBA	2.34	118.96	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b1	613	CLA	O2A-CGA-CBA	2.34	118.96	111.83
31	A	405	CLA	CHD-C1D-ND	-2.34	121.52	124.80
31	c	507	CLA	CHD-C1D-ND	-2.34	121.52	124.80
31	C1	513	CLA	C1C-C2C-C3C	-2.34	104.52	106.98
31	C	513	CLA	CHA-C4D-ND	2.33	137.37	132.55
31	c	504	CLA	CHA-C4D-ND	2.33	137.37	132.55
31	G	613	CLA	CMD-C2D-C3D	-2.33	122.33	127.69
31	G1	613	CLA	C4B-CHC-C1C	2.33	131.74	126.25
31	Y1	608	CLA	C4B-CHC-C1C	2.33	131.74	126.25
31	B	606	CLA	C1D-ND-C4D	-2.33	104.67	106.31
31	B	609	CLA	C1-O2A-CGA	2.33	122.30	116.65
31	S	602	CLA	C4B-CHC-C1C	2.33	131.74	126.25
31	Y1	613	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
31	C	510	CLA	CAA-C2A-C3A	-2.33	106.69	113.00
48	N1	621	LUT	C38-C25-C24	-2.33	117.84	123.36
33	B	618	BCR	C36-C18-C17	-2.33	119.03	122.82
31	B1	603	CLA	C4B-CHC-C1C	2.33	131.74	126.25
31	B1	607	CLA	C4B-CHC-C1C	2.33	131.74	126.25
31	c	503	CLA	O1D-CGD-CBD	-2.33	119.92	124.52
31	b	609	CLA	CMB-C2B-C1B	-2.33	121.87	125.42
31	g	611	CLA	C3B-C4B-NB	-2.33	108.45	110.53
31	A1	410	CLA	C3B-C4B-NB	-2.33	108.45	110.53
31	C1	506	CLA	O2A-CGA-CBA	2.33	118.95	111.83
31	N1	612	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
31	C1	506	CLA	C3D-C2D-C1D	-2.33	102.65	105.83
31	b1	607	CLA	CHA-C4D-ND	2.33	137.36	132.55
31	c1	505	CLA	C4B-CHC-C1C	2.33	131.73	126.25
31	N1	602	CLA	O2D-CGD-O1D	-2.33	119.31	123.85
31	C	507	CLA	O2A-CGA-CBA	2.33	118.94	111.83
47	s	601	CHL	C4C-CHD-C1D	2.33	124.41	116.07
31	R	612	CLA	CHD-C1D-ND	-2.33	121.52	124.80
31	r	612	CLA	CMA-C3A-C4A	2.33	118.04	111.77
31	a1	405	CLA	C1D-ND-C4D	-2.33	104.68	106.31
47	N	606	CHL	C1-C2-C3	-2.33	122.38	126.20
47	G	601	CHL	C1A-CHA-C4D	2.33	122.87	118.98
31	B	611	CLA	CHA-C4D-ND	2.33	137.36	132.55
31	C	503	CLA	C1C-C2C-C3C	-2.33	104.53	106.98
31	D1	402	CLA	CHA-C1A-NA	-2.33	121.11	126.39
31	y1	610	CLA	C4B-CHC-C1C	2.33	131.73	126.25
50	g1	623	NEX	C31-C32-C33	2.33	132.75	126.36
50	s	623	NEX	C4-C3-C2	2.33	115.15	110.79
31	n1	614	CLA	CMD-C2D-C3D	-2.33	122.34	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	Y	609	CHL	CMA-C3A-C4A	2.33	119.63	114.61
47	y	607	CHL	CMA-C3A-C4A	2.33	119.63	114.61
31	a1	410	CLA	C4B-CHC-C1C	2.33	131.73	126.25
31	C	513	CLA	CHD-C1D-ND	-2.33	121.52	124.80
31	Y	602	CLA	C1D-ND-C4D	-2.33	104.68	106.31
31	C1	504	CLA	C1-O2A-CGA	2.33	122.29	116.65
31	c1	511	CLA	CHA-C1A-NA	-2.33	121.11	126.39
34	A	412	SQD	O3-C3-C2	-2.33	104.88	110.38
31	S1	602	CLA	C2C-C1C-NC	2.33	112.43	109.98
31	B1	609	CLA	CHA-C1A-NA	-2.33	121.12	126.39
31	A1	407	CLA	O2A-CGA-CBA	2.33	118.94	111.83
31	N	614	CLA	C4B-CHC-C1C	2.33	131.72	126.25
31	s1	614	CLA	C4B-CHC-C1C	2.33	131.72	126.25
31	s	617	CLA	CHA-C1A-NA	-2.33	121.12	126.39
31	b1	609	CLA	C2A-C1A-CHA	2.33	127.91	123.87
31	R1	609	CLA	CHA-C4D-ND	2.33	137.35	132.55
31	Y	610	CLA	C4B-CHC-C1C	2.33	131.72	126.25
31	r	602	CLA	CHD-C1D-ND	-2.33	121.53	124.80
31	B	604	CLA	CAA-C2A-C3A	-2.33	106.71	113.00
31	Y	611	CLA	CAA-C2A-C3A	-2.33	106.71	113.00
47	y1	601	CHL	C1A-CHA-C4D	2.33	122.87	118.98
31	B	617	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
31	r	608	CLA	O2D-CGD-O1D	-2.33	119.32	123.85
31	B1	616	CLA	C3B-C4B-NB	-2.33	108.45	110.53
31	g1	612	CLA	CMD-C2D-C3D	-2.33	122.35	127.69
47	G1	605	CHL	C4C-CHD-C1D	2.33	124.40	116.07
31	B	612	CLA	C1D-ND-C4D	-2.33	104.68	106.31
31	C	511	CLA	C4B-CHC-C1C	2.33	131.72	126.25
31	Y	603	CLA	C4B-CHC-C1C	2.33	131.72	126.25
31	R1	609	CLA	C4B-CHC-C1C	2.33	131.72	126.25
31	s1	604	CLA	C4B-CHC-C1C	2.33	131.72	126.25
31	N1	602	CLA	C3D-C2D-C1D	-2.33	102.66	105.83
31	n	613	CLA	C2D-C1D-ND	2.33	112.43	110.13
31	y	612	CLA	C3B-C4B-NB	-2.33	108.45	110.53
31	B1	607	CLA	C1C-C2C-C3C	-2.33	104.53	106.98
49	G1	622	XAT	O4-C5-C18	-2.33	112.45	115.05
56	R1	626	ERG	C11-C9-C10	2.33	119.23	113.65
31	C	512	CLA	C4B-CHC-C1C	2.33	131.72	126.25
31	n1	614	CLA	CHD-C1D-ND	-2.33	121.53	124.80
31	G1	602	CLA	C2C-C1C-NC	2.33	112.42	109.98
31	s	602	CLA	CAC-C3C-C4C	2.33	127.82	124.79
33	c1	516	BCR	C34-C9-C10	-2.33	119.05	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c1	507	CLA	CHA-C1A-NA	-2.33	121.12	126.39
31	C	512	CLA	CHA-C1A-NA	-2.33	121.13	126.39
31	N	613	CLA	C4B-CHC-C1C	2.32	131.71	126.25
31	Y1	608	CLA	CHA-C1A-NA	-2.32	121.13	126.39
31	n	613	CLA	CHD-C1D-ND	-2.32	121.53	124.80
31	n	614	CLA	CHD-C1D-ND	-2.32	121.53	124.80
33	C1	516	BCR	C23-C24-C25	-2.32	120.79	127.00
31	s1	617	CLA	C3B-C4B-NB	-2.32	108.46	110.53
31	R	602	CLA	O1D-CGD-CBD	-2.32	119.94	124.52
49	R1	621	XAT	O24-C25-C24	2.32	115.67	113.49
31	c1	513	CLA	C4B-CHC-C1C	2.32	131.71	126.25
31	c	508	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
31	N1	604	CLA	CMD-C2D-C3D	-2.32	122.36	127.69
47	G	601	CHL	C4C-CHD-C1D	2.32	124.38	116.07
48	y1	621	LUT	C10-C11-C12	-2.32	116.47	123.20
31	c1	512	CLA	C4B-CHC-C1C	2.32	131.71	126.25
44	d	405	PL9	C20-C19-C21	2.32	119.26	115.23
31	D1	402	CLA	CHA-C4D-ND	2.32	137.34	132.55
31	B1	617	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
31	G	603	CLA	CAA-C2A-C3A	-2.32	106.72	113.00
31	b1	602	CLA	CHA-C1A-NA	-2.32	121.13	126.39
31	B	615	CLA	C4B-CHC-C1C	2.32	131.71	126.25
31	N1	603	CLA	CHD-C1D-ND	-2.32	121.53	124.80
31	Y	610	CLA	C3B-C4B-NB	-2.32	108.46	110.53
31	Y	614	CLA	O2A-CGA-CBA	2.32	118.91	111.83
31	N1	604	CLA	C1C-C2C-C3C	-2.32	104.54	106.98
31	c1	505	CLA	CHA-C1A-NA	-2.32	121.14	126.39
31	B1	611	CLA	C1-O2A-CGA	2.32	122.27	116.65
33	a1	411	BCR	C35-C13-C12	2.32	121.63	118.09
31	S	603	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
47	S1	601	CHL	CMA-C3A-C4A	2.32	119.61	114.61
31	C	501	CLA	CHD-C1D-ND	-2.32	121.54	124.80
31	c	510	CLA	CHD-C1D-ND	-2.32	121.54	124.80
31	y1	604	CLA	C3B-C4B-NB	-2.32	108.46	110.53
31	C1	512	CLA	CMD-C2D-C3D	-2.32	122.37	127.69
31	R	610	CLA	CHA-C1A-NA	-2.32	121.14	126.39
31	y1	611	CLA	CHA-C1A-NA	-2.32	121.14	126.39
31	a	405	CLA	CHA-C4D-ND	2.32	137.34	132.55
31	G1	603	CLA	O2A-CGA-CBA	2.32	118.91	111.83
31	N	603	CLA	OBD-CAD-C3D	-2.32	122.99	128.42
31	Y1	611	CLA	CHD-C1D-ND	-2.32	121.54	124.80
37	b	620	C7Z	C4-C5-C6	-2.32	115.99	120.76

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	Y	604	CLA	CAA-C2A-C3A	-2.32	106.73	113.00
33	C1	517	BCR	C19-C18-C17	2.32	122.66	119.01
31	b1	602	CLA	O2D-CGD-O1D	-2.32	119.33	123.85
47	n	606	CHL	C4C-CHD-C1D	2.32	124.37	116.07
31	G1	604	CLA	C4B-CHC-C1C	2.32	131.70	126.25
31	B	614	CLA	C2D-C1D-ND	2.32	112.42	110.13
31	C1	512	CLA	C2D-C1D-ND	2.32	112.42	110.13
31	d1	402	CLA	C1D-ND-C4D	-2.32	104.69	106.31
33	C1	514	BCR	C40-C30-C25	-2.32	106.61	110.24
31	B	616	CLA	C4B-CHC-C1C	2.32	131.70	126.25
31	s1	617	CLA	CHA-C4D-ND	2.32	137.33	132.55
31	y1	604	CLA	CHD-C1D-ND	-2.32	121.54	124.80
31	b1	615	CLA	O2A-CGA-CBA	2.32	118.90	111.83
47	G1	606	CHL	C1C-C2C-CMC	2.32	130.98	126.80
31	A1	410	CLA	C2D-C1D-ND	2.32	112.42	110.13
31	G	602	CLA	CHD-C1D-ND	-2.32	121.54	124.80
31	b	613	CLA	C1-C2-C3	-2.32	122.40	126.20
31	G1	602	CLA	CHA-C4D-ND	2.32	137.33	132.55
31	b	602	CLA	CHD-C1D-ND	-2.32	121.54	124.80
31	s1	611	CLA	C2D-C1D-ND	2.32	112.42	110.13
31	n1	611	CLA	O2A-CGA-CBA	2.32	118.90	111.83
31	A1	407	CLA	CMD-C2D-C3D	-2.32	122.38	127.69
31	c1	509	CLA	CMD-C2D-C3D	-2.32	122.38	127.69
31	A1	407	CLA	C3B-C4B-NB	-2.32	108.46	110.53
31	n1	614	CLA	C1-O2A-CGA	2.32	122.26	116.65
47	y	606	CHL	C4C-CHD-C1D	2.32	124.36	116.07
31	Y1	613	CLA	C4B-CHC-C1C	2.32	131.69	126.25
31	b1	603	CLA	C4B-CHC-C1C	2.32	131.69	126.25
31	Y1	614	CLA	CAA-C2A-C3A	-2.32	106.74	113.00
31	b	608	CLA	CHD-C1D-ND	-2.32	121.54	124.80
31	c	501	CLA	CHD-C1D-ND	-2.32	121.54	124.80
31	c1	511	CLA	C1D-ND-C4D	-2.32	104.69	106.31
47	n	601	CHL	CMA-C3A-C4A	2.32	119.60	114.61
31	n1	611	CLA	CMA-C3A-C4A	2.32	118.00	111.77
31	A1	407	CLA	C3D-C2D-C1D	-2.32	102.67	105.83
31	G	604	CLA	C4B-CHC-C1C	2.32	131.69	126.25
31	y1	611	CLA	CMA-C3A-C4A	2.32	118.00	111.77
41	g	624	LHG	C5-O7-C7	-2.32	112.25	117.80
46	h1	101	RRX	C16-C15-C14	2.32	128.26	123.52
31	C	506	CLA	CMD-C2D-C3D	-2.32	122.38	127.69
48	Y1	620	LUT	C22-C23-C24	-2.31	107.75	111.18
31	Y	604	CLA	CMD-C2D-C3D	-2.31	122.38	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	S	604	CLA	C3B-C4B-NB	-2.31	108.46	110.53
31	s	605	CLA	C4B-CHC-C1C	2.31	131.69	126.25
31	C	503	CLA	CHA-C1A-NA	-2.31	121.15	126.39
47	n1	606	CHL	C4C-CHD-C1D	2.31	124.35	116.07
31	Y1	614	CLA	O1D-CGD-CBD	-2.31	119.95	124.52
31	y1	611	CLA	C4B-CHC-C1C	2.31	131.69	126.25
31	S1	605	CLA	C4B-CHC-C1C	2.31	131.69	126.25
31	B1	613	CLA	C1C-C2C-C3C	-2.31	104.55	106.98
47	n	605	CHL	C1-C2-C3	-2.31	122.41	126.20
31	N	611	CLA	O2A-CGA-CBA	2.31	118.89	111.83
31	G1	613	CLA	C1D-ND-C4D	-2.31	104.69	106.31
31	C	513	CLA	O1D-CGD-CBD	-2.31	119.96	124.52
31	y	602	CLA	CBC-CAC-C3C	-2.31	106.15	112.42
31	R	603	CLA	CAC-C3C-C4C	2.31	127.80	124.79
31	B	614	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
31	r	604	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
33	c	514	BCR	C36-C18-C17	-2.31	119.07	122.82
31	S	612	CLA	C2D-C1D-ND	2.31	112.42	110.13
31	C1	503	CLA	C4B-CHC-C1C	2.31	131.69	126.25
31	s1	605	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
31	D1	403	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
31	S1	612	CLA	O2D-CGD-O1D	-2.31	119.35	123.85
50	y	623	NEX	C11-C12-C13	2.31	132.70	126.36
47	R	606	CHL	C1A-CHA-C4D	2.31	122.84	118.98
31	R	603	CLA	O2A-CGA-CBA	2.31	118.88	111.83
31	G	613	CLA	C4B-CHC-C1C	2.31	131.68	126.25
31	a1	405	CLA	CHD-C1D-ND	-2.31	121.55	124.80
31	a	405	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
31	s1	611	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
31	c	511	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
31	Y	610	CLA	CAA-C2A-C3A	-2.31	106.75	113.00
31	G	604	CLA	C3B-C4B-NB	-2.31	108.47	110.53
33	b	618	BCR	C15-C14-C13	-2.31	124.04	127.28
31	r	603	CLA	CHA-C1A-NA	-2.31	121.16	126.39
31	s	609	CLA	CHA-C1A-NA	-2.31	121.16	126.39
31	r1	603	CLA	CHA-C1A-NA	-2.31	121.16	126.39
31	Y	604	CLA	C4B-CHC-C1C	2.31	131.68	126.25
47	G1	606	CHL	C1-O2A-CGA	2.31	122.24	116.65
31	A	410	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
48	Y	621	LUT	C27-C28-C29	-2.31	121.35	126.32
31	r	603	CLA	O2A-CGA-CBA	2.31	118.88	111.83
31	c1	504	CLA	O2A-CGA-CBA	2.31	118.88	111.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	R	610	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
31	S1	614	CLA	C4B-CHC-C1C	2.31	131.68	126.25
31	b1	610	CLA	C4B-CHC-C1C	2.31	131.68	126.25
31	G1	613	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
31	a1	406	CLA	CHA-C4D-ND	2.31	137.31	132.55
48	Y	621	LUT	C10-C11-C12	-2.31	116.51	123.20
31	n	611	CLA	CHA-C1A-NA	-2.31	121.16	126.39
31	B	610	CLA	O2A-CGA-CBA	2.31	118.88	111.83
31	c1	509	CLA	C1D-ND-C4D	-2.31	104.69	106.31
31	s1	612	CLA	C1D-ND-C4D	-2.31	104.69	106.31
31	R1	602	CLA	C2D-C1D-ND	2.31	112.41	110.13
31	S	617	CLA	C3B-C4B-NB	-2.31	108.47	110.53
31	R1	603	CLA	C4B-CHC-C1C	2.31	131.68	126.25
31	r1	609	CLA	C4B-CHC-C1C	2.31	131.68	126.25
31	r1	602	CLA	C1C-C2C-C3C	-2.31	104.55	106.98
31	r1	612	CLA	CMD-C2D-C3D	-2.31	122.39	127.69
31	b	602	CLA	O2A-CGA-CBA	2.31	118.87	111.83
33	B	618	BCR	C33-C5-C4	2.31	118.52	113.60
33	C1	516	BCR	C33-C5-C4	2.31	118.52	113.60
31	n	612	CLA	C2C-C1C-NC	2.31	112.41	109.98
31	s	602	CLA	C4B-CHC-C1C	2.31	131.67	126.25
31	y1	612	CLA	C4B-CHC-C1C	2.31	131.67	126.25
33	b	618	BCR	C32-C1-C6	-2.31	106.62	110.24
31	a1	406	CLA	C2D-C1D-ND	2.31	112.41	110.13
31	C1	508	CLA	CAA-C2A-C3A	-2.31	106.76	113.00
31	B1	614	CLA	CHD-C1D-ND	-2.31	121.56	124.80
31	s1	609	CLA	C4B-CHC-C1C	2.31	131.67	126.25
31	n1	612	CLA	CHD-C1D-ND	-2.31	121.56	124.80
33	D1	404	BCR	C30-C25-C24	2.31	121.91	115.65
48	r	620	LUT	C18-C5-C6	-2.31	121.97	124.48
47	G1	607	CHL	C4C-CHD-C1D	2.31	124.32	116.07
31	c1	511	CLA	C2A-C1A-CHA	2.31	127.87	123.87
31	R	608	CLA	C4B-CHC-C1C	2.31	131.67	126.25
31	r1	612	CLA	C4B-CHC-C1C	2.31	131.67	126.25
31	A	410	CLA	OBD-CAD-C3D	-2.31	123.03	128.42
31	Y	612	CLA	C1D-ND-C4D	-2.31	104.69	106.31
31	A	407	CLA	CMD-C2D-C3D	-2.31	122.40	127.69
31	A	407	CLA	CHD-C1D-ND	-2.31	121.56	124.80
31	b1	609	CLA	C1-O2A-CGA	2.31	122.23	116.65
31	B	610	CLA	CHA-C1A-NA	-2.31	121.17	126.39
31	s	605	CLA	CHA-C1A-NA	-2.31	121.17	126.39
31	S	609	CLA	CMC-C2C-C1C	2.31	128.64	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	603	CLA	CMD-C2D-C3D	-2.30	122.40	127.69
31	C	502	CLA	C1C-C2C-C3C	-2.30	104.56	106.98
31	Y1	610	CLA	C3D-C2D-C1D	-2.30	102.69	105.83
31	a1	406	CLA	CMD-C2D-C3D	-2.30	122.40	127.69
48	S	621	LUT	C27-C28-C29	-2.30	121.37	126.32
31	s1	612	CLA	CMA-C3A-C4A	2.30	117.97	111.77
31	c1	507	CLA	C2C-C1C-NC	2.30	112.40	109.98
33	d1	404	BCR	C27-C26-C25	-2.30	119.59	122.70
31	a1	405	CLA	C2D-C1D-ND	2.30	112.41	110.13
31	b	608	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
31	c1	503	CLA	CAA-C2A-C3A	-2.30	106.78	113.00
31	B1	610	CLA	C1D-ND-C4D	-2.30	104.70	106.31
31	C1	511	CLA	C4B-CHC-C1C	2.30	131.66	126.25
48	S	621	LUT	C26-C27-C28	-2.30	121.00	124.58
31	b	611	CLA	O2A-CGA-CBA	2.30	118.86	111.83
31	c	503	CLA	O2A-CGA-CBA	2.30	118.86	111.83
31	s	602	CLA	CHA-C4D-ND	2.30	137.30	132.55
31	s1	617	CLA	C4B-CHC-C1C	2.30	131.66	126.25
31	n1	614	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
31	S1	614	CLA	CMA-C3A-C4A	2.30	117.96	111.77
44	D	405	PL9	C7-C8-C9	-2.30	122.86	126.83
31	a1	407	CLA	CHA-C4D-ND	2.30	137.30	132.55
31	y1	610	CLA	O1D-CGD-CBD	-2.30	119.98	124.52
46	h1	101	RRX	C15-C14-C13	-2.30	124.05	127.28
31	N	610	CLA	C2D-C1D-ND	2.30	112.40	110.13
31	b1	617	CLA	CHA-C1A-NA	-2.30	121.18	126.39
31	C	505	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
31	B1	602	CLA	CMD-C2D-C3D	-2.30	122.41	127.69
44	d	405	PL9	C27-C28-C29	-2.30	122.36	127.62
31	b1	606	CLA	C4B-CHC-C1C	2.30	131.66	126.25
31	y	604	CLA	CAA-C2A-C3A	-2.30	106.78	113.00
33	c	516	BCR	C27-C26-C25	-2.30	119.59	122.70
31	C	506	CLA	CHA-C1A-NA	-2.30	121.18	126.39
31	n	614	CLA	CHA-C1A-NA	-2.30	121.18	126.39
31	b	612	CLA	CHA-C1A-NA	-2.30	121.18	126.39
31	s	603	CLA	CHA-C1A-NA	-2.30	121.18	126.39
31	Y	608	CLA	CHD-C1D-ND	-2.30	121.57	124.80
31	N1	614	CLA	C3B-C4B-NB	-2.30	108.48	110.53
31	s1	605	CLA	C3B-C4B-NB	-2.30	108.48	110.53
31	N	604	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
47	R1	606	CHL	C1A-CHA-C4D	2.30	122.82	118.98
48	N	621	LUT	C38-C25-C24	-2.30	117.92	123.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	g	604	CLA	O2D-CGD-O1D	-2.30	119.37	123.85
31	N	602	CLA	C2C-C1C-NC	2.30	112.40	109.98
31	b	614	CLA	CHD-C1D-ND	-2.30	121.57	124.80
31	a1	407	CLA	CHD-C1D-ND	-2.30	121.57	124.80
31	b1	614	CLA	CHA-C1A-NA	-2.30	121.19	126.39
31	b1	616	CLA	CHA-C1A-NA	-2.30	121.19	126.39
31	N	602	CLA	C1C-C2C-C3C	-2.30	104.56	106.98
31	b1	608	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
31	b	603	CLA	C2D-C1D-ND	2.30	112.40	110.13
31	B1	607	CLA	CHA-C1A-NA	-2.30	121.19	126.39
44	D	405	PL9	O1-C4-C3	-2.30	118.31	120.73
49	r	622	XAT	O24-C25-C24	2.30	115.64	113.49
31	N1	613	CLA	C4B-CHC-C1C	2.30	131.65	126.25
31	y1	611	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
47	y	609	CHL	C1-C2-C3	-2.30	122.43	126.20
31	r1	610	CLA	O2A-CGA-CBA	2.30	118.84	111.83
31	R1	610	CLA	CHD-C1D-ND	-2.30	121.57	124.80
31	S	609	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
47	S	607	CHL	C4C-CHD-C1D	2.30	124.29	116.07
31	c1	502	CLA	CAA-C2A-C3A	-2.30	106.79	113.00
31	C1	512	CLA	CHA-C1A-NA	-2.30	121.19	126.39
31	R1	603	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
31	a1	405	CLA	CMA-C3A-C4A	2.30	117.95	111.77
31	c	506	CLA	C1-O2A-CGA	2.30	122.21	116.65
31	S	614	CLA	CHD-C1D-ND	-2.30	121.57	124.80
31	c	505	CLA	C1-O2A-CGA	2.30	122.21	116.65
31	N	603	CLA	C4B-CHC-C1C	2.30	131.65	126.25
31	r1	604	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
31	R	611	CLA	CHD-C1D-ND	-2.30	121.57	124.80
31	A	406	CLA	O2A-CGA-CBA	2.30	118.84	111.83
31	b	614	CLA	O2A-CGA-CBA	2.30	118.83	111.83
31	d	402	CLA	C2D-C1D-ND	2.30	112.40	110.13
31	b	608	CLA	C4B-CHC-C1C	2.30	131.65	126.25
31	r1	604	CLA	O2A-CGA-CBA	2.30	118.83	111.83
31	s1	609	CLA	O2A-CGA-CBA	2.30	118.83	111.83
31	n1	610	CLA	CMD-C2D-C3D	-2.30	122.42	127.69
31	R1	609	CLA	C3B-C4B-NB	-2.30	108.48	110.53
47	G	606	CHL	C1C-C2C-CMC	2.30	130.94	126.80
31	b1	604	CLA	O2D-CGD-O1D	-2.29	119.38	123.85
50	G1	623	NEX	C31-C32-C33	2.29	132.65	126.36
31	N1	610	CLA	C4B-CHC-C1C	2.29	131.64	126.25
34	c1	526	SQD	O3-C3-C2	-2.29	104.97	110.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c	506	CLA	C3B-C4B-NB	-2.29	108.48	110.53
31	C	511	CLA	CHA-C1A-NA	-2.29	121.20	126.39
31	b1	611	CLA	CHA-C1A-NA	-2.29	121.20	126.39
33	b	619	BCR	C8-C7-C6	-2.29	120.87	127.00
31	d	402	CLA	O2A-CGA-CBA	2.29	118.83	111.83
31	G1	604	CLA	CHA-C1A-NA	-2.29	121.20	126.39
31	S	605	CLA	CHD-C1D-ND	-2.29	121.58	124.80
31	S	614	CLA	CHA-C1A-NA	-2.29	121.20	126.39
47	n	609	CHL	C3D-C4D-ND	-2.29	109.26	112.94
31	s	612	CLA	C1D-ND-C4D	-2.29	104.70	106.31
31	y1	602	CLA	CHD-C1D-ND	-2.29	121.58	124.80
31	B1	605	CLA	CMA-C3A-C2A	2.29	122.84	113.98
31	a1	406	CLA	O2A-CGA-CBA	2.29	118.82	111.83
31	n1	611	CLA	C4B-CHC-C1C	2.29	131.64	126.25
47	g1	609	CHL	CMA-C3A-C4A	2.29	119.55	114.61
31	B	611	CLA	C4B-CHC-C1C	2.29	131.63	126.25
31	s1	602	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
31	C1	511	CLA	CHD-C1D-ND	-2.29	121.58	124.80
31	N	604	CLA	C4B-CHC-C1C	2.29	131.63	126.25
31	n1	611	CLA	C1D-ND-C4D	-2.29	104.70	106.31
31	c1	507	CLA	OBD-CAD-C3D	-2.29	123.06	128.42
31	b1	612	CLA	CHA-C4D-ND	2.29	137.27	132.55
31	n1	614	CLA	CHA-C1A-NA	-2.29	121.20	126.39
31	S1	617	CLA	C4B-CHC-C1C	2.29	131.63	126.25
34	A1	412	SQD	O3-C3-C2	-2.29	104.98	110.38
32	a1	409	PHO	C2D-C1D-ND	-2.29	107.78	109.43
31	Y	610	CLA	C2C-C1C-NC	2.29	112.39	109.98
31	b	617	CLA	CHA-C1A-NA	-2.29	121.21	126.39
31	B1	602	CLA	O2A-CGA-CBA	2.29	118.82	111.83
31	G	611	CLA	C1C-C2C-C3C	-2.29	104.57	106.98
31	B	609	CLA	OBD-CAD-C3D	-2.29	123.06	128.42
31	C	509	CLA	CHA-C1A-NA	-2.29	121.21	126.39
31	C	502	CLA	CHD-C1D-ND	-2.29	121.58	124.80
31	c	512	CLA	C4B-CHC-C1C	2.29	131.63	126.25
47	g1	608	CHL	C3D-C4D-ND	-2.29	109.27	112.94
31	B	603	CLA	C4B-CHC-C1C	2.29	131.63	126.25
56	r1	626	ERG	C2-C3-C4	2.29	113.51	110.29
31	B	616	CLA	C2D-C1D-ND	2.29	112.39	110.13
45	f	101	HEM	C4D-ND-C1D	2.29	107.92	105.21
31	R	611	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
47	Y	607	CHL	C4C-CHD-C1D	2.29	124.26	116.07
31	R1	602	CLA	C2C-C1C-NC	2.29	112.39	109.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	N	614	CLA	CHD-C1D-ND	-2.29	121.58	124.80
31	R	613	CLA	CHD-C1D-ND	-2.29	121.58	124.80
31	D	403	CLA	C2D-C1D-ND	2.29	112.39	110.13
31	y	611	CLA	C4B-CHC-C1C	2.29	131.63	126.25
31	n1	613	CLA	C4B-CHC-C1C	2.29	131.63	126.25
31	C	509	CLA	CMD-C2D-C3D	-2.29	122.44	127.69
31	y	603	CLA	O2A-CGA-CBA	2.29	118.81	111.83
31	C	507	CLA	C3B-C4B-NB	-2.29	108.49	110.53
31	r1	603	CLA	C1-O2A-CGA	2.29	122.19	116.65
31	N1	611	CLA	CMD-C2D-C3D	-2.29	122.45	127.69
31	b	607	CLA	CAA-C2A-C3A	-2.29	106.82	113.00
31	r1	608	CLA	CHA-C1A-NA	-2.29	121.21	126.39
31	g1	610	CLA	C1D-ND-C4D	-2.29	104.71	106.31
31	C	503	CLA	C2D-C1D-ND	2.29	112.39	110.13
31	y	611	CLA	C3B-C4B-NB	-2.29	108.49	110.53
31	s	609	CLA	CHD-C1D-ND	-2.28	121.59	124.80
31	n1	603	CLA	CHD-C1D-ND	-2.28	121.59	124.80
31	c	502	CLA	C4B-CHC-C1C	2.28	131.62	126.25
31	A	405	CLA	C1C-C2C-C3C	-2.28	104.58	106.98
31	R	612	CLA	C1D-ND-C4D	-2.28	104.71	106.31
31	g1	603	CLA	C1D-ND-C4D	-2.28	104.71	106.31
31	b	615	CLA	C4B-CHC-C1C	2.28	131.62	126.25
48	Y1	620	LUT	C31-C32-C33	-2.28	120.10	126.36
31	b	610	CLA	C4B-CHC-C1C	2.28	131.62	126.25
31	D	403	CLA	CAA-C2A-C3A	-2.28	106.83	113.00
49	y1	622	XAT	C40-C33-C34	-2.28	119.12	122.82
33	c	514	BCR	C38-C26-C27	2.28	118.47	113.60
48	y1	620	LUT	C38-C25-C24	-2.28	117.96	123.36
31	C	506	CLA	O2A-CGA-CBA	2.28	118.80	111.83
31	b1	604	CLA	C4B-CHC-C1C	2.28	131.62	126.25
46	h	101	RRX	C16-C17-C18	-2.28	124.08	127.28
31	B1	603	CLA	O2D-CGD-O1D	-2.28	119.40	123.85
31	y1	612	CLA	O1D-CGD-CBD	-2.28	120.02	124.52
31	G	603	CLA	C2D-C1D-ND	2.28	112.39	110.13
46	h	101	RRX	C20-C21-C22	-2.28	124.08	127.28
31	C1	511	CLA	CAA-CBA-CGA	-2.28	106.73	113.21
31	a1	410	CLA	CHD-C1D-ND	-2.28	121.59	124.80
31	b	605	CLA	O1D-CGD-CBD	-2.28	120.02	124.52
31	S	603	CLA	C4B-CHC-C1C	2.28	131.61	126.25
31	S1	613	CLA	C4B-CHC-C1C	2.28	131.61	126.25
31	R1	610	CLA	CHA-C4D-ND	2.28	137.26	132.55
31	B	607	CLA	CHD-C1D-ND	-2.28	121.59	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	g	614	CLA	CHD-C1D-ND	-2.28	121.59	124.80
31	s1	604	CLA	CHD-C1D-ND	-2.28	121.59	124.80
31	N	613	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
31	b	614	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
31	y1	604	CLA	O1D-CGD-CBD	-2.28	120.02	124.52
31	r	610	CLA	C1C-C2C-C3C	-2.28	104.58	106.98
31	G	602	CLA	C4B-CHC-C1C	2.28	131.61	126.25
31	N1	610	CLA	CAC-C3C-C4C	2.28	127.76	124.79
31	s1	604	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
31	a1	407	CLA	C2D-C1D-ND	2.28	112.38	110.13
31	B1	604	CLA	CAA-C2A-C3A	-2.28	106.84	113.00
31	b1	604	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
31	a1	405	CLA	O2A-CGA-CBA	2.28	118.78	111.83
31	Y1	610	CLA	C2C-C1C-NC	2.28	112.38	109.98
31	y	614	CLA	CMD-C2D-C3D	-2.28	122.46	127.69
31	C1	502	CLA	C1C-C2C-C3C	-2.28	104.58	106.98
31	C	503	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
31	b1	617	CLA	CAA-C2A-C3A	-2.28	106.84	113.00
31	D	402	CLA	CHA-C4D-ND	2.28	137.25	132.55
48	N1	621	LUT	C27-C28-C29	-2.28	121.42	126.32
31	B1	616	CLA	CHD-C1D-ND	-2.28	121.60	124.80
31	Y	603	CLA	O1D-CGD-CBD	-2.28	120.02	124.52
31	S1	609	CLA	C1-C2-C3	-2.28	122.46	126.20
31	y1	614	CLA	O2D-CGD-O1D	-2.28	119.41	123.85
44	D	405	PL9	C27-C28-C29	-2.28	122.41	127.62
33	C1	517	BCR	C4-C5-C6	-2.28	119.63	122.70
31	c1	511	CLA	CHD-C1D-ND	-2.28	121.60	124.80
31	B1	617	CLA	CMA-C3A-C4A	2.28	117.89	111.77
31	b1	614	CLA	C4B-CHC-C1C	2.28	131.60	126.25
31	Y	602	CLA	CHA-C4D-ND	2.28	137.25	132.55
31	b1	614	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
47	g	601	CHL	C1-C2-C3	-2.28	122.47	126.20
31	s	617	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
31	s	603	CLA	O2D-CGD-O1D	-2.28	119.42	123.85
31	n1	613	CLA	O2D-CGD-O1D	-2.28	119.42	123.85
31	y	612	CLA	CHA-C1A-NA	-2.28	121.23	126.39
31	c	506	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
31	g	612	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
33	b1	618	BCR	C1-C6-C7	2.28	121.83	115.65
31	B1	616	CLA	CHA-C1A-NA	-2.28	121.24	126.39
31	Y	611	CLA	C4B-CHC-C1C	2.28	131.60	126.25
31	G1	602	CLA	C6-C5-C3	-2.28	107.92	113.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
49	y1	622	XAT	C19-C9-C10	-2.28	119.13	122.82
48	s	621	LUT	C8-C7-C6	-2.28	120.92	127.00
31	R	612	CLA	CMA-C3A-C4A	2.28	117.89	111.77
31	G1	611	CLA	C4B-CHC-C1C	2.28	131.60	126.25
31	Y	604	CLA	O2A-CGA-CBA	2.28	118.77	111.83
31	C1	510	CLA	O2A-CGA-CBA	2.28	118.77	111.83
31	R1	612	CLA	CMD-C2D-C3D	-2.28	122.47	127.69
31	c	513	CLA	C1C-C2C-C3C	-2.28	104.59	106.98
31	n	604	CLA	C1C-C2C-C3C	-2.28	104.59	106.98
31	r	613	CLA	C4B-CHC-C1C	2.28	131.60	126.25
31	s	604	CLA	O2D-CGD-O1D	-2.27	119.42	123.85
47	Y1	606	CHL	C4C-CHD-C1D	2.27	124.21	116.07
31	s1	609	CLA	CHA-C1A-NA	-2.27	121.24	126.39
31	S1	602	CLA	C4B-CHC-C1C	2.27	131.59	126.25
31	G	610	CLA	CMD-C2D-C3D	-2.27	122.47	127.69
31	b1	617	CLA	CMD-C2D-C3D	-2.27	122.47	127.69
48	g	620	LUT	C38-C25-C24	-2.27	117.98	123.36
31	r	610	CLA	CHA-C1A-NA	-2.27	121.24	126.39
31	r	613	CLA	CHA-C1A-NA	-2.27	121.24	126.39
31	n1	604	CLA	C4B-CHC-C1C	2.27	131.59	126.25
47	G	608	CHL	C4C-CHD-C1D	2.27	124.20	116.07
31	N	602	CLA	CHD-C1D-ND	-2.27	121.60	124.80
35	B1	622	LMG	O7-C10-O9	-2.27	118.39	123.70
31	c	501	CLA	CMA-C3A-C4A	2.27	117.88	111.77
31	G	610	CLA	C1C-C2C-C3C	-2.27	104.59	106.98
31	Y	612	CLA	CHA-C4D-ND	2.27	137.24	132.55
31	r	604	CLA	C4B-CHC-C1C	2.27	131.59	126.25
31	R1	604	CLA	C4B-CHC-C1C	2.27	131.59	126.25
31	C1	504	CLA	C3B-C4B-NB	-2.27	108.50	110.53
31	r1	608	CLA	C3B-C4B-NB	-2.27	108.50	110.53
31	B	608	CLA	CHD-C1D-ND	-2.27	121.60	124.80
31	r	613	CLA	CHD-C1D-ND	-2.27	121.60	124.80
31	S1	604	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
47	n1	608	CHL	C4C-CHD-C1D	2.27	124.20	116.07
31	R	608	CLA	CHA-C1A-NA	-2.27	121.25	126.39
47	n	609	CHL	C4C-CHD-C1D	2.27	124.20	116.07
31	b1	612	CLA	O2D-CGD-O1D	-2.27	119.42	123.85
33	C1	516	BCR	C31-C1-C6	-2.27	106.68	110.24
31	C1	512	CLA	C1D-ND-C4D	-2.27	104.72	106.31
47	G	609	CHL	C1-C2-C3	-2.27	122.47	126.20
31	c	511	CLA	C2C-C1C-NC	2.27	112.37	109.98
31	B	617	CLA	CHA-C1A-NA	-2.27	121.25	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s	602	CLA	C2D-C1D-ND	2.27	112.37	110.13
31	y	604	CLA	C4B-CHC-C1C	2.27	131.59	126.25
31	N1	611	CLA	C4B-CHC-C1C	2.27	131.59	126.25
31	a1	405	CLA	C4B-CHC-C1C	2.27	131.59	126.25
31	R1	612	CLA	CHA-C1A-NA	-2.27	121.25	126.39
46	h1	101	RRX	C2-C1-C6	2.27	113.74	110.44
31	B1	602	CLA	CMA-C3A-C4A	2.27	117.88	111.77
31	c1	507	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
34	b1	626	SQD	O3-C3-C2	-2.27	105.02	110.38
31	S	604	CLA	C4B-CHC-C1C	2.27	131.59	126.25
31	b	617	CLA	C4B-CHC-C1C	2.27	131.59	126.25
31	Y1	611	CLA	C3B-C4B-NB	-2.27	108.50	110.53
31	b	612	CLA	O2A-CGA-CBA	2.27	118.76	111.83
31	R	613	CLA	CHA-C1A-NA	-2.27	121.25	126.39
31	n	612	CLA	CMD-C2D-C3D	-2.27	122.48	127.69
47	Y	609	CHL	C4C-CHD-C1D	2.27	124.19	116.07
45	F	101	HEM	CAC-C3C-C4C	2.27	130.24	124.82
31	N1	610	CLA	C3D-C2D-C1D	-2.27	102.73	105.83
31	C	508	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
31	C1	505	CLA	C4B-CHC-C1C	2.27	131.58	126.25
33	C	515	BCR	C4-C5-C6	-2.27	119.64	122.70
37	B1	620	C7Z	C38-C25-C24	2.27	118.59	114.42
31	R	604	CLA	O1D-CGD-CBD	-2.27	120.04	124.52
31	B	608	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
50	Y	623	NEX	C1-C2-C3	2.27	118.57	113.59
31	Y1	612	CLA	CHA-C1A-NA	-2.27	121.25	126.39
31	C1	508	CLA	C3B-C4B-NB	-2.27	108.50	110.53
31	B1	614	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
31	B1	614	CLA	C4B-CHC-C1C	2.27	131.58	126.25
31	B	604	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
48	Y	621	LUT	C38-C25-C24	-2.27	117.99	123.36
31	g	610	CLA	C4B-CHC-C1C	2.27	131.58	126.25
31	N	603	CLA	CHD-C1D-ND	-2.27	121.61	124.80
31	g1	613	CLA	CHD-C1D-ND	-2.27	121.61	124.80
31	N1	613	CLA	O1D-CGD-CBD	-2.27	120.05	124.52
31	B	613	CLA	O2D-CGD-O1D	-2.27	119.43	123.85
31	b	602	CLA	C1D-ND-C4D	-2.27	104.72	106.31
31	N1	604	CLA	OBD-CAD-C3D	-2.27	123.12	128.42
34	M1	101	SQD	O3-C3-C2	-2.27	105.03	110.38
47	N1	606	CHL	C4C-CHD-C1D	2.27	124.18	116.07
37	b1	620	C7Z	C1-C6-C7	2.27	121.80	115.65
31	A1	410	CLA	CHD-C1D-ND	-2.27	121.61	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	y1	605	CHL	C4C-CHD-C1D	2.27	124.18	116.07
33	d	404	BCR	C35-C13-C12	2.27	121.55	118.09
48	s	621	LUT	C27-C28-C29	-2.27	121.45	126.32
31	a	407	CLA	C1-O2A-CGA	2.27	122.14	116.65
31	c	507	CLA	C4B-CHC-C1C	2.27	131.58	126.25
31	r	609	CLA	C4B-CHC-C1C	2.27	131.58	126.25
31	n	602	CLA	CMC-C2C-C1C	2.27	128.57	125.03
31	C	504	CLA	CHA-C4D-ND	2.27	137.22	132.55
31	s1	603	CLA	CHA-C1A-NA	-2.27	121.26	126.39
31	g	613	CLA	CMD-C2D-C3D	-2.27	122.49	127.69
31	A	406	CLA	C4B-CHC-C1C	2.27	131.57	126.25
31	R1	609	CLA	CHD-C1D-ND	-2.27	121.61	124.80
31	y1	613	CLA	CHD-C1D-ND	-2.27	121.61	124.80
31	R1	609	CLA	O2D-CGD-O1D	-2.27	119.44	123.85
31	S	605	CLA	CHA-C1A-NA	-2.27	121.26	126.39
31	g	610	CLA	C3B-C4B-NB	-2.27	108.51	110.53
31	D	402	CLA	C3D-C2D-C1D	-2.26	102.74	105.83
31	B	615	CLA	CHD-C1D-ND	-2.26	121.61	124.80
31	G	612	CLA	CHA-C1A-NA	-2.26	121.26	126.39
31	b	613	CLA	O1D-CGD-CBD	-2.26	120.05	124.52
31	S	602	CLA	C1C-C2C-C3C	-2.26	104.60	106.98
31	R1	608	CLA	C4B-CHC-C1C	2.26	131.57	126.25
47	G	608	CHL	CMA-C3A-C4A	2.26	119.49	114.61
31	B1	614	CLA	C2D-C1D-ND	2.26	112.37	110.13
31	G1	612	CLA	C2D-C1D-ND	2.26	112.37	110.13
31	S1	614	CLA	CHA-C1A-NA	-2.26	121.26	126.39
31	s1	617	CLA	CHA-C1A-NA	-2.26	121.27	126.39
31	S	613	CLA	C3D-C2D-C1D	-2.26	102.74	105.83
31	s	617	CLA	O2A-CGA-CBA	2.26	118.74	111.83
31	B1	614	CLA	O2A-CGA-CBA	2.26	118.74	111.83
48	N	620	LUT	C10-C11-C12	-2.26	116.64	123.20
31	B	610	CLA	C2D-C1D-ND	2.26	112.37	110.13
31	n	603	CLA	C1D-ND-C4D	-2.26	104.72	106.31
31	c	503	CLA	CHA-C1A-NA	-2.26	121.27	126.39
31	B1	614	CLA	CHA-C1A-NA	-2.26	121.27	126.39
47	g1	609	CHL	C1-O2A-CGA	2.26	122.13	116.65
31	C	512	CLA	O2D-CGD-O1D	-2.26	119.44	123.85
31	c	512	CLA	CHA-C1A-NA	-2.26	121.27	126.39
31	Y1	611	CLA	C4B-CHC-C1C	2.26	131.57	126.25
31	y1	602	CLA	C2D-C1D-ND	2.26	112.36	110.13
31	R	604	CLA	CHD-C1D-ND	-2.26	121.62	124.80
31	g	603	CLA	CHD-C1D-ND	-2.26	121.62	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	512	CLA	CMA-C3A-C4A	2.26	117.85	111.77
40	C1	520	DGD	O6D-C5D-C6D	2.26	111.18	106.69
31	s	605	CLA	CAA-C2A-C3A	-2.26	106.89	113.00
50	R	622	NEX	C40-C33-C34	-2.26	119.15	122.82
31	C	508	CLA	C6-C5-C3	-2.26	107.96	113.47
31	S1	604	CLA	C4B-CHC-C1C	2.26	131.56	126.25
31	g	611	CLA	CHA-C1A-NA	-2.26	121.27	126.39
31	n	612	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
31	y	604	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
31	G	613	CLA	C1C-C2C-C3C	-2.26	104.60	106.98
31	b	605	CLA	C1C-C2C-C3C	-2.26	104.60	106.98
45	f	101	HEM	CHD-C4C-C3C	2.26	129.02	125.21
31	b	614	CLA	C4B-CHC-C1C	2.26	131.56	126.25
31	R1	604	CLA	CHD-C1D-ND	-2.26	121.62	124.80
31	s1	611	CLA	CHD-C1D-ND	-2.26	121.62	124.80
53	Y	625	SPH	C3-C4-C5	-2.26	120.01	124.69
31	B	616	CLA	CMA-C3A-C4A	2.26	117.85	111.77
31	B1	605	CLA	C3D-C2D-C1D	-2.26	102.75	105.83
31	R	613	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
33	b1	619	BCR	C8-C7-C6	-2.26	120.96	127.00
31	G	602	CLA	C3B-C4B-NB	-2.26	108.51	110.53
31	b1	602	CLA	C3B-C4B-NB	-2.26	108.51	110.53
31	G	614	CLA	O2A-CGA-CBA	2.26	118.72	111.83
31	C1	507	CLA	O2A-CGA-CBA	2.26	118.72	111.83
41	G	630	LHG	C6-C5-C4	-2.26	106.52	111.78
50	r1	622	NEX	C26-C27-C28	-2.26	121.22	125.99
31	b	611	CLA	C3D-C2D-C1D	-2.26	102.75	105.83
31	y1	608	CLA	O2A-CGA-CBA	2.26	118.72	111.83
31	Y	602	CLA	CMC-C2C-C1C	2.26	128.56	125.03
31	B	611	CLA	O2A-CGA-CBA	2.26	118.72	111.83
31	B1	612	CLA	CHA-C4D-ND	2.26	137.21	132.55
49	r1	621	XAT	C24-C23-C22	-2.26	106.57	110.79
47	G	605	CHL	C1-O2A-CGA	2.26	123.09	116.67
32	a	408	PHO	C2D-C1D-ND	-2.26	107.80	109.43
31	c1	509	CLA	O2D-CGD-O1D	-2.26	119.45	123.85
31	A	410	CLA	CHD-C1D-ND	-2.26	121.62	124.80
31	a1	405	CLA	C2C-C1C-NC	2.26	112.35	109.98
31	n	613	CLA	CHA-C4D-ND	2.26	137.21	132.55
31	n	614	CLA	C2D-C1D-ND	2.26	112.36	110.13
32	A	408	PHO	O2A-CGA-O1A	-2.26	117.98	123.63
31	y	608	CLA	CHA-C1A-NA	-2.26	121.28	126.39
31	Y	611	CLA	CMD-C2D-C3D	-2.26	122.51	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b1	616	CLA	CMD-C2D-C3D	-2.26	122.51	127.69
31	C	502	CLA	C4B-CHC-C1C	2.26	131.55	126.25
31	G	602	CLA	O1D-CGD-CBD	-2.26	120.07	124.52
31	g1	603	CLA	CHA-C1A-NA	-2.26	121.28	126.39
47	G	609	CHL	C1-O2A-CGA	2.26	122.11	116.65
31	n1	611	CLA	CHD-C1D-ND	-2.26	121.63	124.80
31	s1	604	CLA	O2D-CGD-O1D	-2.26	119.46	123.85
33	D	404	BCR	C33-C5-C6	-2.26	122.02	124.48
31	Y	612	CLA	CHA-C1A-NA	-2.26	121.28	126.39
34	m1	101	SQD	O3-C3-C2	-2.26	105.06	110.38
31	B1	608	CLA	C4B-CHC-C1C	2.26	131.55	126.25
47	S1	601	CHL	C1C-C2C-CMC	2.26	130.87	126.80
31	S1	604	CLA	CHD-C1D-ND	-2.26	121.63	124.80
31	y1	608	CLA	CHA-C1A-NA	-2.26	121.28	126.39
31	g	613	CLA	C4B-CHC-C1C	2.26	131.55	126.25
31	y1	613	CLA	O2D-CGD-O1D	-2.26	119.46	123.85
31	c	506	CLA	O1D-CGD-CBD	-2.26	120.07	124.52
31	Y	614	CLA	CHD-C1D-ND	-2.26	121.63	124.80
31	C1	513	CLA	CHD-C1D-ND	-2.26	121.63	124.80
31	s	614	CLA	C3B-C4B-NB	-2.25	108.52	110.53
31	B	606	CLA	CHA-C1A-NA	-2.25	121.28	126.39
31	S	612	CLA	CHA-C1A-NA	-2.25	121.28	126.39
47	n1	607	CHL	C1A-CHA-C4D	2.25	122.74	118.98
31	n1	604	CLA	CMD-C2D-C3D	-2.25	122.52	127.69
31	C1	503	CLA	CHA-C1A-NA	-2.25	121.29	126.39
31	s	617	CLA	C2D-C1D-ND	2.25	112.36	110.13
31	A1	406	CLA	C2D-C1D-ND	2.25	112.36	110.13
31	C	505	CLA	CMD-C2D-C3D	-2.25	122.52	127.69
34	C	526	SQD	O3-C3-C2	-2.25	105.06	110.38
47	G	609	CHL	C4C-CHD-C1D	2.25	124.13	116.07
31	g	614	CLA	C3B-C4B-NB	-2.25	108.52	110.53
31	Y1	602	CLA	CHA-C1A-NA	-2.25	121.29	126.39
31	y	610	CLA	CMD-C2D-C3D	-2.25	122.52	127.69
31	y	610	CLA	CHA-C1A-NA	-2.25	121.29	126.39
31	d	403	CLA	CAA-C2A-C3A	-2.25	106.91	113.00
31	Y1	610	CLA	CHA-C4D-ND	2.25	137.20	132.55
47	S1	601	CHL	C4C-CHD-C1D	2.25	124.13	116.07
31	Y1	604	CLA	C2D-C1D-ND	2.25	112.36	110.13
47	s	607	CHL	C4C-CHD-C1D	2.25	124.13	116.07
47	g1	607	CHL	C4C-CHD-C1D	2.25	124.13	116.07
31	S1	614	CLA	C3B-C4B-NB	-2.25	108.52	110.53
50	G	623	NEX	O24-C25-C38	-2.25	112.53	115.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s	604	CLA	OBD-CAD-C3D	-2.25	123.16	128.42
31	y	602	CLA	CHD-C1D-ND	-2.25	121.64	124.80
31	D1	403	CLA	CHD-C1D-ND	-2.25	121.64	124.80
31	A	407	CLA	C4B-CHC-C1C	2.25	131.54	126.25
31	c	512	CLA	O2D-CGD-O1D	-2.25	119.47	123.85
31	r1	602	CLA	C2D-C1D-ND	2.25	112.35	110.13
31	N1	602	CLA	CHD-C1D-ND	-2.25	121.64	124.80
31	G	611	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
31	r1	603	CLA	CMA-C3A-C4A	2.25	117.82	111.77
31	D1	402	CLA	C2C-C1C-NC	2.25	112.34	109.98
31	r	608	CLA	CHA-C1A-NA	-2.25	121.30	126.39
47	N	609	CHL	C4C-CHD-C1D	2.25	124.12	116.07
31	a1	407	CLA	C3B-C4B-NB	-2.25	108.52	110.53
31	g1	603	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
32	a1	408	PHO	C1-C2-C3	-2.25	122.51	126.20
31	B1	603	CLA	C2D-C1D-ND	2.25	112.35	110.13
31	n	614	CLA	C1D-ND-C4D	-2.25	104.73	106.31
31	g	614	CLA	CMD-C2D-C3D	-2.25	122.53	127.69
33	a1	411	BCR	C37-C22-C23	2.25	121.52	118.09
31	S1	605	CLA	CHA-C1A-NA	-2.25	121.30	126.39
31	c1	502	CLA	C4B-CHC-C1C	2.25	131.53	126.25
57	Y1	627	PTY	C6-O7-C8	-2.25	113.88	117.85
31	c1	513	CLA	C1D-ND-C4D	-2.25	104.73	106.31
31	B	612	CLA	O2A-CGA-CBA	2.25	118.69	111.83
31	y	613	CLA	C1-O2A-CGA	2.25	122.09	116.65
31	A	405	CLA	C2C-C1C-NC	2.25	112.34	109.98
31	B	607	CLA	CHA-C1A-NA	-2.25	121.30	126.39
31	g1	610	CLA	C6-C5-C3	-2.25	108.00	113.47
31	g	612	CLA	CHD-C1D-ND	-2.25	121.64	124.80
31	R	604	CLA	C4B-CHC-C1C	2.25	131.53	126.25
31	s1	612	CLA	CMD-C2D-C3D	-2.25	122.54	127.69
31	S1	610	CLA	CMC-C2C-C1C	2.25	128.54	125.03
31	b	607	CLA	C4B-CHC-C1C	2.25	131.53	126.25
31	c	510	CLA	O1D-CGD-CBD	-2.25	120.09	124.52
31	C	502	CLA	C3B-C4B-NB	-2.24	108.53	110.53
31	a	405	CLA	C4B-CHC-C1C	2.24	131.52	126.25
31	S	614	CLA	C3B-C4B-NB	-2.24	108.53	110.53
31	r1	602	CLA	C3B-C4B-NB	-2.24	108.53	110.53
31	d	402	CLA	CAC-C3C-C4C	2.24	127.71	124.79
31	B1	611	CLA	CHD-C1D-ND	-2.24	121.64	124.80
33	d1	404	BCR	C30-C25-C24	2.24	121.74	115.65
31	b1	607	CLA	C1D-ND-C4D	-2.24	104.74	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	614	CLA	O2A-CGA-CBA	2.24	118.67	111.83
50	y1	623	NEX	C31-C32-C33	2.24	132.51	126.36
31	S1	612	CLA	C2D-C1D-ND	2.24	112.35	110.13
31	Y1	614	CLA	CHA-C1A-NA	-2.24	121.31	126.39
31	g	610	CLA	CAA-C2A-C3A	-2.24	106.94	113.00
31	c	503	CLA	C4B-CHC-C1C	2.24	131.52	126.25
31	y1	608	CLA	C4B-CHC-C1C	2.24	131.52	126.25
37	b1	620	C7Z	C24-C25-C26	-2.24	116.15	120.76
31	b	609	CLA	CHA-C1A-NA	-2.24	121.31	126.39
34	a1	412	SQD	O3-C3-C2	-2.24	105.09	110.38
33	A1	411	BCR	C4-C5-C6	-2.24	119.67	122.70
31	R	603	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
31	s1	604	CLA	O1D-CGD-CBD	-2.24	120.10	124.52
31	R	603	CLA	C4B-CHC-C1C	2.24	131.52	126.25
31	b1	603	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
47	n1	601	CHL	CMA-C3A-C4A	2.24	119.44	114.61
31	G1	611	CLA	C3B-C4B-NB	-2.24	108.53	110.53
31	b1	610	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
31	B	611	CLA	CHA-C1A-NA	-2.24	121.32	126.39
49	R	621	XAT	C31-C32-C33	2.24	132.51	126.36
31	G	611	CLA	C2D-C1D-ND	2.24	112.34	110.13
31	b	613	CLA	C1C-C2C-C3C	-2.24	104.62	106.98
31	S	609	CLA	O1D-CGD-CBD	-2.24	120.10	124.52
31	b1	609	CLA	CMB-C2B-C1B	-2.24	122.01	125.42
48	N1	620	LUT	C26-C27-C28	-2.24	121.09	124.58
31	b1	615	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
35	w1	201	LMG	C8-O7-C10	-2.24	112.43	117.80
31	Y1	614	CLA	O2A-CGA-CBA	2.24	118.67	111.83
48	n1	621	LUT	C26-C27-C28	-2.24	121.09	124.58
31	a1	405	CLA	C1C-C2C-C3C	-2.24	104.62	106.98
31	N1	612	CLA	CMD-C2D-C3D	-2.24	122.55	127.69
31	S	602	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
31	b	603	CLA	O2D-CGD-O1D	-2.24	119.49	123.85
31	R	612	CLA	OBD-CAD-C3D	-2.24	123.18	128.42
31	b1	606	CLA	CHD-C1D-ND	-2.24	121.65	124.80
31	N1	610	CLA	C3B-C4B-NB	-2.24	108.53	110.53
31	g	603	CLA	CAA-C2A-C3A	-2.24	106.95	113.00
31	s1	610	CLA	C4B-CHC-C1C	2.24	131.51	126.25
33	a	411	BCR	C36-C18-C17	-2.24	119.19	122.82
31	R	602	CLA	CHD-C1D-ND	-2.24	121.65	124.80
31	r	609	CLA	CHD-C1D-ND	-2.24	121.65	124.80
31	B1	603	CLA	O1D-CGD-CBD	-2.24	120.10	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	s	614	CLA	C4B-CHC-C1C	2.24	131.51	126.25
31	n1	614	CLA	C1D-ND-C4D	-2.24	104.74	106.31
31	B	605	CLA	CHA-C1A-NA	-2.24	121.32	126.39
31	n1	612	CLA	CHA-C1A-NA	-2.24	121.32	126.39
47	S	607	CHL	C1C-C2C-CMC	2.24	130.84	126.80
49	N1	622	XAT	O24-C25-C24	2.24	115.59	113.49
31	b1	614	CLA	CHD-C1D-ND	-2.24	121.65	124.80
32	a	409	PHO	CBC-CAC-C3C	2.24	116.08	112.87
41	N	624	LHG	O7-C7-O9	-2.24	118.47	123.70
33	C	516	BCR	C36-C18-C17	-2.24	119.19	122.82
31	r1	608	CLA	O2A-CGA-CBA	2.24	118.66	111.83
31	B	610	CLA	C1-O2A-CGA	2.24	122.06	116.65
31	n1	610	CLA	CHA-C1A-NA	-2.24	121.33	126.39
31	G1	610	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
31	s1	613	CLA	CMD-C2D-C3D	-2.24	122.56	127.69
31	Y1	611	CLA	O2A-CGA-CBA	2.24	118.65	111.83
31	g1	613	CLA	C1D-ND-C4D	-2.24	104.74	106.31
31	G	611	CLA	CHD-C1D-ND	-2.24	121.66	124.80
31	s1	613	CLA	CHD-C1D-ND	-2.24	121.66	124.80
31	B	617	CLA	OBD-CAD-C3D	-2.24	123.19	128.42
49	G1	622	XAT	O24-C26-C27	-2.24	110.47	116.88
31	Y1	603	CLA	CHA-C1A-NA	-2.24	121.33	126.39
49	N1	622	XAT	O4-C5-C4	-2.24	111.40	113.49
31	a	407	CLA	CHD-C1D-ND	-2.24	121.66	124.80
31	c1	507	CLA	CHD-C1D-ND	-2.24	121.66	124.80
31	B1	616	CLA	O2D-CGD-O1D	-2.23	119.50	123.85
31	R1	612	CLA	C1-O2A-CGA	2.23	122.06	116.65
47	N1	607	CHL	C4C-CHD-C1D	2.23	124.06	116.07
31	r1	610	CLA	CHA-C1A-NA	-2.23	121.33	126.39
31	G	603	CLA	O2A-CGA-CBA	2.23	118.65	111.83
31	b1	607	CLA	C4B-CHC-C1C	2.23	131.50	126.25
35	b1	622	LMG	C9-C8-C7	-2.23	106.58	111.78
31	b1	613	CLA	C4B-CHC-C1C	2.23	131.50	126.25
37	B	620	C7Z	C18-C5-C4	2.23	118.53	114.42
31	y	612	CLA	O1D-CGD-CBD	-2.23	120.11	124.52
31	B	603	CLA	CHA-C1A-NA	-2.23	121.33	126.39
31	a1	405	CLA	CHA-C1A-NA	-2.23	121.33	126.39
31	s	609	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
31	c1	513	CLA	C2D-C1D-ND	2.23	112.33	110.13
31	Y	610	CLA	C1D-ND-C4D	-2.23	104.75	106.31
31	B	602	CLA	CMD-C2D-C3D	-2.23	122.57	127.69
48	g1	621	LUT	C31-C32-C33	-2.23	120.24	126.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
44	D	405	PL9	C42-C43-C44	-2.23	122.52	127.62
31	Y	603	CLA	O2A-CGA-CBA	2.23	118.64	111.83
31	B	610	CLA	C4B-CHC-C1C	2.23	131.49	126.25
48	n	621	LUT	C35-C34-C33	-2.23	124.15	127.28
48	S	621	LUT	C1-C6-C5	-2.23	119.59	122.64
48	S	620	LUT	C10-C11-C12	-2.23	116.74	123.20
31	B	612	CLA	CHA-C1A-NA	-2.23	121.34	126.39
31	R1	609	CLA	C1D-ND-C4D	-2.23	104.75	106.31
48	N	621	LUT	C31-C30-C29	-2.23	124.15	127.28
31	C	510	CLA	CHD-C1D-ND	-2.23	121.66	124.80
31	B1	604	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
31	c1	504	CLA	C2D-C1D-ND	2.23	112.33	110.13
31	s1	612	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
31	y1	612	CLA	CHA-C1A-NA	-2.23	121.34	126.39
31	g1	611	CLA	C3B-C4B-NB	-2.23	108.54	110.53
31	b	603	CLA	C1D-ND-C4D	-2.23	104.75	106.31
31	c1	504	CLA	C1D-ND-C4D	-2.23	104.75	106.31
37	b1	620	C7Z	C21-C26-C27	2.23	121.70	115.65
31	G1	603	CLA	CHA-C1A-NA	-2.23	121.34	126.39
31	y1	610	CLA	CHA-C1A-NA	-2.23	121.34	126.39
31	S1	602	CLA	CHD-C1D-ND	-2.23	121.67	124.80
31	C1	506	CLA	C4B-CHC-C1C	2.23	131.49	126.25
31	N1	603	CLA	O2A-CGA-CBA	2.23	118.63	111.83
49	g	622	XAT	C19-C9-C8	2.23	121.49	118.09
31	G	611	CLA	O1D-CGD-CBD	-2.23	120.12	124.52
31	n1	602	CLA	C1D-ND-C4D	-2.23	104.75	106.31
44	D1	405	PL9	C32-C33-C34	-2.23	122.53	127.62
47	N	606	CHL	CMA-C3A-C4A	2.23	119.41	114.61
47	R	606	CHL	CMA-C3A-C4A	2.23	119.41	114.61
31	N1	613	CLA	CHA-C1A-NA	-2.23	121.35	126.39
31	A	407	CLA	C3B-C4B-NB	-2.23	108.54	110.53
31	n1	603	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
47	g1	605	CHL	C1-O2A-CGA	2.23	123.00	116.67
31	c	511	CLA	CHD-C1D-ND	-2.23	121.67	124.80
31	d1	402	CLA	CHD-C1D-ND	-2.23	121.67	124.80
47	N	601	CHL	C4C-CHD-C1D	2.23	124.03	116.07
31	b	611	CLA	CHA-C1A-NA	-2.23	121.35	126.39
48	n	621	LUT	C38-C25-C24	-2.23	118.09	123.36
31	R	604	CLA	CMA-C3A-C4A	2.23	117.76	111.77
31	Y	610	CLA	CHD-C1D-ND	-2.23	121.67	124.80
31	A1	410	CLA	CMA-C3A-C2A	2.23	122.59	113.98
31	B1	604	CLA	C1C-C2C-C3C	-2.23	104.64	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	r	612	CLA	CMD-C2D-C3D	-2.23	122.58	127.69
48	G1	620	LUT	C22-C23-C24	-2.23	107.88	111.18
56	R1	626	ERG	C16-C17-C13	2.22	106.46	103.84
31	S	610	CLA	CHA-C1A-NA	-2.22	121.35	126.39
31	Y	604	CLA	C1D-ND-C4D	-2.22	104.75	106.31
31	a1	410	CLA	CMD-C2D-C3D	-2.22	122.59	127.69
47	y	609	CHL	C4C-CHD-C1D	2.22	124.03	116.07
31	b1	617	CLA	O2D-CGD-O1D	-2.22	119.52	123.85
31	S	617	CLA	CHA-C1A-NA	-2.22	121.35	126.39
31	C1	511	CLA	CHA-C1A-NA	-2.22	121.36	126.39
31	b	614	CLA	C2D-C1D-ND	2.22	112.33	110.13
31	g1	603	CLA	CAA-C2A-C3A	-2.22	106.99	113.00
31	R1	602	CLA	C3B-C4B-NB	-2.22	108.55	110.53
48	r1	620	LUT	C11-C12-C13	-2.22	120.27	126.36
34	B1	621	SQD	O3-C3-C2	-2.22	105.14	110.38
33	B	618	BCR	C34-C9-C10	-2.22	119.21	122.82
50	n1	623	NEX	C11-C12-C13	2.22	132.46	126.36
31	B1	605	CLA	C4B-CHC-C1C	2.22	131.47	126.25
47	g	606	CHL	CMA-C3A-C4A	2.22	119.40	114.61
31	s1	610	CLA	CHA-C1A-NA	-2.22	121.36	126.39
31	Y	613	CLA	C3B-C4B-NB	-2.22	108.55	110.53
31	b1	608	CLA	C4B-CHC-C1C	2.22	131.47	126.25
31	y1	613	CLA	C4B-CHC-C1C	2.22	131.47	126.25
31	n	612	CLA	CHA-C4D-ND	2.22	137.13	132.55
48	G	621	LUT	C35-C15-C14	-2.22	118.97	123.52
31	c1	509	CLA	C1C-C2C-C3C	-2.22	104.64	106.98
31	B	609	CLA	CHA-C1A-NA	-2.22	121.36	126.39
31	Y1	611	CLA	CHA-C1A-NA	-2.22	121.36	126.39
31	Y1	603	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
50	N1	623	NEX	C26-C27-C28	-2.22	121.30	125.99
47	Y1	607	CHL	C1-O2A-CGA	2.22	122.03	116.65
50	n	623	NEX	C40-C33-C34	-2.22	119.22	122.82
31	S1	609	CLA	CHA-C1A-NA	-2.22	121.36	126.39
31	G	604	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
48	y	620	LUT	C20-C13-C12	2.22	121.48	118.09
48	S	621	LUT	C18-C5-C4	2.22	118.50	114.42
31	c1	508	CLA	CHA-C4D-ND	2.22	137.13	132.55
33	B	619	BCR	C31-C1-C6	-2.22	106.76	110.24
31	S	610	CLA	CMD-C2D-C3D	-2.22	122.60	127.69
48	R1	620	LUT	C31-C32-C33	-2.22	120.28	126.36
31	c1	509	CLA	CHD-C1D-ND	-2.22	121.68	124.80
31	r1	610	CLA	CHD-C1D-ND	-2.22	121.68	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	S	611	CLA	CHA-C1A-NA	-2.22	121.36	126.39
31	C	513	CLA	C2D-C1D-ND	2.22	112.32	110.13
33	c1	515	BCR	C38-C26-C25	-2.22	122.06	124.48
31	n1	604	CLA	CHA-C1A-NA	-2.22	121.36	126.39
31	S	612	CLA	C3B-C4B-NB	-2.22	108.55	110.53
40	C	519	DGD	O3G-C1D-C2D	2.22	111.64	108.27
31	c	504	CLA	C4B-CHC-C1C	2.22	131.47	126.25
56	r1	626	ERG	C15-C14-C13	2.22	106.20	104.21
31	B1	617	CLA	CAA-C2A-C3A	-2.22	107.00	113.00
31	B1	610	CLA	C2D-C1D-ND	2.22	112.32	110.13
31	g1	602	CLA	C2D-C1D-ND	2.22	112.32	110.13
31	b	604	CLA	C4B-CHC-C1C	2.22	131.46	126.25
34	c	626	SQD	O3-C3-C2	-2.22	105.15	110.38
31	B1	617	CLA	C1C-C2C-C3C	-2.22	104.65	106.98
31	C	511	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
31	C	507	CLA	CHD-C1D-ND	-2.22	121.68	124.80
31	B	603	CLA	C3B-C4B-NB	-2.22	108.55	110.53
45	F	101	HEM	CHC-C1C-NC	2.22	126.87	124.45
34	b1	621	SQD	O3-C3-C2	-2.22	105.15	110.38
31	r	603	CLA	C4B-CHC-C1C	2.22	131.46	126.25
31	G	614	CLA	C1D-ND-C4D	-2.22	104.76	106.31
31	C1	513	CLA	C2C-C1C-NC	2.22	112.31	109.98
31	S	611	CLA	O1D-CGD-CBD	-2.22	120.14	124.52
47	n	608	CHL	C1A-CHA-C4D	2.22	122.68	118.98
31	S1	611	CLA	CHA-C1A-NA	-2.22	121.37	126.39
31	n1	613	CLA	C2D-C1D-ND	2.22	112.32	110.13
31	B	614	CLA	CHD-C1D-ND	-2.22	121.68	124.80
31	y	608	CLA	O2A-CGA-CBA	2.22	118.59	111.83
31	b1	614	CLA	O2A-CGA-CBA	2.22	118.59	111.83
49	G	622	XAT	O24-C26-C27	-2.22	110.53	116.88
31	n	604	CLA	O1D-CGD-CBD	-2.22	120.15	124.52
31	N	613	CLA	CHD-C1D-ND	-2.22	121.68	124.80
31	G	604	CLA	CHD-C1D-ND	-2.22	121.68	124.80
31	n1	604	CLA	CMA-C3A-C4A	2.22	117.73	111.77
31	b	604	CLA	CMD-C2D-C3D	-2.22	122.61	127.69
31	N1	603	CLA	O2D-CGD-O1D	-2.22	119.54	123.85
31	R1	610	CLA	O2D-CGD-O1D	-2.22	119.54	123.85
31	n1	604	CLA	CHD-C1D-ND	-2.22	121.69	124.80
31	N	610	CLA	C1D-ND-C4D	-2.21	104.76	106.31
31	A1	405	CLA	O2D-CGD-O1D	-2.21	119.54	123.85
31	b1	612	CLA	C4B-CHC-C1C	2.21	131.46	126.25
31	b1	617	CLA	C4B-CHC-C1C	2.21	131.46	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	N	612	CLA	CHA-C1A-NA	-2.21	121.38	126.39
31	R1	604	CLA	C3B-C4B-NB	-2.21	108.55	110.53
31	s1	602	CLA	C2C-C1C-NC	2.21	112.31	109.98
48	N1	620	LUT	C20-C13-C12	2.21	121.47	118.09
31	N1	614	CLA	CAA-C2A-C3A	-2.21	107.02	113.00
31	b	607	CLA	C1C-C2C-C3C	-2.21	104.65	106.98
47	s1	608	CHL	C4C-CHD-C1D	2.21	123.99	116.07
31	G1	610	CLA	CHA-C4D-ND	2.21	137.12	132.55
31	a1	407	CLA	CMD-C2D-C3D	-2.21	122.61	127.69
31	g1	603	CLA	O2A-CGA-CBA	2.21	118.58	111.83
31	C	502	CLA	C2D-C1D-ND	2.21	112.32	110.13
31	N	604	CLA	C2D-C1D-ND	2.21	112.32	110.13
31	G1	614	CLA	C2D-C1D-ND	2.21	112.32	110.13
33	d1	404	BCR	C36-C18-C17	-2.21	119.23	122.82
31	b1	609	CLA	CMD-C2D-C3D	-2.21	122.61	127.69
31	A1	407	CLA	C2D-C1D-ND	2.21	112.32	110.13
35	D	411	LMG	O6-C5-C6	2.21	111.92	106.44
31	c1	508	CLA	CHD-C1D-ND	-2.21	121.69	124.80
31	n	603	CLA	C3B-C4B-NB	-2.21	108.56	110.53
31	B1	609	CLA	C3B-C4B-NB	-2.21	108.56	110.53
31	C1	508	CLA	CHA-C4D-ND	2.21	137.11	132.55
31	g1	604	CLA	O2A-CGA-CBA	2.21	118.58	111.83
31	B	616	CLA	C2A-C1A-CHA	2.21	127.71	123.87
31	R	611	CLA	C1D-ND-C4D	-2.21	104.76	106.31
31	r1	610	CLA	CAA-C2A-C3A	-2.21	107.02	113.00
31	b	603	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
31	s	602	CLA	C3B-C4B-NB	-2.21	108.56	110.53
31	y	611	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
31	B1	610	CLA	CMA-C3A-C4A	2.21	117.72	111.77
31	R1	608	CLA	CHA-C1A-NA	-2.21	121.38	126.39
31	g1	614	CLA	CHA-C1A-NA	-2.21	121.38	126.39
47	G	605	CHL	C4C-CHD-C1D	2.21	123.98	116.07
31	C	503	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
31	Y	610	CLA	C2D-C1D-ND	2.21	112.31	110.13
31	g1	613	CLA	C2D-C1D-ND	2.21	112.31	110.13
31	G	602	CLA	C1-O2A-CGA	2.21	122.00	116.65
31	b	611	CLA	CHD-C1D-ND	-2.21	121.69	124.80
48	g	621	LUT	C27-C28-C29	-2.21	121.57	126.32
37	b	620	C7Z	C28-C27-C26	-2.21	121.09	127.00
31	Y	612	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
31	S1	603	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
31	c1	506	CLA	C4B-CHC-C1C	2.21	131.44	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	614	CLA	CHA-C1A-NA	-2.21	121.39	126.39
31	r	609	CLA	CHA-C1A-NA	-2.21	121.39	126.39
31	C	511	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
31	C	504	CLA	CAA-C2A-C3A	-2.21	107.03	113.00
31	b1	605	CLA	CMA-C3A-C2A	2.21	122.53	113.98
31	b1	603	CLA	CHA-C1A-NA	-2.21	121.39	126.39
31	c1	512	CLA	CHA-C1A-NA	-2.21	121.39	126.39
31	g1	610	CLA	CHA-C1A-NA	-2.21	121.39	126.39
31	S1	613	CLA	O2D-CGD-O1D	-2.21	119.55	123.85
31	y	611	CLA	CHD-C1D-ND	-2.21	121.69	124.80
31	B1	604	CLA	C2C-C1C-NC	2.21	112.30	109.98
31	R1	609	CLA	C2D-C1D-ND	2.21	112.31	110.13
49	r1	621	XAT	C32-C33-C34	2.21	122.48	119.01
31	G1	610	CLA	C3D-C2D-C1D	-2.21	102.82	105.83
31	S	602	CLA	O2A-CGA-CBA	2.21	118.57	111.83
31	G	603	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
31	g	602	CLA	CMD-C2D-C3D	-2.21	122.62	127.69
31	R	608	CLA	CHD-C1D-ND	-2.21	121.69	124.80
31	Y	614	CLA	CHA-C1A-NA	-2.21	121.39	126.39
31	R1	610	CLA	O1D-CGD-CBD	-2.21	120.16	124.52
31	Y1	610	CLA	C3B-C4B-NB	-2.21	108.56	110.53
31	n	611	CLA	C1D-ND-C4D	-2.21	104.76	106.31
31	N1	612	CLA	C1D-ND-C4D	-2.21	104.76	106.31
47	g	607	CHL	C4C-CHD-C1D	2.21	123.97	116.07
31	B	613	CLA	C4B-CHC-C1C	2.21	131.44	126.25
31	b1	608	CLA	C1-O2A-CGA	2.21	121.99	116.65
31	g	603	CLA	C3D-C2D-C1D	-2.21	102.82	105.83
31	n	614	CLA	C1-O2A-CGA	2.21	121.99	116.65
31	b1	606	CLA	O1D-CGD-CBD	-2.21	120.17	124.52
49	G	622	XAT	O24-C25-C24	2.21	115.56	113.49
31	n1	610	CLA	C2A-C1A-CHA	2.21	127.70	123.87
47	Y1	607	CHL	C4C-CHD-C1D	2.21	123.96	116.07
31	B1	603	CLA	CAA-C2A-C3A	-2.21	107.04	113.00
33	c	515	BCR	C35-C13-C12	2.21	121.46	118.09
31	Y1	610	CLA	CHD-C1D-ND	-2.21	121.70	124.80
31	G1	603	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
31	d1	403	CLA	O2D-CGD-O1D	-2.20	119.56	123.85
33	C	514	BCR	C38-C26-C25	-2.20	122.08	124.48
31	C1	512	CLA	C3D-C2D-C1D	-2.20	102.82	105.83
33	c1	515	BCR	C15-C14-C13	-2.20	124.19	127.28
31	r	603	CLA	CHD-C1D-ND	-2.20	121.70	124.80
31	A	405	CLA	C4B-CHC-C1C	2.20	131.43	126.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	R1	609	CLA	CHA-C1A-NA	-2.20	121.40	126.39
31	C1	508	CLA	C1-O2A-CGA	2.20	121.99	116.65
31	c	501	CLA	O1D-CGD-CBD	-2.20	120.17	124.52
31	g1	613	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
31	y1	603	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
31	R	603	CLA	CHA-C1A-NA	-2.20	121.40	126.39
37	b1	620	C7Z	C31-C32-C33	-2.20	120.32	126.36
31	r1	610	CLA	O1D-CGD-CBD	-2.20	120.17	124.52
47	N	608	CHL	C4C-CHD-C1D	2.20	123.95	116.07
31	y1	603	CLA	O1D-CGD-CBD	-2.20	120.17	124.52
31	a	407	CLA	CHA-C1A-NA	-2.20	121.40	126.39
31	s1	604	CLA	CHA-C1A-NA	-2.20	121.40	126.39
31	a1	410	CLA	CAA-C2A-C3A	-2.20	107.05	113.00
48	s1	620	LUT	C38-C25-C24	-2.20	118.15	123.36
31	C1	503	CLA	C3B-C4B-NB	-2.20	108.56	110.53
31	A1	407	CLA	CHA-C1A-NA	-2.20	121.40	126.39
31	C1	507	CLA	CHA-C1A-NA	-2.20	121.40	126.39
47	N	606	CHL	C1C-C2C-CMC	2.20	130.77	126.80
31	s	617	CLA	C4B-CHC-C1C	2.20	131.43	126.25
41	S1	624	LHG	O7-C7-O9	-2.20	118.56	123.70
47	n1	605	CHL	C4C-CHD-C1D	2.20	123.95	116.07
50	Y1	623	NEX	C26-C27-C28	-2.20	121.34	125.99
48	N	620	LUT	C38-C25-C24	-2.20	118.15	123.36
31	G1	610	CLA	C3B-C4B-NB	-2.20	108.56	110.53
31	s	603	CLA	CHD-C1D-ND	-2.20	121.70	124.80
31	G1	603	CLA	CHD-C1D-ND	-2.20	121.70	124.80
31	G1	612	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
31	Y	608	CLA	CAA-C2A-C3A	-2.20	107.05	113.00
31	b1	602	CLA	CMD-C2D-C3D	-2.20	122.64	127.69
44	d	405	PL9	C36-C34-C33	-2.20	116.23	121.17
34	C1	526	SQD	O3-C3-C2	-2.20	105.19	110.38
47	s1	608	CHL	C1-O2A-CGA	2.20	121.97	116.65
31	D1	403	CLA	CAA-C2A-C3A	-2.20	107.06	113.00
31	b	610	CLA	CHA-C1A-NA	-2.20	121.41	126.39
31	Y1	612	CLA	C1D-ND-C4D	-2.20	104.77	106.31
48	G	620	LUT	C26-C27-C28	-2.20	121.16	124.58
31	n1	604	CLA	C3B-C4B-NB	-2.20	108.57	110.53
31	N1	604	CLA	CHD-C1D-ND	-2.20	121.71	124.80
31	S1	617	CLA	CHA-C1A-NA	-2.20	121.41	126.39
31	Y	610	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
31	C	504	CLA	O1D-CGD-CBD	-2.20	120.18	124.52
33	b	619	BCR	C15-C14-C13	-2.20	124.19	127.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	r1	609	CLA	C3B-C4B-NB	-2.20	108.57	110.53
31	d	402	CLA	O2D-CGD-O1D	-2.20	119.57	123.85
49	N1	622	XAT	C28-C29-C30	2.20	122.47	119.01
31	c1	502	CLA	C11-C12-C13	-2.20	108.66	115.97
31	B1	605	CLA	C1D-ND-C4D	-2.20	104.77	106.31
31	c1	501	CLA	C1D-ND-C4D	-2.20	104.77	106.31
31	c1	503	CLA	C1D-ND-C4D	-2.20	104.77	106.31
31	n	611	CLA	CHD-C1D-ND	-2.20	121.71	124.80
33	c	517	BCR	C33-C5-C4	2.20	118.28	113.60
31	b	612	CLA	CHA-C4D-ND	2.20	137.08	132.55
31	s1	614	CLA	C3B-C4B-NB	-2.20	108.57	110.53
31	n1	610	CLA	CMA-C3A-C4A	2.20	117.68	111.77
31	B1	604	CLA	C1D-ND-C4D	-2.20	104.77	106.31
48	S	621	LUT	C1-C6-C7	2.20	121.61	115.65
31	B1	615	CLA	CHA-C1A-NA	-2.20	121.42	126.39
47	s1	608	CHL	C1-C2-C3	-2.20	122.60	126.20
31	s1	610	CLA	CMD-C2D-C3D	-2.20	122.65	127.69
31	g	612	CLA	O1D-CGD-CBD	-2.20	120.19	124.52
48	G1	621	LUT	C27-C28-C29	-2.20	121.60	126.32
45	f1	101	HEM	C3D-C4D-ND	-2.20	107.76	110.17
31	R	612	CLA	CHA-C1A-NA	-2.20	121.42	126.39
31	g1	612	CLA	CHA-C1A-NA	-2.20	121.42	126.39
31	n1	611	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
46	H1	101	RRX	C8-C7-C6	-2.20	121.13	127.00
47	Y	606	CHL	C4C-CHD-C1D	2.19	123.92	116.07
31	C	513	CLA	C1D-ND-C4D	-2.19	104.77	106.31
31	Y	612	CLA	O1D-CGD-CBD	-2.19	120.19	124.52
31	s1	610	CLA	O2A-CGA-CBA	2.19	118.53	111.83
31	G1	604	CLA	O2A-CGA-CBA	2.19	118.53	111.83
48	Y	621	LUT	C22-C23-C24	-2.19	107.92	111.18
31	G	611	CLA	CAA-C2A-C3A	-2.19	107.07	113.00
50	S	622	NEX	C19-C9-C10	-2.19	119.26	122.82
50	S1	623	NEX	C4-C3-C2	2.19	114.89	110.79
33	B1	618	BCR	C36-C18-C17	-2.19	119.26	122.82
31	c	513	CLA	C2D-C1D-ND	2.19	112.30	110.13
41	D	408	LHG	C6-C5-C4	-2.19	106.67	111.78
31	S1	602	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
31	B	606	CLA	CMA-C3A-C4A	2.19	117.67	111.77
31	Y	604	CLA	CMA-C3A-C4A	2.19	117.67	111.77
47	g	608	CHL	C4C-CHD-C1D	2.19	123.91	116.07
33	C1	516	BCR	C19-C18-C17	2.19	122.46	119.01
31	n1	611	CLA	CHA-C1A-NA	-2.19	121.43	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
41	D1	409	LHG	O7-C7-O9	-2.19	118.58	123.70
34	B1	626	SQD	O3-C3-C2	-2.19	105.21	110.38
31	n1	602	CLA	O1D-CGD-CBD	-2.19	120.19	124.52
47	R1	607	CHL	C4C-CHD-C1D	2.19	123.91	116.07
31	Y1	602	CLA	CAA-C2A-C3A	-2.19	107.08	113.00
31	s1	610	CLA	CHD-C1D-ND	-2.19	121.72	124.80
33	C	514	BCR	C33-C5-C4	2.19	118.27	113.60
31	c1	513	CLA	C1C-C2C-C3C	-2.19	104.67	106.98
31	n1	604	CLA	O2A-CGA-CBA	2.19	118.52	111.83
31	s	613	CLA	C4B-CHC-C1C	2.19	131.40	126.25
32	a1	409	PHO	O2A-CGA-O1A	-2.19	118.15	123.63
31	b1	602	CLA	O2A-CGA-CBA	2.19	118.52	111.83
31	Y1	608	CLA	CHD-C1D-ND	-2.19	121.72	124.80
33	b1	619	BCR	C39-C30-C25	-2.19	106.81	110.24
31	y1	603	CLA	C2D-C1D-ND	2.19	112.29	110.13
31	D1	402	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
50	Y1	623	NEX	C4-C3-C2	2.19	114.89	110.79
47	g	605	CHL	C4C-CHD-C1D	2.19	123.90	116.07
31	B1	605	CLA	CHD-C1D-ND	-2.19	121.72	124.80
31	R1	610	CLA	C3B-C4B-NB	-2.19	108.58	110.53
31	B	611	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
31	a1	407	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
31	B	604	CLA	CMC-C2C-C1C	2.19	128.45	125.03
33	c	516	BCR	C31-C1-C6	-2.19	106.81	110.24
48	N	621	LUT	C20-C13-C12	2.19	121.43	118.09
31	B1	616	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
47	s1	606	CHL	C4C-CHD-C1D	2.19	123.90	116.07
31	D	402	CLA	O2A-CGA-CBA	2.19	118.51	111.83
31	g1	602	CLA	C1C-C2C-C3C	-2.19	104.68	106.98
31	b	612	CLA	O1D-CGD-CBD	-2.19	120.20	124.52
31	s	611	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
48	R	620	LUT	C11-C12-C13	-2.19	120.36	126.36
31	B1	614	CLA	C3D-C2D-C1D	-2.19	102.85	105.83
31	C	508	CLA	CHA-C1A-NA	-2.19	121.44	126.39
31	s	609	CLA	CAA-C2A-C3A	-2.19	107.09	113.00
31	c	505	CLA	C4B-CHC-C1C	2.19	131.39	126.25
31	c1	502	CLA	C2D-C1D-ND	2.19	112.29	110.13
48	y1	621	LUT	C38-C25-C24	-2.19	118.19	123.36
31	B1	613	CLA	CHA-C1A-NA	-2.19	121.44	126.39
31	c1	510	CLA	CHA-C1A-NA	-2.19	121.44	126.39
31	S1	603	CLA	CMD-C2D-C3D	-2.19	122.67	127.69
33	c1	514	BCR	C36-C18-C17	-2.19	119.27	122.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
45	F	101	HEM	C4D-ND-C1D	2.19	107.80	105.21
31	B1	610	CLA	CHD-C1D-ND	-2.19	121.73	124.80
47	G1	601	CHL	C3D-C4D-ND	-2.19	109.43	112.94
31	R	611	CLA	CHA-C1A-NA	-2.19	121.44	126.39
31	B1	611	CLA	CHA-C1A-NA	-2.19	121.44	126.39
31	G1	611	CLA	CHA-C1A-NA	-2.19	121.44	126.39
31	b	607	CLA	C3B-C4B-NB	-2.19	108.58	110.53
31	N	602	CLA	C2D-C1D-ND	2.19	112.29	110.13
49	g	622	XAT	C18-C5-C6	-2.19	118.70	122.30
31	S	604	CLA	CHA-C1A-NA	-2.19	121.44	126.39
31	n	604	CLA	C1D-ND-C4D	-2.18	104.78	106.31
31	g1	604	CLA	O1D-CGD-CBD	-2.18	120.21	124.52
47	g1	608	CHL	CMD-C2D-C3D	2.18	129.05	124.68
48	y	621	LUT	C31-C32-C33	-2.18	120.37	126.36
47	S1	608	CHL	C3D-C4D-ND	-2.18	109.43	112.94
48	r1	620	LUT	C1-C6-C5	-2.18	119.65	122.64
31	N	604	CLA	C2C-C1C-NC	2.18	112.28	109.98
31	c	508	CLA	O2A-CGA-CBA	2.18	118.49	111.83
31	r	602	CLA	CHA-C1A-NA	-2.18	121.45	126.39
31	C1	502	CLA	CHA-C1A-NA	-2.18	121.45	126.39
31	b	605	CLA	C4B-CHC-C1C	2.18	131.38	126.25
31	s1	602	CLA	O1D-CGD-CBD	-2.18	120.21	124.52
34	b	621	SQD	O3-C3-C2	-2.18	105.23	110.38
31	a	410	CLA	CHA-C1A-NA	-2.18	121.45	126.39
41	n	624	LHG	O8-C23-C24	2.18	118.49	111.83
31	G	613	CLA	CAA-C2A-C3A	-2.18	107.10	113.00
31	n	612	CLA	C1C-C2C-C3C	-2.18	104.69	106.98
31	g	604	CLA	C1D-ND-C4D	-2.18	104.78	106.31
31	g	611	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
31	N1	603	CLA	CHA-C1A-NA	-2.18	121.45	126.39
48	G	620	LUT	C31-C32-C33	-2.18	120.38	126.36
31	c	507	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
33	C1	515	BCR	C4-C5-C6	-2.18	119.76	122.70
31	G	611	CLA	CHA-C1A-NA	-2.18	121.45	126.39
31	g1	604	CLA	CHA-C1A-NA	-2.18	121.45	126.39
31	r1	610	CLA	C2D-C1D-ND	2.18	112.28	110.13
31	r	611	CLA	CHD-C1D-ND	-2.18	121.73	124.80
44	d1	405	PL9	O2-C1-C2	-2.18	116.87	121.83
31	S1	613	CLA	C3B-C4B-NB	-2.18	108.58	110.53
31	C1	512	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
31	C	507	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
35	b	622	LMG	O7-C10-O9	-2.18	118.61	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	Y	603	CLA	CMD-C2D-C3D	-2.18	122.69	127.69
31	R	602	CLA	CHA-C1A-NA	-2.18	121.45	126.39
31	b1	605	CLA	CHD-C1D-ND	-2.18	121.73	124.80
31	N1	602	CLA	CHA-C4D-ND	2.18	137.05	132.55
31	c1	507	CLA	C1C-C2C-C3C	-2.18	104.69	106.98
31	R	613	CLA	O1D-CGD-CBD	-2.18	120.22	124.52
47	g	606	CHL	C4C-CHD-C1D	2.18	123.86	116.07
31	y1	610	CLA	C1C-C2C-C3C	-2.18	104.69	106.98
31	S1	603	CLA	C1-O2A-CGA	2.18	121.92	116.65
31	S1	603	CLA	O2A-CGA-CBA	2.18	118.48	111.83
31	A	407	CLA	CHA-C1A-NA	-2.18	121.46	126.39
35	A1	413	LMG	O7-C10-O9	-2.18	118.61	123.70
34	B	621	SQD	O3-C3-C2	-2.18	105.24	110.38
47	g1	609	CHL	C4C-CHD-C1D	2.18	123.86	116.07
31	c1	506	CLA	CHD-C1D-ND	-2.18	121.74	124.80
33	c1	517	BCR	C29-C30-C25	2.18	113.60	110.44
31	a	406	CLA	O2A-CGA-CBA	2.18	118.47	111.83
31	Y1	608	CLA	O2A-CGA-CBA	2.18	118.47	111.83
50	g	623	NEX	C26-C27-C28	-2.18	121.39	125.99
31	B1	602	CLA	CHD-C1D-ND	-2.18	121.74	124.80
37	b	620	C7Z	C31-C32-C33	-2.18	120.39	126.36
31	S	614	CLA	C4B-CHC-C1C	2.18	131.37	126.25
31	s1	617	CLA	CMD-C2D-C3D	-2.18	122.70	127.69
31	y1	612	CLA	CMD-C2D-C3D	-2.18	122.70	127.69
41	n	624	LHG	O7-C7-O9	-2.18	118.62	123.70
31	R	611	CLA	C2D-C1D-ND	2.18	112.28	110.13
31	B	611	CLA	C1C-C2C-C3C	-2.18	104.69	106.98
31	b1	607	CLA	C1-C2-C3	-2.18	122.63	126.20
31	b	616	CLA	C4B-CHC-C1C	2.18	131.36	126.25
31	n1	602	CLA	CHA-C1A-NA	-2.17	121.47	126.39
31	C1	502	CLA	O2A-CGA-CBA	2.17	118.47	111.83
31	b1	602	CLA	CHD-C1D-ND	-2.17	121.74	124.80
31	b1	616	CLA	CMA-C3A-C4A	2.17	117.62	111.77
31	Y	602	CLA	C2C-C1C-NC	2.17	112.27	109.98
31	S1	609	CLA	C2D-C1D-ND	2.17	112.28	110.13
31	s1	613	CLA	C4B-CHC-C1C	2.17	131.36	126.25
31	b	617	CLA	C3B-C4B-NB	-2.17	108.59	110.53
31	B	602	CLA	CHD-C1D-ND	-2.17	121.74	124.80
31	r1	612	CLA	CHD-C1D-ND	-2.17	121.74	124.80
31	G1	614	CLA	CHA-C1A-NA	-2.17	121.47	126.39
31	d	402	CLA	CAA-C2A-C3A	-2.17	107.12	113.00
31	y	611	CLA	O1D-CGD-CBD	-2.17	120.23	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C1	501	CLA	CHD-C1D-ND	-2.17	121.74	124.80
31	b	602	CLA	CAA-C2A-C3A	-2.17	107.13	113.00
31	y	610	CLA	C3B-C4B-NB	-2.17	108.59	110.53
47	g	601	CHL	C4C-CHD-C1D	2.17	123.84	116.07
31	R1	603	CLA	CMA-C3A-C4A	2.17	117.61	111.77
31	G	613	CLA	CHA-C1A-NA	-2.17	121.47	126.39
31	B	606	CLA	O2D-CGD-O1D	-2.17	119.62	123.85
31	s1	603	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
31	c	512	CLA	C2D-C1D-ND	2.17	112.28	110.13
31	c	507	CLA	CMA-C3A-C2A	2.17	122.38	113.98
31	S1	610	CLA	C1-O2A-CGA	2.17	121.91	116.65
31	g1	611	CLA	CHA-C1A-NA	-2.17	121.47	126.39
49	r	622	XAT	C31-C32-C33	2.17	132.32	126.36
31	S1	617	CLA	C1D-ND-C4D	-2.17	104.79	106.31
31	g1	611	CLA	C1D-ND-C4D	-2.17	104.79	106.31
47	Y	606	CHL	CMA-C3A-C4A	2.17	119.29	114.61
48	Y1	620	LUT	C39-C29-C28	2.17	121.41	118.09
31	b1	611	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
31	c1	502	CLA	CHD-C1D-ND	-2.17	121.75	124.80
31	s	614	CLA	CHA-C1A-NA	-2.17	121.47	126.39
31	c1	502	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
31	C	508	CLA	O2A-CGA-CBA	2.17	118.46	111.83
31	c1	511	CLA	O1D-CGD-CBD	-2.17	120.23	124.52
31	n	604	CLA	C2D-C1D-ND	2.17	112.28	110.13
47	s	606	CHL	C4C-CHD-C1D	2.17	123.84	116.07
31	c1	505	CLA	CMD-C2D-C3D	-2.17	122.71	127.69
31	g	602	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
31	B1	608	CLA	CHA-C1A-NA	-2.17	121.47	126.39
31	R1	602	CLA	CHA-C1A-NA	-2.17	121.47	126.39
31	N1	602	CLA	C2C-C1C-NC	2.17	112.26	109.98
46	h	101	RRX	C36-C18-C19	2.17	121.40	118.09
31	R1	608	CLA	C1D-ND-C4D	-2.17	104.79	106.31
31	c	509	CLA	CHD-C1D-ND	-2.17	121.75	124.80
31	A1	410	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
31	a1	406	CLA	C6-C5-C3	-2.17	108.18	113.47
31	n1	604	CLA	C2D-C1D-ND	2.17	112.27	110.13
31	B1	609	CLA	C2A-C1A-CHA	2.17	127.63	123.87
31	y	611	CLA	CHA-C1A-NA	-2.17	121.48	126.39
31	y	603	CLA	CAA-C2A-C3A	-2.17	107.14	113.00
31	C	512	CLA	O1D-CGD-CBD	-2.17	120.24	124.52
31	S1	603	CLA	CHD-C1D-ND	-2.17	121.75	124.80
31	r1	602	CLA	CHD-C1D-ND	-2.17	121.75	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	617	CLA	C2D-C1D-ND	2.17	112.27	110.13
31	B1	606	CLA	C4B-CHC-C1C	2.17	131.35	126.25
47	g1	609	CHL	C1-C2-C3	-2.17	122.64	126.20
31	S1	611	CLA	CAC-C3C-C4C	2.17	127.61	124.79
31	b	610	CLA	CHD-C1D-ND	-2.17	121.75	124.80
31	b1	616	CLA	CHD-C1D-ND	-2.17	121.75	124.80
31	D	402	CLA	O2D-CGD-O1D	-2.17	119.63	123.85
31	s1	614	CLA	O2D-CGD-O1D	-2.17	119.63	123.85
31	b1	614	CLA	CMA-C3A-C4A	2.17	117.60	111.77
31	G	602	CLA	C2D-C1D-ND	2.17	112.27	110.13
31	R1	602	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
44	D1	405	PL9	C37-C38-C39	-2.17	122.66	127.62
31	N1	614	CLA	C1-O2A-CGA	2.17	121.90	116.65
31	B1	617	CLA	CMD-C2D-C3D	-2.17	122.72	127.69
31	B	607	CLA	C4B-CHC-C1C	2.17	131.34	126.25
31	b1	607	CLA	C1C-C2C-C3C	-2.17	104.70	106.98
31	C1	508	CLA	CHD-C1D-ND	-2.17	121.75	124.80
53	a1	414	SPH	C3-C4-C5	-2.17	120.20	124.69
56	r1	626	ERG	C12-C13-C17	-2.17	113.41	116.60
31	B1	608	CLA	C1-O2A-CGA	2.17	121.90	116.65
31	Y	610	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
31	G	614	CLA	C3B-C4B-NB	-2.17	108.60	110.53
31	g1	604	CLA	CHD-C1D-ND	-2.17	121.75	124.80
31	b1	615	CLA	C4B-CHC-C1C	2.17	131.34	126.25
31	g	610	CLA	C1C-C2C-C3C	-2.17	104.70	106.98
48	s	620	LUT	C36-C21-C22	-2.17	105.37	109.41
31	G	613	CLA	C1-O2A-CGA	2.17	121.89	116.65
31	C	508	CLA	CHD-C1D-ND	-2.17	121.75	124.80
31	b1	610	CLA	C3B-C4B-NB	-2.17	108.60	110.53
45	f	101	HEM	C3B-C4B-NB	-2.17	107.91	109.47
31	B	617	CLA	C4B-CHC-C1C	2.16	131.34	126.25
31	N	613	CLA	C1D-ND-C4D	-2.16	104.79	106.31
31	C1	501	CLA	O2D-CGD-O1D	-2.16	119.63	123.85
37	b	620	C7Z	C11-C12-C13	-2.16	120.43	126.36
31	d	403	CLA	CHA-C1A-NA	-2.16	121.49	126.39
40	C1	519	DGD	O1G-C1A-O1A	-2.16	118.21	123.63
35	c1	521	LMG	O7-C10-O9	-2.16	118.64	123.70
53	y	625	SPH	C1-C2-C3	-2.16	108.53	113.00
31	s	603	CLA	O2A-CGA-CBA	2.16	118.43	111.83
31	Y	613	CLA	C2D-C1D-ND	2.16	112.27	110.13
31	C1	501	CLA	O1D-CGD-CBD	-2.16	120.25	124.52
31	g	613	CLA	O2D-CGD-O1D	-2.16	119.64	123.85

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	b	605	CLA	O2A-CGA-CBA	2.16	118.43	111.83
31	c	506	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
31	r	604	CLA	O2A-CGA-CBA	2.16	118.43	111.83
31	C	504	CLA	CMD-C2D-C3D	-2.16	122.73	127.69
31	N	604	CLA	C1D-ND-C4D	-2.16	104.80	106.31
31	R	609	CLA	CMA-C3A-C4A	2.16	117.58	111.77
31	b1	614	CLA	C3B-C4B-NB	-2.16	108.60	110.53
31	a	407	CLA	O2A-CGA-CBA	2.16	118.43	111.83
31	b1	608	CLA	CHD-C1D-ND	-2.16	121.76	124.80
31	b1	615	CLA	CHD-C1D-ND	-2.16	121.76	124.80
47	S	601	CHL	C4C-CHD-C1D	2.16	123.80	116.07
31	b	602	CLA	CHA-C1A-NA	-2.16	121.50	126.39
31	c	513	CLA	O1D-CGD-CBD	-2.16	120.25	124.52
31	c1	513	CLA	CHD-C1D-ND	-2.16	121.76	124.80
31	B1	613	CLA	O2A-CGA-CBA	2.16	118.42	111.83
31	B1	606	CLA	CHA-C1A-NA	-2.16	121.50	126.39
31	S1	617	CLA	CHD-C1D-ND	-2.16	121.76	124.80
33	a	411	BCR	C4-C5-C6	-2.16	119.78	122.70
31	a1	406	CLA	C4B-CHC-C1C	2.16	131.33	126.25
47	s	601	CHL	C3D-C4D-ND	-2.16	109.47	112.94
31	N	611	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
31	g1	611	CLA	O2A-CGA-CBA	2.16	118.42	111.83
31	C1	510	CLA	O2D-CGD-O1D	-2.16	119.64	123.85
31	S	602	CLA	C1D-ND-C4D	-2.16	104.80	106.31
31	S	605	CLA	C1D-ND-C4D	-2.16	104.80	106.31
31	S	609	CLA	C1D-ND-C4D	-2.16	104.80	106.31
47	R1	606	CHL	C3D-C4D-ND	-2.16	109.47	112.94
31	c	511	CLA	C1C-C2C-C3C	-2.16	104.71	106.98
31	b1	607	CLA	C2D-C1D-ND	2.16	112.26	110.13
47	g1	601	CHL	C4C-CHD-C1D	2.16	123.79	116.07
31	r1	612	CLA	O2A-CGA-CBA	2.16	118.42	111.83
31	n	611	CLA	O2A-CGA-CBA	2.16	118.41	111.83
31	C1	503	CLA	CHD-C1D-ND	-2.16	121.77	124.80
31	c1	510	CLA	CHD-C1D-ND	-2.16	121.77	124.80
31	y1	612	CLA	CHD-C1D-ND	-2.16	121.77	124.80
33	c	516	BCR	C35-C13-C12	2.16	121.38	118.09
47	S	608	CHL	C1-C2-C3	-2.16	122.66	126.20
31	A	405	CLA	CAA-CBA-CGA	-2.16	107.08	113.21
44	D1	405	PL9	C27-C28-C29	-2.16	122.69	127.62
31	a	410	CLA	C3B-C2B-C1B	-2.16	104.63	107.17
41	c1	525	LHG	C6-C5-C4	-2.16	106.76	111.78
33	d1	404	BCR	C33-C5-C6	-2.16	122.13	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	Y1	620	LUT	C31-C30-C29	-2.16	124.25	127.28
31	g	611	CLA	C2D-C1D-ND	2.16	112.26	110.13
31	b1	607	CLA	O1D-CGD-CBD	-2.16	120.27	124.52
31	N	610	CLA	C1-C2-C3	-2.16	122.67	126.20
31	Y1	608	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
31	a	407	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
31	B1	616	CLA	C1D-ND-C4D	-2.15	104.80	106.31
50	n	623	NEX	C11-C10-C9	2.15	130.30	127.28
31	S1	613	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
47	R	607	CHL	C1C-C2C-CMC	2.15	130.69	126.80
49	R1	621	XAT	C24-C23-C22	-2.15	106.76	110.79
48	y1	621	LUT	C40-C33-C34	-2.15	119.33	122.82
50	S	622	NEX	C40-C33-C34	-2.15	119.33	122.82
31	G	604	CLA	CAA-C2A-C3A	-2.15	107.18	113.00
31	c	508	CLA	CAA-C2A-C3A	-2.15	107.18	113.00
48	r	620	LUT	C31-C32-C33	-2.15	120.46	126.36
48	S1	620	LUT	C27-C28-C29	-2.15	121.69	126.32
47	s	608	CHL	CMD-C2D-C3D	2.15	128.99	124.68
31	C	501	CLA	OBD-CAD-C3D	-2.15	123.38	128.42
31	R	604	CLA	CHA-C1A-NA	-2.15	121.51	126.39
31	y1	608	CLA	C3D-C2D-C1D	-2.15	102.89	105.83
31	B1	603	CLA	C1D-ND-C4D	-2.15	104.80	106.31
31	C1	505	CLA	CHD-C1D-ND	-2.15	121.77	124.80
31	B1	615	CLA	C3B-C4B-NB	-2.15	108.61	110.53
31	s1	609	CLA	C1-O2A-CGA	2.15	121.86	116.65
31	b	607	CLA	CHA-C1A-NA	-2.15	121.52	126.39
47	S	608	CHL	CMD-C2D-C3D	2.15	128.99	124.68
31	B	602	CLA	CMA-C3A-C2A	2.15	122.31	113.98
31	c1	508	CLA	O2D-CGD-O1D	-2.15	119.66	123.85
47	Y1	605	CHL	C4C-CHD-C1D	2.15	123.77	116.07
31	y	604	CLA	CHA-C1A-NA	-2.15	121.52	126.39
31	d1	402	CLA	CHA-C1A-NA	-2.15	121.52	126.39
31	C1	511	CLA	C6-C5-C3	-2.15	108.22	113.47
47	g	608	CHL	CMD-C2D-C3D	2.15	128.98	124.68
31	g	612	CLA	C1D-ND-C4D	-2.15	104.80	106.31
31	n	604	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
31	c	512	CLA	C3B-C4B-NB	-2.15	108.61	110.53
48	g1	620	LUT	C35-C15-C14	-2.15	119.12	123.52
47	y	601	CHL	C3D-C4D-ND	-2.15	109.49	112.94
31	b1	609	CLA	OBD-CAD-C3D	-2.15	123.39	128.42
50	N1	623	NEX	C4-C3-C2	2.15	114.81	110.79
31	B	608	CLA	CHA-C1A-NA	-2.15	121.52	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B1	605	CLA	CHA-C1A-NA	-2.15	121.52	126.39
31	n	613	CLA	CMD-C2D-C3D	-2.15	122.75	127.69
31	B1	604	CLA	C2D-C1D-ND	2.15	112.25	110.13
31	n	611	CLA	C1-O2A-CGA	2.15	121.86	116.65
31	N	603	CLA	O2A-CGA-CBA	2.15	118.39	111.83
31	Y1	602	CLA	C1D-ND-C4D	-2.15	104.80	106.31
31	B1	602	CLA	CHA-C1A-NA	-2.15	121.52	126.39
31	b1	604	CLA	CHA-C1A-NA	-2.15	121.52	126.39
31	a	410	CLA	CHD-C1D-ND	-2.15	121.78	124.80
33	D	404	BCR	C30-C25-C26	-2.15	119.70	122.64
31	n1	612	CLA	CMD-C2D-C3D	-2.15	122.76	127.69
31	b	604	CLA	CHA-C1A-NA	-2.15	121.52	126.39
47	G	601	CHL	C4D-CHA-CBD	-2.15	106.80	108.97
31	G	612	CLA	CHD-C1D-ND	-2.15	121.78	124.80
31	S	609	CLA	CHD-C1D-ND	-2.15	121.78	124.80
31	B1	607	CLA	CHD-C1D-ND	-2.15	121.78	124.80
47	y1	607	CHL	CMA-C3A-C4A	2.15	119.24	114.61
44	d	405	PL9	O2-C1-C6	2.15	123.90	120.48
31	Y1	604	CLA	C6-C7-C8	-2.15	108.82	115.97
31	B1	617	CLA	C1-O2A-CGA	2.15	121.85	116.65
33	C	515	BCR	C8-C7-C6	-2.15	121.26	127.00
31	Y1	610	CLA	C6-C5-C3	-2.15	108.23	113.47
48	n1	621	LUT	C10-C11-C12	-2.15	116.97	123.20
47	s	607	CHL	CMD-C2D-C3D	2.15	128.98	124.68
31	N	611	CLA	CHA-C1A-NA	-2.15	121.52	126.39
43	d	401	BCT	O3-C-O1	-2.15	114.18	119.68
31	r	613	CLA	CMD-C2D-C3D	-2.15	122.76	127.69
31	y	614	CLA	CHA-C1A-NA	-2.15	121.53	126.39
31	b	615	CLA	C2A-C1A-CHA	2.15	127.60	123.87
31	C1	505	CLA	CMA-C3A-C4A	2.15	117.55	111.77
31	s	617	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
31	N1	614	CLA	CMD-C2D-C3D	-2.15	122.76	127.69
48	N	620	LUT	C39-C29-C28	2.15	121.37	118.09
31	B1	604	CLA	CHA-C1A-NA	-2.15	121.53	126.39
31	c1	506	CLA	CHA-C1A-NA	-2.15	121.53	126.39
31	s1	612	CLA	CHA-C1A-NA	-2.15	121.53	126.39
47	R1	606	CHL	CMA-C3A-C4A	2.15	119.24	114.61
31	Y	613	CLA	CAA-C2A-C3A	-2.15	107.19	113.00
31	N1	610	CLA	C2C-C1C-NC	2.15	112.24	109.98
31	n1	612	CLA	C1D-ND-C4D	-2.15	104.81	106.31
47	R1	607	CHL	CMD-C2D-C3D	2.15	128.97	124.68
31	n	612	CLA	C3D-C2D-C1D	-2.15	102.90	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
48	N1	620	LUT	C30-C31-C32	-2.15	116.98	123.20
35	C1	521	LMG	O8-C28-O10	-2.15	118.26	123.63
31	c	512	CLA	CMA-C3A-C4A	2.15	117.55	111.77
31	R	604	CLA	C1-O2A-CGA	2.15	121.85	116.65
31	g	614	CLA	CHA-C1A-NA	-2.15	121.53	126.39
31	b	615	CLA	CHD-C1D-ND	-2.15	121.78	124.80
31	G1	604	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
47	Y	606	CHL	CMD-C2D-C3D	2.15	128.97	124.68
31	c1	511	CLA	CMA-C3A-C4A	2.15	117.54	111.77
31	n1	603	CLA	O1D-CGD-CBD	-2.15	120.28	124.52
40	c1	519	DGD	C2G-O2G-C1B	-2.15	112.66	117.80
31	N	610	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
50	g	623	NEX	C31-C32-C33	2.15	132.25	126.36
31	S	611	CLA	C4B-CHC-C1C	2.15	131.29	126.25
31	g1	602	CLA	CHA-C1A-NA	-2.15	121.53	126.39
31	b1	611	CLA	CHD-C1D-ND	-2.15	121.78	124.80
31	s1	617	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
35	C	521	LMG	O7-C10-O9	-2.15	118.69	123.70
31	N1	614	CLA	CHA-C1A-NA	-2.15	121.53	126.39
48	s1	621	LUT	C1-C6-C7	2.15	121.47	115.65
31	N	614	CLA	C2D-C1D-ND	2.15	112.25	110.13
31	Y	602	CLA	CHD-C1D-ND	-2.14	121.78	124.80
31	B	604	CLA	CHA-C1A-NA	-2.14	121.53	126.39
31	Y	608	CLA	CHA-C1A-NA	-2.14	121.53	126.39
49	G	622	XAT	C19-C9-C10	-2.14	119.34	122.82
35	D	411	LMG	C8-O7-C10	-2.14	112.67	117.80
37	B1	620	C7Z	C20-C13-C14	-2.14	119.34	122.82
31	s	610	CLA	C1D-ND-C4D	-2.14	104.81	106.31
31	C	507	CLA	CMA-C3A-C4A	2.14	117.53	111.77
31	c1	501	CLA	CHA-C1A-NA	-2.14	121.54	126.39
31	G	613	CLA	C2D-C1D-ND	2.14	112.25	110.13
31	S	604	CLA	C2D-C1D-ND	2.14	112.25	110.13
31	g1	603	CLA	C2D-C1D-ND	2.14	112.25	110.13
33	c	516	BCR	C1-C6-C7	2.14	121.46	115.65
31	D	403	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
31	b	605	CLA	CHA-C1A-NA	-2.14	121.54	126.39
31	n	612	CLA	O1D-CGD-CBD	-2.14	120.29	124.52
31	s	612	CLA	C2D-C1D-ND	2.14	112.25	110.13
40	C	523	DGD	O1G-C1A-O1A	-2.14	118.27	123.63
31	S	604	CLA	CMD-C2D-C3D	-2.14	122.78	127.69
31	b	616	CLA	C3B-C4B-NB	-2.14	108.62	110.53
31	R	609	CLA	OBD-CAD-C3D	-2.14	123.41	128.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C	502	CLA	O2A-CGA-CBA	2.14	118.36	111.83
31	Y	614	CLA	O1D-CGD-CBD	-2.14	120.29	124.52
31	B	605	CLA	CHD-C1D-ND	-2.14	121.79	124.80
31	B1	612	CLA	CHD-C1D-ND	-2.14	121.79	124.80
31	s	602	CLA	O2D-CGD-O1D	-2.14	119.68	123.85
31	G	603	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
31	b1	604	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
47	y	607	CHL	C1-C2-C3	-2.14	122.69	126.20
31	R1	612	CLA	C2D-C1D-ND	2.14	112.25	110.13
31	b1	606	CLA	CHA-C1A-NA	-2.14	121.54	126.39
33	b	619	BCR	C1-C6-C5	-2.14	119.71	122.64
48	G1	620	LUT	C10-C11-C12	-2.14	117.00	123.20
44	D1	405	PL9	C40-C39-C41	2.14	118.94	115.23
31	c	511	CLA	CAA-C2A-C3A	-2.14	107.22	113.00
31	B	609	CLA	C2A-C1A-CHA	2.14	127.58	123.87
31	C	502	CLA	C1D-ND-C4D	-2.14	104.81	106.31
31	n	612	CLA	C1D-ND-C4D	-2.14	104.81	106.31
31	b	603	CLA	CHA-C1A-NA	-2.14	121.55	126.39
31	B	616	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
31	c	503	CLA	CAA-CBA-CGA	-2.14	107.14	113.21
31	r	611	CLA	CHA-C1A-NA	-2.14	121.55	126.39
48	n1	620	LUT	C26-C27-C28	-2.14	121.25	124.58
31	a	406	CLA	CHD-C1D-ND	-2.14	121.79	124.80
31	g	604	CLA	C3B-C4B-NB	-2.14	108.62	110.53
31	C1	513	CLA	C3B-C4B-NB	-2.14	108.62	110.53
31	G	610	CLA	CMA-C3A-C4A	2.14	117.52	111.77
31	C1	501	CLA	CHA-C1A-NA	-2.14	121.55	126.39
31	n	614	CLA	CAA-C2A-C3A	-2.14	107.22	113.00
50	r1	622	NEX	C40-C33-C34	-2.14	119.35	122.82
31	c	506	CLA	C2D-C1D-ND	2.14	112.24	110.13
31	g1	604	CLA	C2D-C1D-ND	2.14	112.24	110.13
31	C1	510	CLA	CHA-C1A-NA	-2.14	121.55	126.39
31	C1	504	CLA	O2A-CGA-CBA	2.14	118.35	111.83
47	S1	608	CHL	CMD-C2D-C3D	2.14	128.95	124.68
31	g	602	CLA	C4B-CHC-C1C	2.14	131.27	126.25
31	y1	604	CLA	C1D-ND-C4D	-2.14	104.81	106.31
31	S1	604	CLA	C1-O2A-CGA	2.14	121.82	116.65
33	c1	514	BCR	C29-C28-C27	2.14	115.97	111.28
31	r1	602	CLA	CMD-C2D-C3D	-2.14	122.79	127.69
31	y	608	CLA	O2D-CGD-O1D	-2.14	119.69	123.85
45	F	101	HEM	C3C-C2C-C1C	2.14	109.07	107.05
31	G1	611	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	S	609	CLA	CHA-C1A-NA	-2.14	121.55	126.39
31	n	614	CLA	C3D-C2D-C1D	-2.14	102.92	105.83
31	A1	406	CLA	C3D-C2D-C1D	-2.14	102.92	105.83
40	c	519	DGD	O1G-C1A-O1A	-2.14	118.28	123.63
31	c1	503	CLA	C2D-C1D-ND	2.14	112.24	110.13
47	y	609	CHL	C1C-C2C-CMC	2.14	130.65	126.80
49	n	622	XAT	O4-C5-C18	-2.14	112.66	115.05
31	Y	603	CLA	CHA-C1A-NA	-2.14	121.56	126.39
31	G1	604	CLA	CMD-C2D-C3D	-2.14	122.79	127.69
47	y	601	CHL	CMD-C2D-C3D	2.13	128.95	124.68
31	N	614	CLA	CHA-C1A-NA	-2.13	121.56	126.39
44	D	405	PL9	C37-C38-C39	-2.13	122.74	127.62
33	c1	516	BCR	C35-C13-C12	2.13	121.35	118.09
48	N	620	LUT	C20-C13-C12	2.13	121.35	118.09
31	C1	507	CLA	C3B-C4B-NB	-2.13	108.62	110.53
31	r	602	CLA	C1D-ND-C4D	-2.13	104.81	106.31
31	c1	502	CLA	C11-C10-C8	-2.13	108.88	115.97
31	R	603	CLA	CHD-C1D-ND	-2.13	121.80	124.80
31	S	602	CLA	CHD-C1D-ND	-2.13	121.80	124.80
31	b	607	CLA	CHD-C1D-ND	-2.13	121.80	124.80
47	N1	609	CHL	CMD-C2D-C3D	2.13	128.94	124.68
31	g	610	CLA	C2C-C1C-NC	2.13	112.22	109.98
31	g	610	CLA	CHA-C1A-NA	-2.13	121.56	126.39
49	G1	622	XAT	O4-C6-C7	-2.13	110.77	116.88
31	r1	602	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
47	N1	607	CHL	C3D-C4D-ND	-2.13	109.52	112.94
49	n1	622	XAT	O4-C5-C18	-2.13	112.67	115.05
31	N	603	CLA	CMD-C2D-C3D	-2.13	122.80	127.69
47	s1	601	CHL	CMD-C2D-C3D	2.13	128.94	124.68
31	y1	611	CLA	O2A-CGA-CBA	2.13	118.34	111.83
47	N	605	CHL	C4C-CHD-C1D	2.13	123.70	116.07
31	n	602	CLA	CHA-C1A-NA	-2.13	121.56	126.39
31	S1	614	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
31	g	612	CLA	C2D-C1D-ND	2.13	112.24	110.13
31	S1	610	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
31	D	403	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
31	G	614	CLA	O1D-CGD-CBD	-2.13	120.31	124.52
48	n1	621	LUT	C20-C13-C12	2.13	121.34	118.09
31	B1	617	CLA	CHA-C1A-NA	-2.13	121.56	126.39
31	Y	613	CLA	C1D-ND-C4D	-2.13	104.82	106.31
31	s	609	CLA	C1D-ND-C4D	-2.13	104.82	106.31
31	y	614	CLA	CHD-C1D-ND	-2.13	121.80	124.80

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	R	602	CLA	C3B-C4B-NB	-2.13	108.63	110.53
31	S1	604	CLA	O1D-CGD-CBD	-2.13	120.32	124.52
31	Y1	604	CLA	CAA-C2A-C3A	-2.13	107.24	113.00
47	N1	607	CHL	CMD-C2D-C3D	2.13	128.94	124.68
31	b1	605	CLA	CHA-C1A-NA	-2.13	121.57	126.39
31	g1	604	CLA	OBD-CAD-C3D	-2.13	123.44	128.42
31	G	602	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
33	c1	517	BCR	C8-C7-C6	-2.13	121.31	127.00
31	s1	609	CLA	CHD-C1D-ND	-2.13	121.81	124.80
31	Y1	612	CLA	C2D-C1D-ND	2.13	112.23	110.13
31	N1	611	CLA	CMA-C3A-C4A	2.13	117.50	111.77
31	S1	611	CLA	C3B-C4B-NB	-2.13	108.63	110.53
49	R	621	XAT	O24-C26-C27	-2.13	110.78	116.88
31	R1	608	CLA	C2D-C1D-ND	2.13	112.23	110.13
49	r1	621	XAT	C27-C28-C29	2.13	128.83	125.53
31	B1	603	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
31	b	610	CLA	CMD-C2D-C3D	-2.13	122.81	127.69
31	G	602	CLA	C1D-ND-C4D	-2.13	104.82	106.31
31	B	609	CLA	O2A-CGA-CBA	2.13	118.32	111.83
31	g	603	CLA	O2A-CGA-CBA	2.13	118.32	111.83
48	R1	620	LUT	C1-C6-C5	-2.13	119.73	122.64
31	s	610	CLA	CHA-C1A-NA	-2.13	121.57	126.39
31	g1	612	CLA	CHD-C1D-ND	-2.13	121.81	124.80
31	B1	613	CLA	C4B-CHC-C1C	2.13	131.25	126.25
47	g	607	CHL	CMA-C3A-C4A	2.13	119.19	114.61
31	b	611	CLA	O1D-CGD-CBD	-2.13	120.32	124.52
48	g	621	LUT	C38-C25-C24	-2.13	118.33	123.36
31	B	614	CLA	CHA-C1A-NA	-2.13	121.58	126.39
31	b	604	CLA	CAA-C2A-C3A	-2.13	107.25	113.00
31	y	602	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
31	c	502	CLA	CHD-C1D-ND	-2.13	121.81	124.80
31	a1	407	CLA	O2D-CGD-O1D	-2.13	119.71	123.85
31	g1	602	CLA	O1D-CGD-CBD	-2.13	120.32	124.52
31	N	613	CLA	CHA-C1A-NA	-2.13	121.58	126.39
31	y1	604	CLA	CHA-C1A-NA	-2.13	121.58	126.39
31	s1	609	CLA	C3B-C4B-NB	-2.13	108.63	110.53
31	S1	604	CLA	CHA-C1A-NA	-2.13	121.58	126.39
40	B1	623	DGD	O2G-C1B-O1B	-2.13	118.73	123.70
31	B	617	CLA	C1-O2A-CGA	2.13	121.80	116.65
31	r	603	CLA	O2D-CGD-O1D	-2.13	119.71	123.85
31	R1	608	CLA	O2D-CGD-O1D	-2.13	119.71	123.85
31	G	613	CLA	C1D-ND-C4D	-2.13	104.82	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	S	604	CLA	C1D-ND-C4D	-2.13	104.82	106.31
31	G1	612	CLA	CHA-C1A-NA	-2.13	121.58	126.39
31	Y1	603	CLA	C1-O2A-CGA	2.12	121.79	116.65
31	C	504	CLA	O2A-CGA-CBA	2.12	118.31	111.83
31	y	604	CLA	CMD-C2D-C3D	-2.12	122.82	127.69
31	r	610	CLA	C3D-C2D-C1D	-2.12	102.93	105.83
31	N1	603	CLA	C1-O2A-CGA	2.12	121.79	116.65
47	g1	601	CHL	C3D-C4D-ND	-2.12	109.53	112.94
31	s	604	CLA	CHA-C1A-NA	-2.12	121.58	126.39
31	B1	614	CLA	C1D-ND-C4D	-2.12	104.82	106.31
45	f	101	HEM	CAC-C3C-C4C	2.12	129.89	124.82
31	B	605	CLA	CMB-C2B-C1B	2.12	128.65	125.42
31	N	604	CLA	CHA-C1A-NA	-2.12	121.58	126.39
31	n1	603	CLA	CHA-C1A-NA	-2.12	121.58	126.39
47	g1	608	CHL	C4C-CHD-C1D	2.12	123.67	116.07
33	C1	515	BCR	C1-C6-C7	2.12	121.41	115.65
49	N	622	XAT	C26-C27-C28	-2.12	121.50	125.99
31	C	511	CLA	C3D-C2D-C1D	-2.12	102.93	105.83
31	N	604	CLA	C3D-C2D-C1D	-2.12	102.93	105.83
31	y1	614	CLA	O1D-CGD-CBD	-2.12	120.33	124.52
47	n1	606	CHL	CMD-C2D-C3D	2.12	128.93	124.68
31	b	615	CLA	CHA-C1A-NA	-2.12	121.58	126.39
31	B	616	CLA	O1D-CGD-CBD	-2.12	120.33	124.52
47	G1	601	CHL	C4C-CHD-C1D	2.12	123.66	116.07
48	S1	621	LUT	C31-C32-C33	-2.12	120.54	126.36
31	c	502	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
31	C1	503	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
31	c1	513	CLA	CMD-C2D-C3D	-2.12	122.82	127.69
31	y	603	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
31	g1	604	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
31	g1	613	CLA	CAA-C2A-C3A	-2.12	107.27	113.00
31	B	605	CLA	C4B-CHC-C1C	2.12	131.24	126.25
31	R1	608	CLA	O2A-CGA-CBA	2.12	118.30	111.83
31	c1	501	CLA	CMD-C2D-C3D	-2.12	122.83	127.69
33	D	404	BCR	C33-C5-C4	2.12	118.12	113.60
31	C	510	CLA	C2D-C1D-ND	2.12	112.22	110.13
31	S1	605	CLA	CAA-C2A-C3A	-2.12	107.27	113.00
49	r	622	XAT	C30-C31-C32	-2.12	117.06	123.20
31	B	610	CLA	C1D-ND-C4D	-2.12	104.82	106.31
49	g1	622	XAT	O4-C5-C18	-2.12	112.68	115.05
33	a	411	BCR	C38-C26-C25	-2.12	122.17	124.48
35	a	413	LMG	O7-C10-O9	-2.12	118.75	123.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	y1	602	CLA	CMD-C2D-C3D	-2.12	122.83	127.69
47	n1	601	CHL	C1-C2-C3	-2.12	122.72	126.20
31	y1	614	CLA	O2A-CGA-CBA	2.12	118.30	111.83
31	S1	612	CLA	CHD-C1D-ND	-2.12	121.82	124.80
31	s1	610	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
31	C	507	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
49	n	622	XAT	C20-C13-C14	-2.12	119.38	122.82
33	c	514	BCR	C23-C24-C25	-2.12	121.34	127.00
31	N1	613	CLA	O2D-CGD-O1D	-2.12	119.72	123.85
47	r1	607	CHL	CMD-C2D-C3D	2.12	128.92	124.68
48	r1	620	LUT	C31-C32-C33	-2.12	120.56	126.36
31	y1	614	CLA	CHA-C1A-NA	-2.12	121.59	126.39
31	r	604	CLA	C2D-C1D-ND	2.12	112.22	110.13
31	N1	604	CLA	C2D-C1D-ND	2.12	112.22	110.13
31	n1	614	CLA	C2D-C1D-ND	2.12	112.22	110.13
31	S1	609	CLA	O1D-CGD-CBD	-2.12	120.34	124.52
48	S1	620	LUT	C20-C13-C12	2.12	121.32	118.09
31	S1	610	CLA	CHA-C1A-NA	-2.12	121.60	126.39
31	S	617	CLA	C1-O2A-CGA	2.12	121.78	116.65
31	s	602	CLA	CMD-C2D-C3D	-2.12	122.83	127.69
31	Y1	604	CLA	CMD-C2D-C3D	-2.12	122.83	127.69
31	g1	614	CLA	CMD-C2D-C3D	-2.12	122.83	127.69
31	c	504	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
49	N	622	XAT	O24-C25-C24	2.12	115.47	113.49
47	N1	608	CHL	C3D-C4D-ND	-2.12	109.54	112.94
31	b	609	CLA	O2A-CGA-CBA	2.12	118.29	111.83
31	r	602	CLA	CAA-C2A-C3A	-2.12	107.28	113.00
33	A	411	BCR	C33-C5-C4	2.12	118.11	113.60
31	B	614	CLA	O2D-CGD-O1D	-2.12	119.73	123.85
31	g1	602	CLA	CHD-C1D-ND	-2.12	121.82	124.80
47	Y	605	CHL	C4C-CHD-C1D	2.12	123.64	116.07
31	b1	604	CLA	CAA-C2A-C3A	-2.12	107.28	113.00
31	c	513	CLA	CHA-C1A-NA	-2.12	121.60	126.39
31	A1	405	CLA	C4B-CHC-C1C	2.12	131.22	126.25
31	y1	604	CLA	C2D-C1D-ND	2.12	112.22	110.13
31	y1	604	CLA	CMD-C2D-C3D	-2.12	122.84	127.69
31	s	604	CLA	CAC-C3C-C4C	2.12	127.54	124.79
50	R1	622	NEX	C5-C6-C1	2.12	121.80	119.70
31	C1	509	CLA	C4B-CHC-C1C	2.12	131.22	126.25
31	Y	611	CLA	CHD-C1D-ND	-2.12	121.83	124.80
31	c1	504	CLA	CMD-C2D-C3D	-2.11	122.84	127.69
31	b1	606	CLA	CMA-C3A-C4A	2.11	117.46	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	y	602	CLA	CHA-C4D-ND	2.11	136.91	132.55
31	b1	612	CLA	O1D-CGD-CBD	-2.11	120.35	124.52
33	C1	514	BCR	C19-C18-C17	2.11	122.33	119.01
31	Y	613	CLA	C1-O2A-CGA	2.11	121.77	116.65
31	r	609	CLA	CMD-C2D-C3D	-2.11	122.84	127.69
31	S1	611	CLA	CMD-C2D-C3D	-2.11	122.84	127.69
31	N	603	CLA	CHA-C1A-NA	-2.11	121.60	126.39
31	r1	608	CLA	CHD-C1D-ND	-2.11	121.83	124.80
31	G1	604	CLA	C2D-C1D-ND	2.11	112.22	110.13
31	Y1	603	CLA	C1D-ND-C4D	-2.11	104.83	106.31
31	b1	615	CLA	OBD-CAD-C3D	-2.11	123.48	128.42
31	g	612	CLA	CHA-C1A-NA	-2.11	121.61	126.39
33	C1	516	BCR	C1-C6-C7	2.11	121.38	115.65
31	S1	610	CLA	C3B-C4B-NB	-2.11	108.64	110.53
31	D	403	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
31	b1	610	CLA	CHA-C1A-NA	-2.11	121.61	126.39
31	b	612	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
31	n1	614	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
44	d	405	PL9	C42-C43-C44	-2.11	122.79	127.62
31	N	611	CLA	CMD-C2D-C3D	-2.11	122.85	127.69
31	c	513	CLA	CBB-CAB-C3B	-2.11	116.97	127.53
31	r1	608	CLA	O2D-CGD-O1D	-2.11	119.74	123.85
31	Y1	612	CLA	CMA-C3A-C4A	2.11	117.45	111.77
48	y	621	LUT	C10-C11-C12	-2.11	117.08	123.20
31	c	504	CLA	CMD-C2D-C3D	-2.11	122.85	127.69
31	C	506	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
44	d1	405	PL9	O1-C4-C3	-2.11	118.50	120.73
31	s	612	CLA	CHA-C1A-NA	-2.11	121.61	126.39
31	a1	407	CLA	C1D-ND-C4D	-2.11	104.83	106.31
31	C	508	CLA	C1C-C2C-C3C	-2.11	104.76	106.98
31	r	602	CLA	C2D-C1D-ND	2.11	112.22	110.13
31	C	507	CLA	C2A-C1A-CHA	2.11	127.53	123.87
31	c1	513	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
31	s	613	CLA	C3B-C4B-NB	-2.11	108.65	110.53
31	C1	506	CLA	CHA-C1A-NA	-2.11	121.61	126.39
31	s1	613	CLA	CHA-C1A-NA	-2.11	121.61	126.39
31	B1	604	CLA	CHD-C1D-ND	-2.11	121.83	124.80
45	F	101	HEM	CAB-C3B-C2B	-2.11	121.57	128.43
50	n1	623	NEX	C40-C33-C34	-2.11	119.40	122.82
33	C	516	BCR	C33-C5-C4	2.11	118.09	113.60
31	R	613	CLA	C1D-ND-C4D	-2.11	104.83	106.31
31	n1	613	CLA	C1D-ND-C4D	-2.11	104.83	106.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	g1	607	CHL	CMD-C2D-C3D	2.11	128.90	124.68
31	g	602	CLA	CBC-CAC-C3C	-2.11	106.70	112.42
41	c	625	LHG	O8-C23-O10	-2.11	118.35	123.63
31	n1	613	CLA	C2A-C1A-CHA	2.11	127.53	123.87
31	R	609	CLA	O2D-CGD-O1D	-2.11	119.74	123.85
47	S	607	CHL	CMD-C2D-C3D	2.11	128.90	124.68
31	y1	602	CLA	CHA-C1A-NA	-2.11	121.62	126.39
31	b1	617	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
50	s	623	NEX	C39-C29-C30	-2.11	119.40	122.82
31	S	605	CLA	C2A-C1A-CHA	2.11	127.53	123.87
31	b1	616	CLA	C1-O2A-CGA	2.11	121.75	116.65
31	N	602	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
31	s	611	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
46	h	101	RRX	C1-C6-C7	2.11	121.37	115.65
31	R1	603	CLA	CHD-C1D-ND	-2.11	121.84	124.80
31	B1	610	CLA	CMD-C2D-C3D	-2.11	122.86	127.69
31	a	405	CLA	CAC-C3C-C4C	2.11	127.53	124.79
31	c1	503	CLA	CHA-C1A-NA	-2.11	121.62	126.39
47	G1	608	CHL	CMD-C2D-C3D	2.11	128.89	124.68
31	n1	603	CLA	O2A-CGA-CBA	2.11	118.26	111.83
31	a	407	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
31	s1	604	CLA	C3B-C4B-NB	-2.11	108.65	110.53
33	C1	517	BCR	C31-C1-C6	-2.11	106.94	110.24
31	b1	614	CLA	O2D-CGD-O1D	-2.11	119.75	123.85
31	Y	608	CLA	C4B-CHC-C1C	2.11	131.20	126.25
31	N	610	CLA	CBA-CAA-C2A	2.11	120.06	113.79
31	B	607	CLA	O1D-CGD-CBD	-2.11	120.36	124.52
31	A1	407	CLA	C1D-ND-C4D	-2.11	104.83	106.31
31	G1	612	CLA	C1D-ND-C4D	-2.11	104.83	106.31
47	S	606	CHL	C4C-CHD-C1D	2.11	123.61	116.07
31	d	402	CLA	CMD-C2D-C3D	-2.11	122.86	127.69
50	Y1	623	NEX	C5-C6-C1	2.11	121.79	119.70
31	g1	610	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
31	b1	607	CLA	C3B-C4B-NB	-2.11	108.65	110.53
48	n	620	LUT	C10-C11-C12	-2.11	117.10	123.20
33	C	516	BCR	C35-C13-C12	2.11	121.31	118.09
31	d	402	CLA	CHD-C1D-ND	-2.11	121.84	124.80
31	s1	613	CLA	C1-O2A-CGA	2.11	121.75	116.65
33	D	404	BCR	C4-C5-C6	-2.11	119.86	122.70
47	r1	606	CHL	CMD-C2D-C3D	2.11	128.89	124.68
31	G	613	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
31	g	602	CLA	C3D-C2D-C1D	-2.11	102.96	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	C1	509	CLA	CBC-CAC-C3C	-2.11	106.71	112.42
47	N1	605	CHL	CMA-C3A-C4A	2.11	119.15	114.61
31	b1	613	CLA	CHD-C1D-ND	-2.11	121.84	124.80
31	C	512	CLA	C3B-C4B-NB	-2.10	108.65	110.53
33	c1	516	BCR	C35-C13-C14	-2.10	119.41	122.82
50	s	623	NEX	C40-C33-C34	-2.10	119.41	122.82
41	d1	408	LHG	C5-O7-C7	-2.10	112.76	117.80
31	S1	617	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
31	R1	610	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
47	n1	607	CHL	CMD-C2D-C3D	2.10	128.89	124.68
31	s	604	CLA	C3B-C4B-NB	-2.10	108.65	110.53
31	c1	513	CLA	CAA-C2A-C1A	2.10	118.87	111.97
31	S1	602	CLA	OBD-CAD-C3D	-2.10	123.50	128.42
31	c1	511	CLA	C2D-C1D-ND	2.10	112.21	110.13
31	C1	509	CLA	C1D-ND-C4D	-2.10	104.84	106.31
31	R1	602	CLA	C1D-ND-C4D	-2.10	104.84	106.31
31	D1	403	CLA	CHA-C1A-NA	-2.10	121.63	126.39
33	b	619	BCR	C28-C27-C26	-2.10	110.31	114.06
31	b1	609	CLA	CMB-C2B-C3B	2.10	131.50	126.55
31	A	410	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
31	b	603	CLA	O1D-CGD-CBD	-2.10	120.37	124.52
47	S	608	CHL	C4C-CHD-C1D	2.10	123.59	116.07
46	h	101	RRX	C38-C26-C27	2.10	118.29	114.42
31	S1	602	CLA	CHA-C1A-NA	-2.10	121.63	126.39
47	N	605	CHL	CMD-C2D-C3D	2.10	128.88	124.68
31	C1	508	CLA	O2D-CGD-O1D	-2.10	119.75	123.85
48	Y1	620	LUT	C20-C13-C12	2.10	121.30	118.09
31	B1	603	CLA	CHA-C1A-NA	-2.10	121.63	126.39
31	N	614	CLA	C1D-ND-C4D	-2.10	104.84	106.31
31	R1	610	CLA	C1C-C2C-C3C	-2.10	104.77	106.98
31	R	602	CLA	C1-O2A-CGA	2.10	121.74	116.65
47	n1	608	CHL	CMD-C2D-C3D	2.10	128.88	124.68
31	C1	511	CLA	O2D-CGD-O1D	-2.10	119.76	123.85
31	S1	603	CLA	C2A-C1A-CHA	2.10	127.51	123.87
31	S1	612	CLA	O1D-CGD-CBD	-2.10	120.37	124.52
31	Y1	612	CLA	CHD-C1D-ND	-2.10	121.85	124.80
31	B1	614	CLA	O2D-CGD-O1D	-2.10	119.76	123.85
31	C	513	CLA	C3B-C4B-NB	-2.10	108.66	110.53
48	n1	620	LUT	C37-C21-C26	2.10	112.73	109.55
47	g1	606	CHL	C1C-C2C-CMC	2.10	130.59	126.80
31	C	502	CLA	CHA-C1A-NA	-2.10	121.64	126.39
31	b	605	CLA	CMC-C2C-C3C	2.10	131.83	126.15

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	A1	405	CLA	C1-O2A-CGA	2.10	121.73	116.65
31	D	402	CLA	CMD-C2D-C3D	-2.10	122.87	127.69
31	S	613	CLA	CMD-C2D-C3D	-2.10	122.87	127.69
31	b	609	CLA	CHD-C1D-ND	-2.10	121.85	124.80
47	N1	607	CHL	C1C-C2C-CMC	2.10	130.59	126.80
47	r	606	CHL	CMD-C2D-C3D	2.10	128.88	124.68
47	y	605	CHL	CMD-C2D-C3D	2.10	128.88	124.68
48	g	620	LUT	C31-C32-C33	-2.10	120.61	126.36
47	G1	609	CHL	C4C-CHD-C1D	2.10	123.58	116.07
50	y1	623	NEX	C11-C12-C13	2.10	132.12	126.36
31	r	610	CLA	CHD-C1D-ND	-2.10	121.85	124.80
31	S1	609	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
31	c	503	CLA	O2D-CGD-O1D	-2.10	119.76	123.85
48	y	620	LUT	C28-C29-C30	-2.10	115.71	119.01
31	S1	603	CLA	C2D-C1D-ND	2.10	112.20	110.13
47	N1	608	CHL	CMD-C2D-C3D	2.10	128.88	124.68
31	c1	505	CLA	OBD-CAD-C3D	-2.10	123.51	128.42
33	c	516	BCR	C36-C18-C17	-2.10	119.42	122.82
31	s	612	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
33	c1	514	BCR	C1-C6-C5	-2.10	119.77	122.64
31	n1	612	CLA	C2D-C1D-ND	2.10	112.20	110.13
47	n	609	CHL	C1-O2A-CGA	2.10	121.73	116.65
31	n	613	CLA	C1C-C2C-C3C	-2.10	104.77	106.98
31	Y1	604	CLA	C6-C5-C3	-2.10	108.36	113.47
31	C	512	CLA	CHD-C1D-ND	-2.10	121.85	124.80
31	C	502	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
31	R1	612	CLA	C3D-C2D-C1D	-2.10	102.97	105.83
31	a1	410	CLA	CHA-C1A-NA	-2.10	121.64	126.39
50	n1	623	NEX	C28-C29-C30	2.10	122.31	119.01
43	D1	401	BCT	O3-C-O1	-2.10	114.31	119.68
31	c	512	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
31	r	602	CLA	CMD-C2D-C3D	-2.10	122.88	127.69
47	N1	608	CHL	C4C-CHD-C1D	2.10	123.57	116.07
31	r1	609	CLA	CHA-C1A-NA	-2.10	121.64	126.39
32	a1	408	PHO	C2D-C1D-ND	-2.10	107.92	109.43
33	d1	404	BCR	C38-C26-C27	2.10	118.06	113.60
32	a1	409	PHO	C1-C2-C3	-2.10	122.76	126.20
31	N1	612	CLA	CHD-C1D-ND	-2.10	121.85	124.80
47	N	608	CHL	CMD-C2D-C3D	2.10	128.87	124.68
48	G	621	LUT	C8-C7-C6	-2.10	121.40	127.00
31	S1	610	CLA	C2D-C1D-ND	2.10	112.20	110.13
48	Y1	621	LUT	C26-C27-C28	-2.10	121.32	124.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	G	610	CLA	CHA-C1A-NA	-2.10	121.65	126.39
31	g1	614	CLA	CHD-C1D-ND	-2.09	121.86	124.80
37	b1	620	C7Z	C20-C13-C14	-2.09	119.42	122.82
49	g1	622	XAT	C19-C9-C10	-2.09	119.42	122.82
31	B1	610	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
31	c1	502	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
31	d	403	CLA	CHD-C1D-ND	-2.09	121.86	124.80
31	c1	508	CLA	O2A-CGA-CBA	2.09	118.22	111.83
31	R1	612	CLA	C1D-ND-C4D	-2.09	104.84	106.31
31	g1	610	CLA	C3B-C4B-NB	-2.09	108.66	110.53
31	B	608	CLA	C3D-C2D-C1D	-2.09	102.97	105.83
33	B1	618	BCR	C19-C18-C17	2.09	122.30	119.01
31	S	611	CLA	CMD-C2D-C3D	-2.09	122.89	127.69
31	s1	611	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
31	r	612	CLA	CHD-C1D-ND	-2.09	121.86	124.80
31	n	613	CLA	O1D-CGD-CBD	-2.09	120.39	124.52
33	c1	517	BCR	C4-C5-C6	-2.09	119.88	122.70
31	C1	510	CLA	C4B-CHC-C1C	2.09	131.17	126.25
31	c1	501	CLA	C2D-C1D-ND	2.09	112.20	110.13
53	y1	625	SPH	C3-C4-C5	-2.09	120.35	124.69
33	C	517	BCR	C36-C18-C17	-2.09	119.43	122.82
48	N	620	LUT	C15-C35-C34	-2.09	119.24	123.52
31	g1	610	CLA	O2D-CGD-O1D	-2.09	119.78	123.85
31	n	610	CLA	C3B-C4B-NB	-2.09	108.66	110.53
31	s1	605	CLA	C2A-C1A-CHA	2.09	127.50	123.87
50	y1	623	NEX	C4-C3-C2	2.09	114.70	110.79
31	S	612	CLA	C1D-ND-C4D	-2.09	104.84	106.31
31	G	610	CLA	C2C-C1C-NC	2.09	112.18	109.98
47	y	601	CHL	C4C-CHD-C1D	2.09	123.55	116.07
33	B1	618	BCR	C37-C22-C21	-2.09	119.43	122.82
31	c1	512	CLA	C2A-C1A-CHA	2.09	127.50	123.87
31	a1	410	CLA	C3B-C4B-NB	-2.09	108.66	110.53
31	y	603	CLA	CHD-C1D-ND	-2.09	121.86	124.80
48	G1	620	LUT	C38-C25-C24	-2.09	118.41	123.36
31	S1	612	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
31	r	612	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
31	b1	607	CLA	CHA-C1A-NA	-2.09	121.66	126.39
31	y1	613	CLA	CHA-C1A-NA	-2.09	121.66	126.39
31	c1	506	CLA	CMD-C2D-C3D	-2.09	122.90	127.69
31	c	512	CLA	CHD-C1D-ND	-2.09	121.86	124.80
31	n	602	CLA	C2D-C1D-ND	2.09	112.19	110.13
31	n	603	CLA	C2D-C1D-ND	2.09	112.19	110.13

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	y1	608	CLA	C1D-ND-C4D	-2.09	104.85	106.31
31	s	602	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
31	B	605	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
48	n1	621	LUT	C3-C4-C5	-2.09	106.98	112.18
31	c1	513	CLA	C2A-C1A-CHA	2.09	127.49	123.87
31	G1	604	CLA	CHD-C1D-ND	-2.09	121.86	124.80
44	D	405	PL9	C36-C34-C33	-2.09	116.48	121.17
31	D	402	CLA	CAA-CBA-CGA	-2.09	107.28	113.21
31	r1	604	CLA	CHA-C1A-NA	-2.09	121.66	126.39
31	B	608	CLA	C3B-C4B-NB	-2.09	108.67	110.53
33	c1	517	BCR	C23-C22-C21	2.09	122.29	119.01
47	Y1	605	CHL	CMD-C2D-C3D	2.09	128.85	124.68
33	c1	517	BCR	C34-C9-C10	-2.09	119.43	122.82
31	Y	610	CLA	CHA-C1A-NA	-2.09	121.66	126.39
31	B	604	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
31	g	604	CLA	CHA-C1A-NA	-2.09	121.67	126.39
31	C1	513	CLA	CMD-C2D-C3D	-2.09	122.90	127.69
31	c	503	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
50	N1	623	NEX	C20-C13-C14	-2.09	119.44	122.82
31	N	603	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
47	N1	601	CHL	CMA-C3A-C4A	2.09	119.11	114.61
47	n	608	CHL	C3D-C4D-ND	-2.09	109.59	112.94
31	R1	610	CLA	C2C-C1C-NC	2.09	112.17	109.98
35	J	101	LMG	C8-O7-C10	-2.09	112.80	117.80
31	B	603	CLA	O1D-CGD-CBD	-2.09	120.40	124.52
33	b	618	BCR	C36-C18-C17	-2.09	119.44	122.82
31	b	608	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
31	Y1	603	CLA	C2D-C1D-ND	2.09	112.19	110.13
47	s	606	CHL	CMD-C2D-C3D	2.09	128.85	124.68
31	N1	603	CLA	C1D-ND-C4D	-2.09	104.85	106.31
31	y1	610	CLA	C1D-ND-C4D	-2.09	104.85	106.31
31	C1	508	CLA	C1C-C2C-C3C	-2.09	104.79	106.98
31	c1	503	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
41	D1	408	LHG	O7-C7-O9	-2.08	118.83	123.70
31	s	614	CLA	CBC-CAC-C3C	-2.08	106.77	112.42
31	y	610	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
31	g1	613	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
47	y	607	CHL	CMD-C2D-C3D	2.08	128.85	124.68
31	c1	512	CLA	C3B-C4B-NB	-2.08	108.67	110.53
47	N1	605	CHL	C4C-CHD-C1D	2.08	123.52	116.07
31	r	609	CLA	C1-O2A-CGA	2.08	121.69	116.65
40	c1	518	DGD	O6D-C5D-C6D	2.08	110.83	106.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
50	s	623	NEX	C20-C13-C14	-2.08	119.44	122.82
31	B	605	CLA	CMA-C3A-C2A	2.08	122.03	113.98
50	N	623	NEX	C1-C2-C3	2.08	118.16	113.59
48	y1	620	LUT	C30-C31-C32	-2.08	117.17	123.20
31	N	611	CLA	C2D-C1D-ND	2.08	112.19	110.13
31	s	605	CLA	CMD-C2D-C3D	-2.08	122.92	127.69
47	g	605	CHL	C1-O2A-CGA	2.08	122.58	116.67
31	c	507	CLA	CMA-C3A-C4A	2.08	117.37	111.77
31	n	610	CLA	CHA-C4D-ND	2.08	136.84	132.55
33	C1	514	BCR	C31-C1-C6	-2.08	106.98	110.24
31	g1	612	CLA	O1D-CGD-CBD	-2.08	120.41	124.52
47	N1	601	CHL	C3D-C4D-ND	-2.08	109.60	112.94
31	a	406	CLA	CHA-C1A-NA	-2.08	121.68	126.39
31	A1	410	CLA	CHA-C1A-NA	-2.08	121.68	126.39
31	r1	602	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
48	n	620	LUT	C18-C5-C4	2.08	118.25	114.42
31	g1	602	CLA	CAC-C3C-C4C	2.08	127.50	124.79
37	B1	620	C7Z	C8-C7-C6	-2.08	121.44	127.00
31	B1	605	CLA	C2A-C1A-CHA	2.08	127.48	123.87
31	d	402	CLA	CHA-C1A-NA	-2.08	121.68	126.39
37	B	620	C7Z	C20-C13-C14	-2.08	119.45	122.82
49	G	622	XAT	C40-C33-C34	-2.08	119.45	122.82
31	c1	503	CLA	CMA-C3A-C4A	2.08	117.36	111.77
31	g1	612	CLA	C1D-ND-C4D	-2.08	104.85	106.31
47	G	605	CHL	CMD-C2D-C3D	2.08	128.84	124.68
31	Y	610	CLA	CMA-C3A-C4A	2.08	117.36	111.77
47	Y1	609	CHL	CMD-C2D-C3D	2.08	128.84	124.68
31	b	608	CLA	CHA-C1A-NA	-2.08	121.68	126.39
48	G	621	LUT	C31-C32-C33	-2.08	120.66	126.36
47	n	607	CHL	C1C-C2C-CMC	2.08	130.55	126.80
31	s	603	CLA	CMD-C2D-C3D	-2.08	122.92	127.69
31	B1	607	CLA	CAA-C2A-C3A	-2.08	107.38	113.00
31	c1	510	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
31	s	603	CLA	C3B-C4B-NB	-2.08	108.67	110.53
55	R1	625	LMT	C1'-O5'-C5'	-2.08	109.66	113.72
44	d	405	PL9	C12-C13-C14	-2.08	122.87	127.62
31	B	613	CLA	CHA-C1A-NA	-2.08	121.69	126.39
33	c	515	BCR	C3-C4-C5	-2.08	110.35	114.06
31	a1	405	CLA	C3B-C4B-NB	-2.08	108.68	110.53
47	Y1	606	CHL	CMD-C2D-C3D	2.08	128.83	124.68
44	D	405	PL9	O2-C1-C6	2.08	123.78	120.48
31	b1	603	CLA	C3D-C2D-C1D	-2.08	103.00	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	G	603	CLA	CHA-C1A-NA	-2.08	121.69	126.39
31	G1	613	CLA	C2D-C1D-ND	2.08	112.18	110.13
47	Y	607	CHL	C3D-C4D-ND	-2.08	109.61	112.94
48	S	621	LUT	C38-C25-C24	-2.08	118.45	123.36
31	S1	611	CLA	C2A-C1A-CHA	2.08	127.47	123.87
31	b1	605	CLA	CMD-C2D-C3D	-2.08	122.93	127.69
47	N1	609	CHL	C1-C2-C3	-2.08	122.80	126.20
37	b1	620	C7Z	C4-C5-C6	-2.08	116.49	120.76
31	a	410	CLA	CMD-C2D-C3D	-2.08	122.93	127.69
31	N1	613	CLA	CMD-C2D-C3D	-2.08	122.93	127.69
31	c	502	CLA	CHA-C1A-NA	-2.08	121.69	126.39
47	s1	607	CHL	C1C-C2C-CMC	2.08	130.54	126.80
31	Y1	613	CLA	CMC-C2C-C1C	2.08	128.28	125.03
31	y1	603	CLA	C1-O2A-CGA	2.08	121.67	116.65
31	G	612	CLA	CMD-C2D-C3D	-2.08	122.93	127.69
31	y1	602	CLA	O1D-CGD-CBD	-2.08	120.42	124.52
31	s1	602	CLA	CHA-C1A-NA	-2.08	121.69	126.39
40	c1	519	DGD	O2G-C1B-O1B	-2.07	118.85	123.70
31	b1	611	CLA	CMA-C3A-C4A	2.07	117.35	111.77
31	A	405	CLA	O2D-CGD-O1D	-2.07	119.81	123.85
31	C1	508	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
33	b	618	BCR	C35-C13-C12	2.07	121.26	118.09
33	A1	411	BCR	C35-C13-C12	2.07	121.26	118.09
48	s	620	LUT	C1-C6-C7	2.07	121.28	115.65
31	n1	602	CLA	C2D-C1D-ND	2.07	112.18	110.13
31	S	602	CLA	CMD-C2D-C3D	-2.07	122.93	127.69
47	g1	609	CHL	CMD-C2D-C3D	2.07	128.83	124.68
33	c1	515	BCR	C36-C18-C17	-2.07	119.46	122.82
31	C	505	CLA	C1D-ND-C4D	-2.07	104.86	106.31
31	S1	613	CLA	O2A-CGA-CBA	2.07	118.16	111.83
33	D	404	BCR	C35-C13-C12	2.07	121.25	118.09
33	c	515	BCR	C37-C22-C23	2.07	121.25	118.09
31	R	611	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
31	b	616	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
48	s	620	LUT	C31-C32-C33	-2.07	120.68	126.36
31	n1	602	CLA	CMA-C3A-C4A	2.07	117.34	111.77
48	Y	620	LUT	C26-C27-C28	-2.07	121.35	124.58
31	r	604	CLA	C3B-C4B-NB	-2.07	108.68	110.53
31	G	611	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
48	R	620	LUT	C19-C9-C10	-2.07	119.46	122.82
31	R1	610	CLA	CHA-C1A-NA	-2.07	121.70	126.39
47	Y	605	CHL	CMD-C2D-C3D	2.07	128.82	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	N	610	CLA	C2C-C1C-NC	2.07	112.16	109.98
31	B	616	CLA	CHD-C1D-ND	-2.07	121.89	124.80
31	A1	405	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
31	s1	603	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
46	H	101	RRX	C1-C6-C7	2.07	121.27	115.65
31	r1	612	CLA	CMA-C3A-C4A	2.07	117.34	111.77
31	B1	605	CLA	C3B-C4B-NB	-2.07	108.68	110.53
47	g	605	CHL	CMD-C2D-C3D	2.07	128.82	124.68
31	S	611	CLA	CHD-C1D-ND	-2.07	121.89	124.80
31	C	511	CLA	C1D-ND-C4D	-2.07	104.86	106.31
31	c1	511	CLA	C1-O2A-CGA	2.07	121.66	116.65
33	d	404	BCR	C15-C14-C13	2.07	130.18	127.28
31	n	610	CLA	CBA-CAA-C2A	2.07	119.95	113.79
31	b	603	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
47	s1	607	CHL	CMD-C2D-C3D	2.07	128.82	124.68
31	S	604	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
44	d	405	PL9	O2-C1-C2	-2.07	117.12	121.83
31	s	610	CLA	O2D-CGD-O1D	-2.07	119.82	123.85
31	a	405	CLA	CHA-C1A-NA	-2.07	121.70	126.39
31	d1	403	CLA	CAA-C2A-C3A	-2.07	107.41	113.00
31	r	602	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
31	S	602	CLA	C2D-C1D-ND	2.07	112.17	110.13
31	N	602	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
31	B1	617	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
31	S1	612	CLA	CMD-C2D-C3D	-2.07	122.94	127.69
31	S	610	CLA	OBD-CAD-C3D	-2.07	123.58	128.42
48	G1	621	LUT	C38-C25-C24	-2.07	118.47	123.36
31	c	511	CLA	C2D-C1D-ND	2.07	112.17	110.13
47	R1	606	CHL	CMD-C2D-C3D	2.07	128.82	124.68
31	Y1	614	CLA	CHD-C1D-ND	-2.07	121.89	124.80
31	y1	613	CLA	C1D-ND-C4D	-2.07	104.86	106.31
48	r	620	LUT	C3-C4-C5	-2.07	107.03	112.18
47	S1	607	CHL	CMD-C2D-C3D	2.07	128.81	124.68
31	D	402	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
31	C1	503	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
31	g1	610	CLA	CAA-C2A-C3A	-2.07	107.41	113.00
47	G1	605	CHL	CMD-C2D-C3D	2.07	128.81	124.68
31	B	614	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
31	R	612	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
31	Y	603	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
47	g	609	CHL	CMD-C2D-C3D	2.07	128.81	124.68
31	r1	602	CLA	CHA-C1A-NA	-2.07	121.71	126.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	G1	614	CLA	C1D-ND-C4D	-2.07	104.86	106.31
31	S	613	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
31	g1	604	CLA	CMD-C2D-C3D	-2.07	122.95	127.69
31	s	605	CLA	CHD-C1D-ND	-2.07	121.89	124.80
31	G	613	CLA	C3B-C4B-NB	-2.07	108.69	110.53
31	G1	611	CLA	CAC-C3C-C4C	2.07	127.48	124.79
31	g1	604	CLA	C1D-ND-C4D	-2.07	104.86	106.31
31	S	610	CLA	O1D-CGD-CBD	-2.07	120.44	124.52
31	G1	602	CLA	CAC-C3C-C4C	2.06	127.48	124.79
31	b	616	CLA	CHD-C1D-ND	-2.06	121.90	124.80
31	b1	602	CLA	C2A-C1A-CHA	2.06	127.45	123.87
31	c1	509	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
33	a	411	BCR	C29-C28-C27	2.06	115.82	111.28
31	r1	612	CLA	C1-O2A-CGA	2.06	121.65	116.65
50	Y1	623	NEX	C31-C32-C33	2.06	132.02	126.36
44	D1	405	PL9	O2-C1-C6	2.06	123.76	120.48
50	R	622	NEX	C39-C29-C30	-2.06	119.47	122.82
31	C	506	CLA	C3B-C4B-NB	-2.06	108.69	110.53
31	B	613	CLA	CHD-C1D-ND	-2.06	121.90	124.80
31	c	508	CLA	CHD-C1D-ND	-2.06	121.90	124.80
31	B1	611	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
31	n1	604	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
31	c1	502	CLA	C6-C5-C3	-2.06	108.44	113.47
31	C	508	CLA	CAA-C2A-C3A	-2.06	107.43	113.00
49	G1	622	XAT	C18-C5-C6	-2.06	118.91	122.30
47	y	601	CHL	CMA-C3A-C4A	2.06	119.05	114.61
31	C	504	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
31	N1	614	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
47	g	607	CHL	C3D-C4D-ND	-2.06	109.63	112.94
31	N	604	CLA	CMA-C3A-C4A	2.06	117.31	111.77
31	n	612	CLA	CMA-C3A-C4A	2.06	117.31	111.77
31	D1	402	CLA	O1D-CGD-CBD	-2.06	120.45	124.52
47	y	606	CHL	CMD-C2D-C3D	2.06	128.80	124.68
31	B1	614	CLA	OBD-CAD-C3D	-2.06	123.60	128.42
41	D1	409	LHG	O8-C23-O10	-2.06	118.47	123.63
31	Y1	612	CLA	CMD-C2D-C3D	-2.06	122.96	127.69
31	R	610	CLA	C2D-C1D-ND	2.06	112.17	110.13
31	S	603	CLA	C2D-C1D-ND	2.06	112.17	110.13
31	B1	602	CLA	C2D-C1D-ND	2.06	112.17	110.13
31	N	614	CLA	CAA-C2A-C3A	-2.06	107.43	113.00
31	B	604	CLA	C3B-C4B-NB	-2.06	108.69	110.53
31	C	504	CLA	C3B-C4B-NB	-2.06	108.69	110.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	D1	402	CLA	O2D-CGD-O1D	-2.06	119.84	123.85
31	s	604	CLA	C1D-ND-C4D	-2.06	104.87	106.31
31	Y1	613	CLA	C1D-ND-C4D	-2.06	104.87	106.31
47	Y1	601	CHL	CMD-C2D-C3D	2.06	128.80	124.68
48	Y	620	LUT	C11-C10-C9	-2.06	124.39	127.28
33	D	404	BCR	C8-C9-C10	2.06	122.25	119.01
47	G	608	CHL	CMD-C2D-C3D	2.06	128.80	124.68
31	b1	608	CLA	C2D-C1D-ND	2.06	112.17	110.13
31	r1	609	CLA	CMD-C2D-C3D	-2.06	122.97	127.69
31	C1	509	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
47	g1	605	CHL	CMD-C2D-C3D	2.06	128.80	124.68
45	f	101	HEM	CBD-CAD-C3D	-2.06	106.84	112.53
31	B1	607	CLA	O2D-CGD-O1D	-2.06	119.84	123.85
31	N	614	CLA	CMD-C2D-C3D	-2.06	122.97	127.69
31	b	616	CLA	CMD-C2D-C3D	-2.06	122.97	127.69
31	G1	602	CLA	C3B-C4B-NB	-2.06	108.69	110.53
31	S	613	CLA	C2A-C1A-CHA	2.06	127.44	123.87
47	N1	606	CHL	CMD-C2D-C3D	2.06	128.80	124.68
50	Y	623	NEX	C28-C29-C30	2.06	122.25	119.01
31	S	612	CLA	O1D-CGD-CBD	-2.06	120.46	124.52
31	a1	405	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
31	d1	403	CLA	C1-O2A-CGA	2.06	121.63	116.65
33	B1	618	BCR	C1-C6-C7	2.06	121.23	115.65
31	s1	611	CLA	CMD-C2D-C3D	-2.06	122.97	127.69
31	n	613	CLA	C1-C2-C3	-2.06	122.83	126.20
31	y1	608	CLA	O2D-CGD-O1D	-2.06	119.84	123.85
31	c1	502	CLA	C1D-ND-C4D	-2.06	104.87	106.31
50	n	623	NEX	C1-C2-C3	2.06	118.11	113.59
31	g	611	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
31	d1	402	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
31	r1	612	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
47	g	607	CHL	CMD-C2D-C3D	2.06	128.79	124.68
47	Y	606	CHL	C1C-C2C-CMC	2.06	130.51	126.80
31	b	616	CLA	C2D-C1D-ND	2.06	112.16	110.13
48	Y1	621	LUT	C10-C11-C12	-2.06	117.24	123.20
31	n1	604	CLA	C1D-ND-C4D	-2.06	104.87	106.31
31	Y	610	CLA	OBD-CAD-C3D	-2.06	123.61	128.42
31	N1	610	CLA	C2D-C1D-ND	2.06	112.16	110.13
50	N	623	NEX	C40-C33-C32	2.06	121.23	118.09
31	r	613	CLA	C3B-C4B-NB	-2.06	108.69	110.53
31	R1	602	CLA	CAC-C3C-C4C	2.06	127.46	124.79
31	B1	616	CLA	C3D-C2D-C1D	-2.06	103.03	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	Y1	602	CLA	C3D-C2D-C1D	-2.06	103.03	105.83
31	A	410	CLA	CHA-C1A-NA	-2.06	121.74	126.39
31	B	616	CLA	CMA-C3A-C2A	2.06	121.93	113.98
31	b	605	CLA	C2A-C1A-CHA	2.05	127.43	123.87
47	R	607	CHL	CMD-C2D-C3D	2.05	128.79	124.68
31	B1	603	CLA	C3B-C4B-NB	-2.05	108.70	110.53
31	g1	602	CLA	CMD-C2D-C3D	-2.05	122.98	127.69
31	c1	503	CLA	CMA-C3A-C2A	2.05	121.92	113.98
31	N1	611	CLA	CAA-C2A-C3A	-2.05	107.45	113.00
31	c	509	CLA	CMA-C3A-C4A	2.05	117.29	111.77
31	c	511	CLA	C6-C5-C3	-2.05	108.47	113.47
31	B	606	CLA	C1-O2A-CGA	2.05	121.62	116.65
47	Y1	607	CHL	CMD-C2D-C3D	2.05	128.79	124.68
31	c	505	CLA	CMD-C2D-C3D	-2.05	122.98	127.69
33	B	618	BCR	C38-C26-C25	-2.05	122.24	124.48
47	r1	607	CHL	C1C-C2C-CMC	2.05	130.50	126.80
33	B1	618	BCR	C40-C30-C25	-2.05	107.02	110.24
40	b1	623	DGD	O1G-C1A-O1A	-2.05	118.49	123.63
31	n	612	CLA	C2D-C1D-ND	2.05	112.16	110.13
47	G1	609	CHL	C3D-C4D-ND	-2.05	109.65	112.94
31	r	610	CLA	C2A-C1A-CHA	2.05	127.43	123.87
48	n1	621	LUT	C18-C5-C4	2.05	118.19	114.42
49	N	622	XAT	O4-C6-C7	-2.05	111.00	116.88
31	C	509	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
31	n	604	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
31	c1	501	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
31	n1	602	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
31	G1	604	CLA	CAA-C2A-C3A	-2.05	107.45	113.00
31	s1	613	CLA	O2A-CGA-CBA	2.05	118.09	111.83
31	y1	603	CLA	O2A-CGA-CBA	2.05	118.09	111.83
31	B1	613	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
47	n	608	CHL	CMD-C2D-C3D	2.05	128.78	124.68
47	n1	601	CHL	CMD-C2D-C3D	2.05	128.78	124.68
47	s1	608	CHL	CMD-C2D-C3D	2.05	128.78	124.68
31	C	508	CLA	CMD-C2D-C3D	-2.05	122.98	127.69
31	n1	603	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
31	n1	604	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
31	C	510	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
31	S1	610	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
31	c	511	CLA	CHA-C1A-NA	-2.05	121.75	126.39
47	y1	605	CHL	CMD-C2D-C3D	2.05	128.78	124.68
47	S1	607	CHL	C4C-CHD-C1D	2.05	123.41	116.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
33	a1	411	BCR	C34-C9-C10	-2.05	119.49	122.82
31	y	614	CLA	O1D-CGD-CBD	-2.05	120.47	124.52
31	g	612	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
47	N	606	CHL	CMD-C2D-C3D	2.05	128.78	124.68
47	G1	608	CHL	C4C-CHD-C1D	2.05	123.40	116.07
47	Y1	609	CHL	C3D-C4D-ND	-2.05	109.65	112.94
31	G1	613	CLA	CAA-C2A-C3A	-2.05	107.46	113.00
31	N1	603	CLA	C2D-C1D-ND	2.05	112.16	110.13
31	C1	502	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
31	r1	604	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
31	c	503	CLA	C1D-ND-C4D	-2.05	104.87	106.31
47	N	607	CHL	CMD-C2D-C3D	2.05	128.78	124.68
50	S1	623	NEX	O24-C25-C38	-2.05	112.76	115.05
48	S	620	LUT	C36-C21-C26	2.05	112.65	109.55
31	S	617	CLA	C2D-C1D-ND	2.05	112.15	110.13
31	S1	613	CLA	CHD-C1D-ND	-2.05	121.92	124.80
47	y1	609	CHL	CMD-C2D-C3D	2.05	128.78	124.68
31	C	505	CLA	C4D-C3D-CAD	2.05	110.33	108.11
47	S1	608	CHL	C4C-CHD-C1D	2.05	123.40	116.07
47	N	601	CHL	CMD-C2D-C3D	2.05	128.78	124.68
31	N1	612	CLA	CHA-C1A-NA	-2.05	121.75	126.39
31	N	614	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
31	s1	603	CLA	C2D-C1D-ND	2.05	112.15	110.13
31	C	505	CLA	CAA-C2A-C3A	-2.05	107.47	113.00
31	B1	607	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
31	B1	617	CLA	C3B-C4B-NB	-2.05	108.70	110.53
31	B1	611	CLA	CMD-C2D-C3D	-2.05	122.99	127.69
47	n1	609	CHL	C4C-CHD-C1D	2.05	123.39	116.07
48	s	620	LUT	C1-C6-C5	-2.05	119.84	122.64
31	g1	613	CLA	C1-O2A-CGA	2.05	121.61	116.65
31	G	602	CLA	CHA-C1A-NA	-2.05	121.76	126.39
31	s1	614	CLA	CHA-C1A-NA	-2.05	121.76	126.39
31	S	612	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
48	G	621	LUT	C16-C1-C6	-2.05	107.03	110.24
31	G1	604	CLA	O1D-CGD-CBD	-2.05	120.48	124.52
31	S	609	CLA	O2A-CGA-CBA	2.05	118.07	111.83
31	s1	603	CLA	C2A-C1A-CHA	2.05	127.42	123.87
31	g1	614	CLA	C2D-C1D-ND	2.05	112.15	110.13
31	R	603	CLA	C6-C5-C3	-2.05	108.48	113.47
49	n1	622	XAT	C26-C27-C28	-2.05	121.67	125.99
31	R	613	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
31	Y1	604	CLA	O1D-CGD-CBD	-2.05	120.48	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	n	607	CHL	CMD-C2D-C3D	2.05	128.77	124.68
31	D	403	CLA	CHA-C1A-NA	-2.05	121.76	126.39
31	b1	608	CLA	CHA-C1A-NA	-2.05	121.76	126.39
31	b	606	CLA	CAC-C3C-C4C	2.05	127.45	124.79
32	A1	408	PHO	O2A-CGA-O1A	-2.05	118.51	123.63
31	N1	604	CLA	CMA-C3A-C4A	2.05	117.27	111.77
47	y1	607	CHL	CMD-C2D-C3D	2.05	128.77	124.68
31	y	608	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
47	G1	608	CHL	C3D-C4D-ND	-2.05	109.66	112.94
31	n1	604	CLA	OBD-CAD-C3D	-2.05	123.64	128.42
40	C	519	DGD	O1G-C1A-O1A	-2.04	118.51	123.63
31	S1	611	CLA	CHD-C1D-ND	-2.04	121.92	124.80
31	s1	605	CLA	CHD-C1D-ND	-2.04	121.92	124.80
31	Y	613	CLA	CHA-C1A-NA	-2.04	121.76	126.39
31	S1	613	CLA	CHA-C1A-NA	-2.04	121.76	126.39
31	A1	407	CLA	C1-O2A-CGA	2.04	121.60	116.65
47	G1	609	CHL	CMD-C2D-C3D	2.04	128.77	124.68
31	C1	506	CLA	C1D-ND-C4D	-2.04	104.88	106.31
31	a1	410	CLA	C1D-ND-C4D	-2.04	104.88	106.31
47	r	607	CHL	CMD-C2D-C3D	2.04	128.77	124.68
31	c1	505	CLA	C1-O2A-CGA	2.04	121.60	116.65
31	n	604	CLA	CHA-C1A-NA	-2.04	121.76	126.39
47	n	601	CHL	CMD-C2D-C3D	2.04	128.77	124.68
31	a	410	CLA	C6-C5-C3	-2.04	108.49	113.47
31	C1	513	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
38	c1	524	DGA	CG2-OG2-CB1	-2.04	112.91	117.80
31	B	615	CLA	C2A-C1A-CHA	2.04	127.41	123.87
31	y	611	CLA	O2A-CGA-CBA	2.04	118.06	111.83
31	S	617	CLA	CHD-C1D-ND	-2.04	121.93	124.80
31	N1	604	CLA	C4B-CHC-C1C	2.04	131.05	126.25
31	C1	512	CLA	C1-O2A-CGA	2.04	121.59	116.65
31	R1	602	CLA	CAA-C2A-C3A	-2.04	107.48	113.00
48	s	620	LUT	C36-C21-C26	2.04	112.64	109.55
31	B1	606	CLA	CMA-C3A-C4A	2.04	117.26	111.77
49	Y	622	XAT	O24-C25-C38	-2.04	112.77	115.05
31	r	611	CLA	C1D-ND-C4D	-2.04	104.88	106.31
31	B1	605	CLA	CMD-C2D-C3D	-2.04	123.01	127.69
31	Y1	612	CLA	O1D-CGD-CBD	-2.04	120.49	124.52
31	n1	613	CLA	CHD-C1D-ND	-2.04	121.93	124.80
47	n	605	CHL	CMD-C2D-C3D	2.04	128.76	124.68
50	G1	623	NEX	C28-C29-C30	2.04	122.22	119.01
31	b1	614	CLA	C3D-C2D-C1D	-2.04	103.05	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
47	g	606	CHL	C1C-C2C-CMC	2.04	130.48	126.80
31	A1	407	CLA	C2A-C1A-CHA	2.04	127.41	123.87
31	B	611	CLA	CHD-C1D-ND	-2.04	121.93	124.80
31	B1	610	CLA	CHA-C1A-NA	-2.04	121.77	126.39
47	G1	606	CHL	CMD-C2D-C3D	2.04	128.76	124.68
33	c	514	BCR	C4-C5-C6	-2.04	119.95	122.70
31	n1	612	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	g1	603	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	S	614	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
48	G1	621	LUT	C20-C13-C12	2.04	121.20	118.09
31	b1	603	CLA	C2D-C1D-ND	2.04	112.14	110.13
31	R	602	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	B1	608	CLA	CAC-C3C-C4C	2.04	127.44	124.79
31	C1	513	CLA	CHA-C1A-NA	-2.04	121.78	126.39
47	G	609	CHL	C1C-C2C-CMC	-2.04	123.13	126.80
31	r1	612	CLA	O1D-CGD-CBD	-2.04	120.50	124.52
33	C1	514	BCR	C4-C5-C6	-2.04	119.95	122.70
31	y	613	CLA	CHA-C1A-NA	-2.04	121.78	126.39
46	H	101	RRX	C8-C7-C6	-2.04	121.55	127.00
33	C	516	BCR	C30-C25-C24	2.04	121.18	115.65
31	s1	609	CLA	C2A-C1A-CHA	2.04	127.40	123.87
31	R	609	CLA	CAA-C2A-C3A	-2.04	107.49	113.00
31	r1	610	CLA	O2D-CGD-O1D	-2.04	119.88	123.85
47	g	601	CHL	CMD-C2D-C3D	2.04	128.75	124.68
31	b	609	CLA	CHB-C1B-NB	2.04	127.11	124.05
31	c	512	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
31	B1	609	CLA	C4B-CHC-C1C	2.04	131.04	126.25
31	S1	605	CLA	CHD-C1D-ND	-2.04	121.94	124.80
31	s	602	CLA	C1-O2A-CGA	2.04	121.58	116.65
31	R	610	CLA	O2D-CGD-O1D	-2.04	119.89	123.85
31	C	512	CLA	C2D-C1D-ND	2.04	112.14	110.13
31	C1	502	CLA	C2D-C1D-ND	2.04	112.14	110.13
31	a	405	CLA	O2A-CGA-CBA	2.04	118.04	111.83
31	B	609	CLA	C4B-CHC-C1C	2.04	131.03	126.25
31	B	616	CLA	C1D-ND-C4D	-2.04	104.88	106.31
31	y	613	CLA	C1D-ND-C4D	-2.04	104.88	106.31
31	C	506	CLA	C1-O2A-CGA	2.04	121.58	116.65
33	c	515	BCR	C15-C14-C13	-2.04	124.42	127.28
31	c1	502	CLA	CMC-C2C-C3C	2.03	131.65	126.15
31	s1	602	CLA	C3D-C2D-C1D	-2.03	103.05	105.83
31	B	609	CLA	CHD-C1D-ND	-2.03	121.94	124.80
31	s1	614	CLA	CMD-C2D-C3D	-2.03	123.02	127.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	c1	509	CLA	CHA-C1A-NA	-2.03	121.78	126.39
31	A1	410	CLA	C3B-C2B-C1B	-2.03	104.77	107.17
31	A1	406	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
31	s1	617	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
33	b1	618	BCR	C34-C9-C10	-2.03	119.52	122.82
31	c1	504	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
31	g	613	CLA	CHD-C1D-ND	-2.03	121.94	124.80
47	s	608	CHL	C3D-C4D-ND	-2.03	109.67	112.94
31	A	407	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
31	G	602	CLA	O2A-CGA-CBA	2.03	118.04	111.83
31	g1	602	CLA	C2C-C1C-NC	2.03	112.12	109.98
31	Y	604	CLA	C1-O2A-CGA	2.03	121.57	116.65
47	N1	608	CHL	C1-O2A-CGA	2.03	121.57	116.65
31	b	609	CLA	C2A-C1A-CHA	2.03	127.40	123.87
31	y1	603	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
47	y	605	CHL	C4C-CHD-C1D	2.03	123.34	116.07
31	r	609	CLA	O2D-CGD-O1D	-2.03	119.89	123.85
31	B	605	CLA	C3B-C4B-NB	-2.03	108.72	110.53
31	c1	510	CLA	C3B-C4B-NB	-2.03	108.72	110.53
37	B	620	C7Z	C17-C1-C6	-2.03	107.06	110.24
31	c	503	CLA	C2D-C1D-ND	2.03	112.14	110.13
33	B1	619	BCR	C1-C6-C7	2.03	121.16	115.65
31	G1	614	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
31	Y1	604	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
37	b	620	C7Z	C7-C6-C5	-2.03	116.87	121.56
31	r1	604	CLA	C1D-ND-C4D	-2.03	104.89	106.31
41	C	525	LHG	C5-O7-C7	-2.03	112.93	117.80
47	S	601	CHL	C3D-C4D-ND	-2.03	109.68	112.94
31	R1	609	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
48	Y	620	LUT	C30-C31-C32	-2.03	117.31	123.20
47	y	607	CHL	CMA-C3A-C2A	2.03	121.97	114.13
31	G1	610	CLA	C1C-C2C-C3C	-2.03	104.84	106.98
47	S1	606	CHL	CMD-C2D-C3D	2.03	128.74	124.68
31	y	603	CLA	CHA-C1A-NA	-2.03	121.79	126.39
31	n	604	CLA	C2A-C1A-CHA	2.03	127.39	123.87
31	d1	403	CLA	O1D-CGD-CBD	-2.03	120.51	124.52
31	R	613	CLA	C2D-C1D-ND	2.03	112.14	110.13
31	C1	502	CLA	CMD-C2D-C3D	-2.03	123.03	127.69
47	Y	609	CHL	CMD-C2D-C3D	2.03	128.74	124.68
47	y	606	CHL	C3D-C4D-ND	-2.03	109.68	112.94
49	Y1	622	XAT	O24-C26-C27	-2.03	111.06	116.88
46	h1	101	RRX	C30-C29-C28	-2.03	109.14	113.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	n1	613	CLA	CMD-C2D-C3D	-2.03	123.03	127.69
31	r1	602	CLA	CMC-C2C-C1C	2.03	128.21	125.03
47	R	607	CHL	CMA-C3A-C4A	2.03	118.98	114.61
31	C	502	CLA	CMD-C2D-C3D	-2.03	123.04	127.69
31	C1	509	CLA	C2D-C1D-ND	2.03	112.13	110.13
33	B1	619	BCR	C37-C22-C21	-2.03	119.53	122.82
47	G	606	CHL	CMD-C2D-C3D	2.03	128.74	124.68
31	g	604	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
31	c1	508	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
31	N	602	CLA	C6-C5-C3	-2.03	108.53	113.47
31	R	608	CLA	O2A-CGA-CBA	2.03	118.02	111.83
31	B	607	CLA	CAC-C3C-C4C	2.03	127.43	124.79
47	N	607	CHL	C3D-C4D-ND	-2.03	109.69	112.94
31	b	612	CLA	CHD-C1D-ND	-2.03	121.95	124.80
32	A	409	PHO	O2A-CGA-O1A	-2.03	118.56	123.63
31	b	614	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
31	c	508	CLA	O1D-CGD-CBD	-2.03	120.52	124.52
31	B	615	CLA	CHA-C1A-NA	-2.03	121.80	126.39
47	y1	606	CHL	C4C-CHD-C1D	2.03	123.32	116.07
47	n1	605	CHL	CMD-C2D-C3D	2.03	128.73	124.68
31	S1	605	CLA	C2A-C1A-CHA	2.03	127.39	123.87
33	C	517	BCR	C2-C3-C4	-2.03	106.82	111.28
31	G1	604	CLA	OBD-CAD-C3D	-2.03	123.68	128.42
31	b	604	CLA	CHD-C1D-ND	-2.03	121.95	124.80
31	n	603	CLA	CHA-C1A-NA	-2.03	121.80	126.39
33	C	514	BCR	C4-C5-C6	-2.03	119.97	122.70
31	N1	612	CLA	C2D-C1D-ND	2.03	112.13	110.13
50	S	622	NEX	C1-C2-C3	2.03	118.04	113.59
31	C1	502	CLA	CHD-C1D-ND	-2.03	121.95	124.80
45	F1	101	HEM	CAC-C3C-C4C	-2.03	119.98	124.82
31	B	617	CLA	C1C-C2C-C3C	-2.03	104.85	106.98
31	r	610	CLA	CMD-C2D-C3D	-2.03	123.04	127.69
31	N	611	CLA	CHD-C1D-ND	-2.03	121.95	124.80
31	s	605	CLA	C2A-C1A-CHA	2.03	127.38	123.87
31	Y1	603	CLA	CMD-C2D-C3D	-2.03	123.05	127.69
56	R1	626	ERG	C11-C12-C13	2.02	116.16	112.74
31	R	602	CLA	C2D-C1D-ND	2.02	112.13	110.13
50	G	623	NEX	C16-C1-C6	-2.02	108.66	110.47
31	b1	612	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
50	g	623	NEX	C38-C25-C26	-2.02	118.97	122.30
31	g	602	CLA	C1-O2A-CGA	2.02	121.55	116.65
31	R1	602	CLA	C1C-C2C-C3C	-2.02	104.85	106.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	g1	613	CLA	O2D-CGD-O1D	-2.02	119.91	123.85
31	g	614	CLA	C1D-ND-C4D	-2.02	104.89	106.31
31	B1	613	CLA	C2D-C1D-ND	2.02	112.13	110.13
31	B1	612	CLA	CHA-C1A-NA	-2.02	121.81	126.39
31	B1	617	CLA	CHD-C1D-ND	-2.02	121.95	124.80
31	S1	610	CLA	CAC-C3C-C4C	2.02	127.42	124.79
31	R1	612	CLA	O2A-CGA-CBA	2.02	118.00	111.83
31	c	502	CLA	CMD-C2D-C3D	-2.02	123.05	127.69
47	S	606	CHL	C1C-C2C-CMC	2.02	130.45	126.80
31	G	613	CLA	CAC-C3C-C2C	-2.02	123.84	127.56
31	Y1	604	CLA	CHA-C1A-NA	-2.02	121.81	126.39
31	B	603	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
31	R	602	CLA	CMD-C2D-C3D	-2.02	123.05	127.69
31	b	616	CLA	CAC-C3C-C4C	2.02	127.42	124.79
31	G1	603	CLA	C1D-ND-C4D	-2.02	104.89	106.31
31	C1	510	CLA	OBD-CAD-C3D	-2.02	123.69	128.42
31	D	402	CLA	C2C-C1C-NC	2.02	112.11	109.98
45	f	101	HEM	C3C-C2C-C1C	2.02	108.96	107.05
31	A1	406	CLA	C3B-C4B-NB	-2.02	108.72	110.53
31	n1	610	CLA	C3B-C4B-NB	-2.02	108.72	110.53
31	S	617	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
33	c1	517	BCR	C19-C18-C17	2.02	122.19	119.01
50	S	622	NEX	C11-C10-C9	2.02	130.11	127.28
47	g	608	CHL	C3D-C4D-ND	-2.02	109.69	112.94
31	B1	615	CLA	O2A-CGA-CBA	2.02	118.00	111.83
47	g1	601	CHL	C1C-C2C-CMC	2.02	130.44	126.80
35	C1	523	LMG	O7-C10-O9	-2.02	118.98	123.70
48	n	621	LUT	C16-C1-C6	-2.02	107.07	110.24
31	A	406	CLA	CHA-C1A-NA	-2.02	121.81	126.39
47	S	606	CHL	CMD-C2D-C3D	2.02	128.72	124.68
31	S	603	CLA	CHD-C1D-ND	-2.02	121.96	124.80
48	N	620	LUT	C35-C15-C14	-2.02	119.39	123.52
31	G	614	CLA	CHA-C1A-NA	-2.02	121.82	126.39
31	C	513	CLA	CMD-C2D-C3D	-2.02	123.06	127.69
31	g	610	CLA	C2D-C1D-ND	2.02	112.12	110.13
47	s	608	CHL	C4C-CHD-C1D	2.02	123.30	116.07
31	C	510	CLA	C3B-C4B-NB	-2.02	108.73	110.53
31	b1	606	CLA	C1D-ND-C4D	-2.02	104.89	106.31
31	y1	611	CLA	O2D-CGD-O1D	-2.02	119.92	123.85
31	R1	604	CLA	O2A-CGA-CBA	2.02	117.99	111.83
31	b1	612	CLA	CHA-C1A-NA	-2.02	121.82	126.39
31	a	405	CLA	CMC-C2C-C1C	2.02	128.19	125.03

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	B	616	CLA	CMD-C2D-C3D	-2.02	123.06	127.69
33	C	514	BCR	C35-C13-C12	2.02	121.17	118.09
31	r1	604	CLA	C2D-C1D-ND	2.02	112.12	110.13
31	A	405	CLA	C6-C7-C8	-2.02	109.25	115.97
31	s	617	CLA	O1D-CGD-CBD	-2.02	120.54	124.52
31	s1	604	CLA	CAA-C2A-C3A	-2.02	107.55	113.00
48	n1	620	LUT	C38-C25-C24	-2.02	118.58	123.36
31	B1	604	CLA	O1D-CGD-CBD	-2.02	120.54	124.52
31	g1	603	CLA	O1D-CGD-CBD	-2.02	120.54	124.52
31	S	603	CLA	CMD-C2D-C3D	-2.02	123.06	127.69
31	c	510	CLA	C11-C10-C8	-2.02	109.26	115.97
48	N1	620	LUT	C19-C9-C8	2.02	121.17	118.09
48	y1	621	LUT	C20-C13-C12	2.02	121.17	118.09
31	r	613	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
31	r	612	CLA	C1-O2A-CGA	2.02	121.53	116.65
31	r1	612	CLA	CAC-C3C-C4C	2.02	127.41	124.79
47	r	607	CHL	C1C-C2C-CMC	2.02	130.44	126.80
31	R	612	CLA	C2D-C1D-ND	2.02	112.12	110.13
31	N	610	CLA	CAC-C3C-C4C	2.02	127.41	124.79
31	C	510	CLA	CHA-C1A-NA	-2.02	121.83	126.39
44	d1	405	PL9	C37-C38-C39	-2.02	123.01	127.62
40	C1	520	DGD	O1G-C1A-O1A	-2.02	118.59	123.63
31	C1	507	CLA	C4B-CHC-C1C	2.02	130.99	126.25
31	R1	608	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
31	b1	608	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
48	s	621	LUT	C38-C25-C24	-2.01	118.59	123.36
47	G1	607	CHL	C3D-C4D-ND	-2.01	109.71	112.94
31	B1	607	CLA	C2A-C1A-CHA	2.01	127.36	123.87
35	w1	201	LMG	O8-C28-O10	-2.01	118.59	123.63
31	C	513	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
31	s1	604	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
31	R	612	CLA	C6-C5-C3	-2.01	108.56	113.47
31	s	602	CLA	CHD-C1D-ND	-2.01	121.97	124.80
33	b	619	BCR	C23-C22-C21	2.01	122.18	119.01
47	n1	606	CHL	C3D-C4D-ND	-2.01	109.71	112.94
45	f	101	HEM	C2B-C1B-NB	-2.01	107.53	109.84
31	a1	406	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
31	c1	503	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
31	B1	612	CLA	CAA-C2A-C3A	-2.01	107.56	113.00
31	B	606	CLA	C2D-C1D-ND	2.01	112.12	110.13
49	Y1	622	XAT	O24-C25-C38	-2.01	112.80	115.05
31	s1	609	CLA	O1D-CGD-CBD	-2.01	120.55	124.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	y1	608	CLA	C2D-C1D-ND	2.01	112.12	110.13
48	N1	620	LUT	C39-C29-C28	2.01	121.16	118.09
31	B1	609	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
48	g1	620	LUT	C38-C25-C24	-2.01	118.60	123.36
31	B1	609	CLA	O2A-CGA-CBA	2.01	117.97	111.83
32	A1	409	PHO	C4D-ND-C1D	-2.01	106.46	108.87
47	Y	607	CHL	CMD-C2D-C3D	2.01	128.70	124.68
47	G1	607	CHL	CMD-C2D-C3D	2.01	128.70	124.68
31	b	602	CLA	C2D-C1D-ND	2.01	112.12	110.13
31	n	614	CLA	O2A-CGA-CBA	2.01	117.97	111.83
47	N1	601	CHL	CMD-C2D-C3D	2.01	128.70	124.68
31	B1	615	CLA	CAC-C3C-C4C	2.01	127.41	124.79
47	y1	605	CHL	C1C-C2C-CMC	2.01	130.43	126.80
31	y1	613	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
31	y1	610	CLA	C2A-C1A-CHA	2.01	127.36	123.87
31	r1	610	CLA	CMD-C2D-C3D	-2.01	123.08	127.69
31	r	609	CLA	O1D-CGD-CBD	-2.01	120.55	124.52
47	G	607	CHL	CMD-C2D-C3D	2.01	128.70	124.68
48	R1	620	LUT	C39-C29-C28	2.01	121.16	118.09
31	B1	617	CLA	C1D-ND-C4D	-2.01	104.90	106.31
47	N1	601	CHL	C4C-CHD-C1D	2.01	123.26	116.07
31	B1	603	CLA	CMD-C2D-C3D	-2.01	123.08	127.69
31	s1	609	CLA	CMD-C2D-C3D	-2.01	123.08	127.69
31	y1	613	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
47	G	609	CHL	C4D-CHA-CBD	-2.01	106.94	108.97
49	G1	622	XAT	O24-C25-C24	2.01	115.37	113.49
32	a1	409	PHO	OBD-CAD-C3D	2.01	131.03	127.89
31	c	504	CLA	CAA-CBA-CGA	-2.01	107.50	113.21
49	y	622	XAT	C20-C13-C14	-2.01	119.56	122.82
31	S1	604	CLA	CAA-C2A-C3A	-2.01	107.57	113.00
31	R1	602	CLA	C2A-C1A-CHA	2.01	127.35	123.87
33	D	404	BCR	C38-C26-C25	-2.01	122.29	124.48
31	Y1	612	CLA	C6-C5-C3	-2.01	108.58	113.47
47	N1	605	CHL	CMD-C2D-C3D	2.01	128.69	124.68
31	r	608	CLA	O2A-CGA-CBA	2.01	117.96	111.83
31	c1	512	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
31	c	501	CLA	CHA-C1A-NA	-2.01	121.85	126.39
55	r1	625	LMT	C3B-C4B-C5B	-2.01	106.59	110.23
49	g	622	XAT	O24-C26-C27	-2.01	111.13	116.88
31	A1	407	CLA	O1D-CGD-CBD	-2.01	120.56	124.52
48	S	620	LUT	C31-C32-C33	-2.01	120.86	126.36
31	R	610	CLA	C3D-C2D-C1D	-2.01	103.09	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	y1	602	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
31	Y1	612	CLA	C1-O2A-CGA	2.01	121.51	116.65
48	G1	620	LUT	C35-C15-C14	-2.01	119.41	123.52
31	s	611	CLA	C2D-C1D-ND	2.01	112.11	110.13
48	g1	621	LUT	C38-C25-C24	-2.01	118.61	123.36
31	S1	617	CLA	C1-O2A-CGA	2.01	121.50	116.65
31	d1	402	CLA	C4-C3-C5	2.01	118.71	115.23
47	S1	601	CHL	CMD-C2D-C3D	2.01	128.69	124.68
31	r1	604	CLA	C3B-C4B-NB	-2.01	108.74	110.53
31	b1	609	CLA	CHD-C1D-ND	-2.00	121.98	124.80
31	s	602	CLA	CHA-C1A-NA	-2.00	121.85	126.39
31	B	616	CLA	O2A-CGA-CBA	2.00	117.95	111.83
31	c	507	CLA	OBD-CAD-C3D	-2.00	123.73	128.42
31	b1	609	CLA	CMA-C3A-C2A	2.00	121.73	113.98
31	b1	615	CLA	C2A-C1A-CHA	2.00	127.35	123.87
31	N1	614	CLA	O1D-CGD-CBD	-2.00	120.56	124.52
41	G1	624	LHG	C6-C5-C4	-2.00	107.11	111.78
31	c	508	CLA	CHA-C1A-NA	-2.00	121.85	126.39
47	G1	601	CHL	CMD-C2D-C3D	2.00	128.69	124.68
47	g1	601	CHL	CMD-C2D-C3D	2.00	128.69	124.68
31	g	613	CLA	C3D-C2D-C1D	-2.00	103.10	105.83
47	N1	606	CHL	C1C-C2C-CMC	2.00	130.41	126.80
31	N	613	CLA	C2D-C1D-ND	2.00	112.11	110.13
31	S	614	CLA	C2D-C1D-ND	2.00	112.11	110.13
31	b1	614	CLA	C2D-C1D-ND	2.00	112.11	110.13
31	c1	504	CLA	CHA-C1A-NA	-2.00	121.85	126.39
31	Y	612	CLA	CHD-C1D-ND	-2.00	121.98	124.80
50	r1	622	NEX	O24-C25-C38	-2.00	112.81	115.05
31	g1	613	CLA	CHA-C1A-NA	-2.00	121.86	126.39
35	h	102	LMG	O7-C10-O9	-2.00	119.02	123.70
49	n1	622	XAT	C20-C13-C14	-2.00	119.57	122.82
31	B	602	CLA	CAA-CBA-CGA	-2.00	107.52	113.21
31	S1	604	CLA	CAA-CBA-CGA	-2.00	107.52	113.21
31	b	611	CLA	CMD-C2D-C3D	-2.00	123.10	127.69
47	y1	606	CHL	CMD-C2D-C3D	2.00	128.69	124.68
31	C1	512	CLA	O2D-CGD-O1D	-2.00	119.95	123.85
48	Y1	620	LUT	C10-C11-C12	-2.00	117.40	123.20
48	S1	621	LUT	C10-C11-C12	-2.00	117.40	123.20
31	b	614	CLA	C3B-C4B-NB	-2.00	108.74	110.53
31	d	403	CLA	CMD-C2D-C3D	-2.00	123.10	127.69
31	B1	617	CLA	O2A-CGA-CBA	2.00	117.94	111.83
31	G	612	CLA	C3D-C2D-C1D	-2.00	103.10	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(^{o})	Ideal(^{o})
31	n1	610	CLA	C1D-ND-C4D	-2.00	104.91	106.31
31	S	611	CLA	CAC-C3C-C4C	2.00	127.39	124.79
35	c	521	LMG	O8-C28-O10	-2.00	118.62	123.63
41	N1	624	LHG	C6-C5-C4	-2.00	107.12	111.78
31	C1	513	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
31	b1	605	CLA	O1D-CGD-CBD	-2.00	120.57	124.52
31	s	603	CLA	C2D-C1D-ND	2.00	112.11	110.13
31	s	605	CLA	C2D-C1D-ND	2.00	112.11	110.13
31	r1	610	CLA	C1-O2A-CGA	2.00	121.49	116.65
31	r	604	CLA	CHA-C1A-NA	-2.00	121.86	126.39
31	s	602	CLA	C2C-C1C-NC	2.00	112.08	109.98
31	b	607	CLA	CGD-CBD-CAD	-2.00	104.37	110.85
31	G	604	CLA	CHA-C1A-NA	-2.00	121.86	126.39
31	G1	602	CLA	CHA-C1A-NA	-2.00	121.86	126.39

All (694) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
31	A	405	CLA	ND
31	A	406	CLA	ND
31	A	407	CLA	ND
31	A	410	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
31	C	501	CLA	ND
31	C	502	CLA	ND
31	C	503	CLA	ND
31	C	504	CLA	ND

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Mol	Chain	Res	Type	Atom
31	C	505	CLA	ND
31	C	506	CLA	ND
31	C	507	CLA	ND
31	C	508	CLA	ND
31	C	509	CLA	ND
31	C	510	CLA	ND
31	C	511	CLA	ND
31	C	512	CLA	ND
31	C	513	CLA	ND
31	D	402	CLA	ND
31	D	403	CLA	ND
31	N	602	CLA	ND
31	N	603	CLA	ND
31	N	604	CLA	ND
31	N	610	CLA	ND
31	N	611	CLA	ND
31	N	612	CLA	ND
31	N	613	CLA	ND
31	N	614	CLA	ND
31	G	602	CLA	ND
31	G	603	CLA	ND
31	G	604	CLA	ND
31	G	610	CLA	ND
31	G	611	CLA	ND
31	G	612	CLA	ND
31	G	613	CLA	ND
31	G	614	CLA	ND
31	R	602	CLA	ND
31	R	603	CLA	ND
31	R	604	CLA	ND
31	R	608	CLA	ND
31	R	609	CLA	ND
31	R	610	CLA	ND
31	R	611	CLA	ND
31	R	612	CLA	ND
31	R	613	CLA	ND
31	S	602	CLA	ND
31	S	603	CLA	ND
31	S	604	CLA	ND
31	S	605	CLA	ND
31	S	609	CLA	ND
31	S	610	CLA	ND

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Mol	Chain	Res	Type	Atom
31	S	611	CLA	ND
31	S	612	CLA	ND
31	S	613	CLA	ND
31	S	614	CLA	ND
31	S	617	CLA	ND
31	Y	602	CLA	ND
31	Y	603	CLA	ND
31	Y	604	CLA	ND
31	Y	608	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	a	405	CLA	ND
31	a	406	CLA	ND
31	a	407	CLA	ND
31	a	410	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
31	c	501	CLA	ND
31	c	502	CLA	ND
31	c	503	CLA	ND
31	c	504	CLA	ND
31	c	505	CLA	ND
31	c	506	CLA	ND
31	c	507	CLA	ND
31	c	508	CLA	ND

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Mol	Chain	Res	Type	Atom
31	c	509	CLA	ND
31	c	510	CLA	ND
31	c	511	CLA	ND
31	c	512	CLA	ND
31	c	513	CLA	ND
31	d	402	CLA	ND
31	d	403	CLA	ND
31	n	602	CLA	ND
31	n	603	CLA	ND
31	n	604	CLA	ND
31	n	610	CLA	ND
31	n	611	CLA	ND
31	n	612	CLA	ND
31	n	613	CLA	ND
31	n	614	CLA	ND
31	g	602	CLA	ND
31	g	603	CLA	ND
31	g	604	CLA	ND
31	g	610	CLA	ND
31	g	611	CLA	ND
31	g	612	CLA	ND
31	g	613	CLA	ND
31	g	614	CLA	ND
31	r	602	CLA	ND
31	r	603	CLA	ND
31	r	604	CLA	ND
31	r	608	CLA	ND
31	r	609	CLA	ND
31	r	610	CLA	ND
31	r	611	CLA	ND
31	r	612	CLA	ND
31	r	613	CLA	ND
31	s	602	CLA	ND
31	s	603	CLA	ND
31	s	604	CLA	ND
31	s	605	CLA	ND
31	s	609	CLA	ND
31	s	610	CLA	ND
31	s	611	CLA	ND
31	s	612	CLA	ND
31	s	613	CLA	ND
31	s	614	CLA	ND

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Mol	Chain	Res	Type	Atom
31	s	617	CLA	ND
31	y	602	CLA	ND
31	y	603	CLA	ND
31	y	604	CLA	ND
31	y	608	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	A1	405	CLA	ND
31	A1	406	CLA	ND
31	A1	407	CLA	ND
31	A1	410	CLA	ND
31	B1	602	CLA	ND
31	B1	603	CLA	ND
31	B1	604	CLA	ND
31	B1	605	CLA	ND
31	B1	606	CLA	ND
31	B1	607	CLA	ND
31	B1	608	CLA	ND
31	B1	609	CLA	ND
31	B1	610	CLA	ND
31	B1	611	CLA	ND
31	B1	612	CLA	ND
31	B1	613	CLA	ND
31	B1	614	CLA	ND
31	B1	615	CLA	ND
31	B1	616	CLA	ND
31	B1	617	CLA	ND
31	C1	501	CLA	ND
31	C1	502	CLA	ND
31	C1	503	CLA	ND
31	C1	504	CLA	ND
31	C1	505	CLA	ND
31	C1	506	CLA	ND
31	C1	507	CLA	ND
31	C1	508	CLA	ND
31	C1	509	CLA	ND
31	C1	510	CLA	ND
31	C1	511	CLA	ND
31	C1	512	CLA	ND

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Mol	Chain	Res	Type	Atom
31	C1	513	CLA	ND
31	D1	402	CLA	ND
31	D1	403	CLA	ND
31	N1	602	CLA	ND
31	N1	603	CLA	ND
31	N1	604	CLA	ND
31	N1	610	CLA	ND
31	N1	611	CLA	ND
31	N1	612	CLA	ND
31	N1	613	CLA	ND
31	N1	614	CLA	ND
31	G1	602	CLA	ND
31	G1	603	CLA	ND
31	G1	604	CLA	ND
31	G1	610	CLA	ND
31	G1	611	CLA	ND
31	G1	612	CLA	ND
31	G1	613	CLA	ND
31	G1	614	CLA	ND
31	R1	602	CLA	ND
31	R1	603	CLA	ND
31	R1	604	CLA	ND
31	R1	608	CLA	ND
31	R1	609	CLA	ND
31	R1	610	CLA	ND
31	R1	612	CLA	ND
31	S1	602	CLA	ND
31	S1	603	CLA	ND
31	S1	604	CLA	ND
31	S1	605	CLA	ND
31	S1	609	CLA	ND
31	S1	610	CLA	ND
31	S1	611	CLA	ND
31	S1	612	CLA	ND
31	S1	613	CLA	ND
31	S1	614	CLA	ND
31	S1	617	CLA	ND
31	Y1	602	CLA	ND
31	Y1	603	CLA	ND
31	Y1	604	CLA	ND
31	Y1	608	CLA	ND
31	Y1	610	CLA	ND

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Mol	Chain	Res	Type	Atom
31	Y1	611	CLA	ND
31	Y1	612	CLA	ND
31	Y1	613	CLA	ND
31	Y1	614	CLA	ND
31	a1	405	CLA	ND
31	a1	406	CLA	ND
31	a1	407	CLA	ND
31	a1	410	CLA	ND
31	b1	602	CLA	ND
31	b1	603	CLA	ND
31	b1	604	CLA	ND
31	b1	605	CLA	ND
31	b1	606	CLA	ND
31	b1	607	CLA	ND
31	b1	608	CLA	ND
31	b1	609	CLA	ND
31	b1	610	CLA	ND
31	b1	611	CLA	ND
31	b1	612	CLA	ND
31	b1	613	CLA	ND
31	b1	614	CLA	ND
31	b1	615	CLA	ND
31	b1	616	CLA	ND
31	b1	617	CLA	ND
31	c1	501	CLA	ND
31	c1	502	CLA	ND
31	c1	503	CLA	ND
31	c1	504	CLA	ND
31	c1	505	CLA	ND
31	c1	506	CLA	ND
31	c1	507	CLA	ND
31	c1	508	CLA	ND
31	c1	509	CLA	ND
31	c1	510	CLA	ND
31	c1	511	CLA	ND
31	c1	512	CLA	ND
31	c1	513	CLA	ND
31	d1	402	CLA	ND
31	d1	403	CLA	ND
31	n1	602	CLA	ND
31	n1	603	CLA	ND
31	n1	604	CLA	ND

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Mol	Chain	Res	Type	Atom
31	n1	610	CLA	ND
31	n1	611	CLA	ND
31	n1	612	CLA	ND
31	n1	613	CLA	ND
31	n1	614	CLA	ND
31	g1	602	CLA	ND
31	g1	603	CLA	ND
31	g1	604	CLA	ND
31	g1	610	CLA	ND
31	g1	611	CLA	ND
31	g1	612	CLA	ND
31	g1	613	CLA	ND
31	g1	614	CLA	ND
31	r1	602	CLA	ND
31	r1	603	CLA	ND
31	r1	604	CLA	ND
31	r1	608	CLA	ND
31	r1	609	CLA	ND
31	r1	610	CLA	ND
31	r1	612	CLA	ND
31	s1	602	CLA	ND
31	s1	603	CLA	ND
31	s1	604	CLA	ND
31	s1	605	CLA	ND
31	s1	609	CLA	ND
31	s1	610	CLA	ND
31	s1	611	CLA	ND
31	s1	612	CLA	ND
31	s1	613	CLA	ND
31	s1	614	CLA	ND
31	s1	617	CLA	ND
31	y1	602	CLA	ND
31	y1	603	CLA	ND
31	y1	604	CLA	ND
31	y1	608	CLA	ND
31	y1	610	CLA	ND
31	y1	611	CLA	ND
31	y1	612	CLA	ND
31	y1	613	CLA	ND
31	y1	614	CLA	ND
37	B	620	C7Z	C3
37	b	620	C7Z	C3

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Mol	Chain	Res	Type	Atom
37	B1	620	C7Z	C3
37	b1	620	C7Z	C3
42	C	527	LMK	C3
42	c	627	LMK	C3
42	C1	527	LMK	C3
42	C1	527	LMK	C8
42	c1	527	LMK	C3
42	c1	527	LMK	C8
46	H	101	RRX	C28
46	h	101	RRX	C28
46	H1	101	RRX	C28
46	h1	101	RRX	C28
47	N	601	CHL	ND
47	N	601	CHL	NA
47	N	601	CHL	NC
47	N	601	CHL	C8
47	N	605	CHL	ND
47	N	605	CHL	NA
47	N	605	CHL	NC
47	N	605	CHL	C8
47	N	606	CHL	ND
47	N	606	CHL	NA
47	N	606	CHL	NC
47	N	606	CHL	C8
47	N	607	CHL	ND
47	N	607	CHL	NA
47	N	607	CHL	NC
47	N	607	CHL	C8
47	N	608	CHL	ND
47	N	608	CHL	NA
47	N	608	CHL	NC
47	N	609	CHL	ND
47	N	609	CHL	NA
47	N	609	CHL	NC
47	N	609	CHL	C8
47	G	601	CHL	ND
47	G	601	CHL	NA
47	G	601	CHL	NC
47	G	601	CHL	C8
47	G	605	CHL	ND
47	G	605	CHL	NA
47	G	605	CHL	NC

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Mol	Chain	Res	Type	Atom
47	G	606	CHL	C3A
47	G	606	CHL	ND
47	G	606	CHL	NA
47	G	606	CHL	NC
47	G	607	CHL	ND
47	G	607	CHL	NA
47	G	607	CHL	NC
47	G	608	CHL	ND
47	G	608	CHL	NA
47	G	608	CHL	NC
47	G	609	CHL	ND
47	G	609	CHL	NA
47	G	609	CHL	NC
47	G	609	CHL	C8
47	R	606	CHL	ND
47	R	606	CHL	NA
47	R	606	CHL	NC
47	R	607	CHL	ND
47	R	607	CHL	NA
47	R	607	CHL	NC
47	S	601	CHL	ND
47	S	601	CHL	NA
47	S	601	CHL	NC
47	S	606	CHL	ND
47	S	606	CHL	NA
47	S	606	CHL	NC
47	S	607	CHL	C3A
47	S	607	CHL	ND
47	S	607	CHL	NA
47	S	607	CHL	NC
47	S	608	CHL	ND
47	S	608	CHL	NA
47	S	608	CHL	NC
47	S	608	CHL	C8
47	Y	601	CHL	ND
47	Y	601	CHL	NA
47	Y	601	CHL	NC
47	Y	601	CHL	C8
47	Y	605	CHL	ND
47	Y	605	CHL	NA
47	Y	605	CHL	NC
47	Y	606	CHL	ND

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Mol	Chain	Res	Type	Atom
47	Y	606	CHL	NA
47	Y	606	CHL	NC
47	Y	606	CHL	C8
47	Y	607	CHL	ND
47	Y	607	CHL	NA
47	Y	607	CHL	NC
47	Y	607	CHL	C8
47	Y	609	CHL	ND
47	Y	609	CHL	NA
47	Y	609	CHL	NC
47	Y	609	CHL	C8
47	n	601	CHL	ND
47	n	601	CHL	NA
47	n	601	CHL	NC
47	n	601	CHL	C8
47	n	605	CHL	ND
47	n	605	CHL	NA
47	n	605	CHL	NC
47	n	605	CHL	C8
47	n	606	CHL	ND
47	n	606	CHL	NA
47	n	606	CHL	NC
47	n	606	CHL	C8
47	n	607	CHL	ND
47	n	607	CHL	NA
47	n	607	CHL	NC
47	n	607	CHL	C8
47	n	608	CHL	ND
47	n	608	CHL	NA
47	n	608	CHL	NC
47	n	609	CHL	ND
47	n	609	CHL	NA
47	n	609	CHL	NC
47	n	609	CHL	C8
47	g	601	CHL	ND
47	g	601	CHL	NA
47	g	601	CHL	NC
47	g	601	CHL	C8
47	g	605	CHL	ND
47	g	605	CHL	NA
47	g	605	CHL	NC
47	g	606	CHL	ND

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Mol	Chain	Res	Type	Atom
47	g	606	CHL	NA
47	g	606	CHL	NC
47	g	607	CHL	ND
47	g	607	CHL	NA
47	g	607	CHL	NC
47	g	608	CHL	ND
47	g	608	CHL	NA
47	g	608	CHL	NC
47	g	609	CHL	ND
47	g	609	CHL	NA
47	g	609	CHL	NC
47	g	609	CHL	C8
47	r	606	CHL	ND
47	r	606	CHL	NA
47	r	606	CHL	NC
47	r	607	CHL	ND
47	r	607	CHL	NA
47	r	607	CHL	NC
47	s	601	CHL	ND
47	s	601	CHL	NA
47	s	601	CHL	NC
47	s	606	CHL	ND
47	s	606	CHL	NA
47	s	606	CHL	NC
47	s	607	CHL	C3A
47	s	607	CHL	ND
47	s	607	CHL	NA
47	s	607	CHL	NC
47	s	608	CHL	ND
47	s	608	CHL	NA
47	s	608	CHL	NC
47	s	608	CHL	C8
47	y	601	CHL	ND
47	y	601	CHL	NA
47	y	601	CHL	NC
47	y	601	CHL	C8
47	y	605	CHL	ND
47	y	605	CHL	NA
47	y	605	CHL	NC
47	y	606	CHL	ND
47	y	606	CHL	NA
47	y	606	CHL	NC

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Mol	Chain	Res	Type	Atom
47	y	606	CHL	C8
47	y	607	CHL	ND
47	y	607	CHL	NA
47	y	607	CHL	NC
47	y	607	CHL	C8
47	y	609	CHL	ND
47	y	609	CHL	NA
47	y	609	CHL	NC
47	y	609	CHL	C8
47	N1	601	CHL	ND
47	N1	601	CHL	NA
47	N1	601	CHL	NC
47	N1	601	CHL	C8
47	N1	605	CHL	ND
47	N1	605	CHL	NA
47	N1	605	CHL	NC
47	N1	605	CHL	C8
47	N1	606	CHL	ND
47	N1	606	CHL	NA
47	N1	606	CHL	NC
47	N1	606	CHL	C8
47	N1	607	CHL	ND
47	N1	607	CHL	NA
47	N1	607	CHL	NC
47	N1	607	CHL	C8
47	N1	608	CHL	ND
47	N1	608	CHL	NA
47	N1	608	CHL	NC
47	N1	609	CHL	ND
47	N1	609	CHL	NA
47	N1	609	CHL	NC
47	N1	609	CHL	C8
47	G1	601	CHL	ND
47	G1	601	CHL	NA
47	G1	601	CHL	NC
47	G1	601	CHL	C8
47	G1	605	CHL	C3A
47	G1	605	CHL	ND
47	G1	605	CHL	NA
47	G1	605	CHL	NC
47	G1	606	CHL	ND
47	G1	606	CHL	NA

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Mol	Chain	Res	Type	Atom
47	G1	606	CHL	NC
47	G1	607	CHL	ND
47	G1	607	CHL	NA
47	G1	607	CHL	NC
47	G1	607	CHL	C8
47	G1	608	CHL	ND
47	G1	608	CHL	NA
47	G1	608	CHL	NC
47	G1	609	CHL	ND
47	G1	609	CHL	NA
47	G1	609	CHL	NC
47	G1	609	CHL	C8
47	R1	606	CHL	ND
47	R1	606	CHL	NA
47	R1	606	CHL	NC
47	R1	607	CHL	ND
47	R1	607	CHL	NA
47	R1	607	CHL	NC
47	S1	601	CHL	ND
47	S1	601	CHL	NA
47	S1	601	CHL	NC
47	S1	606	CHL	ND
47	S1	606	CHL	NA
47	S1	606	CHL	NC
47	S1	607	CHL	ND
47	S1	607	CHL	NA
47	S1	607	CHL	NC
47	S1	608	CHL	ND
47	S1	608	CHL	NA
47	S1	608	CHL	NC
47	S1	608	CHL	C8
47	Y1	601	CHL	ND
47	Y1	601	CHL	NA
47	Y1	601	CHL	NC
47	Y1	601	CHL	C8
47	Y1	605	CHL	ND
47	Y1	605	CHL	NA
47	Y1	605	CHL	NC
47	Y1	606	CHL	ND
47	Y1	606	CHL	NA
47	Y1	606	CHL	NC
47	Y1	606	CHL	C8

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Mol	Chain	Res	Type	Atom
47	Y1	607	CHL	ND
47	Y1	607	CHL	NA
47	Y1	607	CHL	NC
47	Y1	607	CHL	C8
47	Y1	609	CHL	ND
47	Y1	609	CHL	NA
47	Y1	609	CHL	NC
47	Y1	609	CHL	C8
47	n1	601	CHL	ND
47	n1	601	CHL	NA
47	n1	601	CHL	NC
47	n1	601	CHL	C8
47	n1	605	CHL	ND
47	n1	605	CHL	NA
47	n1	605	CHL	NC
47	n1	605	CHL	C8
47	n1	606	CHL	ND
47	n1	606	CHL	NA
47	n1	606	CHL	NC
47	n1	606	CHL	C8
47	n1	607	CHL	ND
47	n1	607	CHL	NA
47	n1	607	CHL	NC
47	n1	607	CHL	C8
47	n1	608	CHL	ND
47	n1	608	CHL	NA
47	n1	608	CHL	NC
47	n1	609	CHL	ND
47	n1	609	CHL	NA
47	n1	609	CHL	NC
47	n1	609	CHL	C8
47	g1	601	CHL	ND
47	g1	601	CHL	NA
47	g1	601	CHL	NC
47	g1	601	CHL	C8
47	g1	605	CHL	C3A
47	g1	605	CHL	ND
47	g1	605	CHL	NA
47	g1	605	CHL	NC
47	g1	606	CHL	ND
47	g1	606	CHL	NA
47	g1	606	CHL	NC

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Mol	Chain	Res	Type	Atom
47	g1	607	CHL	ND
47	g1	607	CHL	NA
47	g1	607	CHL	NC
47	g1	607	CHL	C8
47	g1	608	CHL	ND
47	g1	608	CHL	NA
47	g1	608	CHL	NC
47	g1	609	CHL	ND
47	g1	609	CHL	NA
47	g1	609	CHL	NC
47	g1	609	CHL	C8
47	r1	606	CHL	ND
47	r1	606	CHL	NA
47	r1	606	CHL	NC
47	r1	607	CHL	ND
47	r1	607	CHL	NA
47	r1	607	CHL	NC
47	s1	601	CHL	ND
47	s1	601	CHL	NA
47	s1	601	CHL	NC
47	s1	606	CHL	ND
47	s1	606	CHL	NA
47	s1	606	CHL	NC
47	s1	607	CHL	ND
47	s1	607	CHL	NA
47	s1	607	CHL	NC
47	s1	608	CHL	ND
47	s1	608	CHL	NA
47	s1	608	CHL	NC
47	s1	608	CHL	C8
47	y1	601	CHL	ND
47	y1	601	CHL	NA
47	y1	601	CHL	NC
47	y1	601	CHL	C8
47	y1	605	CHL	ND
47	y1	605	CHL	NA
47	y1	605	CHL	NC
47	y1	606	CHL	ND
47	y1	606	CHL	NA
47	y1	606	CHL	NC
47	y1	606	CHL	C8
47	y1	607	CHL	ND

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Mol	Chain	Res	Type	Atom
47	y1	607	CHL	NA
47	y1	607	CHL	NC
47	y1	607	CHL	C8
47	y1	609	CHL	ND
47	y1	609	CHL	NA
47	y1	609	CHL	NC
47	y1	609	CHL	C8
48	G	621	LUT	C26
48	S	620	LUT	C26
48	Y	621	LUT	C26
48	n	621	LUT	C26
48	s	620	LUT	C26
48	R1	620	LUT	C26
48	g1	621	LUT	C26
49	N	622	XAT	C6
49	G	622	XAT	C26
49	G	622	XAT	C6
49	R	621	XAT	C26
49	Y	622	XAT	C6
49	g	622	XAT	C26
49	g	622	XAT	C6
49	r	622	XAT	C26
49	N1	622	XAT	C6
49	G1	622	XAT	C26
49	Y1	622	XAT	C26
49	Y1	622	XAT	C6
49	n1	622	XAT	C6
49	g1	622	XAT	C26
49	g1	622	XAT	C6
49	r1	621	XAT	C26
56	R1	626	ERG	C9
56	R1	626	ERG	C14
56	R1	626	ERG	C10
56	R1	626	ERG	C24
56	R1	626	ERG	C20
56	r1	626	ERG	C9
56	r1	626	ERG	C14
56	r1	626	ERG	C10
56	r1	626	ERG	C24
56	r1	626	ERG	C20

All (8548) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
31	A	405	CLA	CBD-CGD-O2D-CED
31	A	406	CLA	C1A-C2A-CAA-CBA
31	A	406	CLA	C3A-C2A-CAA-CBA
31	A	407	CLA	C2B-C3B-CAB-CBB
31	A	407	CLA	C4B-C3B-CAB-CBB
31	B	602	CLA	CBD-CGD-O2D-CED
31	B	604	CLA	CBD-CGD-O2D-CED
31	B	605	CLA	C2-C1-O2A-CGA
31	B	605	CLA	CAD-CBD-CGD-O1D
31	B	605	CLA	CAD-CBD-CGD-O2D
31	B	605	CLA	C4-C3-C5-C6
31	B	608	CLA	C1A-C2A-CAA-CBA
31	B	608	CLA	C3A-C2A-CAA-CBA
31	B	608	CLA	C2-C1-O2A-CGA
31	B	608	CLA	CAD-CBD-CGD-O1D
31	B	608	CLA	CAD-CBD-CGD-O2D
31	B	608	CLA	CBD-CGD-O2D-CED
31	B	608	CLA	C2-C3-C5-C6
31	B	608	CLA	C4-C3-C5-C6
31	B	609	CLA	C1A-C2A-CAA-CBA
31	B	609	CLA	CHA-CBD-CGD-O1D
31	B	609	CLA	CHA-CBD-CGD-O2D
31	B	610	CLA	C1A-C2A-CAA-CBA
31	B	610	CLA	C3A-C2A-CAA-CBA
31	B	610	CLA	CAD-CBD-CGD-O2D
31	B	610	CLA	CBD-CGD-O2D-CED
31	B	611	CLA	CHA-CBD-CGD-O1D
31	B	611	CLA	CHA-CBD-CGD-O2D
31	B	612	CLA	C1A-C2A-CAA-CBA
31	B	612	CLA	C2-C1-O2A-CGA
31	B	612	CLA	C2-C3-C5-C6
31	B	612	CLA	C4-C3-C5-C6
31	B	614	CLA	C2-C1-O2A-CGA
31	B	615	CLA	C1A-C2A-CAA-CBA
31	B	615	CLA	CAD-CBD-CGD-O1D
31	B	615	CLA	CAD-CBD-CGD-O2D
31	B	617	CLA	C2B-C3B-CAB-CBB
31	B	617	CLA	C4B-C3B-CAB-CBB
31	C	501	CLA	CHA-CBD-CGD-O1D
31	C	501	CLA	CHA-CBD-CGD-O2D
31	C	502	CLA	CAD-CBD-CGD-O1D
31	C	502	CLA	CAD-CBD-CGD-O2D
31	C	504	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	C	505	CLA	CAD-CBD-CGD-O1D
31	C	505	CLA	CAD-CBD-CGD-O2D
31	C	507	CLA	CHA-CBD-CGD-O1D
31	C	507	CLA	CHA-CBD-CGD-O2D
31	C	513	CLA	C1A-C2A-CAA-CBA
31	C	513	CLA	C11-C10-C8-C9
31	D	402	CLA	C1A-C2A-CAA-CBA
31	D	402	CLA	CBD-CGD-O2D-CED
31	D	402	CLA	C2-C3-C5-C6
31	D	402	CLA	C4-C3-C5-C6
31	D	403	CLA	C2B-C3B-CAB-CBB
31	D	403	CLA	C4B-C3B-CAB-CBB
31	D	403	CLA	CBD-CGD-O2D-CED
31	N	602	CLA	C14-C13-C15-C16
31	N	603	CLA	C3A-C2A-CAA-CBA
31	N	603	CLA	C4B-C3B-CAB-CBB
31	N	610	CLA	C1A-C2A-CAA-CBA
31	N	611	CLA	CHA-CBD-CGD-O1D
31	N	611	CLA	CHA-CBD-CGD-O2D
31	N	613	CLA	C1A-C2A-CAA-CBA
31	N	614	CLA	CBD-CGD-O2D-CED
31	G	602	CLA	C1A-C2A-CAA-CBA
31	G	602	CLA	C3A-C2A-CAA-CBA
31	G	602	CLA	CHA-CBD-CGD-O1D
31	G	602	CLA	CHA-CBD-CGD-O2D
31	G	603	CLA	CBD-CGD-O2D-CED
31	G	612	CLA	CHA-CBD-CGD-O1D
31	G	612	CLA	CHA-CBD-CGD-O2D
31	G	614	CLA	CBD-CGD-O2D-CED
31	R	602	CLA	CHA-CBD-CGD-O1D
31	R	602	CLA	CHA-CBD-CGD-O2D
31	R	603	CLA	C2-C1-O2A-CGA
31	R	604	CLA	CHA-CBD-CGD-O1D
31	R	604	CLA	CHA-CBD-CGD-O2D
31	R	608	CLA	C3A-C2A-CAA-CBA
31	R	608	CLA	C4B-C3B-CAB-CBB
31	R	608	CLA	CBD-CGD-O2D-CED
31	R	609	CLA	C2B-C3B-CAB-CBB
31	R	609	CLA	C4B-C3B-CAB-CBB
31	R	610	CLA	C1A-C2A-CAA-CBA
31	R	611	CLA	CBA-CGA-O2A-C1
31	R	611	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	R	611	CLA	C4B-C3B-CAB-CBB
31	R	611	CLA	CBD-CGD-O2D-CED
31	R	612	CLA	C2-C1-O2A-CGA
31	R	612	CLA	CHA-CBD-CGD-O1D
31	R	612	CLA	CHA-CBD-CGD-O2D
31	R	613	CLA	CBA-CGA-O2A-C1
31	R	613	CLA	CHA-CBD-CGD-O1D
31	R	613	CLA	CHA-CBD-CGD-O2D
31	S	602	CLA	C1A-C2A-CAA-CBA
31	S	602	CLA	C3A-C2A-CAA-CBA
31	S	603	CLA	C2B-C3B-CAB-CBB
31	S	603	CLA	C4B-C3B-CAB-CBB
31	S	605	CLA	C1A-C2A-CAA-CBA
31	S	605	CLA	C3A-C2A-CAA-CBA
31	S	605	CLA	C2-C1-O2A-CGA
31	S	605	CLA	CHA-CBD-CGD-O1D
31	S	605	CLA	CHA-CBD-CGD-O2D
31	S	609	CLA	CBD-CGD-O2D-CED
31	S	610	CLA	C4B-C3B-CAB-CBB
31	S	611	CLA	C2B-C3B-CAB-CBB
31	S	611	CLA	C4B-C3B-CAB-CBB
31	S	611	CLA	CBD-CGD-O2D-CED
31	S	612	CLA	CHA-CBD-CGD-O1D
31	S	612	CLA	CHA-CBD-CGD-O2D
31	S	617	CLA	CBA-CGA-O2A-C1
31	S	617	CLA	O1A-CGA-O2A-C1
31	Y	603	CLA	CHA-CBD-CGD-O2D
31	Y	610	CLA	C2B-C3B-CAB-CBB
31	Y	610	CLA	C4B-C3B-CAB-CBB
31	Y	612	CLA	CHA-CBD-CGD-O1D
31	Y	612	CLA	CHA-CBD-CGD-O2D
31	Y	613	CLA	CBD-CGD-O2D-CED
31	Y	614	CLA	CBD-CGD-O2D-CED
31	a	405	CLA	CBD-CGD-O2D-CED
31	a	406	CLA	C1A-C2A-CAA-CBA
31	a	406	CLA	C3A-C2A-CAA-CBA
31	b	604	CLA	CBD-CGD-O2D-CED
31	b	605	CLA	C2-C1-O2A-CGA
31	b	605	CLA	CAD-CBD-CGD-O2D
31	b	607	CLA	C1A-C2A-CAA-CBA
31	b	608	CLA	C1A-C2A-CAA-CBA
31	b	608	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
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	609	CLA	C2B-C3B-CAB-CBB
31	b	609	CLA	C4B-C3B-CAB-CBB
31	b	609	CLA	CHA-CBD-CGD-O1D
31	b	609	CLA	CHA-CBD-CGD-O2D
31	b	610	CLA	C3A-C2A-CAA-CBA
31	b	610	CLA	CAD-CBD-CGD-O2D
31	b	610	CLA	CBD-CGD-O2D-CED
31	b	611	CLA	CHA-CBD-CGD-O1D
31	b	611	CLA	CHA-CBD-CGD-O2D
31	b	612	CLA	C1A-C2A-CAA-CBA
31	b	612	CLA	CBD-CGD-O2D-CED
31	b	615	CLA	C1A-C2A-CAA-CBA
31	b	615	CLA	CAD-CBD-CGD-O1D
31	b	615	CLA	CAD-CBD-CGD-O2D
31	b	617	CLA	CBA-CGA-O2A-C1
31	b	617	CLA	O1A-CGA-O2A-C1
31	b	617	CLA	C6-C7-C8-C9
31	c	501	CLA	C1A-C2A-CAA-CBA
31	c	501	CLA	C2B-C3B-CAB-CBB
31	c	501	CLA	C4B-C3B-CAB-CBB
31	c	501	CLA	CHA-CBD-CGD-O1D
31	c	501	CLA	CHA-CBD-CGD-O2D
31	c	502	CLA	CBD-CGD-O2D-CED
31	c	503	CLA	C4B-C3B-CAB-CBB
31	c	504	CLA	CBA-CGA-O2A-C1
31	c	504	CLA	O1A-CGA-O2A-C1
31	c	505	CLA	C4B-C3B-CAB-CBB
31	c	505	CLA	CAD-CBD-CGD-O1D
31	c	505	CLA	CAD-CBD-CGD-O2D
31	c	506	CLA	C6-C7-C8-C9
31	c	507	CLA	CHA-CBD-CGD-O1D
31	c	507	CLA	CHA-CBD-CGD-O2D
31	d	403	CLA	CBD-CGD-O2D-CED
31	n	603	CLA	C1A-C2A-CAA-CBA
31	n	603	CLA	CBA-CGA-O2A-C1
31	n	603	CLA	O1A-CGA-O2A-C1
31	n	603	CLA	C4B-C3B-CAB-CBB
31	n	603	CLA	CAD-CBD-CGD-O1D
31	n	603	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	n	603	CLA	CBD-CGD-O2D-CED
31	n	604	CLA	C1A-C2A-CAA-CBA
31	n	604	CLA	C3A-C2A-CAA-CBA
31	n	610	CLA	C1A-C2A-CAA-CBA
31	n	610	CLA	CBD-CGD-O2D-CED
31	n	611	CLA	C1A-C2A-CAA-CBA
31	n	611	CLA	C3A-C2A-CAA-CBA
31	n	611	CLA	C2B-C3B-CAB-CBB
31	n	611	CLA	C4B-C3B-CAB-CBB
31	n	611	CLA	CHA-CBD-CGD-O1D
31	n	611	CLA	CHA-CBD-CGD-O2D
31	n	612	CLA	C2B-C3B-CAB-CBB
31	n	612	CLA	C4B-C3B-CAB-CBB
31	n	612	CLA	CBD-CGD-O2D-CED
31	n	614	CLA	C1A-C2A-CAA-CBA
31	n	614	CLA	CBD-CGD-O2D-CED
31	g	602	CLA	C1A-C2A-CAA-CBA
31	g	602	CLA	C3A-C2A-CAA-CBA
31	g	602	CLA	CHA-CBD-CGD-O1D
31	g	602	CLA	CHA-CBD-CGD-O2D
31	g	603	CLA	C3A-C2A-CAA-CBA
31	g	603	CLA	CBD-CGD-O2D-CED
31	g	604	CLA	C2-C1-O2A-CGA
31	g	604	CLA	CBD-CGD-O2D-CED
31	g	612	CLA	C1A-C2A-CAA-CBA
31	g	612	CLA	CHA-CBD-CGD-O1D
31	g	612	CLA	CHA-CBD-CGD-O2D
31	r	602	CLA	CHA-CBD-CGD-O1D
31	r	602	CLA	CHA-CBD-CGD-O2D
31	r	603	CLA	C2-C1-O2A-CGA
31	r	603	CLA	CBD-CGD-O2D-CED
31	r	604	CLA	C1A-C2A-CAA-CBA
31	r	604	CLA	C3A-C2A-CAA-CBA
31	r	608	CLA	C1A-C2A-CAA-CBA
31	r	608	CLA	C3A-C2A-CAA-CBA
31	r	609	CLA	CBD-CGD-O2D-CED
31	r	610	CLA	C1A-C2A-CAA-CBA
31	r	611	CLA	CBA-CGA-O2A-C1
31	r	611	CLA	C4B-C3B-CAB-CBB
31	r	612	CLA	C2-C1-O2A-CGA
31	r	612	CLA	CHA-CBD-CGD-O1D
31	r	612	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
31	r	613	CLA	CBA-CGA-O2A-C1
31	r	613	CLA	O1A-CGA-O2A-C1
31	r	613	CLA	CHA-CBD-CGD-O1D
31	r	613	CLA	CHA-CBD-CGD-O2D
31	s	602	CLA	C1A-C2A-CAA-CBA
31	s	602	CLA	C3A-C2A-CAA-CBA
31	s	602	CLA	C4B-C3B-CAB-CBB
31	s	603	CLA	CBD-CGD-O2D-CED
31	s	604	CLA	CBD-CGD-O2D-CED
31	s	605	CLA	C1A-C2A-CAA-CBA
31	s	605	CLA	CHA-CBD-CGD-O1D
31	s	605	CLA	CHA-CBD-CGD-O2D
31	s	610	CLA	C1A-C2A-CAA-CBA
31	s	610	CLA	CBD-CGD-O2D-CED
31	s	611	CLA	CBD-CGD-O2D-CED
31	s	612	CLA	CHA-CBD-CGD-O1D
31	s	612	CLA	CHA-CBD-CGD-O2D
31	s	612	CLA	CBD-CGD-O2D-CED
31	s	613	CLA	CHA-CBD-CGD-O1D
31	s	613	CLA	CHA-CBD-CGD-O2D
31	s	614	CLA	CBA-CGA-O2A-C1
31	s	614	CLA	O1A-CGA-O2A-C1
31	s	614	CLA	C2B-C3B-CAB-CBB
31	s	614	CLA	C4B-C3B-CAB-CBB
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	612	CLA	CHA-CBD-CGD-O1D
31	y	612	CLA	CHA-CBD-CGD-O2D
31	y	614	CLA	C2-C1-O2A-CGA
31	A1	405	CLA	C3A-C2A-CAA-CBA
31	A1	405	CLA	CBD-CGD-O2D-CED
31	A1	406	CLA	C1A-C2A-CAA-CBA
31	A1	406	CLA	C3A-C2A-CAA-CBA
31	A1	406	CLA	C2-C1-O2A-CGA
31	A1	407	CLA	C2-C1-O2A-CGA
31	B1	602	CLA	C1A-C2A-CAA-CBA
31	B1	602	CLA	C2-C1-O2A-CGA
31	B1	602	CLA	CAD-CBD-CGD-O1D
31	B1	602	CLA	CAD-CBD-CGD-O2D
31	B1	603	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	B1	604	CLA	C11-C10-C8-C9
31	B1	605	CLA	CAD-CBD-CGD-O1D
31	B1	605	CLA	CAD-CBD-CGD-O2D
31	B1	608	CLA	C1A-C2A-CAA-CBA
31	B1	608	CLA	C3A-C2A-CAA-CBA
31	B1	608	CLA	CAD-CBD-CGD-O2D
31	B1	608	CLA	CBD-CGD-O2D-CED
31	B1	608	CLA	C2-C3-C5-C6
31	B1	608	CLA	C4-C3-C5-C6
31	B1	609	CLA	C1A-C2A-CAA-CBA
31	B1	609	CLA	C3A-C2A-CAA-CBA
31	B1	609	CLA	CHA-CBD-CGD-O1D
31	B1	609	CLA	CHA-CBD-CGD-O2D
31	B1	610	CLA	CAD-CBD-CGD-O1D
31	B1	610	CLA	CAD-CBD-CGD-O2D
31	B1	610	CLA	CBD-CGD-O2D-CED
31	B1	613	CLA	C1A-C2A-CAA-CBA
31	B1	613	CLA	C3A-C2A-CAA-CBA
31	B1	613	CLA	C2-C1-O2A-CGA
31	B1	614	CLA	C2-C1-O2A-CGA
31	B1	614	CLA	CBD-CGD-O2D-CED
31	B1	616	CLA	CBD-CGD-O2D-CED
31	B1	616	CLA	C11-C10-C8-C9
31	B1	617	CLA	CHA-CBD-CGD-O1D
31	B1	617	CLA	CHA-CBD-CGD-O2D
31	B1	617	CLA	CBD-CGD-O2D-CED
31	C1	502	CLA	C4B-C3B-CAB-CBB
31	C1	502	CLA	CAD-CBD-CGD-O2D
31	C1	503	CLA	CBD-CGD-O2D-CED
31	C1	504	CLA	CAD-CBD-CGD-O1D
31	C1	504	CLA	CAD-CBD-CGD-O2D
31	C1	505	CLA	CAD-CBD-CGD-O1D
31	C1	505	CLA	CAD-CBD-CGD-O2D
31	C1	506	CLA	C2-C1-O2A-CGA
31	C1	506	CLA	CAD-CBD-CGD-O1D
31	C1	506	CLA	CAD-CBD-CGD-O2D
31	C1	506	CLA	CBD-CGD-O2D-CED
31	C1	507	CLA	CHA-CBD-CGD-O1D
31	C1	507	CLA	CHA-CBD-CGD-O2D
31	C1	509	CLA	C2-C1-O2A-CGA
31	C1	509	CLA	CBD-CGD-O2D-CED
31	C1	510	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	C1	512	CLA	C1A-C2A-CAA-CBA
31	C1	512	CLA	CBA-CGA-O2A-C1
31	C1	512	CLA	O1A-CGA-O2A-C1
31	C1	512	CLA	CBD-CGD-O2D-CED
31	C1	513	CLA	C1A-C2A-CAA-CBA
31	C1	513	CLA	C3A-C2A-CAA-CBA
31	C1	513	CLA	CBD-CGD-O2D-CED
31	C1	513	CLA	C11-C10-C8-C9
31	D1	402	CLA	CBD-CGD-O2D-CED
31	N1	602	CLA	CBD-CGD-O2D-CED
31	N1	603	CLA	CBD-CGD-O2D-CED
31	N1	604	CLA	C1A-C2A-CAA-CBA
31	N1	604	CLA	C3A-C2A-CAA-CBA
31	N1	610	CLA	C1A-C2A-CAA-CBA
31	N1	610	CLA	C3A-C2A-CAA-CBA
31	N1	611	CLA	C2-C1-O2A-CGA
31	N1	611	CLA	C2B-C3B-CAB-CBB
31	N1	611	CLA	C4B-C3B-CAB-CBB
31	N1	612	CLA	CHA-CBD-CGD-O1D
31	N1	612	CLA	CHA-CBD-CGD-O2D
31	N1	613	CLA	C1A-C2A-CAA-CBA
31	N1	614	CLA	C1A-C2A-CAA-CBA
31	N1	614	CLA	CBD-CGD-O2D-CED
31	G1	602	CLA	C1A-C2A-CAA-CBA
31	G1	602	CLA	C3A-C2A-CAA-CBA
31	G1	602	CLA	CBD-CGD-O2D-CED
31	G1	604	CLA	CBD-CGD-O2D-CED
31	G1	610	CLA	CBD-CGD-O2D-CED
31	G1	610	CLA	O1D-CGD-O2D-CED
31	G1	612	CLA	CHA-CBD-CGD-O1D
31	G1	612	CLA	CHA-CBD-CGD-O2D
31	G1	614	CLA	CBA-CGA-O2A-C1
31	G1	614	CLA	CBD-CGD-O2D-CED
31	R1	602	CLA	CHA-CBD-CGD-O1D
31	R1	602	CLA	CHA-CBD-CGD-O2D
31	R1	603	CLA	C2-C1-O2A-CGA
31	R1	603	CLA	C2B-C3B-CAB-CBB
31	R1	603	CLA	C4B-C3B-CAB-CBB
31	R1	603	CLA	CBD-CGD-O2D-CED
31	R1	604	CLA	C2-C1-O2A-CGA
31	R1	608	CLA	C1A-C2A-CAA-CBA
31	R1	608	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	R1	609	CLA	CBD-CGD-O2D-CED
31	R1	610	CLA	CBD-CGD-O2D-CED
31	R1	612	CLA	C1A-C2A-CAA-CBA
31	R1	612	CLA	C3A-C2A-CAA-CBA
31	R1	612	CLA	CHA-CBD-CGD-O1D
31	R1	612	CLA	CHA-CBD-CGD-O2D
31	R1	612	CLA	CBD-CGD-O2D-CED
31	S1	602	CLA	C2-C1-O2A-CGA
31	S1	602	CLA	CHA-CBD-CGD-O1D
31	S1	602	CLA	CHA-CBD-CGD-O2D
31	S1	603	CLA	C1A-C2A-CAA-CBA
31	S1	603	CLA	C3A-C2A-CAA-CBA
31	S1	603	CLA	CHA-CBD-CGD-O1D
31	S1	603	CLA	CHA-CBD-CGD-O2D
31	S1	604	CLA	CBA-CGA-O2A-C1
31	S1	604	CLA	O1A-CGA-O2A-C1
31	S1	604	CLA	CBD-CGD-O2D-CED
31	S1	605	CLA	C1A-C2A-CAA-CBA
31	S1	605	CLA	CBD-CGD-O2D-CED
31	S1	609	CLA	C1A-C2A-CAA-CBA
31	S1	609	CLA	CBD-CGD-O2D-CED
31	S1	610	CLA	C1A-C2A-CAA-CBA
31	S1	610	CLA	C3A-C2A-CAA-CBA
31	S1	610	CLA	CBD-CGD-O2D-CED
31	S1	611	CLA	C1A-C2A-CAA-CBA
31	S1	611	CLA	C3A-C2A-CAA-CBA
31	S1	612	CLA	CHA-CBD-CGD-O1D
31	S1	612	CLA	CHA-CBD-CGD-O2D
31	S1	613	CLA	CBD-CGD-O2D-CED
31	S1	617	CLA	CBD-CGD-O2D-CED
31	Y1	602	CLA	CHA-CBD-CGD-O1D
31	Y1	602	CLA	CHA-CBD-CGD-O2D
31	Y1	602	CLA	C11-C10-C8-C9
31	Y1	603	CLA	CHA-CBD-CGD-O1D
31	Y1	603	CLA	CHA-CBD-CGD-O2D
31	Y1	603	CLA	C6-C7-C8-C9
31	Y1	608	CLA	CBD-CGD-O2D-CED
31	Y1	611	CLA	CBD-CGD-O2D-CED
31	Y1	612	CLA	C4B-C3B-CAB-CBB
31	Y1	612	CLA	CHA-CBD-CGD-O1D
31	Y1	612	CLA	CHA-CBD-CGD-O2D
31	Y1	613	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	a1	405	CLA	C3A-C2A-CAA-CBA
31	a1	405	CLA	CBD-CGD-O2D-CED
31	a1	406	CLA	C1A-C2A-CAA-CBA
31	a1	406	CLA	C3A-C2A-CAA-CBA
31	b1	603	CLA	C1A-C2A-CAA-CBA
31	b1	605	CLA	C2B-C3B-CAB-CBB
31	b1	605	CLA	C4B-C3B-CAB-CBB
31	b1	605	CLA	CAD-CBD-CGD-O2D
31	b1	607	CLA	CBD-CGD-O2D-CED
31	b1	608	CLA	C1A-C2A-CAA-CBA
31	b1	608	CLA	C3A-C2A-CAA-CBA
31	b1	608	CLA	C2-C1-O2A-CGA
31	b1	608	CLA	CAD-CBD-CGD-O1D
31	b1	608	CLA	CAD-CBD-CGD-O2D
31	b1	608	CLA	CBD-CGD-O2D-CED
31	b1	608	CLA	C2-C3-C5-C6
31	b1	608	CLA	C4-C3-C5-C6
31	b1	609	CLA	C1A-C2A-CAA-CBA
31	b1	609	CLA	C3A-C2A-CAA-CBA
31	b1	609	CLA	CHA-CBD-CGD-O1D
31	b1	609	CLA	CHA-CBD-CGD-O2D
31	b1	610	CLA	C3A-C2A-CAA-CBA
31	b1	610	CLA	CAD-CBD-CGD-O1D
31	b1	610	CLA	CAD-CBD-CGD-O2D
31	b1	611	CLA	CHA-CBD-CGD-O1D
31	b1	611	CLA	CHA-CBD-CGD-O2D
31	b1	611	CLA	CBD-CGD-O2D-CED
31	b1	612	CLA	CBD-CGD-O2D-CED
31	b1	613	CLA	C2-C1-O2A-CGA
31	b1	613	CLA	CAD-CBD-CGD-O1D
31	b1	613	CLA	CAD-CBD-CGD-O2D
31	b1	614	CLA	C2-C1-O2A-CGA
31	b1	614	CLA	CBD-CGD-O2D-CED
31	b1	615	CLA	C1A-C2A-CAA-CBA
31	b1	615	CLA	C3A-C2A-CAA-CBA
31	b1	615	CLA	C2B-C3B-CAB-CBB
31	b1	615	CLA	C4B-C3B-CAB-CBB
31	b1	616	CLA	CBD-CGD-O2D-CED
31	b1	617	CLA	C2-C1-O2A-CGA
31	b1	617	CLA	CBD-CGD-O2D-CED
31	c1	501	CLA	C1A-C2A-CAA-CBA
31	c1	501	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	c1	501	CLA	CAD-CBD-CGD-O2D
31	c1	501	CLA	C4-C3-C5-C6
31	c1	502	CLA	CAD-CBD-CGD-O1D
31	c1	502	CLA	CAD-CBD-CGD-O2D
31	c1	503	CLA	C2B-C3B-CAB-CBB
31	c1	503	CLA	C4B-C3B-CAB-CBB
31	c1	503	CLA	C2-C3-C5-C6
31	c1	503	CLA	C4-C3-C5-C6
31	c1	504	CLA	CAD-CBD-CGD-O1D
31	c1	504	CLA	CAD-CBD-CGD-O2D
31	c1	504	CLA	CBD-CGD-O2D-CED
31	c1	505	CLA	C1A-C2A-CAA-CBA
31	c1	505	CLA	C2B-C3B-CAB-CBB
31	c1	505	CLA	C4B-C3B-CAB-CBB
31	c1	506	CLA	C2-C1-O2A-CGA
31	c1	506	CLA	CAD-CBD-CGD-O1D
31	c1	506	CLA	CAD-CBD-CGD-O2D
31	c1	507	CLA	CHA-CBD-CGD-O1D
31	c1	507	CLA	CHA-CBD-CGD-O2D
31	c1	509	CLA	CHA-CBD-CGD-O1D
31	c1	509	CLA	CHA-CBD-CGD-O2D
31	c1	509	CLA	C6-C7-C8-C9
31	c1	510	CLA	CHA-CBD-CGD-O1D
31	c1	510	CLA	CHA-CBD-CGD-O2D
31	c1	511	CLA	C1A-C2A-CAA-CBA
31	c1	512	CLA	CBA-CGA-O2A-C1
31	c1	512	CLA	O1A-CGA-O2A-C1
31	c1	512	CLA	CBD-CGD-O2D-CED
31	c1	513	CLA	C1A-C2A-CAA-CBA
31	c1	513	CLA	CBD-CGD-O2D-CED
31	d1	403	CLA	CBA-CGA-O2A-C1
31	d1	403	CLA	CBD-CGD-O2D-CED
31	d1	403	CLA	C4-C3-C5-C6
31	n1	604	CLA	C1A-C2A-CAA-CBA
31	n1	604	CLA	C3A-C2A-CAA-CBA
31	n1	610	CLA	C1A-C2A-CAA-CBA
31	n1	611	CLA	C2B-C3B-CAB-CBB
31	n1	611	CLA	C4B-C3B-CAB-CBB
31	n1	612	CLA	CHA-CBD-CGD-O1D
31	n1	612	CLA	CHA-CBD-CGD-O2D
31	n1	613	CLA	C1A-C2A-CAA-CBA
31	n1	614	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	g1	602	CLA	C1A-C2A-CAA-CBA
31	g1	602	CLA	C3A-C2A-CAA-CBA
31	g1	603	CLA	C3A-C2A-CAA-CBA
31	g1	604	CLA	C2-C1-O2A-CGA
31	g1	604	CLA	CBD-CGD-O2D-CED
31	g1	610	CLA	CBD-CGD-O2D-CED
31	g1	611	CLA	CBD-CGD-O2D-CED
31	g1	612	CLA	CHA-CBD-CGD-O1D
31	g1	612	CLA	CHA-CBD-CGD-O2D
31	g1	614	CLA	CBA-CGA-O2A-C1
31	g1	614	CLA	O1A-CGA-O2A-C1
31	r1	602	CLA	CHA-CBD-CGD-O1D
31	r1	602	CLA	CHA-CBD-CGD-O2D
31	r1	603	CLA	C1A-C2A-CAA-CBA
31	r1	603	CLA	C3A-C2A-CAA-CBA
31	r1	603	CLA	CBD-CGD-O2D-CED
31	r1	608	CLA	C1A-C2A-CAA-CBA
31	r1	608	CLA	C3A-C2A-CAA-CBA
31	r1	608	CLA	CBD-CGD-O2D-CED
31	r1	609	CLA	CBD-CGD-O2D-CED
31	r1	612	CLA	C1A-C2A-CAA-CBA
31	r1	612	CLA	C3A-C2A-CAA-CBA
31	r1	612	CLA	CBD-CGD-O2D-CED
31	s1	602	CLA	C2-C1-O2A-CGA
31	s1	602	CLA	CHA-CBD-CGD-O1D
31	s1	602	CLA	CHA-CBD-CGD-O2D
31	s1	603	CLA	C3A-C2A-CAA-CBA
31	s1	603	CLA	CHA-CBD-CGD-O1D
31	s1	603	CLA	CHA-CBD-CGD-O2D
31	s1	604	CLA	CHA-CBD-CGD-O1D
31	s1	604	CLA	CHA-CBD-CGD-O2D
31	s1	605	CLA	C1A-C2A-CAA-CBA
31	s1	605	CLA	CBA-CGA-O2A-C1
31	s1	609	CLA	C3A-C2A-CAA-CBA
31	s1	610	CLA	C1A-C2A-CAA-CBA
31	s1	610	CLA	C3A-C2A-CAA-CBA
31	s1	611	CLA	C1A-C2A-CAA-CBA
31	s1	611	CLA	C3A-C2A-CAA-CBA
31	s1	611	CLA	CBD-CGD-O2D-CED
31	s1	612	CLA	CHA-CBD-CGD-O1D
31	s1	612	CLA	CHA-CBD-CGD-O2D
31	s1	613	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	s1	617	CLA	C2-C1-O2A-CGA
31	y1	602	CLA	CBD-CGD-O2D-CED
31	y1	604	CLA	CHA-CBD-CGD-O1D
31	y1	604	CLA	CHA-CBD-CGD-O2D
31	y1	610	CLA	CBD-CGD-O2D-CED
31	y1	612	CLA	CHA-CBD-CGD-O1D
31	y1	612	CLA	CHA-CBD-CGD-O2D
31	y1	613	CLA	CBD-CGD-O2D-CED
32	A	409	PHO	C3A-C2A-CAA-CBA
32	A1	409	PHO	C1A-C2A-CAA-CBA
32	A1	409	PHO	C3A-C2A-CAA-CBA
32	a1	409	PHO	CBD-CGD-O2D-CED
33	A	411	BCR	C11-C10-C9-C8
33	A	411	BCR	C11-C10-C9-C34
33	A	411	BCR	C10-C11-C12-C13
33	A	411	BCR	C11-C12-C13-C14
33	A	411	BCR	C11-C12-C13-C35
33	A	411	BCR	C17-C18-C19-C20
33	A	411	BCR	C36-C18-C19-C20
33	B	618	BCR	C11-C10-C9-C8
33	B	618	BCR	C11-C10-C9-C34
33	B	618	BCR	C10-C11-C12-C13
33	B	618	BCR	C17-C18-C19-C20
33	B	618	BCR	C36-C18-C19-C20
33	B	618	BCR	C21-C22-C23-C24
33	B	618	BCR	C37-C22-C23-C24
33	C	514	BCR	C11-C10-C9-C8
33	C	514	BCR	C11-C10-C9-C34
33	C	514	BCR	C9-C10-C11-C12
33	C	514	BCR	C10-C11-C12-C13
33	C	515	BCR	C7-C8-C9-C10
33	C	515	BCR	C7-C8-C9-C34
33	C	515	BCR	C11-C10-C9-C34
33	C	515	BCR	C17-C18-C19-C20
33	C	516	BCR	C1-C6-C7-C8
33	C	516	BCR	C5-C6-C7-C8
33	C	516	BCR	C7-C8-C9-C10
33	C	516	BCR	C11-C10-C9-C8
33	C	516	BCR	C11-C10-C9-C34
33	C	516	BCR	C10-C11-C12-C13
33	C	516	BCR	C17-C18-C19-C20
33	C	516	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
33	C	517	BCR	C11-C10-C9-C8
33	C	517	BCR	C11-C10-C9-C34
33	C	517	BCR	C10-C11-C12-C13
33	C	517	BCR	C17-C18-C19-C20
33	C	517	BCR	C36-C18-C19-C20
33	D	404	BCR	C11-C10-C9-C8
33	D	404	BCR	C11-C10-C9-C34
33	D	404	BCR	C10-C11-C12-C13
33	a	411	BCR	C11-C10-C9-C8
33	a	411	BCR	C11-C10-C9-C34
33	a	411	BCR	C10-C11-C12-C13
33	a	411	BCR	C17-C18-C19-C20
33	b	618	BCR	C7-C8-C9-C34
33	b	618	BCR	C11-C10-C9-C8
33	b	618	BCR	C11-C10-C9-C34
33	b	618	BCR	C10-C11-C12-C13
33	b	619	BCR	C11-C10-C9-C8
33	b	619	BCR	C11-C10-C9-C34
33	b	619	BCR	C10-C11-C12-C13
33	b	619	BCR	C21-C22-C23-C24
33	b	619	BCR	C37-C22-C23-C24
33	c	514	BCR	C10-C11-C12-C13
33	c	515	BCR	C11-C10-C9-C8
33	c	515	BCR	C11-C10-C9-C34
33	c	515	BCR	C10-C11-C12-C13
33	c	515	BCR	C17-C18-C19-C20
33	c	515	BCR	C36-C18-C19-C20
33	c	516	BCR	C7-C8-C9-C10
33	c	516	BCR	C7-C8-C9-C34
33	c	516	BCR	C11-C10-C9-C8
33	c	516	BCR	C11-C10-C9-C34
33	c	516	BCR	C10-C11-C12-C13
33	c	516	BCR	C21-C22-C23-C24
33	c	516	BCR	C37-C22-C23-C24
33	c	517	BCR	C11-C10-C9-C8
33	c	517	BCR	C11-C10-C9-C34
33	c	517	BCR	C10-C11-C12-C13
33	c	517	BCR	C36-C18-C19-C20
33	d	404	BCR	C11-C10-C9-C8
33	d	404	BCR	C11-C10-C9-C34
33	d	404	BCR	C10-C11-C12-C13
33	A1	411	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
33	A1	411	BCR	C11-C10-C9-C34
33	A1	411	BCR	C17-C18-C19-C20
33	A1	411	BCR	C36-C18-C19-C20
33	B1	618	BCR	C11-C10-C9-C8
33	B1	618	BCR	C11-C10-C9-C34
33	B1	618	BCR	C9-C10-C11-C12
33	B1	618	BCR	C10-C11-C12-C13
33	B1	618	BCR	C17-C18-C19-C20
33	B1	619	BCR	C7-C8-C9-C10
33	B1	619	BCR	C7-C8-C9-C34
33	B1	619	BCR	C11-C10-C9-C8
33	B1	619	BCR	C11-C10-C9-C34
33	C1	514	BCR	C11-C10-C9-C8
33	C1	514	BCR	C11-C10-C9-C34
33	C1	514	BCR	C9-C10-C11-C12
33	C1	514	BCR	C10-C11-C12-C13
33	C1	515	BCR	C11-C10-C9-C8
33	C1	515	BCR	C11-C10-C9-C34
33	C1	515	BCR	C10-C11-C12-C13
33	C1	516	BCR	C1-C6-C7-C8
33	C1	516	BCR	C5-C6-C7-C8
33	C1	516	BCR	C7-C8-C9-C10
33	C1	516	BCR	C7-C8-C9-C34
33	C1	516	BCR	C11-C10-C9-C8
33	C1	516	BCR	C11-C10-C9-C34
33	C1	516	BCR	C10-C11-C12-C13
33	C1	516	BCR	C11-C12-C13-C14
33	C1	516	BCR	C11-C12-C13-C35
33	C1	516	BCR	C17-C18-C19-C20
33	C1	516	BCR	C21-C22-C23-C24
33	C1	517	BCR	C11-C10-C9-C8
33	C1	517	BCR	C11-C10-C9-C34
33	C1	517	BCR	C17-C18-C19-C20
33	C1	517	BCR	C36-C18-C19-C20
33	C1	517	BCR	C23-C24-C25-C26
33	D1	404	BCR	C11-C10-C9-C8
33	D1	404	BCR	C11-C10-C9-C34
33	D1	404	BCR	C21-C22-C23-C24
33	D1	404	BCR	C37-C22-C23-C24
33	D1	404	BCR	C23-C24-C25-C26
33	D1	404	BCR	C23-C24-C25-C30
33	a1	411	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
33	a1	411	BCR	C11-C10-C9-C34
33	a1	411	BCR	C10-C11-C12-C13
33	a1	411	BCR	C17-C18-C19-C20
33	a1	411	BCR	C36-C18-C19-C20
33	a1	411	BCR	C21-C22-C23-C24
33	b1	618	BCR	C11-C10-C9-C8
33	b1	618	BCR	C11-C10-C9-C34
33	b1	618	BCR	C10-C11-C12-C13
33	b1	618	BCR	C17-C18-C19-C20
33	b1	618	BCR	C36-C18-C19-C20
33	b1	619	BCR	C11-C10-C9-C8
33	b1	619	BCR	C11-C10-C9-C34
33	b1	619	BCR	C10-C11-C12-C13
33	c1	514	BCR	C11-C10-C9-C8
33	c1	514	BCR	C11-C10-C9-C34
33	c1	514	BCR	C10-C11-C12-C13
33	c1	514	BCR	C17-C18-C19-C20
33	c1	515	BCR	C11-C10-C9-C8
33	c1	515	BCR	C11-C10-C9-C34
33	c1	515	BCR	C11-C12-C13-C14
33	c1	515	BCR	C17-C18-C19-C20
33	c1	515	BCR	C36-C18-C19-C20
33	c1	516	BCR	C11-C10-C9-C8
33	c1	516	BCR	C11-C10-C9-C34
33	c1	516	BCR	C17-C18-C19-C20
33	c1	516	BCR	C21-C22-C23-C24
33	c1	516	BCR	C37-C22-C23-C24
33	c1	517	BCR	C11-C10-C9-C8
33	c1	517	BCR	C11-C10-C9-C34
33	c1	517	BCR	C17-C18-C19-C20
33	d1	404	BCR	C11-C10-C9-C8
33	d1	404	BCR	C11-C10-C9-C34
33	d1	404	BCR	C11-C12-C13-C14
33	d1	404	BCR	C21-C22-C23-C24
33	d1	404	BCR	C37-C22-C23-C24
33	d1	404	BCR	C23-C24-C25-C26
33	d1	404	BCR	C23-C24-C25-C30
34	A	412	SQD	O5-C1-O6-C44
34	A	412	SQD	O5-C5-C6-S
34	B	621	SQD	O49-C7-O47-C45
34	B	621	SQD	C8-C7-O47-C45
34	B	621	SQD	O5-C5-C6-S

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Mol	Chain	Res	Type	Atoms
34	C	526	SQD	O5-C5-C6-S
34	C	526	SQD	C5-C6-S-O7
34	C	526	SQD	C5-C6-S-O8
34	C	526	SQD	C5-C6-S-O9
34	a	412	SQD	O5-C1-O6-C44
34	a	412	SQD	O5-C5-C6-S
34	b	621	SQD	O49-C7-O47-C45
34	b	621	SQD	C8-C7-O47-C45
34	c	626	SQD	O5-C5-C6-S
34	c	626	SQD	C5-C6-S-O7
34	c	626	SQD	C5-C6-S-O8
34	c	626	SQD	C5-C6-S-O9
34	B1	621	SQD	O5-C1-O6-C44
34	B1	626	SQD	C5-C6-S-O7
34	B1	626	SQD	C5-C6-S-O8
34	B1	626	SQD	C5-C6-S-O9
34	C1	526	SQD	C5-C6-S-O7
34	C1	526	SQD	C5-C6-S-O9
34	a1	412	SQD	O5-C5-C6-S
34	b1	621	SQD	O5-C1-O6-C44
34	b1	621	SQD	O5-C5-C6-S
34	b1	626	SQD	C2-C1-O6-C44
34	b1	626	SQD	O5-C1-O6-C44
34	b1	626	SQD	C5-C6-S-O7
34	b1	626	SQD	C5-C6-S-O8
34	b1	626	SQD	C5-C6-S-O9
34	m1	101	SQD	O5-C5-C6-S
34	m1	101	SQD	C5-C6-S-O7
34	m1	101	SQD	C5-C6-S-O8
34	m1	101	SQD	C5-C6-S-O9
35	A	413	LMG	C11-C10-O7-C8
35	C	521	LMG	C11-C10-O7-C8
35	J	101	LMG	O6-C1-O1-C7
35	J	101	LMG	O7-C8-C9-O8
35	a	413	LMG	O6-C1-O1-C7
35	b	622	LMG	O9-C10-O7-C8
35	c	521	LMG	O9-C10-O7-C8
35	j	101	LMG	O7-C8-C9-O8
35	A1	413	LMG	O6-C1-O1-C7
35	B1	622	LMG	C2-C1-O1-C7
35	B1	622	LMG	O6-C1-O1-C7
35	B1	622	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
35	W1	201	LMG	C11-C10-O7-C8
35	a1	413	LMG	O6-C1-O1-C7
35	b1	622	LMG	O6-C1-O1-C7
35	b1	622	LMG	O9-C10-O7-C8
35	b1	622	LMG	C11-C10-O7-C8
37	B	620	C7Z	C7-C8-C9-C19
37	B	620	C7Z	C7-C8-C9-C10
37	b	620	C7Z	C9-C10-C11-C12
37	b	620	C7Z	C11-C12-C13-C14
37	B1	620	C7Z	C5-C6-C7-C8
37	b1	620	C7Z	C5-C6-C7-C8
37	b1	620	C7Z	C11-C12-C13-C14
37	b1	620	C7Z	C31-C32-C33-C34
37	b1	620	C7Z	C27-C28-C29-C30
37	b1	620	C7Z	C27-C28-C29-C39
38	B	625	DGA	CG1-CG2-CG3-OXT
38	B	625	DGA	OG2-CG2-CG3-OXT
38	C	524	DGA	CG1-CG2-CG3-OXT
38	C	524	DGA	OG2-CG2-CG3-OXT
38	b	623	DGA	CB2-CB1-OG2-CG2
38	b	623	DGA	CG1-CG2-CG3-OXT
38	b	623	DGA	OG2-CG2-CG3-OXT
38	c	524	DGA	OG2-CG2-CG3-OXT
38	C1	524	DGA	CG1-CG2-CG3-OXT
38	C1	524	DGA	OG2-CG2-CG3-OXT
39	b	625	GOL	O1-C1-C2-O2
39	b	625	GOL	O1-C1-C2-C3
40	C	520	DGD	C2B-C1B-O2G-C2G
40	C	523	DGD	C2A-C1A-O1G-C1G
40	C	523	DGD	O1A-C1A-O1G-C1G
40	C	523	DGD	O1B-C1B-O2G-C2G
40	c	520	DGD	C2B-C1B-O2G-C2G
40	c	523	DGD	C2A-C1A-O1G-C1G
40	c	523	DGD	O1A-C1A-O1G-C1G
40	c	523	DGD	C2B-C1B-O2G-C2G
40	c	523	DGD	O1B-C1B-O2G-C2G
40	B1	623	DGD	C2B-C1B-O2G-C2G
40	B1	623	DGD	O6D-C1D-O3G-C3G
40	B1	623	DGD	C2E-C1E-O5D-C6D
40	B1	623	DGD	O6E-C1E-O5D-C6D
40	b1	623	DGD	C2B-C1B-O2G-C2G
40	b1	623	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
40	b1	623	DGD	O6D-C1D-O3G-C3G
40	b1	623	DGD	C2E-C1E-O5D-C6D
40	b1	623	DGD	O6E-C1E-O5D-C6D
41	C	525	LHG	C1-C2-C3-O3
41	C	525	LHG	C3-O3-P-O4
41	C	525	LHG	C3-O3-P-O6
41	C	525	LHG	C4-O6-P-O3
41	C	525	LHG	C4-O6-P-O4
41	D	408	LHG	C1-C2-C3-O3
41	D	408	LHG	C3-O3-P-O4
41	D	408	LHG	C3-O3-P-O5
41	D	408	LHG	C3-O3-P-O6
41	D	408	LHG	C4-O6-P-O3
41	D	408	LHG	C4-O6-P-O4
41	D	409	LHG	C1-C2-C3-O3
41	D	409	LHG	C3-O3-P-O6
41	D	410	LHG	C3-O3-P-O4
41	D	410	LHG	C3-O3-P-O5
41	D	410	LHG	C3-O3-P-O6
41	D	410	LHG	C4-O6-P-O3
41	D	410	LHG	C4-O6-P-O4
41	D	410	LHG	O6-C4-C5-O7
41	L	101	LHG	C3-O3-P-O4
41	L	101	LHG	C3-O3-P-O5
41	L	101	LHG	C3-O3-P-O6
41	L	101	LHG	C4-O6-P-O5
41	N	624	LHG	C1-C2-C3-O3
41	N	624	LHG	O2-C2-C3-O3
41	N	624	LHG	O9-C7-O7-C5
41	G	630	LHG	O1-C1-C2-C3
41	G	630	LHG	C4-O6-P-O3
41	G	630	LHG	C4-O6-P-O4
41	G	630	LHG	O7-C5-C6-O8
41	G	630	LHG	C8-C7-O7-C5
41	S	624	LHG	C4-O6-P-O3
41	S	624	LHG	O6-C4-C5-O7
41	S	624	LHG	C8-C7-O7-C5
41	Y	624	LHG	C1-C2-C3-O3
41	Y	624	LHG	O2-C2-C3-O3
41	Y	624	LHG	C4-O6-P-O3
41	Y	624	LHG	C4-O6-P-O4
41	Y	624	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
41	Y	624	LHG	O7-C5-C6-O8
41	c	625	LHG	O1-C1-C2-C3
41	c	625	LHG	O2-C2-C3-O3
41	c	625	LHG	C3-O3-P-O5
41	c	625	LHG	C3-O3-P-O6
41	c	625	LHG	C4-O6-P-O3
41	c	625	LHG	C4-O6-P-O4
41	c	625	LHG	C4-O6-P-O5
41	d	408	LHG	O1-C1-C2-C3
41	d	408	LHG	C4-O6-P-O3
41	d	408	LHG	C4-O6-P-O4
41	d	408	LHG	C8-C7-O7-C5
41	d	409	LHG	C1-C2-C3-O3
41	d	410	LHG	C3-O3-P-O4
41	d	410	LHG	C3-O3-P-O5
41	d	410	LHG	C3-O3-P-O6
41	d	410	LHG	C4-O6-P-O3
41	d	410	LHG	C4-O6-P-O5
41	l	101	LHG	C3-O3-P-O6
41	l	101	LHG	C4-O6-P-O3
41	l	101	LHG	C4-O6-P-O5
41	n	624	LHG	O1-C1-C2-O2
41	n	624	LHG	C4-O6-P-O3
41	n	624	LHG	C4-O6-P-O4
41	n	624	LHG	O9-C7-O7-C5
41	g	624	LHG	O1-C1-C2-C3
41	g	624	LHG	C1-C2-C3-O3
41	g	624	LHG	C4-O6-P-O3
41	g	624	LHG	C4-O6-P-O4
41	s	624	LHG	C1-C2-C3-O3
41	s	624	LHG	O2-C2-C3-O3
41	s	624	LHG	C4-O6-P-O3
41	s	624	LHG	C8-C7-O7-C5
41	y	624	LHG	O1-C1-C2-C3
41	y	624	LHG	C3-O3-P-O6
41	y	624	LHG	C4-O6-P-O3
41	y	624	LHG	C4-O6-P-O5
41	C1	525	LHG	C1-C2-C3-O3
41	C1	525	LHG	C3-O3-P-O4
41	C1	525	LHG	C3-O3-P-O6
41	C1	525	LHG	C4-O6-P-O3
41	C1	525	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
41	D1	408	LHG	O1-C1-C2-C3
41	D1	408	LHG	C3-O3-P-O6
41	D1	408	LHG	C4-O6-P-O3
41	D1	408	LHG	C4-O6-P-O5
41	D1	409	LHG	C1-C2-C3-O3
41	D1	410	LHG	O1-C1-C2-O2
41	D1	410	LHG	O1-C1-C2-C3
41	D1	410	LHG	C3-O3-P-O4
41	D1	410	LHG	C3-O3-P-O5
41	D1	410	LHG	C3-O3-P-O6
41	D1	410	LHG	C4-O6-P-O3
41	D1	410	LHG	C4-O6-P-O4
41	D1	410	LHG	C4-O6-P-O5
41	D1	410	LHG	O7-C5-C6-O8
41	L1	101	LHG	O1-C1-C2-C3
41	L1	101	LHG	C3-O3-P-O4
41	L1	101	LHG	C3-O3-P-O6
41	L1	101	LHG	O9-C7-O7-C5
41	L1	101	LHG	C8-C7-O7-C5
41	N1	624	LHG	O1-C1-C2-C3
41	N1	624	LHG	C1-C2-C3-O3
41	N1	624	LHG	O2-C2-C3-O3
41	N1	624	LHG	C4-O6-P-O3
41	N1	624	LHG	C4-O6-P-O5
41	N1	624	LHG	O7-C5-C6-O8
41	G1	624	LHG	C3-O3-P-O5
41	G1	624	LHG	C4-O6-P-O3
41	G1	624	LHG	C4-O6-P-O4
41	G1	624	LHG	O7-C5-C6-O8
41	S1	624	LHG	O1-C1-C2-C3
41	S1	624	LHG	C3-O3-P-O5
41	S1	624	LHG	C4-O6-P-O3
41	S1	624	LHG	C4-O6-P-O4
41	S1	624	LHG	C4-O6-P-O5
41	Y1	624	LHG	C4-O6-P-O3
41	Y1	624	LHG	C4-O6-P-O4
41	Y1	624	LHG	C4-O6-P-O5
41	c1	525	LHG	C4-O6-P-O3
41	c1	525	LHG	C4-O6-P-O4
41	d1	408	LHG	O1-C1-C2-C3
41	d1	408	LHG	C3-O3-P-O5
41	d1	409	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
41	d1	409	LHG	C1-C2-C3-O3
41	d1	409	LHG	C3-O3-P-O5
41	d1	409	LHG	C4-O6-P-O3
41	d1	409	LHG	C4-O6-P-O4
41	d1	410	LHG	C3-O3-P-O5
41	d1	410	LHG	C3-O3-P-O6
41	d1	410	LHG	C4-O6-P-O3
41	d1	410	LHG	C4-O6-P-O4
41	d1	410	LHG	C4-O6-P-O5
41	d1	410	LHG	O7-C5-C6-O8
41	n1	624	LHG	C4-O6-P-O3
41	n1	624	LHG	C4-O6-P-O4
41	n1	624	LHG	O7-C5-C6-O8
41	n1	624	LHG	C8-C7-O7-C5
41	g1	624	LHG	C4-O6-P-O3
41	g1	624	LHG	C4-O6-P-O4
41	g1	624	LHG	O7-C5-C6-O8
41	g1	624	LHG	O9-C7-O7-C5
41	g1	624	LHG	C8-C7-O7-C5
41	s1	624	LHG	O1-C1-C2-C3
41	s1	624	LHG	C3-O3-P-O5
41	s1	624	LHG	C4-O6-P-O3
41	s1	624	LHG	C4-O6-P-O5
41	y1	624	LHG	O1-C1-C2-C3
41	y1	624	LHG	C1-C2-C3-O3
41	y1	624	LHG	O2-C2-C3-O3
41	y1	624	LHG	C3-O3-P-O5
41	y1	624	LHG	C4-O6-P-O5
42	C	527	LMK	O9-C10-C11-C12
42	C	527	LMK	O9-C10-O7-C8
42	C	527	LMK	O1-C1-C2-C3
42	C	527	LMK	O10-C28-O8-C9
42	c	627	LMK	O9-C10-O7-C8
42	c	627	LMK	O10-C28-C29-C30
42	C1	527	LMK	C7-C8-O7-C10
42	C1	527	LMK	O9-C10-O7-C8
42	C1	527	LMK	C1-C2-C3-N4
42	C1	527	LMK	C2-C3-N4-C5
42	C1	527	LMK	C2-C3-N4-C6
42	C1	527	LMK	C2-C3-N4-C46
42	C1	527	LMK	O10-C28-O8-C9
42	c1	527	LMK	O1-C7-C8-O7

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Mol	Chain	Res	Type	Atoms
42	c1	527	LMK	O10-C28-C29-C30
44	D	405	PL9	C7-C8-C9-C11
44	D	405	PL9	C12-C11-C9-C8
44	D	405	PL9	C12-C13-C14-C15
44	D	405	PL9	C37-C38-C39-C41
44	D	405	PL9	C42-C43-C44-C45
44	d	405	PL9	C12-C13-C14-C16
44	D1	405	PL9	C22-C23-C24-C25
44	D1	405	PL9	C37-C38-C39-C40
44	d1	405	PL9	C20-C19-C21-C22
44	d1	405	PL9	C22-C23-C24-C26
44	d1	405	PL9	C32-C33-C34-C35
44	d1	405	PL9	C32-C33-C34-C36
44	d1	405	PL9	C37-C38-C39-C40
46	H	101	RRX	C37-C22-C23-C24
46	H	101	RRX	C21-C22-C23-C24
46	H	101	RRX	C7-C8-C9-C10
46	H	101	RRX	C7-C8-C9-C34
46	h	101	RRX	C7-C8-C9-C10
46	H1	101	RRX	C23-C24-C25-C26
46	h1	101	RRX	C23-C24-C25-C26
46	h1	101	RRX	C17-C18-C19-C20
46	h1	101	RRX	C13-C14-C15-C16
46	h1	101	RRX	C5-C6-C7-C8
47	N	601	CHL	C4-C3-C5-C6
47	N	609	CHL	CHA-CBD-CGD-O1D
47	N	609	CHL	CHA-CBD-CGD-O2D
47	G	606	CHL	C1A-C2A-CAA-CBA
47	G	606	CHL	C3A-C2A-CAA-CBA
47	G	609	CHL	C4C-C3C-CAC-CBC
47	R	606	CHL	CAD-CBD-CGD-O1D
47	R	606	CHL	CAD-CBD-CGD-O2D
47	S	601	CHL	CAD-CBD-CGD-O2D
47	Y	606	CHL	C1A-C2A-CAA-CBA
47	n	609	CHL	C1A-C2A-CAA-CBA
47	n	609	CHL	C4C-C3C-CAC-CBC
47	s	601	CHL	CAD-CBD-CGD-O2D
47	y	601	CHL	C11-C12-C13-C14
47	y	606	CHL	C1A-C2A-CAA-CBA
47	N1	609	CHL	CAD-CBD-CGD-O1D
47	N1	609	CHL	CAD-CBD-CGD-O2D
47	G1	605	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
47	G1	605	CHL	C3A-C2A-CAA-CBA
47	g1	601	CHL	C1A-C2A-CAA-CBA
47	g1	601	CHL	C3A-C2A-CAA-CBA
47	g1	605	CHL	C1A-C2A-CAA-CBA
48	N	620	LUT	C25-C26-C27-C28
48	N	620	LUT	C27-C28-C29-C30
48	N	621	LUT	C21-C26-C27-C28
48	G	620	LUT	C27-C28-C29-C30
48	G	621	LUT	C31-C32-C33-C34
48	R	620	LUT	C25-C26-C27-C28
48	R	620	LUT	C31-C32-C33-C34
48	R	620	LUT	C31-C32-C33-C40
48	S	620	LUT	C21-C26-C27-C28
48	S	620	LUT	C25-C26-C27-C28
48	Y	620	LUT	C27-C28-C29-C30
48	Y	621	LUT	C21-C26-C27-C28
48	n	620	LUT	C25-C26-C27-C28
48	n	620	LUT	C31-C32-C33-C34
48	n	621	LUT	C21-C26-C27-C28
48	g	620	LUT	C31-C32-C33-C34
48	r	620	LUT	C31-C32-C33-C34
48	r	620	LUT	C31-C32-C33-C40
48	r	620	LUT	C33-C34-C35-C15
48	s	620	LUT	C21-C26-C27-C28
48	s	620	LUT	C25-C26-C27-C28
48	s	621	LUT	C25-C26-C27-C28
48	N1	620	LUT	C27-C28-C29-C30
48	N1	621	LUT	C21-C26-C27-C28
48	G1	621	LUT	C21-C26-C27-C28
48	R1	620	LUT	C25-C26-C27-C28
48	R1	620	LUT	C27-C28-C29-C30
48	S1	620	LUT	C25-C26-C27-C28
48	S1	621	LUT	C25-C26-C27-C28
48	Y1	621	LUT	C21-C26-C27-C28
48	n1	621	LUT	C21-C26-C27-C28
48	g1	620	LUT	C27-C28-C29-C30
48	g1	620	LUT	C27-C28-C29-C39
48	g1	621	LUT	C21-C26-C27-C28
48	r1	620	LUT	C7-C8-C9-C10
48	r1	620	LUT	C31-C32-C33-C34
48	r1	620	LUT	C31-C32-C33-C40
48	s1	620	LUT	C21-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
48	s1	621	LUT	C25-C26-C27-C28
48	y1	620	LUT	C27-C28-C29-C30
48	y1	621	LUT	C21-C26-C27-C28
49	R	621	XAT	C9-C10-C11-C12
49	R	621	XAT	C10-C11-C12-C13
49	R	621	XAT	C12-C13-C14-C15
49	R	621	XAT	C20-C13-C14-C15
49	Y	622	XAT	C26-C27-C28-C29
49	r	622	XAT	C7-C8-C9-C10
49	r	622	XAT	C10-C11-C12-C13
49	r	622	XAT	C26-C27-C28-C29
49	y1	622	XAT	C26-C27-C28-C29
50	R	622	NEX	C7-C8-C9-C19
50	R	622	NEX	C12-C13-C14-C15
50	R	622	NEX	C20-C13-C14-C15
50	R	622	NEX	C14-C15-C35-C34
50	S	622	NEX	C11-C10-C9-C8
50	S	622	NEX	C11-C10-C9-C19
50	S	622	NEX	C10-C11-C12-C13
50	S	622	NEX	C11-C12-C13-C14
50	Y	623	NEX	C28-C29-C30-C31
50	Y	623	NEX	C39-C29-C30-C31
50	g	623	NEX	C28-C29-C30-C31
50	g	623	NEX	C39-C29-C30-C31
50	r	623	NEX	C14-C15-C35-C34
50	s	623	NEX	C10-C11-C12-C13
50	y	623	NEX	O24-C26-C27-C28
50	R1	622	NEX	C12-C13-C14-C15
50	R1	622	NEX	C20-C13-C14-C15
50	R1	622	NEX	C14-C15-C35-C34
50	n1	623	NEX	C7-C8-C9-C19
50	r1	622	NEX	C12-C13-C14-C15
50	r1	622	NEX	C20-C13-C14-C15
50	y1	623	NEX	C7-C8-C9-C19
51	S	625	LPX	O1-C3-C4-O5
51	S	625	LPX	C1-O2-P1-O1
51	s	625	LPX	C3-C4-C5-O6
51	s	625	LPX	O1-C3-C4-C5
51	s	625	LPX	C3-O1-P1-O3
51	s	625	LPX	C3-O1-P1-O2
51	s	625	LPX	C1-O2-P1-O1
51	s	625	LPX	C2-C1-O2-P1

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Mol	Chain	Res	Type	Atoms
51	s1	625	LPX	C3-C4-C5-O6
51	s1	625	LPX	O1-C3-C4-O5
51	s1	625	LPX	C3-O1-P1-O3
51	s1	625	LPX	C3-O1-P1-O2
51	s1	625	LPX	C3-O1-P1-O4
52	S	626	3PH	C22-C21-O21-C2
52	i	101	3PH	C1-O11-P-O13
52	i	101	3PH	C1-O11-P-O14
52	i	101	3PH	C1-O11-P-O12
52	s	626	3PH	C1-O11-P-O13
52	s	626	3PH	C1-O11-P-O14
52	s	626	3PH	C1-O11-P-O12
52	s	626	3PH	O21-C2-C3-O31
52	s	626	3PH	C22-C21-O21-C2
52	T1	101	3PH	C1-O11-P-O13
52	T1	101	3PH	C1-O11-P-O14
52	T1	101	3PH	O22-C21-O21-C2
52	T1	101	3PH	C22-C21-O21-C2
52	S1	626	3PH	C1-O11-P-O13
52	S1	626	3PH	C1-O11-P-O14
52	S1	626	3PH	O22-C21-O21-C2
52	b1	624	3PH	C22-C21-O21-C2
52	b1	624	3PH	O32-C31-O31-C3
52	t1	101	3PH	C1-O11-P-O13
52	t1	101	3PH	C1-O11-P-O14
52	t1	101	3PH	C1-O11-P-O12
52	t1	101	3PH	O22-C21-O21-C2
52	s1	626	3PH	C1-O11-P-O13
52	s1	626	3PH	C1-O11-P-O14
52	s1	626	3PH	O22-C21-O21-C2
53	Y	625	SPH	O1-C1-C2-N2
53	Y	625	SPH	O1-C1-C2-C3
53	Y	625	SPH	C1-C2-C3-O3
53	Y	625	SPH	C1-C2-C3-C4
53	Y	625	SPH	N2-C2-C3-C4
53	y	625	SPH	C2-C3-C4-C5
53	A1	414	SPH	O1-C1-C2-N2
53	A1	414	SPH	O1-C1-C2-C3
53	A1	414	SPH	C1-C2-C3-O3
53	A1	414	SPH	C1-C2-C3-C4
53	A1	414	SPH	N2-C2-C3-C4
53	Y1	625	SPH	O1-C1-C2-N2

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Mol	Chain	Res	Type	Atoms
53	Y1	625	SPH	O1-C1-C2-C3
53	Y1	625	SPH	C2-C3-C4-C5
53	Y1	625	SPH	O3-C3-C4-C5
53	a1	414	SPH	C1-C2-C3-O3
53	a1	414	SPH	C1-C2-C3-C4
53	a1	414	SPH	N2-C2-C3-O3
53	a1	414	SPH	N2-C2-C3-C4
53	y1	625	SPH	O1-C1-C2-N2
53	y1	625	SPH	O1-C1-C2-C3
53	y1	625	SPH	C1-C2-C3-O3
53	y1	625	SPH	C1-C2-C3-C4
53	y1	625	SPH	N2-C2-C3-O3
53	y1	625	SPH	N2-C2-C3-C4
53	y1	625	SPH	C2-C3-C4-C5
53	y1	625	SPH	O3-C3-C4-C5
54	I1	102	4RF	C24-C22-O21-C20
54	i1	101	4RF	O18-C19-C20-O21
54	i1	101	4RF	O21-C20-C39-O40
54	i1	101	4RF	C24-C22-O21-C20
54	i1	101	4RF	O23-C22-O21-C20
56	R1	626	ERG	C13-C17-C20-C21
56	R1	626	ERG	C16-C17-C20-C21
56	r1	626	ERG	C13-C17-C20-C21
56	r1	626	ERG	C16-C17-C20-C21
56	r1	626	ERG	C16-C17-C20-C22
57	Y1	626	PTY	N1-C2-C3-O11
57	Y1	626	PTY	C3-O11-P1-O13
57	Y1	626	PTY	C3-O11-P1-O14
57	Y1	627	PTY	N1-C2-C3-O11
57	Y1	627	PTY	C5-O14-P1-O13
57	y1	626	PTY	C5-O14-P1-O11
57	y1	626	PTY	C5-O14-P1-O12
57	y1	627	PTY	C11-C8-O7-C6
57	y1	627	PTY	C3-O11-P1-O12
57	y1	627	PTY	C3-O11-P1-O13
57	y1	627	PTY	C3-O11-P1-O14
57	y1	627	PTY	C5-O14-P1-O11
57	y1	627	PTY	C5-O14-P1-O12
57	y1	627	PTY	C5-O14-P1-O13
31	N	612	CLA	O1D-CGD-O2D-CED
31	G	613	CLA	O1D-CGD-O2D-CED
31	R	603	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	R	608	CLA	O1D-CGD-O2D-CED
31	R	609	CLA	O1D-CGD-O2D-CED
31	y	604	CLA	O1D-CGD-O2D-CED
31	y	608	CLA	O1D-CGD-O2D-CED
31	B1	606	CLA	O1D-CGD-O2D-CED
31	R1	604	CLA	O1D-CGD-O2D-CED
31	R1	608	CLA	O1D-CGD-O2D-CED
31	b1	614	CLA	O1D-CGD-O2D-CED
31	c1	502	CLA	O1D-CGD-O2D-CED
31	n1	610	CLA	O1D-CGD-O2D-CED
31	g1	613	CLA	O1D-CGD-O2D-CED
31	r1	604	CLA	O1D-CGD-O2D-CED
31	r1	609	CLA	O1D-CGD-O2D-CED
31	r1	610	CLA	O1D-CGD-O2D-CED
31	s1	617	CLA	O1D-CGD-O2D-CED
57	Y1	627	PTY	C11-C8-O7-C6
57	y1	627	PTY	O10-C8-O7-C6
31	A	405	CLA	O1D-CGD-O2D-CED
31	N	613	CLA	O1D-CGD-O2D-CED
31	a	405	CLA	O1D-CGD-O2D-CED
31	b	606	CLA	O1D-CGD-O2D-CED
31	c	502	CLA	O1D-CGD-O2D-CED
31	n	610	CLA	O1D-CGD-O2D-CED
31	g	610	CLA	O1D-CGD-O2D-CED
31	g	613	CLA	O1D-CGD-O2D-CED
31	r	603	CLA	O1D-CGD-O2D-CED
31	s	609	CLA	O1D-CGD-O2D-CED
31	s	610	CLA	O1D-CGD-O2D-CED
31	B1	604	CLA	O1D-CGD-O2D-CED
31	B1	607	CLA	O1D-CGD-O2D-CED
31	B1	614	CLA	O1D-CGD-O2D-CED
31	B1	615	CLA	O1D-CGD-O2D-CED
31	C1	511	CLA	O1D-CGD-O2D-CED
31	N1	613	CLA	O1D-CGD-O2D-CED
31	G1	613	CLA	O1D-CGD-O2D-CED
31	R1	603	CLA	O1D-CGD-O2D-CED
31	S1	613	CLA	O1D-CGD-O2D-CED
31	S1	614	CLA	O1D-CGD-O2D-CED
31	Y1	610	CLA	O1D-CGD-O2D-CED
31	a1	405	CLA	O1D-CGD-O2D-CED
31	b1	604	CLA	O1D-CGD-O2D-CED
31	n1	613	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	n1	614	CLA	O1D-CGD-O2D-CED
31	g1	610	CLA	O1D-CGD-O2D-CED
31	r1	608	CLA	O1D-CGD-O2D-CED
31	s1	613	CLA	O1D-CGD-O2D-CED
31	y1	611	CLA	O1D-CGD-O2D-CED
31	A	410	CLA	CBD-CGD-O2D-CED
31	B	606	CLA	CBD-CGD-O2D-CED
31	B	607	CLA	CBD-CGD-O2D-CED
31	B	611	CLA	CBD-CGD-O2D-CED
31	B	614	CLA	CBD-CGD-O2D-CED
31	B	616	CLA	CBD-CGD-O2D-CED
31	B	617	CLA	CBD-CGD-O2D-CED
31	C	503	CLA	CBD-CGD-O2D-CED
31	C	504	CLA	CBD-CGD-O2D-CED
31	C	507	CLA	CBD-CGD-O2D-CED
31	C	511	CLA	CBD-CGD-O2D-CED
31	N	602	CLA	CBD-CGD-O2D-CED
31	N	604	CLA	CBD-CGD-O2D-CED
31	N	612	CLA	CBD-CGD-O2D-CED
31	N	613	CLA	CBD-CGD-O2D-CED
31	G	604	CLA	CBD-CGD-O2D-CED
31	G	610	CLA	CBD-CGD-O2D-CED
31	G	611	CLA	CBD-CGD-O2D-CED
31	G	612	CLA	CBD-CGD-O2D-CED
31	G	613	CLA	CBD-CGD-O2D-CED
31	R	603	CLA	CBD-CGD-O2D-CED
31	R	604	CLA	CBD-CGD-O2D-CED
31	R	609	CLA	CBD-CGD-O2D-CED
31	R	610	CLA	CBD-CGD-O2D-CED
31	R	612	CLA	CBD-CGD-O2D-CED
31	R	613	CLA	CBD-CGD-O2D-CED
31	S	603	CLA	CBD-CGD-O2D-CED
31	S	604	CLA	CBD-CGD-O2D-CED
31	S	605	CLA	CBD-CGD-O2D-CED
31	S	610	CLA	CBD-CGD-O2D-CED
31	S	613	CLA	CBD-CGD-O2D-CED
31	S	617	CLA	CBD-CGD-O2D-CED
31	Y	603	CLA	CBD-CGD-O2D-CED
31	Y	608	CLA	CBD-CGD-O2D-CED
31	Y	610	CLA	CBD-CGD-O2D-CED
31	Y	612	CLA	CBD-CGD-O2D-CED
31	b	602	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	b	603	CLA	CBD-CGD-O2D-CED
31	b	606	CLA	CBD-CGD-O2D-CED
31	b	607	CLA	CBD-CGD-O2D-CED
31	b	608	CLA	CBD-CGD-O2D-CED
31	b	611	CLA	CBD-CGD-O2D-CED
31	b	613	CLA	CBD-CGD-O2D-CED
31	b	614	CLA	CBD-CGD-O2D-CED
31	b	617	CLA	CBD-CGD-O2D-CED
31	c	503	CLA	CBD-CGD-O2D-CED
31	c	504	CLA	CBD-CGD-O2D-CED
31	c	509	CLA	CBD-CGD-O2D-CED
31	c	511	CLA	CBD-CGD-O2D-CED
31	n	602	CLA	CBD-CGD-O2D-CED
31	n	613	CLA	CBD-CGD-O2D-CED
31	g	602	CLA	CBD-CGD-O2D-CED
31	g	610	CLA	CBD-CGD-O2D-CED
31	g	611	CLA	CBD-CGD-O2D-CED
31	g	612	CLA	CBD-CGD-O2D-CED
31	g	613	CLA	CBD-CGD-O2D-CED
31	g	614	CLA	CBD-CGD-O2D-CED
31	r	602	CLA	CBD-CGD-O2D-CED
31	r	604	CLA	CBD-CGD-O2D-CED
31	r	608	CLA	CBD-CGD-O2D-CED
31	r	611	CLA	CBD-CGD-O2D-CED
31	r	612	CLA	CBD-CGD-O2D-CED
31	r	613	CLA	CBD-CGD-O2D-CED
31	s	602	CLA	CBD-CGD-O2D-CED
31	s	609	CLA	CBD-CGD-O2D-CED
31	s	613	CLA	CBD-CGD-O2D-CED
31	s	617	CLA	CBD-CGD-O2D-CED
31	y	602	CLA	CBD-CGD-O2D-CED
31	y	603	CLA	CBD-CGD-O2D-CED
31	y	604	CLA	CBD-CGD-O2D-CED
31	y	608	CLA	CBD-CGD-O2D-CED
31	y	610	CLA	CBD-CGD-O2D-CED
31	y	611	CLA	CBD-CGD-O2D-CED
31	y	613	CLA	CBD-CGD-O2D-CED
31	B1	604	CLA	CBD-CGD-O2D-CED
31	B1	606	CLA	CBD-CGD-O2D-CED
31	B1	607	CLA	CBD-CGD-O2D-CED
31	B1	611	CLA	CBD-CGD-O2D-CED
31	B1	615	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	C1	501	CLA	CBD-CGD-O2D-CED
31	C1	502	CLA	CBD-CGD-O2D-CED
31	C1	504	CLA	CBD-CGD-O2D-CED
31	C1	511	CLA	CBD-CGD-O2D-CED
31	D1	403	CLA	CBD-CGD-O2D-CED
31	N1	610	CLA	CBD-CGD-O2D-CED
31	N1	611	CLA	CBD-CGD-O2D-CED
31	N1	613	CLA	CBD-CGD-O2D-CED
31	G1	603	CLA	CBD-CGD-O2D-CED
31	G1	611	CLA	CBD-CGD-O2D-CED
31	G1	613	CLA	CBD-CGD-O2D-CED
31	R1	604	CLA	CBD-CGD-O2D-CED
31	R1	608	CLA	CBD-CGD-O2D-CED
31	S1	603	CLA	CBD-CGD-O2D-CED
31	S1	611	CLA	CBD-CGD-O2D-CED
31	S1	614	CLA	CBD-CGD-O2D-CED
31	Y1	603	CLA	CBD-CGD-O2D-CED
31	Y1	604	CLA	CBD-CGD-O2D-CED
31	Y1	610	CLA	CBD-CGD-O2D-CED
31	Y1	614	CLA	CBD-CGD-O2D-CED
31	a1	407	CLA	CBD-CGD-O2D-CED
31	a1	410	CLA	CBD-CGD-O2D-CED
31	b1	602	CLA	CBD-CGD-O2D-CED
31	b1	603	CLA	CBD-CGD-O2D-CED
31	b1	604	CLA	CBD-CGD-O2D-CED
31	b1	606	CLA	CBD-CGD-O2D-CED
31	b1	609	CLA	CBD-CGD-O2D-CED
31	b1	610	CLA	CBD-CGD-O2D-CED
31	b1	613	CLA	CBD-CGD-O2D-CED
31	b1	615	CLA	CBD-CGD-O2D-CED
31	c1	501	CLA	CBD-CGD-O2D-CED
31	c1	502	CLA	CBD-CGD-O2D-CED
31	c1	503	CLA	CBD-CGD-O2D-CED
31	c1	507	CLA	CBD-CGD-O2D-CED
31	c1	509	CLA	CBD-CGD-O2D-CED
31	c1	510	CLA	CBD-CGD-O2D-CED
31	c1	511	CLA	CBD-CGD-O2D-CED
31	n1	602	CLA	CBD-CGD-O2D-CED
31	n1	610	CLA	CBD-CGD-O2D-CED
31	n1	611	CLA	CBD-CGD-O2D-CED
31	n1	612	CLA	CBD-CGD-O2D-CED
31	n1	613	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	n1	614	CLA	CBD-CGD-O2D-CED
31	g1	602	CLA	CBD-CGD-O2D-CED
31	g1	603	CLA	CBD-CGD-O2D-CED
31	g1	613	CLA	CBD-CGD-O2D-CED
31	g1	614	CLA	CBD-CGD-O2D-CED
31	r1	604	CLA	CBD-CGD-O2D-CED
31	r1	610	CLA	CBD-CGD-O2D-CED
31	s1	602	CLA	CBD-CGD-O2D-CED
31	s1	605	CLA	CBD-CGD-O2D-CED
31	s1	609	CLA	CBD-CGD-O2D-CED
31	s1	610	CLA	CBD-CGD-O2D-CED
31	s1	612	CLA	CBD-CGD-O2D-CED
31	s1	614	CLA	CBD-CGD-O2D-CED
31	s1	617	CLA	CBD-CGD-O2D-CED
31	y1	603	CLA	CBD-CGD-O2D-CED
31	y1	604	CLA	CBD-CGD-O2D-CED
31	y1	608	CLA	CBD-CGD-O2D-CED
31	y1	611	CLA	CBD-CGD-O2D-CED
31	y1	612	CLA	CBD-CGD-O2D-CED
31	y1	614	CLA	CBD-CGD-O2D-CED
32	a	409	PHO	CBD-CGD-O2D-CED
31	B	617	CLA	O1A-CGA-O2A-C1
31	C	504	CLA	O1A-CGA-O2A-C1
31	N	611	CLA	O1A-CGA-O2A-C1
31	S	603	CLA	O1A-CGA-O2A-C1
31	S	605	CLA	O1A-CGA-O2A-C1
31	c	512	CLA	O1A-CGA-O2A-C1
31	g	614	CLA	O1A-CGA-O2A-C1
31	s	605	CLA	O1A-CGA-O2A-C1
31	y	603	CLA	O1A-CGA-O2A-C1
31	y	611	CLA	O1A-CGA-O2A-C1
31	A1	406	CLA	O1A-CGA-O2A-C1
31	C1	505	CLA	O1A-CGA-O2A-C1
31	G1	611	CLA	O1A-CGA-O2A-C1
31	G1	614	CLA	O1A-CGA-O2A-C1
31	S1	605	CLA	O1A-CGA-O2A-C1
31	S1	613	CLA	O1A-CGA-O2A-C1
31	Y1	611	CLA	O1A-CGA-O2A-C1
31	d1	403	CLA	O1A-CGA-O2A-C1
31	g1	611	CLA	O1A-CGA-O2A-C1
31	s1	605	CLA	O1A-CGA-O2A-C1
31	s1	610	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	y1	612	CLA	O1A-CGA-O2A-C1
52	t1	101	3PH	O32-C31-O31-C3
54	i1	101	4RF	O17-C16-O18-C19
31	R	613	CLA	O1A-CGA-O2A-C1
31	A1	405	CLA	O1D-CGD-O2D-CED
31	B	606	CLA	O1D-CGD-O2D-CED
31	B	614	CLA	O1D-CGD-O2D-CED
31	B	617	CLA	O1D-CGD-O2D-CED
31	C	503	CLA	O1D-CGD-O2D-CED
31	C	511	CLA	O1D-CGD-O2D-CED
31	R	610	CLA	O1D-CGD-O2D-CED
31	S	617	CLA	O1D-CGD-O2D-CED
31	Y	608	CLA	O1D-CGD-O2D-CED
31	b	602	CLA	O1D-CGD-O2D-CED
31	b	614	CLA	O1D-CGD-O2D-CED
31	b	617	CLA	O1D-CGD-O2D-CED
31	c	504	CLA	O1D-CGD-O2D-CED
31	n	613	CLA	O1D-CGD-O2D-CED
31	g	614	CLA	O1D-CGD-O2D-CED
31	r	611	CLA	O1D-CGD-O2D-CED
31	s	617	CLA	O1D-CGD-O2D-CED
31	y	610	CLA	O1D-CGD-O2D-CED
31	C1	501	CLA	O1D-CGD-O2D-CED
31	N1	610	CLA	O1D-CGD-O2D-CED
31	G1	603	CLA	O1D-CGD-O2D-CED
31	b1	602	CLA	O1D-CGD-O2D-CED
31	b1	606	CLA	O1D-CGD-O2D-CED
31	b1	610	CLA	O1D-CGD-O2D-CED
31	b1	615	CLA	O1D-CGD-O2D-CED
31	c1	503	CLA	O1D-CGD-O2D-CED
31	s1	610	CLA	O1D-CGD-O2D-CED
31	y1	608	CLA	O1D-CGD-O2D-CED
31	y1	614	CLA	O1D-CGD-O2D-CED
31	B	617	CLA	CBA-CGA-O2A-C1
31	C	504	CLA	CBA-CGA-O2A-C1
31	C	505	CLA	CBA-CGA-O2A-C1
31	g	614	CLA	CBA-CGA-O2A-C1
31	s	605	CLA	CBA-CGA-O2A-C1
31	A1	406	CLA	CBA-CGA-O2A-C1
31	C1	505	CLA	CBA-CGA-O2A-C1
31	G1	611	CLA	CBA-CGA-O2A-C1
31	S1	605	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	g1	611	CLA	CBA-CGA-O2A-C1
31	y1	604	CLA	CBA-CGA-O2A-C1
35	C1	521	LMG	C29-C28-O8-C9
54	i1	101	4RF	C15-C16-O18-C19
31	B	603	CLA	CBD-CGD-O2D-CED
31	C	509	CLA	CBD-CGD-O2D-CED
31	N	611	CLA	CBD-CGD-O2D-CED
31	G	602	CLA	CBD-CGD-O2D-CED
31	Y	602	CLA	CBD-CGD-O2D-CED
31	n	611	CLA	CBD-CGD-O2D-CED
31	Y1	602	CLA	CBD-CGD-O2D-CED
31	s1	604	CLA	CBD-CGD-O2D-CED
31	A	406	CLA	O1A-CGA-O2A-C1
31	B	603	CLA	O1A-CGA-O2A-C1
31	C	505	CLA	O1A-CGA-O2A-C1
31	G	602	CLA	O1A-CGA-O2A-C1
31	G	613	CLA	O1A-CGA-O2A-C1
31	G	614	CLA	O1A-CGA-O2A-C1
31	S	609	CLA	O1A-CGA-O2A-C1
31	S	613	CLA	O1A-CGA-O2A-C1
31	Y	603	CLA	O1A-CGA-O2A-C1
31	Y	604	CLA	O1A-CGA-O2A-C1
31	Y	611	CLA	O1A-CGA-O2A-C1
31	a	406	CLA	O1A-CGA-O2A-C1
31	b	603	CLA	O1A-CGA-O2A-C1
31	c	505	CLA	O1A-CGA-O2A-C1
31	d	403	CLA	O1A-CGA-O2A-C1
31	g	604	CLA	O1A-CGA-O2A-C1
31	g	613	CLA	O1A-CGA-O2A-C1
31	s	603	CLA	O1A-CGA-O2A-C1
31	y	604	CLA	O1A-CGA-O2A-C1
31	B1	611	CLA	O1A-CGA-O2A-C1
31	G1	602	CLA	O1A-CGA-O2A-C1
31	G1	604	CLA	O1A-CGA-O2A-C1
31	R1	603	CLA	O1A-CGA-O2A-C1
31	S1	609	CLA	O1A-CGA-O2A-C1
31	S1	610	CLA	O1A-CGA-O2A-C1
31	S1	617	CLA	O1A-CGA-O2A-C1
31	Y1	604	CLA	O1A-CGA-O2A-C1
31	a1	406	CLA	O1A-CGA-O2A-C1
31	b1	603	CLA	O1A-CGA-O2A-C1
31	c1	511	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	n1	611	CLA	O1A-CGA-O2A-C1
31	g1	602	CLA	O1A-CGA-O2A-C1
31	g1	604	CLA	O1A-CGA-O2A-C1
31	r1	603	CLA	O1A-CGA-O2A-C1
31	s1	603	CLA	O1A-CGA-O2A-C1
31	s1	604	CLA	O1A-CGA-O2A-C1
31	y1	604	CLA	O1A-CGA-O2A-C1
31	y1	611	CLA	O1A-CGA-O2A-C1
32	A	408	PHO	O1A-CGA-O2A-C1
34	c1	526	SQD	O10-C23-O48-C46
35	J	101	LMG	O10-C28-O8-C9
35	c	521	LMG	O10-C28-O8-C9
35	C1	521	LMG	O10-C28-O8-C9
35	C1	523	LMG	O10-C28-O8-C9
35	W1	201	LMG	O10-C28-O8-C9
35	c1	521	LMG	O10-C28-O8-C9
35	w1	201	LMG	O10-C28-O8-C9
52	S	626	3PH	O32-C31-O31-C3
52	i	101	3PH	O32-C31-O31-C3
52	s	626	3PH	O32-C31-O31-C3
31	r	611	CLA	O1A-CGA-O2A-C1
31	A1	405	CLA	C4C-C3C-CAC-CBC
31	B	602	CLA	O1D-CGD-O2D-CED
31	B	604	CLA	O1D-CGD-O2D-CED
31	N	614	CLA	O1D-CGD-O2D-CED
31	G	610	CLA	O1D-CGD-O2D-CED
31	S	603	CLA	O1D-CGD-O2D-CED
31	S	609	CLA	O1D-CGD-O2D-CED
31	S	613	CLA	O1D-CGD-O2D-CED
31	Y	614	CLA	O1D-CGD-O2D-CED
31	b	610	CLA	O1D-CGD-O2D-CED
31	b	612	CLA	O1D-CGD-O2D-CED
31	c	503	CLA	O1D-CGD-O2D-CED
31	c	511	CLA	O1D-CGD-O2D-CED
31	d	403	CLA	O1D-CGD-O2D-CED
31	g	603	CLA	O1D-CGD-O2D-CED
31	g	611	CLA	O1D-CGD-O2D-CED
31	r	608	CLA	O1D-CGD-O2D-CED
31	r	609	CLA	O1D-CGD-O2D-CED
31	s	603	CLA	O1D-CGD-O2D-CED
31	y	613	CLA	O1D-CGD-O2D-CED
31	C1	506	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	C1	509	CLA	O1D-CGD-O2D-CED
31	C1	512	CLA	O1D-CGD-O2D-CED
31	D1	402	CLA	O1D-CGD-O2D-CED
31	N1	603	CLA	O1D-CGD-O2D-CED
31	R1	609	CLA	O1D-CGD-O2D-CED
31	R1	612	CLA	O1D-CGD-O2D-CED
31	S1	611	CLA	O1D-CGD-O2D-CED
31	S1	617	CLA	O1D-CGD-O2D-CED
31	Y1	613	CLA	O1D-CGD-O2D-CED
31	c1	504	CLA	O1D-CGD-O2D-CED
31	c1	512	CLA	O1D-CGD-O2D-CED
31	s1	611	CLA	O1D-CGD-O2D-CED
31	s1	614	CLA	O1D-CGD-O2D-CED
31	y1	610	CLA	O1D-CGD-O2D-CED
31	A1	405	CLA	C2C-C3C-CAC-CBC
31	B	610	CLA	O1D-CGD-O2D-CED
31	D	402	CLA	O1D-CGD-O2D-CED
31	D	403	CLA	O1D-CGD-O2D-CED
31	Y	613	CLA	O1D-CGD-O2D-CED
31	b	604	CLA	O1D-CGD-O2D-CED
31	n	614	CLA	O1D-CGD-O2D-CED
31	g	604	CLA	O1D-CGD-O2D-CED
31	s	611	CLA	O1D-CGD-O2D-CED
31	B1	603	CLA	O1D-CGD-O2D-CED
31	C1	513	CLA	O1D-CGD-O2D-CED
31	N1	614	CLA	O1D-CGD-O2D-CED
31	G1	604	CLA	O1D-CGD-O2D-CED
31	G1	614	CLA	O1D-CGD-O2D-CED
31	S1	605	CLA	O1D-CGD-O2D-CED
31	S1	609	CLA	O1D-CGD-O2D-CED
31	S1	610	CLA	O1D-CGD-O2D-CED
31	Y1	608	CLA	O1D-CGD-O2D-CED
31	b1	608	CLA	O1D-CGD-O2D-CED
31	b1	612	CLA	O1D-CGD-O2D-CED
31	c1	513	CLA	O1D-CGD-O2D-CED
31	d1	403	CLA	O1D-CGD-O2D-CED
31	g1	604	CLA	O1D-CGD-O2D-CED
31	g1	611	CLA	O1D-CGD-O2D-CED
31	r1	603	CLA	O1D-CGD-O2D-CED
31	r1	612	CLA	O1D-CGD-O2D-CED
31	y1	613	CLA	O1D-CGD-O2D-CED
32	a1	409	PHO	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
55	r1	625	LMT	O5B-C5B-C6B-O6B
31	B	613	CLA	CBD-CGD-O2D-CED
31	B1	612	CLA	CBD-CGD-O2D-CED
31	n1	604	CLA	CBD-CGD-O2D-CED
35	A	413	LMG	O9-C10-O7-C8
35	B	622	LMG	O9-C10-O7-C8
35	C	521	LMG	O9-C10-O7-C8
35	W1	201	LMG	O9-C10-O7-C8
35	c1	521	LMG	O9-C10-O7-C8
38	B	625	DGA	OB1-CB1-OG2-CG2
38	b	623	DGA	OB1-CB1-OG2-CG2
40	C	520	DGD	O1B-C1B-O2G-C2G
40	B1	623	DGD	O1B-C1B-O2G-C2G
41	G	630	LHG	O9-C7-O7-C5
41	S	624	LHG	O9-C7-O7-C5
41	d	408	LHG	O9-C7-O7-C5
41	n1	624	LHG	O9-C7-O7-C5
52	S	626	3PH	O22-C21-O21-C2
52	s	626	3PH	O22-C21-O21-C2
52	b1	624	3PH	O22-C21-O21-C2
54	I1	102	4RF	O23-C22-O21-C20
31	s	612	CLA	O1D-CGD-O2D-CED
31	C1	510	CLA	O1D-CGD-O2D-CED
57	Y1	627	PTY	O10-C8-O7-C6
31	C	512	CLA	C3-C5-C6-C7
31	D	403	CLA	C3-C5-C6-C7
31	N	603	CLA	C3-C5-C6-C7
31	Y	610	CLA	C3-C5-C6-C7
31	Y	613	CLA	C3-C5-C6-C7
31	Y	614	CLA	C3-C5-C6-C7
31	a	405	CLA	C3-C5-C6-C7
31	b	605	CLA	C3-C5-C6-C7
31	b	610	CLA	C3-C5-C6-C7
31	b	612	CLA	C3-C5-C6-C7
31	c	503	CLA	C3-C5-C6-C7
31	d	403	CLA	C3-C5-C6-C7
31	n	602	CLA	C3-C5-C6-C7
31	r	609	CLA	C3-C5-C6-C7
31	y	614	CLA	C3-C5-C6-C7
31	A1	406	CLA	C3-C5-C6-C7
31	B1	604	CLA	C3-C5-C6-C7
31	B1	608	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
31	B1	610	CLA	C3-C5-C6-C7
31	C1	505	CLA	C3-C5-C6-C7
31	C1	506	CLA	C3-C5-C6-C7
31	S1	603	CLA	C3-C5-C6-C7
31	S1	604	CLA	C3-C5-C6-C7
31	S1	610	CLA	C3-C5-C6-C7
31	b1	602	CLA	C3-C5-C6-C7
31	b1	614	CLA	C3-C5-C6-C7
31	b1	617	CLA	C3-C5-C6-C7
31	c1	504	CLA	C3-C5-C6-C7
31	d1	403	CLA	C3-C5-C6-C7
31	n1	604	CLA	C3-C5-C6-C7
31	n1	610	CLA	C3-C5-C6-C7
31	g1	611	CLA	C3-C5-C6-C7
31	r1	608	CLA	C3-C5-C6-C7
31	s1	603	CLA	C3-C5-C6-C7
31	s1	609	CLA	C3-C5-C6-C7
31	s1	610	CLA	C3-C5-C6-C7
31	y1	611	CLA	C3-C5-C6-C7
32	A	408	PHO	C3-C5-C6-C7
32	A	409	PHO	C3-C5-C6-C7
32	a	409	PHO	C3-C5-C6-C7
32	A1	408	PHO	C3-C5-C6-C7
47	Y1	607	CHL	C3-C5-C6-C7
31	G	612	CLA	O1D-CGD-O2D-CED
31	R	611	CLA	O1D-CGD-O2D-CED
31	c	509	CLA	O1D-CGD-O2D-CED
31	n	603	CLA	O1D-CGD-O2D-CED
31	B1	610	CLA	O1D-CGD-O2D-CED
31	R1	610	CLA	O1D-CGD-O2D-CED
31	A	410	CLA	CBA-CGA-O2A-C1
31	B	603	CLA	CBA-CGA-O2A-C1
31	B	608	CLA	CBA-CGA-O2A-C1
31	C	511	CLA	CBA-CGA-O2A-C1
31	C	512	CLA	CBA-CGA-O2A-C1
31	N	611	CLA	CBA-CGA-O2A-C1
31	G	604	CLA	CBA-CGA-O2A-C1
31	G	614	CLA	CBA-CGA-O2A-C1
31	R	608	CLA	CBA-CGA-O2A-C1
31	R	612	CLA	CBA-CGA-O2A-C1
31	S	603	CLA	CBA-CGA-O2A-C1
31	S	605	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	Y	604	CLA	CBA-CGA-O2A-C1
31	Y	611	CLA	CBA-CGA-O2A-C1
31	Y	613	CLA	CBA-CGA-O2A-C1
31	a	406	CLA	CBA-CGA-O2A-C1
31	b	603	CLA	CBA-CGA-O2A-C1
31	b	605	CLA	CBA-CGA-O2A-C1
31	c	505	CLA	CBA-CGA-O2A-C1
31	c	512	CLA	CBA-CGA-O2A-C1
31	d	403	CLA	CBA-CGA-O2A-C1
31	g	613	CLA	CBA-CGA-O2A-C1
31	s	602	CLA	CBA-CGA-O2A-C1
31	s	603	CLA	CBA-CGA-O2A-C1
31	y	603	CLA	CBA-CGA-O2A-C1
31	y	604	CLA	CBA-CGA-O2A-C1
31	y	611	CLA	CBA-CGA-O2A-C1
31	y	612	CLA	CBA-CGA-O2A-C1
31	B1	603	CLA	CBA-CGA-O2A-C1
31	C1	511	CLA	CBA-CGA-O2A-C1
31	G1	602	CLA	CBA-CGA-O2A-C1
31	R1	603	CLA	CBA-CGA-O2A-C1
31	R1	609	CLA	CBA-CGA-O2A-C1
31	S1	613	CLA	CBA-CGA-O2A-C1
31	Y1	602	CLA	CBA-CGA-O2A-C1
31	Y1	604	CLA	CBA-CGA-O2A-C1
31	Y1	611	CLA	CBA-CGA-O2A-C1
31	a1	406	CLA	CBA-CGA-O2A-C1
31	b1	606	CLA	CBA-CGA-O2A-C1
31	n1	611	CLA	CBA-CGA-O2A-C1
31	r1	603	CLA	CBA-CGA-O2A-C1
31	s1	604	CLA	CBA-CGA-O2A-C1
31	s1	610	CLA	CBA-CGA-O2A-C1
31	y1	611	CLA	CBA-CGA-O2A-C1
31	y1	612	CLA	CBA-CGA-O2A-C1
32	A	408	PHO	CBA-CGA-O2A-C1
34	c1	526	SQD	C24-C23-O48-C46
35	J	101	LMG	C29-C28-O8-C9
35	c	521	LMG	C29-C28-O8-C9
35	W1	201	LMG	C29-C28-O8-C9
35	w1	201	LMG	C29-C28-O8-C9
52	s	626	3PH	C32-C31-O31-C3
52	b1	624	3PH	C32-C31-O31-C3
52	t1	101	3PH	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
57	y1	626	PTY	C31-C30-O4-C1
31	C	501	CLA	CBD-CGD-O2D-CED
31	C	502	CLA	CBD-CGD-O2D-CED
31	C	506	CLA	CBD-CGD-O2D-CED
31	C	510	CLA	CBD-CGD-O2D-CED
31	C	513	CLA	CBD-CGD-O2D-CED
31	N	603	CLA	CBD-CGD-O2D-CED
31	N	610	CLA	CBD-CGD-O2D-CED
31	R	602	CLA	CBD-CGD-O2D-CED
31	S	612	CLA	CBD-CGD-O2D-CED
31	S	614	CLA	CBD-CGD-O2D-CED
31	a	410	CLA	CBD-CGD-O2D-CED
31	b	609	CLA	CBD-CGD-O2D-CED
31	b	616	CLA	CBD-CGD-O2D-CED
31	c	501	CLA	CBD-CGD-O2D-CED
31	c	507	CLA	CBD-CGD-O2D-CED
31	c	510	CLA	CBD-CGD-O2D-CED
31	c	513	CLA	CBD-CGD-O2D-CED
31	r	610	CLA	CBD-CGD-O2D-CED
31	s	605	CLA	CBD-CGD-O2D-CED
31	y	612	CLA	CBD-CGD-O2D-CED
31	y	614	CLA	CBD-CGD-O2D-CED
31	A1	407	CLA	CBD-CGD-O2D-CED
31	A1	410	CLA	CBD-CGD-O2D-CED
31	B1	609	CLA	CBD-CGD-O2D-CED
31	B1	613	CLA	CBD-CGD-O2D-CED
31	C1	507	CLA	CBD-CGD-O2D-CED
31	N1	604	CLA	CBD-CGD-O2D-CED
31	N1	612	CLA	CBD-CGD-O2D-CED
31	G1	612	CLA	CBD-CGD-O2D-CED
31	R1	602	CLA	CBD-CGD-O2D-CED
31	S1	602	CLA	CBD-CGD-O2D-CED
31	S1	612	CLA	CBD-CGD-O2D-CED
31	Y1	612	CLA	CBD-CGD-O2D-CED
31	d1	402	CLA	CBD-CGD-O2D-CED
31	n1	603	CLA	CBD-CGD-O2D-CED
31	g1	612	CLA	CBD-CGD-O2D-CED
31	r1	602	CLA	CBD-CGD-O2D-CED
31	s1	603	CLA	CBD-CGD-O2D-CED
35	b	622	LMG	C11-C10-O7-C8
35	c	521	LMG	C11-C10-O7-C8
35	B1	622	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
35	c1	521	LMG	C11-C10-O7-C8
38	B	625	DGA	CB2-CB1-OG2-CG2
40	C	523	DGD	C2B-C1B-O2G-C2G
41	N	624	LHG	C8-C7-O7-C5
41	n	624	LHG	C8-C7-O7-C5
52	t1	101	3PH	C22-C21-O21-C2
31	B	608	CLA	O1D-CGD-O2D-CED
31	B	611	CLA	O1D-CGD-O2D-CED
31	G	603	CLA	O1D-CGD-O2D-CED
31	G	614	CLA	O1D-CGD-O2D-CED
31	S	611	CLA	O1D-CGD-O2D-CED
31	Y	612	CLA	O1D-CGD-O2D-CED
31	n	602	CLA	O1D-CGD-O2D-CED
31	n	612	CLA	O1D-CGD-O2D-CED
31	r	602	CLA	O1D-CGD-O2D-CED
31	r	613	CLA	O1D-CGD-O2D-CED
31	s	604	CLA	O1D-CGD-O2D-CED
31	B1	608	CLA	O1D-CGD-O2D-CED
31	B1	611	CLA	O1D-CGD-O2D-CED
31	B1	616	CLA	O1D-CGD-O2D-CED
31	B1	617	CLA	O1D-CGD-O2D-CED
31	C1	502	CLA	O1D-CGD-O2D-CED
31	C1	503	CLA	O1D-CGD-O2D-CED
31	N1	602	CLA	O1D-CGD-O2D-CED
31	G1	602	CLA	O1D-CGD-O2D-CED
31	Y1	604	CLA	O1D-CGD-O2D-CED
31	Y1	611	CLA	O1D-CGD-O2D-CED
31	b1	607	CLA	O1D-CGD-O2D-CED
31	b1	611	CLA	O1D-CGD-O2D-CED
31	b1	616	CLA	O1D-CGD-O2D-CED
31	b1	617	CLA	O1D-CGD-O2D-CED
31	c1	501	CLA	O1D-CGD-O2D-CED
31	c1	510	CLA	O1D-CGD-O2D-CED
31	y1	602	CLA	O1D-CGD-O2D-CED
31	y1	612	CLA	O1D-CGD-O2D-CED
31	S	602	CLA	O1A-CGA-O2A-C1
31	N1	611	CLA	O1A-CGA-O2A-C1
31	N	604	CLA	O1D-CGD-O2D-CED
31	S1	604	CLA	O1D-CGD-O2D-CED
31	B	606	CLA	C4-C3-C5-C6
31	C	501	CLA	C4-C3-C5-C6
31	C	503	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	C	513	CLA	C4-C3-C5-C6
31	R	610	CLA	C4-C3-C5-C6
31	b	606	CLA	C4-C3-C5-C6
31	b	607	CLA	C4-C3-C5-C6
31	b	608	CLA	C4-C3-C5-C6
31	b	612	CLA	C4-C3-C5-C6
31	c	501	CLA	C4-C3-C5-C6
31	c	512	CLA	C4-C3-C5-C6
31	d	402	CLA	C4-C3-C5-C6
31	r	610	CLA	C4-C3-C5-C6
31	s	603	CLA	C4-C3-C5-C6
31	B1	604	CLA	C4-C3-C5-C6
31	B1	615	CLA	C4-C3-C5-C6
31	C1	505	CLA	C4-C3-C5-C6
31	D1	402	CLA	C4-C3-C5-C6
31	c1	504	CLA	C4-C3-C5-C6
31	d1	402	CLA	C4-C3-C5-C6
31	r1	608	CLA	C4-C3-C5-C6
44	D1	405	PL9	C20-C19-C21-C22
44	d1	405	PL9	C35-C34-C36-C37
47	G	601	CHL	C4-C3-C5-C6
47	G	609	CHL	C4-C3-C5-C6
47	Y	601	CHL	C4-C3-C5-C6
47	Y	606	CHL	C4-C3-C5-C6
47	g	609	CHL	C4-C3-C5-C6
47	y	601	CHL	C4-C3-C5-C6
47	N1	606	CHL	C4-C3-C5-C6
47	g1	609	CHL	C4-C3-C5-C6
31	B	605	CLA	C2-C3-C5-C6
31	B	606	CLA	C2-C3-C5-C6
31	C	501	CLA	C2-C3-C5-C6
31	C	503	CLA	C2-C3-C5-C6
31	C	504	CLA	C2-C3-C5-C6
31	R	610	CLA	C2-C3-C5-C6
31	b	606	CLA	C2-C3-C5-C6
31	b	608	CLA	C2-C3-C5-C6
31	c	512	CLA	C2-C3-C5-C6
31	r	610	CLA	C2-C3-C5-C6
31	s	603	CLA	C2-C3-C5-C6
31	B1	604	CLA	C2-C3-C5-C6
31	B1	615	CLA	C2-C3-C5-C6
31	D1	402	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	c1	501	CLA	C2-C3-C5-C6
31	d1	402	CLA	C2-C3-C5-C6
31	d1	403	CLA	C2-C3-C5-C6
31	r1	608	CLA	C2-C3-C5-C6
47	N	601	CHL	C2-C3-C5-C6
47	Y	601	CHL	C2-C3-C5-C6
47	g	609	CHL	C2-C3-C5-C6
47	N1	606	CHL	C2-C3-C5-C6
57	Y1	627	PTY	O30-C30-O4-C1
31	c	506	CLA	CBD-CGD-O2D-CED
31	G	611	CLA	O1D-CGD-O2D-CED
31	R	613	CLA	O1D-CGD-O2D-CED
31	Y	610	CLA	O1D-CGD-O2D-CED
31	r	604	CLA	O1D-CGD-O2D-CED
31	s	602	CLA	O1D-CGD-O2D-CED
31	S1	603	CLA	O1D-CGD-O2D-CED
31	Y1	614	CLA	O1D-CGD-O2D-CED
31	c1	509	CLA	O1D-CGD-O2D-CED
31	n1	612	CLA	O1D-CGD-O2D-CED
31	g1	614	CLA	O1D-CGD-O2D-CED
31	s1	612	CLA	O1D-CGD-O2D-CED
31	n	603	CLA	C2A-CAA-CBA-CGA
31	N1	611	CLA	C2A-CAA-CBA-CGA
31	c1	507	CLA	C2A-CAA-CBA-CGA
31	s1	617	CLA	C2A-CAA-CBA-CGA
31	r	609	CLA	O1A-CGA-O2A-C1
31	N1	603	CLA	O1A-CGA-O2A-C1
31	y1	608	CLA	O1A-CGA-O2A-C1
54	I1	102	4RF	O17-C16-O18-C19
31	B	605	CLA	C3-C5-C6-C7
31	B	612	CLA	C3-C5-C6-C7
31	C	504	CLA	C3-C5-C6-C7
31	C	510	CLA	C3-C5-C6-C7
31	N	610	CLA	C3-C5-C6-C7
31	G	603	CLA	C3-C5-C6-C7
31	b	608	CLA	C3-C5-C6-C7
31	n	613	CLA	C3-C5-C6-C7
31	s	611	CLA	C3-C5-C6-C7
31	y	611	CLA	C3-C5-C6-C7
31	B1	609	CLA	C3-C5-C6-C7
31	B1	614	CLA	C3-C5-C6-C7
31	G1	611	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
31	R1	602	CLA	C3-C5-C6-C7
31	S1	609	CLA	C3-C5-C6-C7
31	Y1	604	CLA	C3-C5-C6-C7
31	c1	505	CLA	C3-C5-C6-C7
31	c1	506	CLA	C3-C5-C6-C7
31	n1	613	CLA	C3-C5-C6-C7
31	s1	604	CLA	C3-C5-C6-C7
32	A1	409	PHO	C3-C5-C6-C7
32	a1	409	PHO	C3-C5-C6-C7
31	A	406	CLA	CBA-CGA-O2A-C1
31	C	510	CLA	CBA-CGA-O2A-C1
31	D	403	CLA	CBA-CGA-O2A-C1
31	G	602	CLA	CBA-CGA-O2A-C1
31	G	613	CLA	CBA-CGA-O2A-C1
31	R	603	CLA	CBA-CGA-O2A-C1
31	R	609	CLA	CBA-CGA-O2A-C1
31	S	609	CLA	CBA-CGA-O2A-C1
31	S	613	CLA	CBA-CGA-O2A-C1
31	Y	603	CLA	CBA-CGA-O2A-C1
31	Y	612	CLA	CBA-CGA-O2A-C1
31	a	405	CLA	CBA-CGA-O2A-C1
31	b	602	CLA	CBA-CGA-O2A-C1
31	b	608	CLA	CBA-CGA-O2A-C1
31	c	511	CLA	CBA-CGA-O2A-C1
31	g	604	CLA	CBA-CGA-O2A-C1
31	r	603	CLA	CBA-CGA-O2A-C1
31	r	608	CLA	CBA-CGA-O2A-C1
31	r	609	CLA	CBA-CGA-O2A-C1
31	r	612	CLA	CBA-CGA-O2A-C1
31	s	613	CLA	CBA-CGA-O2A-C1
31	y	614	CLA	CBA-CGA-O2A-C1
31	B1	611	CLA	CBA-CGA-O2A-C1
31	B1	613	CLA	CBA-CGA-O2A-C1
31	C1	506	CLA	CBA-CGA-O2A-C1
31	C1	509	CLA	CBA-CGA-O2A-C1
31	C1	513	CLA	CBA-CGA-O2A-C1
31	G1	604	CLA	CBA-CGA-O2A-C1
31	G1	613	CLA	CBA-CGA-O2A-C1
31	S1	602	CLA	CBA-CGA-O2A-C1
31	S1	609	CLA	CBA-CGA-O2A-C1
31	S1	610	CLA	CBA-CGA-O2A-C1
31	S1	614	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	S1	617	CLA	CBA-CGA-O2A-C1
31	b1	608	CLA	CBA-CGA-O2A-C1
31	c1	506	CLA	CBA-CGA-O2A-C1
31	c1	509	CLA	CBA-CGA-O2A-C1
31	c1	511	CLA	CBA-CGA-O2A-C1
31	n1	602	CLA	CBA-CGA-O2A-C1
31	g1	602	CLA	CBA-CGA-O2A-C1
31	g1	604	CLA	CBA-CGA-O2A-C1
31	r1	602	CLA	CBA-CGA-O2A-C1
31	r1	604	CLA	CBA-CGA-O2A-C1
31	r1	609	CLA	CBA-CGA-O2A-C1
31	s1	602	CLA	CBA-CGA-O2A-C1
31	s1	603	CLA	CBA-CGA-O2A-C1
31	s1	613	CLA	CBA-CGA-O2A-C1
31	y1	602	CLA	CBA-CGA-O2A-C1
31	y1	603	CLA	CBA-CGA-O2A-C1
31	y1	608	CLA	CBA-CGA-O2A-C1
34	M1	101	SQD	C24-C23-O48-C46
35	C1	523	LMG	C29-C28-O8-C9
35	c1	521	LMG	C29-C28-O8-C9
40	c1	520	DGD	C2A-C1A-O1G-C1G
52	S	626	3PH	C32-C31-O31-C3
52	i	101	3PH	C32-C31-O31-C3
52	T1	101	3PH	C32-C31-O31-C3
35	C	521	LMG	C35-C36-C37-C38
35	j	101	LMG	C17-C18-C19-C20
35	C1	523	LMG	C41-C42-C43-C44
35	a1	413	LMG	C35-C36-C37-C38
35	d1	411	LMG	C17-C18-C19-C20
35	h1	102	LMG	C38-C39-C40-C41
40	C	520	DGD	CBB-CCB-CDB-CEB
40	c1	519	DGD	C8A-C9A-CAA-CBA
41	L1	101	LHG	C7-C8-C9-C10
57	Y1	627	PTY	C31-C30-O4-C1
35	C1	521	LMG	C35-C36-C37-C38
35	W1	201	LMG	C38-C39-C40-C41
40	C	518	DGD	C8B-C9B-CAB-CBB
44	D	405	PL9	C12-C13-C14-C16
44	D	405	PL9	C42-C43-C44-C46
44	D1	405	PL9	C22-C23-C24-C26
44	D1	405	PL9	C37-C38-C39-C41
44	d1	405	PL9	C37-C38-C39-C41

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Mol	Chain	Res	Type	Atoms
35	H	102	LMG	C38-C39-C40-C41
35	J	101	LMG	C20-C21-C22-C23
35	a1	413	LMG	C17-C18-C19-C20
35	a1	413	LMG	C38-C39-C40-C41
35	c1	521	LMG	C17-C18-C19-C20
40	c	520	DGD	CBB-CCB-CDB-CEB
40	C1	519	DGD	C8A-C9A-CAA-CBA
33	c	514	BCR	C9-C10-C11-C12
33	C1	515	BCR	C9-C10-C11-C12
33	C1	515	BCR	C19-C20-C21-C22
33	D1	404	BCR	C19-C20-C21-C22
33	b1	618	BCR	C9-C10-C11-C12
33	c1	514	BCR	C9-C10-C11-C12
33	c1	517	BCR	C9-C10-C11-C12
37	b1	620	C7Z	C29-C30-C31-C32
46	H	101	RRX	C19-C20-C21-C22
46	H	101	RRX	C13-C14-C15-C16
46	H	101	RRX	C9-C10-C11-C12
48	n	621	LUT	C33-C34-C35-C15
49	R	621	XAT	C13-C14-C15-C35
49	r	622	XAT	C13-C14-C15-C35
31	B	611	CLA	O1A-CGA-O2A-C1
31	C	511	CLA	O1A-CGA-O2A-C1
31	C	512	CLA	O1A-CGA-O2A-C1
31	D	403	CLA	O1A-CGA-O2A-C1
31	R	603	CLA	O1A-CGA-O2A-C1
31	R	612	CLA	O1A-CGA-O2A-C1
31	Y	612	CLA	O1A-CGA-O2A-C1
31	Y	613	CLA	O1A-CGA-O2A-C1
31	b	602	CLA	O1A-CGA-O2A-C1
31	b	605	CLA	O1A-CGA-O2A-C1
31	c	511	CLA	O1A-CGA-O2A-C1
31	s	602	CLA	O1A-CGA-O2A-C1
31	s	609	CLA	O1A-CGA-O2A-C1
31	s	617	CLA	O1A-CGA-O2A-C1
31	y	612	CLA	O1A-CGA-O2A-C1
31	B1	603	CLA	O1A-CGA-O2A-C1
31	C1	506	CLA	O1A-CGA-O2A-C1
31	C1	509	CLA	O1A-CGA-O2A-C1
31	C1	511	CLA	O1A-CGA-O2A-C1
31	G1	613	CLA	O1A-CGA-O2A-C1
31	S1	602	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	Y1	602	CLA	O1A-CGA-O2A-C1
31	Y1	608	CLA	O1A-CGA-O2A-C1
31	Y1	613	CLA	O1A-CGA-O2A-C1
31	b1	606	CLA	O1A-CGA-O2A-C1
31	c1	506	CLA	O1A-CGA-O2A-C1
31	c1	509	CLA	O1A-CGA-O2A-C1
31	n1	603	CLA	O1A-CGA-O2A-C1
31	g1	613	CLA	O1A-CGA-O2A-C1
31	r1	608	CLA	O1A-CGA-O2A-C1
31	r1	609	CLA	O1A-CGA-O2A-C1
31	s1	602	CLA	O1A-CGA-O2A-C1
31	s1	617	CLA	O1A-CGA-O2A-C1
31	y1	603	CLA	O1A-CGA-O2A-C1
52	T1	101	3PH	O32-C31-O31-C3
57	y1	626	PTY	O30-C30-O4-C1
40	c	520	DGD	O1B-C1B-O2G-C2G
41	s	624	LHG	O9-C7-O7-C5
31	b	607	CLA	O1D-CGD-O2D-CED
35	c	521	LMG	C17-C18-C19-C20
35	A1	413	LMG	C17-C18-C19-C20
35	b1	622	LMG	C17-C18-C19-C20
40	C	519	DGD	C8B-C9B-CAB-CBB
40	C	523	DGD	CEB-CFB-CGB-CHB
35	A	413	LMG	C17-C18-C19-C20
35	A	413	LMG	C35-C36-C37-C38
35	A	413	LMG	C38-C39-C40-C41
35	B	622	LMG	C17-C18-C19-C20
35	C	521	LMG	C17-C18-C19-C20
35	D	411	LMG	C17-C18-C19-C20
35	D	411	LMG	C20-C21-C22-C23
35	J	101	LMG	C17-C18-C19-C20
35	a	413	LMG	C17-C18-C19-C20
35	a	413	LMG	C35-C36-C37-C38
35	a	413	LMG	C38-C39-C40-C41
35	b	622	LMG	C17-C18-C19-C20
35	c	521	LMG	C35-C36-C37-C38
35	d	411	LMG	C17-C18-C19-C20
35	d	411	LMG	C20-C21-C22-C23
35	h	102	LMG	C38-C39-C40-C41
35	j	101	LMG	C20-C21-C22-C23
35	A1	413	LMG	C38-C39-C40-C41
35	B1	622	LMG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
35	C1	521	LMG	C17-C18-C19-C20
35	C1	523	LMG	C17-C18-C19-C20
35	D1	411	LMG	C17-C18-C19-C20
35	D1	411	LMG	C20-C21-C22-C23
35	H1	102	LMG	C38-C39-C40-C41
35	W1	201	LMG	C35-C36-C37-C38
35	c1	521	LMG	C35-C36-C37-C38
35	c1	523	LMG	C17-C18-C19-C20
35	c1	523	LMG	C41-C42-C43-C44
35	w1	201	LMG	C35-C36-C37-C38
35	w1	201	LMG	C38-C39-C40-C41
40	C	519	DGD	C8A-C9A-CAA-CBA
40	C	523	DGD	CBA-CCA-CDA-CEA
40	c	518	DGD	C8B-C9B-CAB-CBB
40	c	519	DGD	C8A-C9A-CAA-CBA
40	c	519	DGD	C8B-C9B-CAB-CBB
40	c	523	DGD	CBA-CCA-CDA-CEA
40	c	523	DGD	CEB-CFB-CGB-CHB
40	C1	518	DGD	C8B-C9B-CAB-CBB
40	C1	519	DGD	CBB-CCB-CDB-CEB
40	C1	520	DGD	CBB-CCB-CDB-CEB
40	c1	518	DGD	C8B-C9B-CAB-CBB
40	c1	519	DGD	CBB-CCB-CDB-CEB
40	c1	520	DGD	CBB-CCB-CDB-CEB
31	C	507	CLA	O1D-CGD-O2D-CED
31	N	602	CLA	O1D-CGD-O2D-CED
31	G	604	CLA	O1D-CGD-O2D-CED
31	S	604	CLA	O1D-CGD-O2D-CED
31	D1	403	CLA	O1D-CGD-O2D-CED
31	N1	611	CLA	O1D-CGD-O2D-CED
31	b1	613	CLA	O1D-CGD-O2D-CED
31	s1	605	CLA	O1D-CGD-O2D-CED
31	C	501	CLA	C3-C5-C6-C7
31	Y	603	CLA	C3-C5-C6-C7
31	y	610	CLA	C3-C5-C6-C7
31	Y1	611	CLA	C3-C5-C6-C7
31	r1	612	CLA	C3-C5-C6-C7
31	y1	614	CLA	C3-C5-C6-C7
31	B	609	CLA	CBD-CGD-O2D-CED
32	a	408	PHO	CBD-CGD-O2D-CED
35	A1	413	LMG	C35-C36-C37-C38
35	d1	411	LMG	C20-C21-C22-C23

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Mol	Chain	Res	Type	Atoms
41	C	525	LHG	O2-C2-C3-O3
41	G	630	LHG	O2-C2-C3-O3
41	S	624	LHG	O2-C2-C3-O3
41	d	409	LHG	O2-C2-C3-O3
41	l	101	LHG	O2-C2-C3-O3
41	g	624	LHG	O2-C2-C3-O3
41	y	624	LHG	O2-C2-C3-O3
41	C1	525	LHG	O2-C2-C3-O3
41	D1	409	LHG	O2-C2-C3-O3
41	L1	101	LHG	O2-C2-C3-O3
41	S1	624	LHG	O2-C2-C3-O3
41	Y1	624	LHG	O2-C2-C3-O3
41	d1	409	LHG	O2-C2-C3-O3
41	n1	624	LHG	O2-C2-C3-O3
41	g1	624	LHG	O2-C2-C3-O3
41	s1	624	LHG	O2-C2-C3-O3
51	s	625	LPX	O1-C3-C4-O5
51	S1	625	LPX	O1-C3-C4-O5
31	B	607	CLA	O1D-CGD-O2D-CED
31	C	504	CLA	O1D-CGD-O2D-CED
31	S	605	CLA	O1D-CGD-O2D-CED
31	b	608	CLA	O1D-CGD-O2D-CED
31	b	613	CLA	O1D-CGD-O2D-CED
31	r	612	CLA	O1D-CGD-O2D-CED
31	s	613	CLA	O1D-CGD-O2D-CED
31	y	603	CLA	O1D-CGD-O2D-CED
31	y	611	CLA	O1D-CGD-O2D-CED
31	a1	407	CLA	O1D-CGD-O2D-CED
31	n1	611	CLA	O1D-CGD-O2D-CED
31	g1	602	CLA	O1D-CGD-O2D-CED
31	g1	603	CLA	O1D-CGD-O2D-CED
31	y1	603	CLA	O1D-CGD-O2D-CED
32	a	409	PHO	O1D-CGD-O2D-CED
31	B	605	CLA	CBA-CGA-O2A-C1
31	B	606	CLA	CBA-CGA-O2A-C1
31	C	506	CLA	CBA-CGA-O2A-C1
31	N	603	CLA	CBA-CGA-O2A-C1
31	S	602	CLA	CBA-CGA-O2A-C1
31	b	611	CLA	CBA-CGA-O2A-C1
31	s	609	CLA	CBA-CGA-O2A-C1
31	A1	407	CLA	CBA-CGA-O2A-C1
31	C1	504	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	D1	403	CLA	CBA-CGA-O2A-C1
31	N1	610	CLA	CBA-CGA-O2A-C1
31	N1	611	CLA	CBA-CGA-O2A-C1
31	R1	608	CLA	CBA-CGA-O2A-C1
31	Y1	603	CLA	CBA-CGA-O2A-C1
31	Y1	608	CLA	CBA-CGA-O2A-C1
31	Y1	612	CLA	CBA-CGA-O2A-C1
31	a1	407	CLA	CBA-CGA-O2A-C1
31	a1	410	CLA	CBA-CGA-O2A-C1
31	b1	614	CLA	CBA-CGA-O2A-C1
31	n1	603	CLA	CBA-CGA-O2A-C1
31	s1	617	CLA	CBA-CGA-O2A-C1
35	j	101	LMG	C29-C28-O8-C9
38	c1	524	DGA	CA2-CA1-OG1-CG1
40	c	520	DGD	C2A-C1A-O1G-C1G
31	A	410	CLA	O1A-CGA-O2A-C1
31	B	608	CLA	O1A-CGA-O2A-C1
31	G	604	CLA	O1A-CGA-O2A-C1
31	R	608	CLA	O1A-CGA-O2A-C1
31	R	609	CLA	O1A-CGA-O2A-C1
31	b	611	CLA	O1A-CGA-O2A-C1
31	r	612	CLA	O1A-CGA-O2A-C1
31	B1	613	CLA	O1A-CGA-O2A-C1
31	R1	609	CLA	O1A-CGA-O2A-C1
31	n1	602	CLA	O1A-CGA-O2A-C1
31	r1	602	CLA	O1A-CGA-O2A-C1
31	s1	613	CLA	O1A-CGA-O2A-C1
34	M1	101	SQD	O10-C23-O48-C46
51	s	625	LPX	O5-C4-C5-O6
31	A	410	CLA	O1D-CGD-O2D-CED
31	R	604	CLA	O1D-CGD-O2D-CED
31	S	610	CLA	O1D-CGD-O2D-CED
31	g	602	CLA	O1D-CGD-O2D-CED
31	C1	504	CLA	O1D-CGD-O2D-CED
31	c1	511	CLA	O1D-CGD-O2D-CED
31	n1	602	CLA	O1D-CGD-O2D-CED
31	s1	609	CLA	O1D-CGD-O2D-CED
35	d1	411	LMG	O6-C5-C6-O5
55	r1	625	LMT	C4B-C5B-C6B-O6B
31	s	614	CLA	CBD-CGD-O2D-CED
34	b1	626	SQD	C8-C7-O47-C45
35	B	622	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
38	b1	625	DGA	CB2-CB1-OG2-CG2
40	C	519	DGD	C2B-C1B-O2G-C2G
31	A1	407	CLA	O1A-CGA-O2A-C1
44	D	405	PL9	C47-C48-C49-C50
31	b	611	CLA	O1D-CGD-O2D-CED
31	y	602	CLA	O1D-CGD-O2D-CED
31	G1	611	CLA	O1D-CGD-O2D-CED
31	Y1	603	CLA	O1D-CGD-O2D-CED
31	b1	603	CLA	O1D-CGD-O2D-CED
31	c1	507	CLA	O1D-CGD-O2D-CED
31	C	502	CLA	C3-C5-C6-C7
31	b	602	CLA	C3-C5-C6-C7
31	s	604	CLA	C3-C5-C6-C7
31	C1	509	CLA	C3-C5-C6-C7
31	a1	406	CLA	C3-C5-C6-C7
31	s1	613	CLA	C3-C5-C6-C7
31	C	508	CLA	CBD-CGD-O2D-CED
31	C1	508	CLA	CBD-CGD-O2D-CED
31	B	616	CLA	O1D-CGD-O2D-CED
31	C	509	CLA	O1D-CGD-O2D-CED
31	R	612	CLA	O1D-CGD-O2D-CED
31	b	603	CLA	O1D-CGD-O2D-CED
31	b1	609	CLA	O1D-CGD-O2D-CED
31	s1	602	CLA	O1D-CGD-O2D-CED
31	B	611	CLA	CBA-CGA-O2A-C1
31	c	510	CLA	CBA-CGA-O2A-C1
31	s	617	CLA	CBA-CGA-O2A-C1
31	B1	610	CLA	CBA-CGA-O2A-C1
31	N1	603	CLA	CBA-CGA-O2A-C1
31	Y1	613	CLA	CBA-CGA-O2A-C1
31	b1	603	CLA	CBA-CGA-O2A-C1
31	g1	613	CLA	CBA-CGA-O2A-C1
31	r1	608	CLA	CBA-CGA-O2A-C1
54	I1	102	4RF	C15-C16-O18-C19
31	b	604	CLA	C4-C3-C5-C6
31	c	503	CLA	C4-C3-C5-C6
31	g	602	CLA	C4-C3-C5-C6
31	C1	503	CLA	C4-C3-C5-C6
31	b1	615	CLA	C4-C3-C5-C6
31	r1	610	CLA	C4-C3-C5-C6
47	n	601	CHL	C4-C3-C5-C6
31	C	513	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	b	607	CLA	C2-C3-C5-C6
31	b	612	CLA	C2-C3-C5-C6
31	c	501	CLA	C2-C3-C5-C6
31	g	602	CLA	C2-C3-C5-C6
31	C1	504	CLA	C2-C3-C5-C6
31	b1	615	CLA	C2-C3-C5-C6
44	d1	405	PL9	C33-C34-C36-C37
47	n	601	CHL	C2-C3-C5-C6
47	y	601	CHL	C2-C3-C5-C6
47	g1	609	CHL	C2-C3-C5-C6
31	B	605	CLA	O1A-CGA-O2A-C1
31	B	606	CLA	O1A-CGA-O2A-C1
31	C	510	CLA	O1A-CGA-O2A-C1
31	r	608	CLA	O1A-CGA-O2A-C1
31	s	613	CLA	O1A-CGA-O2A-C1
31	y	614	CLA	O1A-CGA-O2A-C1
31	C1	504	CLA	O1A-CGA-O2A-C1
31	C1	513	CLA	O1A-CGA-O2A-C1
31	D1	403	CLA	O1A-CGA-O2A-C1
31	S1	614	CLA	O1A-CGA-O2A-C1
31	a1	407	CLA	O1A-CGA-O2A-C1
31	a1	410	CLA	O1A-CGA-O2A-C1
31	b1	608	CLA	O1A-CGA-O2A-C1
31	b1	614	CLA	O1A-CGA-O2A-C1
35	j	101	LMG	O10-C28-O8-C9
40	c1	520	DGD	O1A-C1A-O1G-C1G
38	b1	625	DGA	OB1-CB1-OG2-CG2
40	C	519	DGD	O1B-C1B-O2G-C2G
55	r1	625	LMT	O5'-C5'-C6'-O6'
31	g	612	CLA	O1D-CGD-O2D-CED
44	D	405	PL9	C34-C36-C37-C38
44	D1	405	PL9	C19-C21-C22-C23
44	d1	405	PL9	C29-C31-C32-C33
31	Y	604	CLA	CBD-CGD-O2D-CED
35	d	411	LMG	O6-C5-C6-O5
45	F	101	HEM	C3D-CAD-CBD-CGD
45	F1	101	HEM	C3D-CAD-CBD-CGD
31	S	617	CLA	C2A-CAA-CBA-CGA
31	c	504	CLA	C2A-CAA-CBA-CGA
31	C1	502	CLA	C2A-CAA-CBA-CGA
32	a	408	PHO	C2A-CAA-CBA-CGA
47	N	605	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
47	N1	605	CHL	C2A-CAA-CBA-CGA
47	G1	605	CHL	C2A-CAA-CBA-CGA
47	n1	605	CHL	C2A-CAA-CBA-CGA
47	n1	606	CHL	C2A-CAA-CBA-CGA
47	s1	601	CHL	C2A-CAA-CBA-CGA
31	B	603	CLA	O1D-CGD-O2D-CED
31	Y	603	CLA	O1D-CGD-O2D-CED
31	n	611	CLA	O1D-CGD-O2D-CED
31	a1	410	CLA	O1D-CGD-O2D-CED
31	y1	604	CLA	O1D-CGD-O2D-CED
31	C	506	CLA	O1A-CGA-O2A-C1
31	N	603	CLA	O1A-CGA-O2A-C1
31	a	405	CLA	O1A-CGA-O2A-C1
31	b	608	CLA	O1A-CGA-O2A-C1
31	c	510	CLA	O1A-CGA-O2A-C1
31	r	603	CLA	O1A-CGA-O2A-C1
31	B1	610	CLA	O1A-CGA-O2A-C1
31	N1	610	CLA	O1A-CGA-O2A-C1
31	Y1	603	CLA	O1A-CGA-O2A-C1
31	Y1	612	CLA	O1A-CGA-O2A-C1
31	r1	604	CLA	O1A-CGA-O2A-C1
31	y1	602	CLA	O1A-CGA-O2A-C1
38	c1	524	DGA	OA1-CA1-OG1-CG1
40	c	519	DGD	O1A-C1A-O1G-C1G
31	N	602	CLA	C3-C5-C6-C7
31	b	614	CLA	C3-C5-C6-C7
34	B1	626	SQD	O5-C1-O6-C44
35	C	521	LMG	O6-C1-O1-C7
35	c	521	LMG	O6-C1-O1-C7
40	C	519	DGD	O6E-C1E-O5D-C6D
40	C	523	DGD	O6E-C1E-O5D-C6D
40	c	519	DGD	O6E-C1E-O5D-C6D
40	c	523	DGD	O6E-C1E-O5D-C6D
40	C1	520	DGD	O6E-C5E-C6E-O5E
31	Y	602	CLA	O1D-CGD-O2D-CED
31	B1	612	CLA	O1D-CGD-O2D-CED
31	b	606	CLA	CBA-CGA-O2A-C1
31	g	602	CLA	CBA-CGA-O2A-C1
31	r	604	CLA	CBA-CGA-O2A-C1
31	B1	608	CLA	CBA-CGA-O2A-C1
31	c1	508	CLA	CBA-CGA-O2A-C1
35	c1	523	LMG	C29-C28-O8-C9

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Mol	Chain	Res	Type	Atoms
40	c	519	DGD	C2A-C1A-O1G-C1G
41	L1	101	LHG	C24-C23-O8-C6
31	d	402	CLA	CBD-CGD-O2D-CED
31	B1	602	CLA	CBD-CGD-O2D-CED
31	c1	506	CLA	CBD-CGD-O2D-CED
44	d1	405	PL9	C22-C23-C24-C25
31	R1	608	CLA	O1A-CGA-O2A-C1
40	c	520	DGD	O1A-C1A-O1G-C1G
31	B	613	CLA	O1D-CGD-O2D-CED
31	N	611	CLA	O1D-CGD-O2D-CED
31	G	602	CLA	O1D-CGD-O2D-CED
31	R	602	CLA	O1D-CGD-O2D-CED
31	s1	604	CLA	O1D-CGD-O2D-CED
31	Y	611	CLA	CBD-CGD-O2D-CED
34	m1	101	SQD	C8-C7-O47-C45
38	B1	625	DGA	CB2-CB1-OG2-CG2
31	c1	511	CLA	C3-C5-C6-C7
33	c1	515	BCR	C9-C10-C11-C12
46	h	101	RRX	C19-C20-C21-C22
48	Y	621	LUT	C29-C30-C31-C32
31	A	405	CLA	O1A-CGA-O2A-C1
31	b	606	CLA	O1A-CGA-O2A-C1
31	g	602	CLA	O1A-CGA-O2A-C1
31	r	604	CLA	O1A-CGA-O2A-C1
31	B1	608	CLA	O1A-CGA-O2A-C1
31	y1	610	CLA	O1A-CGA-O2A-C1
35	c1	523	LMG	O10-C28-O8-C9
41	L1	101	LHG	O10-C23-O8-C6
34	m1	101	SQD	O49-C7-O47-C45
41	L	101	LHG	C1-C2-C3-O3
41	G	630	LHG	C1-C2-C3-O3
41	l	101	LHG	C1-C2-C3-O3
41	L1	101	LHG	C1-C2-C3-O3
41	G1	624	LHG	C1-C2-C3-O3
41	Y1	624	LHG	C1-C2-C3-O3
41	c1	525	LHG	C1-C2-C3-O3
41	g1	624	LHG	C1-C2-C3-O3
51	S	625	LPX	O1-C3-C4-C5
51	S1	625	LPX	O1-C3-C4-C5
31	A	405	CLA	CBA-CGA-O2A-C1
31	B	612	CLA	CBA-CGA-O2A-C1
31	B	614	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	C	509	CLA	CBA-CGA-O2A-C1
31	G	603	CLA	CBA-CGA-O2A-C1
31	S	604	CLA	CBA-CGA-O2A-C1
31	Y	614	CLA	CBA-CGA-O2A-C1
31	a	410	CLA	CBA-CGA-O2A-C1
31	b	604	CLA	CBA-CGA-O2A-C1
31	b	613	CLA	CBA-CGA-O2A-C1
31	b	614	CLA	CBA-CGA-O2A-C1
31	c	503	CLA	CBA-CGA-O2A-C1
31	c	506	CLA	CBA-CGA-O2A-C1
31	c	507	CLA	CBA-CGA-O2A-C1
31	n	611	CLA	CBA-CGA-O2A-C1
31	g	603	CLA	CBA-CGA-O2A-C1
31	s	611	CLA	CBA-CGA-O2A-C1
31	B1	602	CLA	CBA-CGA-O2A-C1
31	B1	604	CLA	CBA-CGA-O2A-C1
31	B1	614	CLA	CBA-CGA-O2A-C1
31	B1	617	CLA	CBA-CGA-O2A-C1
31	N1	602	CLA	CBA-CGA-O2A-C1
31	R1	602	CLA	CBA-CGA-O2A-C1
31	R1	604	CLA	CBA-CGA-O2A-C1
31	a1	405	CLA	CBA-CGA-O2A-C1
31	b1	604	CLA	CBA-CGA-O2A-C1
31	b1	613	CLA	CBA-CGA-O2A-C1
31	y1	610	CLA	CBA-CGA-O2A-C1
34	b	621	SQD	C24-C23-O48-C46
34	m1	101	SQD	C24-C23-O48-C46
35	B1	622	LMG	C29-C28-O8-C9
40	C	519	DGD	C2A-C1A-O1G-C1G
40	C	520	DGD	C2A-C1A-O1G-C1G
40	c	518	DGD	C2A-C1A-O1G-C1G
40	C1	518	DGD	C2A-C1A-O1G-C1G
41	c1	525	LHG	C24-C23-O8-C6
52	S1	626	3PH	C32-C31-O31-C3
31	C	510	CLA	O1D-CGD-O2D-CED
31	S	612	CLA	O1D-CGD-O2D-CED
31	c	501	CLA	O1D-CGD-O2D-CED
31	c	507	CLA	O1D-CGD-O2D-CED
31	c	510	CLA	O1D-CGD-O2D-CED
31	C1	507	CLA	O1D-CGD-O2D-CED
31	Y1	602	CLA	O1D-CGD-O2D-CED
31	Y1	612	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	n1	604	CLA	O1D-CGD-O2D-CED
55	R1	625	LMT	C4B-C5B-C6B-O6B
31	B1	614	CLA	O1A-CGA-O2A-C1
31	S1	612	CLA	O1D-CGD-O2D-CED
31	C1	504	CLA	C4-C3-C5-C6
31	N1	610	CLA	C4-C3-C5-C6
31	b1	604	CLA	C4-C3-C5-C6
31	b1	606	CLA	C4-C3-C5-C6
31	c	503	CLA	C2-C3-C5-C6
31	d	402	CLA	C2-C3-C5-C6
31	C1	503	CLA	C2-C3-C5-C6
31	C1	505	CLA	C2-C3-C5-C6
31	N1	610	CLA	C2-C3-C5-C6
31	b1	604	CLA	C2-C3-C5-C6
31	b1	606	CLA	C2-C3-C5-C6
31	c1	504	CLA	C2-C3-C5-C6
31	r1	610	CLA	C2-C3-C5-C6
47	G	601	CHL	C2-C3-C5-C6
47	G	609	CHL	C2-C3-C5-C6
47	Y	606	CHL	C2-C3-C5-C6
31	r	608	CLA	C3-C5-C6-C7
31	s	603	CLA	C3-C5-C6-C7
31	y	613	CLA	C3-C5-C6-C7
31	B1	603	CLA	C3-C5-C6-C7
31	B	612	CLA	CBD-CGD-O2D-CED
31	B	612	CLA	C11-C12-C13-C14
31	B	616	CLA	C6-C7-C8-C9
31	C	501	CLA	C11-C12-C13-C14
31	C	506	CLA	C11-C12-C13-C14
31	C	507	CLA	C11-C10-C8-C9
31	G	602	CLA	C14-C13-C15-C16
31	R	603	CLA	C11-C10-C8-C9
31	Y	602	CLA	C14-C13-C15-C16
31	b	604	CLA	C14-C13-C15-C16
31	c	502	CLA	C6-C7-C8-C9
31	c	507	CLA	C11-C10-C8-C9
31	c	513	CLA	C11-C10-C8-C9
31	d	402	CLA	C6-C7-C8-C9
31	r	603	CLA	C11-C10-C8-C9
31	r	610	CLA	C11-C10-C8-C9
31	y	602	CLA	C11-C10-C8-C9
31	D1	402	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	R1	602	CLA	C6-C7-C8-C9
31	R1	610	CLA	C6-C7-C8-C9
31	R1	612	CLA	C6-C7-C8-C9
31	Y1	604	CLA	C11-C10-C8-C9
31	a1	406	CLA	C14-C13-C15-C16
31	b1	605	CLA	C6-C7-C8-C9
31	b1	607	CLA	C14-C13-C15-C16
31	b1	612	CLA	C11-C12-C13-C14
31	b1	617	CLA	C14-C13-C15-C16
31	c1	505	CLA	C6-C7-C8-C9
31	c1	511	CLA	C6-C7-C8-C9
31	c1	513	CLA	C11-C10-C8-C9
31	d1	402	CLA	C6-C7-C8-C9
31	n1	613	CLA	C14-C13-C15-C16
31	r1	612	CLA	C6-C7-C8-C9
31	s1	609	CLA	C11-C10-C8-C9
31	y1	604	CLA	C6-C7-C8-C9
31	y1	611	CLA	C11-C12-C13-C14
32	A	409	PHO	C6-C7-C8-C9
32	a	409	PHO	C6-C7-C8-C9
32	a1	409	PHO	C6-C7-C8-C9
47	Y	601	CHL	C11-C10-C8-C9
47	Y	607	CHL	C11-C10-C8-C9
47	Y	607	CHL	C14-C13-C15-C16
47	n	605	CHL	C11-C10-C8-C9
47	g	609	CHL	C11-C10-C8-C9
47	y	601	CHL	C11-C10-C8-C9
47	N1	606	CHL	C14-C13-C15-C16
47	G1	601	CHL	C14-C13-C15-C16
47	G1	607	CHL	C11-C10-C8-C9
47	Y1	607	CHL	C14-C13-C15-C16
47	Y1	609	CHL	C11-C12-C13-C14
47	n1	606	CHL	C14-C13-C15-C16
47	n1	607	CHL	C14-C13-C15-C16
47	g1	601	CHL	C14-C13-C15-C16
47	y1	609	CHL	C11-C12-C13-C14
31	C	502	CLA	O1D-CGD-O2D-CED
31	C	513	CLA	O1D-CGD-O2D-CED
31	S	614	CLA	O1D-CGD-O2D-CED
31	b	609	CLA	O1D-CGD-O2D-CED
31	b	616	CLA	O1D-CGD-O2D-CED
31	s	605	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
31	B1	609	CLA	O1D-CGD-O2D-CED
31	B1	613	CLA	O1D-CGD-O2D-CED
31	N1	604	CLA	O1D-CGD-O2D-CED
31	g1	612	CLA	O1D-CGD-O2D-CED
31	r1	602	CLA	O1D-CGD-O2D-CED
34	A	412	SQD	C2-C1-O6-C44
34	B1	626	SQD	C2-C1-O6-C44
34	b1	621	SQD	C2-C1-O6-C44
35	C	521	LMG	C2-C1-O1-C7
35	c	521	LMG	C2-C1-O1-C7
40	C	519	DGD	C2E-C1E-O5D-C6D
40	C	523	DGD	C2E-C1E-O5D-C6D
40	c	519	DGD	C2E-C1E-O5D-C6D
40	c	523	DGD	C2E-C1E-O5D-C6D
41	s	624	LHG	C7-C8-C9-C10
41	D	409	LHG	O2-C2-C3-O3
41	L	101	LHG	O2-C2-C3-O3
41	c1	525	LHG	O2-C2-C3-O3
31	G1	612	CLA	O1D-CGD-O2D-CED
56	R1	626	ERG	C17-C20-C22-C23
56	r1	626	ERG	C17-C20-C22-C23
31	Y	614	CLA	O1A-CGA-O2A-C1
31	b	613	CLA	O1A-CGA-O2A-C1
31	c	503	CLA	O1A-CGA-O2A-C1
31	g	603	CLA	O1A-CGA-O2A-C1
34	b	621	SQD	O10-C23-O48-C46
40	C1	518	DGD	O1A-C1A-O1G-C1G
31	N	610	CLA	O1D-CGD-O2D-CED
31	c	513	CLA	O1D-CGD-O2D-CED
31	y	614	CLA	O1D-CGD-O2D-CED
31	S1	602	CLA	O1D-CGD-O2D-CED
33	B	619	BCR	C37-C22-C23-C24
33	C	515	BCR	C36-C18-C19-C20
33	C	516	BCR	C7-C8-C9-C34
33	a	411	BCR	C36-C18-C19-C20
33	b	618	BCR	C36-C18-C19-C20
33	B1	618	BCR	C36-C18-C19-C20
33	C1	515	BCR	C7-C8-C9-C34
33	C1	516	BCR	C36-C18-C19-C20
33	C1	517	BCR	C37-C22-C23-C24
33	a1	411	BCR	C37-C22-C23-C24
33	c1	514	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
33	c1	516	BCR	C7-C8-C9-C34
33	c1	516	BCR	C36-C18-C19-C20
33	c1	517	BCR	C36-C18-C19-C20
33	d1	404	BCR	C11-C12-C13-C35
37	B	620	C7Z	C31-C32-C33-C40
37	b	620	C7Z	C11-C12-C13-C20
37	b	620	C7Z	C31-C32-C33-C40
37	B1	620	C7Z	C7-C8-C9-C19
37	b1	620	C7Z	C7-C8-C9-C19
37	b1	620	C7Z	C11-C12-C13-C20
37	b1	620	C7Z	C31-C32-C33-C40
46	h	101	RRX	C36-C18-C19-C20
46	h	101	RRX	C7-C8-C9-C34
46	h1	101	RRX	C36-C18-C19-C20
48	N	620	LUT	C27-C28-C29-C39
48	G	620	LUT	C27-C28-C29-C39
48	G	621	LUT	C31-C32-C33-C40
48	R	620	LUT	C7-C8-C9-C19
48	Y	620	LUT	C27-C28-C29-C39
48	n	620	LUT	C31-C32-C33-C40
48	g	620	LUT	C31-C32-C33-C40
48	r	620	LUT	C7-C8-C9-C19
48	y	621	LUT	C31-C32-C33-C40
48	N1	620	LUT	C27-C28-C29-C39
48	R1	620	LUT	C27-C28-C29-C39
48	Y1	620	LUT	C27-C28-C29-C39
48	n1	620	LUT	C27-C28-C29-C39
48	r1	620	LUT	C7-C8-C9-C19
48	y1	620	LUT	C27-C28-C29-C39
49	R	621	XAT	C7-C8-C9-C19
49	r	622	XAT	C7-C8-C9-C19
49	Y1	622	XAT	C27-C28-C29-C39
49	n1	622	XAT	C27-C28-C29-C39
49	y1	622	XAT	C27-C28-C29-C39
50	S	622	NEX	C11-C12-C13-C20
35	a1	413	LMG	O6-C5-C6-O5
40	c1	520	DGD	O6E-C5E-C6E-O5E
55	R1	625	LMT	O5'-C5'-C6'-O6'
33	B	619	BCR	C21-C22-C23-C24
33	b	618	BCR	C7-C8-C9-C10
33	c	517	BCR	C17-C18-C19-C20
33	C1	515	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
33	C1	517	BCR	C21-C22-C23-C24
33	c1	516	BCR	C7-C8-C9-C10
37	B	620	C7Z	C31-C32-C33-C34
37	b	620	C7Z	C31-C32-C33-C34
37	B1	620	C7Z	C7-C8-C9-C10
37	b1	620	C7Z	C7-C8-C9-C10
48	R	620	LUT	C7-C8-C9-C10
48	r	620	LUT	C7-C8-C9-C10
31	n	611	CLA	C2A-CAA-CBA-CGA
31	r	609	CLA	C2A-CAA-CBA-CGA
31	N1	604	CLA	C2A-CAA-CBA-CGA
31	G1	613	CLA	C2A-CAA-CBA-CGA
31	b1	604	CLA	C2A-CAA-CBA-CGA
31	s1	614	CLA	C2A-CAA-CBA-CGA
32	A1	409	PHO	C2A-CAA-CBA-CGA
38	C	524	DGA	CB1-CB2-CB3-CB4
31	s1	603	CLA	O1D-CGD-O2D-CED
31	C	509	CLA	O1A-CGA-O2A-C1
31	a	410	CLA	O1A-CGA-O2A-C1
31	c	506	CLA	O1A-CGA-O2A-C1
31	n	611	CLA	O1A-CGA-O2A-C1
31	B1	617	CLA	O1A-CGA-O2A-C1
31	R1	604	CLA	O1A-CGA-O2A-C1
31	C	507	CLA	C3-C5-C6-C7
31	C	511	CLA	C3-C5-C6-C7
47	g1	601	CHL	C3-C5-C6-C7
34	B1	621	SQD	C8-C7-O47-C45
38	c	524	DGA	CB2-CB1-OG2-CG2
40	c	519	DGD	C2B-C1B-O2G-C2G
35	a	413	LMG	O1-C7-C8-O7
41	g	624	LHG	O7-C5-C6-O8
31	B	602	CLA	CBA-CGA-O2A-C1
31	b	612	CLA	CBA-CGA-O2A-C1
31	c1	504	CLA	CBA-CGA-O2A-C1
38	b	623	DGA	CA2-CA1-OG1-CG1
31	d	402	CLA	C15-C16-C17-C18
31	g	613	CLA	C8-C10-C11-C12
31	B1	604	CLA	C10-C11-C12-C13
31	B1	608	CLA	C10-C11-C12-C13
31	s1	610	CLA	C8-C10-C11-C12
41	c	625	LHG	C23-C24-C25-C26
31	A	406	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
31	B	602	CLA	C2-C1-O2A-CGA
31	B	613	CLA	C2-C1-O2A-CGA
31	C	506	CLA	C2-C1-O2A-CGA
31	C	509	CLA	C2-C1-O2A-CGA
31	C	512	CLA	C2-C1-O2A-CGA
31	N	603	CLA	C2-C1-O2A-CGA
31	N	611	CLA	C2-C1-O2A-CGA
31	G	614	CLA	C2-C1-O2A-CGA
31	R	609	CLA	C2-C1-O2A-CGA
31	Y	603	CLA	C2-C1-O2A-CGA
31	Y	608	CLA	C2-C1-O2A-CGA
31	Y	614	CLA	C2-C1-O2A-CGA
31	a	406	CLA	C2-C1-O2A-CGA
31	b	602	CLA	C2-C1-O2A-CGA
31	b	608	CLA	C2-C1-O2A-CGA
31	b	612	CLA	C2-C1-O2A-CGA
31	b	613	CLA	C2-C1-O2A-CGA
31	b	614	CLA	C2-C1-O2A-CGA
31	c	506	CLA	C2-C1-O2A-CGA
31	c	509	CLA	C2-C1-O2A-CGA
31	n	613	CLA	C2-C1-O2A-CGA
31	g	602	CLA	C2-C1-O2A-CGA
31	r	609	CLA	C2-C1-O2A-CGA
31	s	610	CLA	C2-C1-O2A-CGA
31	y	604	CLA	C2-C1-O2A-CGA
31	B1	603	CLA	C2-C1-O2A-CGA
31	B1	608	CLA	C2-C1-O2A-CGA
31	C1	502	CLA	C2-C1-O2A-CGA
31	C1	503	CLA	C2-C1-O2A-CGA
31	C1	510	CLA	C2-C1-O2A-CGA
31	N1	603	CLA	C2-C1-O2A-CGA
31	N1	613	CLA	C2-C1-O2A-CGA
31	G1	604	CLA	C2-C1-O2A-CGA
31	Y1	603	CLA	C2-C1-O2A-CGA
31	Y1	604	CLA	C2-C1-O2A-CGA
31	Y1	608	CLA	C2-C1-O2A-CGA
31	Y1	614	CLA	C2-C1-O2A-CGA
31	a1	406	CLA	C2-C1-O2A-CGA
31	a1	407	CLA	C2-C1-O2A-CGA
31	c1	502	CLA	C2-C1-O2A-CGA
31	c1	509	CLA	C2-C1-O2A-CGA
31	n1	611	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
31	r1	603	CLA	C2-C1-O2A-CGA
31	r1	608	CLA	C2-C1-O2A-CGA
31	y1	603	CLA	C2-C1-O2A-CGA
31	y1	608	CLA	C2-C1-O2A-CGA
40	C	519	DGD	O1A-C1A-O1G-C1G
31	N	603	CLA	O1D-CGD-O2D-CED
31	a	410	CLA	O1D-CGD-O2D-CED
31	r	610	CLA	O1D-CGD-O2D-CED
31	y	612	CLA	O1D-CGD-O2D-CED
31	A1	410	CLA	O1D-CGD-O2D-CED
31	n1	603	CLA	O1D-CGD-O2D-CED
31	B	611	CLA	C15-C16-C17-C18
31	N	602	CLA	C5-C6-C7-C8
31	G	602	CLA	C13-C15-C16-C17
31	S	613	CLA	C5-C6-C7-C8
31	a	410	CLA	C8-C10-C11-C12
31	b	603	CLA	C10-C11-C12-C13
31	y	604	CLA	C15-C16-C17-C18
31	B1	609	CLA	C5-C6-C7-C8
31	N1	602	CLA	C8-C10-C11-C12
31	N1	602	CLA	C10-C11-C12-C13
31	G1	603	CLA	C15-C16-C17-C18
31	b1	602	CLA	C8-C10-C11-C12
31	d1	403	CLA	C8-C10-C11-C12
31	s1	604	CLA	C5-C6-C7-C8
31	N1	612	CLA	O1D-CGD-O2D-CED
41	c	625	LHG	O1-C1-C2-O2
41	d	408	LHG	O1-C1-C2-O2
41	g1	624	LHG	O1-C1-C2-O2
31	B	614	CLA	C3-C5-C6-C7
31	N1	610	CLA	C3-C5-C6-C7
34	B1	621	SQD	C23-C24-C25-C26
35	b	622	LMG	C10-C11-C12-C13
35	h	102	LMG	C28-C29-C30-C31
40	B1	623	DGD	C1B-C2B-C3B-C4B
41	C	525	LHG	C23-C24-C25-C26
31	C	506	CLA	O1D-CGD-O2D-CED
31	R1	602	CLA	O1D-CGD-O2D-CED
31	d1	402	CLA	O1D-CGD-O2D-CED
31	B	603	CLA	C5-C6-C7-C8
31	B	613	CLA	C5-C6-C7-C8
31	b	602	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
31	B1	603	CLA	C10-C11-C12-C13
31	B1	604	CLA	C8-C10-C11-C12
31	B1	604	CLA	C15-C16-C17-C18
31	c	509	CLA	C11-C10-C8-C7
31	B1	602	CLA	C11-C10-C8-C7
31	r1	610	CLA	C11-C10-C8-C7
31	C1	503	CLA	CBA-CGA-O2A-C1
40	C	518	DGD	C2A-C1A-O1G-C1G
40	C1	518	DGD	O6E-C5E-C6E-O5E
31	Y1	613	CLA	C5-C6-C7-C8
31	g1	611	CLA	C15-C16-C17-C18
38	j1	101	DGA	CA1-CA2-CA3-CA4
41	C	525	LHG	C7-C8-C9-C10
41	Y	624	LHG	C7-C8-C9-C10
54	I1	102	4RF	C13-C14-C15-C16
33	A	411	BCR	C9-C10-C11-C12
33	C	517	BCR	C9-C10-C11-C12
33	c	516	BCR	C19-C20-C21-C22
33	B1	619	BCR	C19-C20-C21-C22
46	h	101	RRX	C9-C10-C11-C12
46	H1	101	RRX	C9-C10-C11-C12
46	h1	101	RRX	C15-C16-C17-C18
48	G	621	LUT	C33-C34-C35-C15
44	D1	405	PL9	C47-C48-C49-C51
34	B1	621	SQD	O49-C7-O47-C45
34	b1	626	SQD	O49-C7-O47-C45
38	B1	625	DGA	OB1-CB1-OG2-CG2
44	d	405	PL9	C39-C41-C42-C43
44	D1	405	PL9	C29-C31-C32-C33
44	D1	405	PL9	C39-C41-C42-C43
44	d1	405	PL9	C34-C36-C37-C38
44	d1	405	PL9	C39-C41-C42-C43
40	C1	520	DGD	C4E-C5E-C6E-O5E
31	a	410	CLA	C3-C5-C6-C7
31	B	609	CLA	C8-C10-C11-C12
31	B	614	CLA	C8-C10-C11-C12
31	C	502	CLA	C5-C6-C7-C8
31	n	602	CLA	C5-C6-C7-C8
31	y	611	CLA	C10-C11-C12-C13
31	S1	604	CLA	C5-C6-C7-C8
31	S1	611	CLA	C5-C6-C7-C8
31	Y1	611	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	c1	513	CLA	C8-C10-C11-C12
31	g1	603	CLA	C13-C15-C16-C17
31	s1	602	CLA	C10-C11-C12-C13
35	H	102	LMG	O6-C5-C6-O5
34	M1	101	SQD	C7-C8-C9-C10
35	a	413	LMG	C28-C29-C30-C31
35	A1	413	LMG	C10-C11-C12-C13
35	H1	102	LMG	C28-C29-C30-C31
38	B	625	DGA	CA1-CA2-CA3-CA4
38	J1	101	DGA	CB1-CB2-CB3-CB4
38	b1	625	DGA	CB1-CB2-CB3-CB4
40	c	520	DGD	C1A-C2A-C3A-C4A
41	D	408	LHG	C7-C8-C9-C10
41	L	101	LHG	C7-C8-C9-C10
41	c	625	LHG	C7-C8-C9-C10
41	C1	525	LHG	C23-C24-C25-C26
41	D1	410	LHG	C23-C24-C25-C26
41	N1	624	LHG	C7-C8-C9-C10
41	d1	408	LHG	C23-C24-C25-C26
54	K1	101	4RF	C41-C43-C44-C45
57	y1	626	PTY	C8-C11-C12-C13
31	B	602	CLA	O1A-CGA-O2A-C1
31	B	612	CLA	O1A-CGA-O2A-C1
31	b	614	CLA	O1A-CGA-O2A-C1
31	s	611	CLA	O1A-CGA-O2A-C1
31	B1	604	CLA	O1A-CGA-O2A-C1
31	N1	602	CLA	O1A-CGA-O2A-C1
34	m1	101	SQD	O10-C23-O48-C46
35	B1	622	LMG	O10-C28-O8-C9
40	c	518	DGD	O1A-C1A-O1G-C1G
41	g	624	LHG	C8-C7-O7-C5
57	Y1	626	PTY	C11-C8-O7-C6
31	C	501	CLA	O1D-CGD-O2D-CED
31	B	604	CLA	C13-C15-C16-C17
31	B	608	CLA	C13-C15-C16-C17
31	B	614	CLA	C5-C6-C7-C8
31	B	617	CLA	C5-C6-C7-C8
31	C	502	CLA	C8-C10-C11-C12
31	C	507	CLA	C15-C16-C17-C18
31	N	602	CLA	C15-C16-C17-C18
31	N	603	CLA	C10-C11-C12-C13
31	N	604	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
31	R	612	CLA	C10-C11-C12-C13
31	S	611	CLA	C15-C16-C17-C18
31	b	603	CLA	C13-C15-C16-C17
31	b	607	CLA	C10-C11-C12-C13
31	c	501	CLA	C5-C6-C7-C8
31	c	503	CLA	C15-C16-C17-C18
31	c	506	CLA	C5-C6-C7-C8
31	c	507	CLA	C15-C16-C17-C18
31	d	403	CLA	C10-C11-C12-C13
31	y	603	CLA	C15-C16-C17-C18
31	y	614	CLA	C10-C11-C12-C13
31	y	614	CLA	C13-C15-C16-C17
31	A1	406	CLA	C15-C16-C17-C18
31	B1	610	CLA	C5-C6-C7-C8
31	B1	610	CLA	C15-C16-C17-C18
31	B1	616	CLA	C8-C10-C11-C12
31	B1	617	CLA	C8-C10-C11-C12
31	D1	402	CLA	C15-C16-C17-C18
31	G1	602	CLA	C8-C10-C11-C12
31	Y1	602	CLA	C13-C15-C16-C17
31	Y1	610	CLA	C15-C16-C17-C18
31	Y1	612	CLA	C13-C15-C16-C17
31	b1	605	CLA	C5-C6-C7-C8
31	b1	608	CLA	C13-C15-C16-C17
31	b1	616	CLA	C13-C15-C16-C17
31	c1	503	CLA	C5-C6-C7-C8
31	c1	510	CLA	C15-C16-C17-C18
31	g1	603	CLA	C15-C16-C17-C18
31	r1	608	CLA	C10-C11-C12-C13
31	s1	609	CLA	C5-C6-C7-C8
31	s1	610	CLA	C10-C11-C12-C13
31	s1	611	CLA	C8-C10-C11-C12
31	y1	604	CLA	C8-C10-C11-C12
31	y1	610	CLA	C5-C6-C7-C8
31	y1	613	CLA	C8-C10-C11-C12
47	N1	606	CHL	C5-C6-C7-C8
31	B	605	CLA	C2A-CAA-CBA-CGA
31	N	614	CLA	C2A-CAA-CBA-CGA
31	G	613	CLA	C2A-CAA-CBA-CGA
31	R	603	CLA	C2A-CAA-CBA-CGA
31	R	609	CLA	C2A-CAA-CBA-CGA
31	S	614	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
31	b	602	CLA	C2A-CAA-CBA-CGA
31	b	605	CLA	C2A-CAA-CBA-CGA
31	b	612	CLA	C2A-CAA-CBA-CGA
31	n	604	CLA	C2A-CAA-CBA-CGA
31	g	613	CLA	C2A-CAA-CBA-CGA
31	r	602	CLA	C2A-CAA-CBA-CGA
31	A1	407	CLA	C2A-CAA-CBA-CGA
31	R1	609	CLA	C2A-CAA-CBA-CGA
31	S1	602	CLA	C2A-CAA-CBA-CGA
31	Y1	613	CLA	C2A-CAA-CBA-CGA
31	a1	407	CLA	C2A-CAA-CBA-CGA
31	b1	603	CLA	C2A-CAA-CBA-CGA
31	b1	611	CLA	C2A-CAA-CBA-CGA
31	c1	502	CLA	C2A-CAA-CBA-CGA
31	n1	604	CLA	C2A-CAA-CBA-CGA
31	g1	613	CLA	C2A-CAA-CBA-CGA
31	g1	614	CLA	C2A-CAA-CBA-CGA
31	r1	609	CLA	C2A-CAA-CBA-CGA
31	s1	602	CLA	C2A-CAA-CBA-CGA
31	s1	609	CLA	C2A-CAA-CBA-CGA
31	y1	608	CLA	C2A-CAA-CBA-CGA
47	n	609	CHL	C2A-CAA-CBA-CGA
47	g	606	CHL	C2A-CAA-CBA-CGA
47	y	605	CHL	C2A-CAA-CBA-CGA
47	Y1	605	CHL	C2A-CAA-CBA-CGA
47	Y1	607	CHL	C2A-CAA-CBA-CGA
47	n1	608	CHL	C2A-CAA-CBA-CGA
47	g1	601	CHL	C2A-CAA-CBA-CGA
47	y1	605	CHL	C2A-CAA-CBA-CGA
33	B1	619	BCR	C10-C11-C12-C13
50	r	623	NEX	C30-C31-C32-C33
50	Y1	623	NEX	C10-C11-C12-C13
31	A	410	CLA	C10-C11-C12-C13
31	B	604	CLA	C5-C6-C7-C8
31	B	612	CLA	C15-C16-C17-C18
31	C	503	CLA	C15-C16-C17-C18
31	C	507	CLA	C5-C6-C7-C8
31	G	603	CLA	C15-C16-C17-C18
31	R	609	CLA	C5-C6-C7-C8
31	Y	613	CLA	C8-C10-C11-C12
31	b	605	CLA	C15-C16-C17-C18
31	b	611	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
31	b	613	CLA	C10-C11-C12-C13
31	c	503	CLA	C10-C11-C12-C13
31	n	604	CLA	C10-C11-C12-C13
31	g	603	CLA	C5-C6-C7-C8
31	g	603	CLA	C10-C11-C12-C13
31	y	611	CLA	C8-C10-C11-C12
31	B1	608	CLA	C5-C6-C7-C8
31	B1	615	CLA	C5-C6-C7-C8
31	C1	513	CLA	C8-C10-C11-C12
31	N1	602	CLA	C13-C15-C16-C17
31	N1	613	CLA	C8-C10-C11-C12
31	G1	603	CLA	C8-C10-C11-C12
31	G1	611	CLA	C15-C16-C17-C18
31	R1	608	CLA	C5-C6-C7-C8
31	S1	602	CLA	C10-C11-C12-C13
31	S1	603	CLA	C13-C15-C16-C17
31	S1	611	CLA	C8-C10-C11-C12
31	a1	406	CLA	C5-C6-C7-C8
31	b1	610	CLA	C5-C6-C7-C8
31	c1	503	CLA	C8-C10-C11-C12
31	c1	503	CLA	C15-C16-C17-C18
31	c1	508	CLA	C5-C6-C7-C8
31	c1	508	CLA	C13-C15-C16-C17
31	c1	509	CLA	C15-C16-C17-C18
31	g1	613	CLA	C15-C16-C17-C18
31	s1	609	CLA	C8-C10-C11-C12
31	y1	603	CLA	C10-C11-C12-C13
31	y1	604	CLA	C5-C6-C7-C8
31	y1	611	CLA	C5-C6-C7-C8
34	b1	621	SQD	C23-C24-C25-C26
34	m1	101	SQD	C7-C8-C9-C10
35	C	521	LMG	C10-C11-C12-C13
38	c	524	DGA	CB1-CB2-CB3-CB4
40	c1	518	DGD	C1B-C2B-C3B-C4B
41	S	624	LHG	C23-C24-C25-C26
41	d	408	LHG	C7-C8-C9-C10
41	D1	408	LHG	C7-C8-C9-C10
41	G1	624	LHG	C7-C8-C9-C10
41	c1	525	LHG	C23-C24-C25-C26
41	d1	409	LHG	C7-C8-C9-C10
41	d1	409	LHG	C23-C24-C25-C26
41	d1	410	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
41	n1	624	LHG	C7-C8-C9-C10
52	b1	624	3PH	C31-C32-C33-C34
54	i1	101	4RF	C41-C43-C44-C45
31	c	506	CLA	O1D-CGD-O2D-CED
31	B	614	CLA	O1A-CGA-O2A-C1
31	G	603	CLA	O1A-CGA-O2A-C1
31	S	604	CLA	O1A-CGA-O2A-C1
31	b	604	CLA	O1A-CGA-O2A-C1
31	B1	602	CLA	O1A-CGA-O2A-C1
31	R1	602	CLA	O1A-CGA-O2A-C1
31	b1	604	CLA	O1A-CGA-O2A-C1
31	b1	613	CLA	O1A-CGA-O2A-C1
52	S1	626	3PH	O32-C31-O31-C3
31	c	511	CLA	C3-C5-C6-C7
34	m1	101	SQD	O5-C1-O6-C44
40	C1	519	DGD	O6E-C1E-O5D-C6D
41	y	624	LHG	C33-C34-C35-C36
55	R1	625	LMT	O5B-C5B-C6B-O6B
31	B	607	CLA	C10-C11-C12-C13
31	B	608	CLA	C8-C10-C11-C12
31	B	612	CLA	C8-C10-C11-C12
31	B	613	CLA	C13-C15-C16-C17
31	B	615	CLA	C8-C10-C11-C12
31	C	502	CLA	C15-C16-C17-C18
31	C	506	CLA	C5-C6-C7-C8
31	R	612	CLA	C8-C10-C11-C12
31	Y	610	CLA	C15-C16-C17-C18
31	Y	611	CLA	C5-C6-C7-C8
31	b	603	CLA	C8-C10-C11-C12
31	b	604	CLA	C5-C6-C7-C8
31	b	604	CLA	C8-C10-C11-C12
31	b	608	CLA	C5-C6-C7-C8
31	b	614	CLA	C5-C6-C7-C8
31	c	502	CLA	C8-C10-C11-C12
31	c	505	CLA	C13-C15-C16-C17
31	c	506	CLA	C8-C10-C11-C12
31	c	507	CLA	C5-C6-C7-C8
31	c	513	CLA	C10-C11-C12-C13
31	n	610	CLA	C15-C16-C17-C18
31	g	602	CLA	C13-C15-C16-C17
31	g	603	CLA	C8-C10-C11-C12
31	g	610	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	g	613	CLA	C15-C16-C17-C18
31	r	608	CLA	C5-C6-C7-C8
31	r	608	CLA	C10-C11-C12-C13
31	y	610	CLA	C13-C15-C16-C17
31	y	614	CLA	C15-C16-C17-C18
31	B1	602	CLA	C13-C15-C16-C17
31	B1	606	CLA	C5-C6-C7-C8
31	B1	608	CLA	C13-C15-C16-C17
31	B1	616	CLA	C13-C15-C16-C17
31	C1	504	CLA	C10-C11-C12-C13
31	N1	603	CLA	C13-C15-C16-C17
31	N1	613	CLA	C5-C6-C7-C8
31	G1	611	CLA	C10-C11-C12-C13
31	G1	611	CLA	C13-C15-C16-C17
31	R1	603	CLA	C5-C6-C7-C8
31	R1	603	CLA	C10-C11-C12-C13
31	S1	610	CLA	C5-C6-C7-C8
31	S1	610	CLA	C10-C11-C12-C13
31	Y1	611	CLA	C5-C6-C7-C8
31	Y1	614	CLA	C5-C6-C7-C8
31	a1	406	CLA	C15-C16-C17-C18
31	a1	410	CLA	C5-C6-C7-C8
31	b1	602	CLA	C10-C11-C12-C13
31	b1	604	CLA	C10-C11-C12-C13
31	b1	608	CLA	C8-C10-C11-C12
31	b1	611	CLA	C15-C16-C17-C18
31	b1	612	CLA	C13-C15-C16-C17
31	n1	603	CLA	C5-C6-C7-C8
31	n1	604	CLA	C8-C10-C11-C12
31	g1	602	CLA	C10-C11-C12-C13
31	r1	608	CLA	C8-C10-C11-C12
31	r1	609	CLA	C5-C6-C7-C8
31	r1	610	CLA	C5-C6-C7-C8
31	s1	609	CLA	C10-C11-C12-C13
31	s1	611	CLA	C13-C15-C16-C17
31	y1	604	CLA	C15-C16-C17-C18
31	y1	612	CLA	C10-C11-C12-C13
31	y1	613	CLA	C15-C16-C17-C18
41	C1	525	LHG	C33-C34-C35-C36
41	S1	624	LHG	C26-C27-C28-C29
41	d1	410	LHG	C29-C30-C31-C32
52	S1	626	3PH	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
54	k1	101	4RF	C46-C47-C48-C49
41	D	408	LHG	O2-C2-C3-O3
41	G1	624	LHG	O2-C2-C3-O3
31	A1	407	CLA	O1D-CGD-O2D-CED
31	C	503	CLA	CBA-CGA-O2A-C1
31	S1	603	CLA	CBA-CGA-O2A-C1
31	c1	503	CLA	CBA-CGA-O2A-C1
31	c1	510	CLA	CBA-CGA-O2A-C1
31	r1	612	CLA	CBA-CGA-O2A-C1
35	D	411	LMG	C35-C36-C37-C38
35	d	411	LMG	C35-C36-C37-C38
31	c	507	CLA	O1A-CGA-O2A-C1
31	a1	405	CLA	O1A-CGA-O2A-C1
31	c1	508	CLA	O1A-CGA-O2A-C1
40	C	520	DGD	O1A-C1A-O1G-C1G
34	b	621	SQD	C23-C24-C25-C26
41	D	408	LHG	C23-C24-C25-C26
41	D	410	LHG	C23-C24-C25-C26
41	G	630	LHG	C23-C24-C25-C26
41	n	624	LHG	C7-C8-C9-C10
41	L1	101	LHG	C23-C24-C25-C26
41	c1	525	LHG	C7-C8-C9-C10
41	g1	624	LHG	C7-C8-C9-C10
41	s1	624	LHG	C23-C24-C25-C26
31	B	602	CLA	C10-C11-C12-C13
31	B	612	CLA	C10-C11-C12-C13
31	D	403	CLA	C15-C16-C17-C18
31	N	613	CLA	C8-C10-C11-C12
31	Y	610	CLA	C5-C6-C7-C8
31	b	613	CLA	C15-C16-C17-C18
31	n	610	CLA	C5-C6-C7-C8
31	r	608	CLA	C8-C10-C11-C12
31	s	603	CLA	C15-C16-C17-C18
31	y	602	CLA	C10-C11-C12-C13
31	B1	611	CLA	C5-C6-C7-C8
31	N1	604	CLA	C10-C11-C12-C13
31	G1	613	CLA	C13-C15-C16-C17
31	Y1	604	CLA	C13-C15-C16-C17
31	g1	602	CLA	C13-C15-C16-C17
34	b1	621	SQD	O49-C7-O47-C45
38	c	524	DGA	OB1-CB1-OG2-CG2
35	b1	622	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
41	L	101	LHG	C11-C10-C9-C8
41	l	101	LHG	C11-C10-C9-C8
31	B	608	CLA	C3-C5-C6-C7
31	B	609	CLA	O1D-CGD-O2D-CED
31	A	410	CLA	C5-C6-C7-C8
31	B	607	CLA	C8-C10-C11-C12
31	B	617	CLA	C13-C15-C16-C17
31	C	513	CLA	C8-C10-C11-C12
31	R	602	CLA	C10-C11-C12-C13
31	Y	614	CLA	C8-C10-C11-C12
31	Y	614	CLA	C10-C11-C12-C13
31	b	614	CLA	C10-C11-C12-C13
31	c	511	CLA	C13-C15-C16-C17
31	g	610	CLA	C5-C6-C7-C8
31	A1	405	CLA	C5-C6-C7-C8
31	B1	614	CLA	C8-C10-C11-C12
31	c1	503	CLA	C13-C15-C16-C17
31	r1	602	CLA	C8-C10-C11-C12
31	s1	611	CLA	C15-C16-C17-C18
31	b	612	CLA	O1A-CGA-O2A-C1
31	b	604	CLA	C2-C3-C5-C6
51	S1	625	LPX	O5-C4-C5-O6
35	d1	411	LMG	C4-C5-C6-O5
41	G1	624	LHG	C23-C24-C25-C26
52	s1	626	3PH	C31-C32-C33-C34
54	I1	102	4RF	C22-C24-C25-C26
31	B	614	CLA	C15-C16-C17-C18
31	B	616	CLA	C15-C16-C17-C18
31	N	604	CLA	C10-C11-C12-C13
31	R	602	CLA	C8-C10-C11-C12
31	Y	610	CLA	C13-C15-C16-C17
31	Y	614	CLA	C5-C6-C7-C8
31	b	602	CLA	C10-C11-C12-C13
31	b	615	CLA	C8-C10-C11-C12
31	b	617	CLA	C15-C16-C17-C18
31	c	509	CLA	C15-C16-C17-C18
31	g	613	CLA	C10-C11-C12-C13
31	r	612	CLA	C10-C11-C12-C13
31	s	610	CLA	C5-C6-C7-C8
31	y	604	CLA	C8-C10-C11-C12
31	y	612	CLA	C15-C16-C17-C18
31	A1	410	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
31	B1	603	CLA	C5-C6-C7-C8
31	b1	613	CLA	C10-C11-C12-C13
31	b1	614	CLA	C15-C16-C17-C18
31	d1	402	CLA	C15-C16-C17-C18
31	n1	603	CLA	C8-C10-C11-C12
31	y1	610	CLA	C8-C10-C11-C12
31	C1	510	CLA	CBA-CGA-O2A-C1
31	R1	610	CLA	CBA-CGA-O2A-C1
31	g1	603	CLA	CBA-CGA-O2A-C1
31	g1	610	CLA	CBA-CGA-O2A-C1
31	b1	605	CLA	CBD-CGD-O2D-CED
34	M1	101	SQD	C8-C7-O47-C45
34	b1	621	SQD	C8-C7-O47-C45
35	C1	521	LMG	C11-C10-O7-C8
35	C1	523	LMG	C11-C10-O7-C8
41	S1	624	LHG	C8-C7-O7-C5
31	C1	503	CLA	O1A-CGA-O2A-C1
31	c1	504	CLA	O1A-CGA-O2A-C1
38	b	623	DGA	OA1-CA1-OG1-CG1
31	b	608	CLA	C15-C16-C17-C18
31	Y1	614	CLA	C3-C5-C6-C7
31	c1	508	CLA	C3-C5-C6-C7
47	G1	608	CHL	C2A-CAA-CBA-CGA
33	A1	411	BCR	C9-C10-C11-C12
33	C1	517	BCR	C9-C10-C11-C12
37	B	620	C7Z	C9-C10-C11-C12
37	b	620	C7Z	C29-C30-C31-C32
50	S	622	NEX	C13-C14-C15-C35
31	B	604	CLA	C10-C11-C12-C13
31	Y	611	CLA	C10-C11-C12-C13
31	c	505	CLA	C10-C11-C12-C13
31	B1	607	CLA	C10-C11-C12-C13
31	C1	512	CLA	C15-C16-C17-C18
34	M1	101	SQD	O49-C7-O47-C45
35	C1	521	LMG	O9-C10-O7-C8
35	C1	523	LMG	O9-C10-O7-C8
40	c	519	DGD	O1B-C1B-O2G-C2G
41	g	624	LHG	O9-C7-O7-C5
57	Y1	626	PTY	O10-C8-O7-C6
41	c	625	LHG	C1-C2-C3-O3
41	y	624	LHG	C1-C2-C3-O3
41	S1	624	LHG	C1-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
31	R	602	CLA	C2A-CAA-CBA-CGA
31	S	609	CLA	C2A-CAA-CBA-CGA
31	g	614	CLA	C2A-CAA-CBA-CGA
31	s	617	CLA	C2A-CAA-CBA-CGA
31	B1	603	CLA	C2A-CAA-CBA-CGA
31	C1	507	CLA	C2A-CAA-CBA-CGA
31	G1	614	CLA	C2A-CAA-CBA-CGA
31	y1	610	CLA	C2A-CAA-CBA-CGA
47	G	605	CHL	C2A-CAA-CBA-CGA
47	Y1	606	CHL	C2A-CAA-CBA-CGA
31	B	613	CLA	CBA-CGA-O2A-C1
31	C	507	CLA	CBA-CGA-O2A-C1
31	R	602	CLA	CBA-CGA-O2A-C1
31	R	604	CLA	CBA-CGA-O2A-C1
31	Y	602	CLA	CBA-CGA-O2A-C1
31	g	610	CLA	CBA-CGA-O2A-C1
31	Y1	610	CLA	CBA-CGA-O2A-C1
31	b1	611	CLA	CBA-CGA-O2A-C1
31	b1	612	CLA	CBA-CGA-O2A-C1
31	y1	614	CLA	CBA-CGA-O2A-C1
41	d1	410	LHG	C24-C23-O8-C6
51	S	625	LPX	C7-C6-O6-C5
31	B	609	CLA	C5-C6-C7-C8
31	B	614	CLA	C13-C15-C16-C17
31	C	504	CLA	C8-C10-C11-C12
31	C	506	CLA	C8-C10-C11-C12
31	C	506	CLA	C10-C11-C12-C13
31	C	507	CLA	C13-C15-C16-C17
31	S	604	CLA	C5-C6-C7-C8
31	Y	604	CLA	C8-C10-C11-C12
31	Y	612	CLA	C10-C11-C12-C13
31	b	617	CLA	C5-C6-C7-C8
31	c	506	CLA	C13-C15-C16-C17
31	c	508	CLA	C15-C16-C17-C18
31	g	610	CLA	C15-C16-C17-C18
31	y	612	CLA	C5-C6-C7-C8
31	B1	602	CLA	C15-C16-C17-C18
31	C1	506	CLA	C5-C6-C7-C8
31	D1	403	CLA	C8-C10-C11-C12
31	N1	603	CLA	C5-C6-C7-C8
31	G1	602	CLA	C13-C15-C16-C17
31	R1	612	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	Y1	604	CLA	C8-C10-C11-C12
31	Y1	610	CLA	C8-C10-C11-C12
31	Y1	611	CLA	C15-C16-C17-C18
31	Y1	613	CLA	C10-C11-C12-C13
31	b1	605	CLA	C8-C10-C11-C12
31	b1	607	CLA	C8-C10-C11-C12
31	b1	608	CLA	C15-C16-C17-C18
31	c1	504	CLA	C10-C11-C12-C13
31	c1	505	CLA	C10-C11-C12-C13
31	g1	611	CLA	C5-C6-C7-C8
31	y1	603	CLA	C15-C16-C17-C18
31	y1	610	CLA	C13-C15-C16-C17
47	n1	609	CHL	C15-C16-C17-C18
54	k1	101	4RF	C48-C49-C50-C51
32	a	408	PHO	O1D-CGD-O2D-CED
31	A	406	CLA	CBD-CGD-O2D-CED
41	c1	525	LHG	O10-C23-O8-C6
31	c1	512	CLA	C3-C5-C6-C7
35	h1	102	LMG	C15-C16-C17-C18
41	D	410	LHG	C7-C8-C9-C10
31	B	610	CLA	C15-C16-C17-C18
31	C	507	CLA	C8-C10-C11-C12
31	C	509	CLA	C13-C15-C16-C17
31	R	608	CLA	C5-C6-C7-C8
31	S	602	CLA	C10-C11-C12-C13
31	b	604	CLA	C15-C16-C17-C18
31	b	614	CLA	C15-C16-C17-C18
31	c	508	CLA	C8-C10-C11-C12
31	d	403	CLA	C15-C16-C17-C18
31	C1	507	CLA	C13-C15-C16-C17
31	N1	603	CLA	C8-C10-C11-C12
31	Y1	603	CLA	C8-C10-C11-C12
31	b1	602	CLA	C13-C15-C16-C17
31	b1	607	CLA	C13-C15-C16-C17
31	c1	505	CLA	C5-C6-C7-C8
31	n1	602	CLA	C5-C6-C7-C8
31	n1	603	CLA	C13-C15-C16-C17
47	g1	607	CHL	C5-C6-C7-C8
31	B	602	CLA	C5-C6-C7-C8
31	C	503	CLA	C5-C6-C7-C8
31	C	505	CLA	C13-C15-C16-C17
31	C	509	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	N	603	CLA	C5-C6-C7-C8
31	G	613	CLA	C13-C15-C16-C17
31	R	608	CLA	C8-C10-C11-C12
31	Y	602	CLA	C13-C15-C16-C17
31	b	616	CLA	C5-C6-C7-C8
31	c	506	CLA	C10-C11-C12-C13
31	B1	608	CLA	C8-C10-C11-C12
31	B1	612	CLA	C15-C16-C17-C18
31	B1	613	CLA	C10-C11-C12-C13
31	C1	505	CLA	C8-C10-C11-C12
31	C1	508	CLA	C10-C11-C12-C13
31	C1	508	CLA	C13-C15-C16-C17
31	C1	510	CLA	C15-C16-C17-C18
31	R1	602	CLA	C10-C11-C12-C13
31	R1	609	CLA	C10-C11-C12-C13
31	Y1	612	CLA	C5-C6-C7-C8
31	b1	615	CLA	C10-C11-C12-C13
31	c1	506	CLA	C5-C6-C7-C8
31	r1	612	CLA	C10-C11-C12-C13
31	s1	613	CLA	C5-C6-C7-C8
31	G1	603	CLA	CBA-CGA-O2A-C1
31	Y1	614	CLA	CBA-CGA-O2A-C1
41	d	410	LHG	C24-C23-O8-C6
51	s1	625	LPX	C7-C6-O6-C5
31	c	513	CLA	C4-C3-C5-C6
31	n	603	CLA	C4-C3-C5-C6
47	n1	601	CHL	C4-C3-C5-C6
44	D1	405	PL9	C18-C19-C21-C22
47	n1	601	CHL	C2-C3-C5-C6
42	C	527	LMK	O7-C10-C11-C12
42	c	627	LMK	O8-C28-C29-C30
53	y	625	SPH	O3-C3-C4-C5
31	b	608	CLA	C8-C10-C11-C12
31	R1	608	CLA	C10-C11-C12-C13
56	R1	626	ERG	C13-C17-C20-C22
56	R1	626	ERG	C16-C17-C20-C22
56	r1	626	ERG	C13-C17-C20-C22
35	A1	413	LMG	C11-C10-O7-C8
41	D	408	LHG	C8-C7-O7-C5
41	D1	409	LHG	C8-C7-O7-C5
41	N1	624	LHG	C8-C7-O7-C5
41	G1	624	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
31	D	402	CLA	C6-C7-C8-C9
31	r1	608	CLA	C11-C10-C8-C9
51	S1	625	LPX	C3-C4-C5-O6
31	d	402	CLA	O1D-CGD-O2D-CED
31	s	614	CLA	O1D-CGD-O2D-CED
41	s	624	LHG	C30-C31-C32-C33
35	A1	413	LMG	O9-C10-O7-C8
41	D	408	LHG	O9-C7-O7-C5
41	D1	409	LHG	O9-C7-O7-C5
41	G1	624	LHG	O9-C7-O7-C5
41	S1	624	LHG	O9-C7-O7-C5
34	B1	621	SQD	C2-C1-O6-C44
34	m1	101	SQD	C2-C1-O6-C44
35	A1	413	LMG	C2-C1-O1-C7
35	b1	622	LMG	C2-C1-O1-C7
35	c1	523	LMG	C2-C1-O1-C7
40	C1	519	DGD	C2E-C1E-O5D-C6D
40	c1	519	DGD	C2E-C1E-O5D-C6D
31	c	507	CLA	C13-C15-C16-C17
31	B1	608	CLA	C15-C16-C17-C18
31	b1	617	CLA	C5-C6-C7-C8
34	b1	626	SQD	C23-C24-C25-C26
31	B1	606	CLA	CBA-CGA-O2A-C1
41	C	525	LHG	C24-C23-O8-C6
41	C1	525	LHG	C24-C23-O8-C6
41	D1	410	LHG	C24-C23-O8-C6
54	i1	101	4RF	C43-C41-O40-C39
31	B	604	CLA	C16-C17-C18-C20
31	S	613	CLA	C6-C7-C8-C10
31	s	613	CLA	C6-C7-C8-C10
31	C1	507	CLA	C16-C17-C18-C20
31	y1	614	CLA	C16-C17-C18-C19
41	S	624	LHG	C30-C31-C32-C33
41	c1	525	LHG	C33-C34-C35-C36
31	B	616	CLA	C5-C6-C7-C8
31	c	507	CLA	C8-C10-C11-C12
31	C	507	CLA	O1A-CGA-O2A-C1
31	R1	610	CLA	O1A-CGA-O2A-C1
40	C	518	DGD	O1A-C1A-O1G-C1G
33	c	514	BCR	C11-C10-C9-C34
49	R	621	XAT	C40-C33-C34-C35
49	r	622	XAT	C20-C13-C14-C15

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Mol	Chain	Res	Type	Atoms
49	r	622	XAT	C40-C33-C34-C35
49	R1	621	XAT	C20-C13-C14-C15
50	G	623	NEX	C39-C29-C30-C31
50	R	622	NEX	C39-C29-C30-C31
50	R	622	NEX	C40-C33-C34-C35
50	S	622	NEX	C40-C33-C34-C35
50	r	623	NEX	C20-C13-C14-C15
50	r	623	NEX	C39-C29-C30-C31
50	N1	623	NEX	C39-C29-C30-C31
50	R1	622	NEX	C39-C29-C30-C31
50	Y1	623	NEX	C11-C10-C9-C19
50	Y1	623	NEX	C20-C13-C14-C15
50	g1	623	NEX	C39-C29-C30-C31
50	r1	622	NEX	C39-C29-C30-C31
50	r1	622	NEX	C40-C33-C34-C35
50	s1	623	NEX	C39-C29-C30-C31
50	y1	623	NEX	C39-C29-C30-C31
31	n	604	CLA	C3-C5-C6-C7
54	k1	101	4RF	C41-C43-C44-C45
41	d	410	LHG	C25-C26-C27-C28
31	B	606	CLA	C15-C16-C17-C18
31	Y	611	CLA	C8-C10-C11-C12
31	y	610	CLA	C10-C11-C12-C13
31	C1	508	CLA	C15-C16-C17-C18
31	d1	402	CLA	C13-C15-C16-C17
47	G1	607	CHL	C5-C6-C7-C8
33	C	514	BCR	C11-C12-C13-C35
33	c	515	BCR	C7-C8-C9-C34
33	B1	618	BCR	C37-C22-C23-C24
33	C1	514	BCR	C36-C18-C19-C20
33	C1	516	BCR	C37-C22-C23-C24
33	C1	517	BCR	C7-C8-C9-C34
33	a1	411	BCR	C7-C8-C9-C34
33	c1	515	BCR	C7-C8-C9-C34
33	c1	515	BCR	C11-C12-C13-C35
41	C1	525	LHG	C2-C3-O3-P
46	H1	101	RRX	C7-C8-C9-C34
46	h1	101	RRX	C11-C12-C13-C35
49	Y	622	XAT	C27-C28-C29-C39
49	y	622	XAT	C11-C12-C13-C20
50	s	623	NEX	C11-C12-C13-C20
33	c1	515	BCR	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
46	h	101	RRX	C17-C18-C19-C20
46	H1	101	RRX	C7-C8-C9-C10
46	h1	101	RRX	C11-C12-C13-C14
48	y	621	LUT	C31-C32-C33-C34
48	n1	620	LUT	C27-C28-C29-C30
49	R	621	XAT	C7-C8-C9-C10
49	Y1	622	XAT	C27-C28-C29-C30
31	g	610	CLA	O1A-CGA-O2A-C1
31	b1	611	CLA	O1A-CGA-O2A-C1
31	C	505	CLA	C2A-CAA-CBA-CGA
31	N	602	CLA	C2A-CAA-CBA-CGA
31	N	612	CLA	C2A-CAA-CBA-CGA
31	R	612	CLA	C2A-CAA-CBA-CGA
31	S	604	CLA	C2A-CAA-CBA-CGA
31	S	613	CLA	C2A-CAA-CBA-CGA
31	Y	613	CLA	C2A-CAA-CBA-CGA
31	a	407	CLA	C2A-CAA-CBA-CGA
31	b	617	CLA	C2A-CAA-CBA-CGA
31	c	505	CLA	C2A-CAA-CBA-CGA
31	c	512	CLA	C2A-CAA-CBA-CGA
31	g	604	CLA	C2A-CAA-CBA-CGA
31	r	612	CLA	C2A-CAA-CBA-CGA
31	y	610	CLA	C2A-CAA-CBA-CGA
31	B1	602	CLA	C2A-CAA-CBA-CGA
31	B1	613	CLA	C2A-CAA-CBA-CGA
31	R1	602	CLA	C2A-CAA-CBA-CGA
31	R1	610	CLA	C2A-CAA-CBA-CGA
31	Y1	602	CLA	C2A-CAA-CBA-CGA
31	b1	613	CLA	C2A-CAA-CBA-CGA
31	b1	617	CLA	C2A-CAA-CBA-CGA
31	n1	602	CLA	C2A-CAA-CBA-CGA
31	g1	602	CLA	C2A-CAA-CBA-CGA
31	r1	610	CLA	C2A-CAA-CBA-CGA
31	y1	602	CLA	C2A-CAA-CBA-CGA
47	Y	607	CHL	C2A-CAA-CBA-CGA
47	n	606	CHL	C2A-CAA-CBA-CGA
47	y	607	CHL	C2A-CAA-CBA-CGA
31	A	406	CLA	C5-C6-C7-C8
31	B	602	CLA	C13-C15-C16-C17
31	B	614	CLA	C10-C11-C12-C13
31	c1	506	CLA	C15-C16-C17-C18
31	r1	610	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
51	s1	625	LPX	O5-C4-C5-O6
41	C	525	LHG	O1-C1-C2-C3
41	D	409	LHG	O1-C1-C2-C3
41	L	101	LHG	O1-C1-C2-C3
41	N	624	LHG	O1-C1-C2-C3
41	S	624	LHG	O1-C1-C2-C3
41	Y	624	LHG	O1-C1-C2-C3
41	d	409	LHG	O1-C1-C2-C3
41	l	101	LHG	O1-C1-C2-C3
41	n	624	LHG	O1-C1-C2-C3
41	C1	525	LHG	O1-C1-C2-C3
41	D1	409	LHG	O1-C1-C2-C3
41	G1	624	LHG	O1-C1-C2-C3
41	Y1	624	LHG	O1-C1-C2-C3
41	c1	525	LHG	O1-C1-C2-C3
41	g1	624	LHG	O1-C1-C2-C3
38	C1	524	DGA	CB1-CB2-CB3-CB4
33	b1	619	BCR	C19-C20-C21-C22
48	n1	621	LUT	C29-C30-C31-C32
48	g1	621	LUT	C29-C30-C31-C32
31	B	617	CLA	C16-C17-C18-C19
31	C	513	CLA	C16-C17-C18-C20
31	G	602	CLA	C16-C17-C18-C19
31	R	603	CLA	C11-C12-C13-C15
31	S	602	CLA	C11-C12-C13-C15
31	S	604	CLA	C6-C7-C8-C9
31	Y	602	CLA	C16-C17-C18-C20
31	c	504	CLA	C16-C17-C18-C20
31	c	507	CLA	C16-C17-C18-C20
31	c	513	CLA	C16-C17-C18-C19
31	r	609	CLA	C11-C12-C13-C15
31	s	613	CLA	C6-C7-C8-C9
31	y	610	CLA	C16-C17-C18-C20
31	B1	609	CLA	C16-C17-C18-C19
31	C1	501	CLA	C16-C17-C18-C19
31	b1	602	CLA	C16-C17-C18-C20
31	c1	501	CLA	C16-C17-C18-C20
31	c1	507	CLA	C16-C17-C18-C19
31	n1	602	CLA	C16-C17-C18-C19
54	I1	102	4RF	C33-C34-C35-C36
54	i1	101	4RF	C33-C34-C35-C36
31	C	503	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	R	602	CLA	O1A-CGA-O2A-C1
31	S1	603	CLA	O1A-CGA-O2A-C1
31	c1	503	CLA	O1A-CGA-O2A-C1
31	r1	612	CLA	O1A-CGA-O2A-C1
31	B	607	CLA	C13-C15-C16-C17
31	b	614	CLA	C8-C10-C11-C12
31	N1	603	CLA	C15-C16-C17-C18
31	Y1	612	CLA	C10-C11-C12-C13
31	a1	405	CLA	C10-C11-C12-C13
31	r1	610	CLA	C8-C10-C11-C12
33	C	515	BCR	C11-C10-C9-C8
33	c	514	BCR	C11-C10-C9-C8
49	R	621	XAT	C32-C33-C34-C35
49	r	622	XAT	C12-C13-C14-C15
49	r	622	XAT	C32-C33-C34-C35
49	R1	621	XAT	C12-C13-C14-C15
50	G	623	NEX	C28-C29-C30-C31
50	R	622	NEX	C28-C29-C30-C31
50	R	622	NEX	C32-C33-C34-C35
50	S	622	NEX	C32-C33-C34-C35
50	r	623	NEX	C12-C13-C14-C15
50	r	623	NEX	C28-C29-C30-C31
50	N1	623	NEX	C28-C29-C30-C31
50	R1	622	NEX	C28-C29-C30-C31
50	Y1	623	NEX	C11-C10-C9-C8
50	Y1	623	NEX	C12-C13-C14-C15
50	g1	623	NEX	C28-C29-C30-C31
50	r1	622	NEX	C28-C29-C30-C31
50	r1	622	NEX	C32-C33-C34-C35
50	s1	623	NEX	C28-C29-C30-C31
50	y1	623	NEX	C28-C29-C30-C31
38	C1	524	DGA	CCB-CDB-CEB-CFB
41	C1	525	LHG	O9-C7-O7-C5
41	N1	624	LHG	O9-C7-O7-C5
34	c	626	SQD	O5-C1-O6-C44
34	a1	412	SQD	O5-C1-O6-C44
35	c1	523	LMG	O6-C1-O1-C7
40	c1	519	DGD	O6E-C1E-O5D-C6D
41	Y	624	LHG	C8-C7-O7-C5
41	d	410	LHG	C8-C7-O7-C5
31	r1	603	CLA	C8-C10-C11-C12
40	B1	623	DGD	C4D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
31	C	508	CLA	O1D-CGD-O2D-CED
31	b1	612	CLA	O1A-CGA-O2A-C1
54	K1	101	4RF	C15-C16-O18-C19
31	G	613	CLA	C8-C10-C11-C12
31	S	609	CLA	C10-C11-C12-C13
31	Y	612	CLA	C8-C10-C11-C12
31	B1	611	CLA	C15-C16-C17-C18
31	n1	613	CLA	C13-C15-C16-C17
31	y1	602	CLA	C13-C15-C16-C17
34	C	526	SQD	C7-C8-C9-C10
41	d	410	LHG	C7-C8-C9-C10
31	B	603	CLA	C2-C1-O2A-CGA
31	C	503	CLA	C2-C1-O2A-CGA
31	N	613	CLA	C2-C1-O2A-CGA
31	N	614	CLA	C2-C1-O2A-CGA
31	G	604	CLA	C2-C1-O2A-CGA
31	R	604	CLA	C2-C1-O2A-CGA
31	S	603	CLA	C2-C1-O2A-CGA
31	S	609	CLA	C2-C1-O2A-CGA
31	S	614	CLA	C2-C1-O2A-CGA
31	b	603	CLA	C2-C1-O2A-CGA
31	b	607	CLA	C2-C1-O2A-CGA
31	b	611	CLA	C2-C1-O2A-CGA
31	g	614	CLA	C2-C1-O2A-CGA
31	y	603	CLA	C2-C1-O2A-CGA
31	B1	611	CLA	C2-C1-O2A-CGA
31	B1	616	CLA	C2-C1-O2A-CGA
31	B1	617	CLA	C2-C1-O2A-CGA
31	C1	507	CLA	C2-C1-O2A-CGA
31	G1	611	CLA	C2-C1-O2A-CGA
31	G1	613	CLA	C2-C1-O2A-CGA
31	R1	612	CLA	C2-C1-O2A-CGA
31	S1	614	CLA	C2-C1-O2A-CGA
31	a1	405	CLA	C2-C1-O2A-CGA
31	c1	503	CLA	C2-C1-O2A-CGA
31	n1	603	CLA	C2-C1-O2A-CGA
31	g1	611	CLA	C2-C1-O2A-CGA
31	g1	613	CLA	C2-C1-O2A-CGA
31	s1	614	CLA	C2-C1-O2A-CGA
31	y1	604	CLA	C2-C1-O2A-CGA
31	B	604	CLA	C16-C17-C18-C19
31	C	504	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
31	C	513	CLA	C16-C17-C18-C19
31	R	603	CLA	C11-C12-C13-C14
31	R	608	CLA	C11-C12-C13-C15
31	S	602	CLA	C11-C12-C13-C14
31	S	604	CLA	C6-C7-C8-C10
31	S	609	CLA	C11-C12-C13-C14
31	Y	602	CLA	C16-C17-C18-C19
31	n	602	CLA	C16-C17-C18-C20
31	n	604	CLA	C16-C17-C18-C20
31	g	602	CLA	C16-C17-C18-C20
31	r	609	CLA	C11-C12-C13-C14
31	y	604	CLA	C16-C17-C18-C20
31	y	610	CLA	C16-C17-C18-C19
31	C1	507	CLA	C16-C17-C18-C19
31	C1	513	CLA	C16-C17-C18-C19
31	D1	402	CLA	C16-C17-C18-C19
31	R1	608	CLA	C11-C12-C13-C14
31	S1	602	CLA	C11-C12-C13-C14
31	Y1	614	CLA	C16-C17-C18-C19
31	b1	602	CLA	C16-C17-C18-C19
31	n1	602	CLA	C16-C17-C18-C20
47	s1	608	CHL	C11-C12-C13-C14
31	B	613	CLA	O1A-CGA-O2A-C1
31	Y1	610	CLA	O1A-CGA-O2A-C1
31	y1	614	CLA	O1A-CGA-O2A-C1
31	c	509	CLA	C8-C10-C11-C12
31	s	610	CLA	C10-C11-C12-C13
31	G1	602	CLA	C15-C16-C17-C18
31	b1	610	CLA	C13-C15-C16-C17
47	s	608	CHL	C5-C6-C7-C8
35	H1	102	LMG	C30-C31-C32-C33
38	C1	524	DGA	CA9-CAA-CBA-CCA
38	J1	101	DGA	CA6-CA7-CA8-CA9
40	C	519	DGD	C2B-C3B-C4B-C5B
41	d	408	LHG	C25-C26-C27-C28
41	y	624	LHG	C11-C10-C9-C8
42	C1	527	LMK	C12-C13-C14-C15
50	r1	622	NEX	C14-C15-C35-C34
34	C	526	SQD	C32-C33-C34-C35
35	C	521	LMG	C29-C30-C31-C32
35	W1	201	LMG	C32-C33-C34-C35
40	c1	520	DGD	CCB-CDB-CEB-CFB

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Mol	Chain	Res	Type	Atoms
41	c	625	LHG	C34-C35-C36-C37
41	n	624	LHG	C13-C14-C15-C16
41	C1	525	LHG	C29-C30-C31-C32
41	D1	408	LHG	C30-C31-C32-C33
41	L1	101	LHG	C28-C29-C30-C31
41	Y1	624	LHG	C29-C30-C31-C32
41	d1	409	LHG	C25-C26-C27-C28
52	S	626	3PH	C22-C23-C24-C25
52	T1	101	3PH	C28-C29-C2A-C2B
52	S1	626	3PH	C24-C25-C26-C27
52	t1	101	3PH	C35-C36-C37-C38
53	Y1	625	SPH	C14-C15-C16-C17
55	R1	625	LMT	C4-C5-C6-C7
31	C1	508	CLA	O1D-CGD-O2D-CED
41	D1	409	LHG	C7-C8-C9-C10
31	B1	615	CLA	C10-C11-C12-C13
38	b	623	DGA	CDB-CEB-CFB-CGB
38	J1	101	DGA	CB7-CB8-CB9-CAB
41	l	101	LHG	C11-C12-C13-C14
52	S	626	3PH	C25-C26-C27-C28
31	C1	510	CLA	O1A-CGA-O2A-C1
31	c1	510	CLA	O1A-CGA-O2A-C1
31	g1	610	CLA	O1A-CGA-O2A-C1
31	Y	604	CLA	O1D-CGD-O2D-CED
35	B	622	LMG	C15-C16-C17-C18
35	c	521	LMG	C11-C12-C13-C14
38	b	623	DGA	CA6-CA7-CA8-CA9
38	c	524	DGA	CB4-CB5-CB6-CB7
38	c	524	DGA	CB5-CB6-CB7-CB8
38	J1	101	DGA	CB3-CB4-CB5-CB6
40	C1	520	DGD	C4B-C5B-C6B-C7B
41	d	408	LHG	C33-C34-C35-C36
41	l	101	LHG	C25-C26-C27-C28
41	D1	408	LHG	C29-C30-C31-C32
52	S	626	3PH	C35-C36-C37-C38
52	S	626	3PH	C3E-C3F-C3G-C3H
52	t1	101	3PH	C27-C28-C29-C2A
52	s1	626	3PH	C2A-C2B-C2C-C2D
53	y1	625	SPH	C11-C10-C9-C8
55	r1	625	LMT	C11-C10-C9-C8
41	D	409	LHG	O1-C1-C2-O2
41	L	101	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
41	S	624	LHG	O1-C1-C2-O2
41	d	409	LHG	O1-C1-C2-O2
41	l	101	LHG	O1-C1-C2-O2
41	y	624	LHG	O1-C1-C2-O2
41	C1	525	LHG	O1-C1-C2-O2
41	D1	408	LHG	O1-C1-C2-O2
41	L1	101	LHG	O1-C1-C2-O2
41	N1	624	LHG	O1-C1-C2-O2
41	G1	624	LHG	O1-C1-C2-O2
41	S1	624	LHG	O1-C1-C2-O2
41	d1	409	LHG	O1-C1-C2-O2
41	s1	624	LHG	O1-C1-C2-O2
41	y1	624	LHG	O1-C1-C2-O2
34	b	621	SQD	C30-C31-C32-C33
34	C1	526	SQD	C11-C10-C9-C8
35	H1	102	LMG	C13-C14-C15-C16
38	B	625	DGA	CB7-CB8-CB9-CAB
38	j1	101	DGA	CA2-CA3-CA4-CA5
40	c	519	DGD	C9B-CAB-CBB-CCB
41	d	408	LHG	C28-C29-C30-C31
41	D1	408	LHG	C28-C29-C30-C31
41	S1	624	LHG	C28-C29-C30-C31
57	Y1	626	PTY	C40-C41-C42-C43
31	B	603	CLA	C4B-C3B-CAB-CBB
31	B	605	CLA	C4B-C3B-CAB-CBB
31	B	609	CLA	C4B-C3B-CAB-CBB
31	C	505	CLA	C4B-C3B-CAB-CBB
31	N	610	CLA	C4B-C3B-CAB-CBB
31	N	611	CLA	C4B-C3B-CAB-CBB
31	N	612	CLA	C4B-C3B-CAB-CBB
31	N	614	CLA	C4B-C3B-CAB-CBB
31	G	610	CLA	C4B-C3B-CAB-CBB
31	G	611	CLA	C4B-C3B-CAB-CBB
31	G	612	CLA	C4B-C3B-CAB-CBB
31	R	603	CLA	C4B-C3B-CAB-CBB
31	S	604	CLA	C4B-C3B-CAB-CBB
31	S	613	CLA	C4B-C3B-CAB-CBB
31	Y	603	CLA	C4B-C3B-CAB-CBB
31	Y	604	CLA	C4B-C3B-CAB-CBB
31	Y	608	CLA	C4B-C3B-CAB-CBB
31	Y	611	CLA	C4B-C3B-CAB-CBB
31	Y	612	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	a	407	CLA	C4B-C3B-CAB-CBB
31	b	602	CLA	C4B-C3B-CAB-CBB
31	b	603	CLA	C4B-C3B-CAB-CBB
31	b	604	CLA	C4B-C3B-CAB-CBB
31	b	606	CLA	C4B-C3B-CAB-CBB
31	b	607	CLA	C4B-C3B-CAB-CBB
31	c	511	CLA	C4B-C3B-CAB-CBB
31	c	513	CLA	C4B-C3B-CAB-CBB
31	g	611	CLA	C4B-C3B-CAB-CBB
31	g	612	CLA	C4B-C3B-CAB-CBB
31	r	603	CLA	C4B-C3B-CAB-CBB
31	r	612	CLA	C4B-C3B-CAB-CBB
31	s	605	CLA	C4B-C3B-CAB-CBB
31	s	610	CLA	C4B-C3B-CAB-CBB
31	s	613	CLA	C4B-C3B-CAB-CBB
31	y	602	CLA	C4B-C3B-CAB-CBB
31	y	608	CLA	C4B-C3B-CAB-CBB
31	y	612	CLA	C4B-C3B-CAB-CBB
31	B1	603	CLA	C4B-C3B-CAB-CBB
31	B1	604	CLA	C4B-C3B-CAB-CBB
31	B1	606	CLA	C4B-C3B-CAB-CBB
31	C1	504	CLA	C4B-C3B-CAB-CBB
31	D1	403	CLA	C4B-C3B-CAB-CBB
31	N1	610	CLA	C4B-C3B-CAB-CBB
31	N1	612	CLA	C4B-C3B-CAB-CBB
31	G1	611	CLA	C4B-C3B-CAB-CBB
31	G1	612	CLA	C4B-C3B-CAB-CBB
31	G1	613	CLA	C4B-C3B-CAB-CBB
31	G1	614	CLA	C4B-C3B-CAB-CBB
31	R1	604	CLA	C4B-C3B-CAB-CBB
31	S1	605	CLA	C4B-C3B-CAB-CBB
31	S1	609	CLA	C4B-C3B-CAB-CBB
31	S1	613	CLA	C4B-C3B-CAB-CBB
31	S1	617	CLA	C4B-C3B-CAB-CBB
31	Y1	608	CLA	C4B-C3B-CAB-CBB
31	Y1	611	CLA	C4B-C3B-CAB-CBB
31	Y1	614	CLA	C4B-C3B-CAB-CBB
31	b1	610	CLA	C4B-C3B-CAB-CBB
31	b1	613	CLA	C4B-C3B-CAB-CBB
31	n1	612	CLA	C4B-C3B-CAB-CBB
31	n1	613	CLA	C4B-C3B-CAB-CBB
31	g1	612	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	g1	614	CLA	C4B-C3B-CAB-CBB
31	r1	609	CLA	C4B-C3B-CAB-CBB
31	r1	612	CLA	C4B-C3B-CAB-CBB
31	s1	604	CLA	C4B-C3B-CAB-CBB
31	s1	605	CLA	C4B-C3B-CAB-CBB
31	s1	610	CLA	C4B-C3B-CAB-CBB
31	s1	611	CLA	C4B-C3B-CAB-CBB
31	s1	613	CLA	C4B-C3B-CAB-CBB
31	y1	603	CLA	C4B-C3B-CAB-CBB
31	y1	614	CLA	C4B-C3B-CAB-CBB
41	D	409	LHG	C7-C8-C9-C10
34	b1	621	SQD	C10-C11-C12-C13
38	C1	524	DGA	CA2-CA3-CA4-CA5
41	D	408	LHG	C13-C14-C15-C16
41	G	630	LHG	C31-C32-C33-C34
41	Y	624	LHG	C11-C12-C13-C14
41	c1	525	LHG	C29-C30-C31-C32
54	k1	101	4RF	C32-C33-C34-C35
31	B	617	CLA	C16-C17-C18-C20
31	C	504	CLA	C16-C17-C18-C19
31	G	602	CLA	C16-C17-C18-C20
31	G	613	CLA	C16-C17-C18-C19
31	R	608	CLA	C11-C12-C13-C14
31	R	609	CLA	C11-C12-C13-C14
31	R	609	CLA	C11-C12-C13-C15
31	c	504	CLA	C16-C17-C18-C19
31	c	507	CLA	C16-C17-C18-C19
31	c	513	CLA	C16-C17-C18-C20
31	n	602	CLA	C16-C17-C18-C19
31	n	604	CLA	C16-C17-C18-C19
31	g	602	CLA	C16-C17-C18-C19
31	y	604	CLA	C16-C17-C18-C19
31	B1	609	CLA	C16-C17-C18-C20
31	C1	501	CLA	C16-C17-C18-C20
31	C1	513	CLA	C16-C17-C18-C20
31	D1	402	CLA	C16-C17-C18-C20
31	Y1	613	CLA	C16-C17-C18-C20
31	c1	507	CLA	C16-C17-C18-C20
31	c1	509	CLA	C16-C17-C18-C19
31	c1	509	CLA	C16-C17-C18-C20
31	g1	602	CLA	C16-C17-C18-C20
31	r1	608	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
31	g	610	CLA	C2A-CAA-CBA-CGA
31	r1	604	CLA	C2A-CAA-CBA-CGA
47	n	605	CHL	C2A-CAA-CBA-CGA
47	S1	608	CHL	C2A-CAA-CBA-CGA
35	b1	622	LMG	C12-C13-C14-C15
41	y	624	LHG	C30-C31-C32-C33
41	D1	408	LHG	C33-C34-C35-C36
31	C	506	CLA	C13-C15-C16-C17
31	b	607	CLA	C8-C10-C11-C12
31	c	512	CLA	C8-C10-C11-C12
31	C1	501	CLA	C15-C16-C17-C18
31	s1	603	CLA	C5-C6-C7-C8
31	y1	612	CLA	C5-C6-C7-C8
47	y	606	CHL	C15-C16-C17-C18
35	a	413	LMG	C11-C10-O7-C8
38	c1	524	DGA	CB2-CB1-OG2-CG2
41	C1	525	LHG	C8-C7-O7-C5
41	D1	408	LHG	C8-C7-O7-C5
54	k1	101	4RF	C24-C22-O21-C20
35	C1	523	LMG	C18-C19-C20-C21
38	C	524	DGA	CCB-CDB-CEB-CFB
52	S1	626	3PH	C2B-C2C-C2D-C2E
31	A	405	CLA	C11-C12-C13-C15
31	Y	611	CLA	C11-C10-C8-C7
31	b	602	CLA	C6-C7-C8-C10
31	s	610	CLA	C11-C12-C13-C15
31	B1	607	CLA	C11-C12-C13-C15
41	G	630	LHG	C7-C8-C9-C10
41	D1	410	LHG	C7-C8-C9-C10
41	Y1	624	LHG	C23-C24-C25-C26
41	d1	408	LHG	C7-C8-C9-C10
31	N	614	CLA	CBA-CGA-O2A-C1
31	g	602	CLA	C15-C16-C17-C18
31	g	603	CLA	C15-C16-C17-C18
31	r	603	CLA	C8-C10-C11-C12
31	n1	613	CLA	C10-C11-C12-C13
31	g1	602	CLA	C5-C6-C7-C8
31	g1	603	CLA	C8-C10-C11-C12
31	s1	603	CLA	C15-C16-C17-C18
34	A1	412	SQD	C13-C14-C15-C16
38	C	524	DGA	CB4-CB5-CB6-CB7
38	B1	625	DGA	CA7-CA8-CA9-CAA

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Mol	Chain	Res	Type	Atoms
38	c1	524	DGA	CB7-CB8-CB9-CAB
40	C	523	DGD	C7B-C8B-C9B-CAB
41	D	409	LHG	C13-C14-C15-C16
41	N	624	LHG	C15-C16-C17-C18
41	N1	624	LHG	C33-C34-C35-C36
41	y1	624	LHG	C16-C17-C18-C19
41	y1	624	LHG	C29-C30-C31-C32
52	s	626	3PH	C3B-C3C-C3D-C3E
54	K1	101	4RF	C44-C45-C46-C47
31	R	604	CLA	O1A-CGA-O2A-C1
31	g1	603	CLA	O1A-CGA-O2A-C1
31	d	402	CLA	C3-C5-C6-C7
47	n	601	CHL	C3-C5-C6-C7
31	B	609	CLA	C3A-C2A-CAA-CBA
31	B	615	CLA	C3A-C2A-CAA-CBA
31	C	513	CLA	C3A-C2A-CAA-CBA
31	D	402	CLA	C3A-C2A-CAA-CBA
31	N	612	CLA	C3A-C2A-CAA-CBA
31	G	603	CLA	C3A-C2A-CAA-CBA
31	G	611	CLA	C3A-C2A-CAA-CBA
31	Y	603	CLA	C3A-C2A-CAA-CBA
31	a	405	CLA	C3A-C2A-CAA-CBA
31	b	609	CLA	C3A-C2A-CAA-CBA
31	b	615	CLA	C3A-C2A-CAA-CBA
31	n	603	CLA	C3A-C2A-CAA-CBA
31	g	611	CLA	C3A-C2A-CAA-CBA
31	g	612	CLA	C3A-C2A-CAA-CBA
31	r	610	CLA	C3A-C2A-CAA-CBA
31	y	603	CLA	C3A-C2A-CAA-CBA
31	C1	507	CLA	C3A-C2A-CAA-CBA
31	C1	512	CLA	C3A-C2A-CAA-CBA
31	D1	402	CLA	C3A-C2A-CAA-CBA
31	N1	603	CLA	C3A-C2A-CAA-CBA
31	N1	604	CLA	C4-C3-C5-C6
31	N1	613	CLA	C3A-C2A-CAA-CBA
31	G1	603	CLA	C3A-C2A-CAA-CBA
31	Y1	603	CLA	C3A-C2A-CAA-CBA
31	b1	603	CLA	C3A-C2A-CAA-CBA
31	c1	507	CLA	C3A-C2A-CAA-CBA
31	c1	511	CLA	C3A-C2A-CAA-CBA
31	c1	512	CLA	C3A-C2A-CAA-CBA
31	c1	513	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	n1	603	CLA	C3A-C2A-CAA-CBA
31	n1	610	CLA	C3A-C2A-CAA-CBA
31	n1	613	CLA	C3A-C2A-CAA-CBA
31	n1	614	CLA	C3A-C2A-CAA-CBA
31	s1	605	CLA	C3A-C2A-CAA-CBA
31	y1	603	CLA	C3A-C2A-CAA-CBA
32	a1	409	PHO	C3A-C2A-CAA-CBA
47	G	607	CHL	C3A-C2A-CAA-CBA
47	Y	606	CHL	C3A-C2A-CAA-CBA
47	n	609	CHL	C3A-C2A-CAA-CBA
47	g	607	CHL	C3A-C2A-CAA-CBA
47	y	605	CHL	C3A-C2A-CAA-CBA
47	y	606	CHL	C3A-C2A-CAA-CBA
47	N1	607	CHL	C3A-C2A-CAA-CBA
47	g1	605	CHL	C3A-C2A-CAA-CBA
47	g1	607	CHL	C3A-C2A-CAA-CBA
38	C1	524	DGA	CEA-CFA-CGA-CHA
41	S1	624	LHG	C11-C12-C13-C14
41	d1	408	LHG	C11-C12-C13-C14
41	s1	624	LHG	C11-C12-C13-C14
52	T1	101	3PH	C38-C39-C3A-C3B
52	t1	101	3PH	C22-C23-C24-C25
53	Y1	625	SPH	C11-C10-C9-C8
44	d1	405	PL9	C18-C19-C21-C22
34	B1	626	SQD	C13-C14-C15-C16
41	N1	624	LHG	C28-C29-C30-C31
41	c1	525	LHG	C28-C29-C30-C31
31	N	613	CLA	C10-C11-C12-C13
31	G	603	CLA	C8-C10-C11-C12
31	C1	511	CLA	C5-C6-C7-C8
31	c1	509	CLA	C10-C11-C12-C13
31	c1	510	CLA	C8-C10-C11-C12
31	c1	513	CLA	C10-C11-C12-C13
31	B1	602	CLA	O1D-CGD-O2D-CED
41	N	624	LHG	C7-C8-C9-C10
33	b	618	BCR	C9-C10-C11-C12
33	c	514	BCR	C13-C14-C15-C16
33	c	517	BCR	C9-C10-C11-C12
33	d1	404	BCR	C19-C20-C21-C22
46	H	101	RRX	C15-C16-C17-C18
48	n	620	LUT	C29-C30-C31-C32
31	C	507	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
31	G	613	CLA	C16-C17-C18-C20
31	y	611	CLA	C16-C17-C18-C19
31	B1	602	CLA	C16-C17-C18-C19
31	B1	611	CLA	C16-C17-C18-C20
31	G1	602	CLA	C16-C17-C18-C19
31	R1	608	CLA	C11-C12-C13-C15
31	Y1	613	CLA	C16-C17-C18-C19
31	r1	608	CLA	C11-C12-C13-C14
31	y1	613	CLA	C16-C17-C18-C19
31	y1	613	CLA	C16-C17-C18-C20
47	s1	608	CHL	C11-C12-C13-C15
31	Y	602	CLA	O1A-CGA-O2A-C1
31	B1	606	CLA	O1A-CGA-O2A-C1
51	S	625	LPX	O7-C6-O6-C5
35	D1	411	LMG	C29-C30-C31-C32
40	c	520	DGD	CAB-CBB-CCB-CDB
41	G	630	LHG	C25-C26-C27-C28
41	c1	525	LHG	C13-C14-C15-C16
41	s1	624	LHG	C9-C10-C11-C12
42	C1	527	LMK	C31-C32-C33-C34
55	r1	625	LMT	C3-C4-C5-C6
31	B	603	CLA	C13-C15-C16-C17
31	S1	611	CLA	C10-C11-C12-C13
34	b	621	SQD	C26-C27-C28-C29
34	A1	412	SQD	C12-C13-C14-C15
41	c1	525	LHG	C14-C15-C16-C17
41	y1	624	LHG	C13-C14-C15-C16
54	k1	101	4RF	C43-C44-C45-C46
40	C1	520	DGD	C2A-C1A-O1G-C1G
35	B1	622	LMG	C7-C8-C9-O8
38	j1	101	DGA	OG1-CG1-CG2-CG3
41	d	408	LHG	C4-C5-C6-O8
38	B	625	DGA	CDA-CEA-CFA-CGA
38	C1	524	DGA	CBB-CAB-CB9-CB8
41	d	410	LHG	C26-C27-C28-C29
52	S1	626	3PH	C22-C23-C24-C25
54	K1	101	4RF	C45-C46-C47-C48
31	B	603	CLA	C3-C5-C6-C7
31	C1	512	CLA	C3-C5-C6-C7
31	R1	612	CLA	C3-C5-C6-C7
41	D	409	LHG	C23-C24-C25-C26
41	d	408	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
31	s	604	CLA	C5-C6-C7-C8
31	B1	603	CLA	C15-C16-C17-C18
34	B	621	SQD	C29-C30-C31-C32
34	b	621	SQD	C14-C15-C16-C17
35	J	101	LMG	C29-C30-C31-C32
35	h1	102	LMG	C11-C12-C13-C14
38	B	625	DGA	CB5-CB6-CB7-CB8
38	C	524	DGA	CA4-CA5-CA6-CA7
38	c1	524	DGA	CA4-CA5-CA6-CA7
40	c	523	DGD	C2A-C3A-C4A-C5A
41	D	408	LHG	C29-C30-C31-C32
41	D	408	LHG	C33-C34-C35-C36
41	D	409	LHG	C18-C19-C20-C21
41	L	101	LHG	C9-C10-C11-C12
41	N	624	LHG	C13-C14-C15-C16
41	G	630	LHG	C28-C29-C30-C31
41	d	408	LHG	C29-C30-C31-C32
41	g	624	LHG	C31-C32-C33-C34
41	G1	624	LHG	C13-C14-C15-C16
41	c1	525	LHG	C11-C12-C13-C14
41	d1	409	LHG	C34-C35-C36-C37
41	y1	624	LHG	C15-C16-C17-C18
41	y1	624	LHG	C31-C32-C33-C34
52	S1	626	3PH	C25-C26-C27-C28
54	K1	101	4RF	C26-C27-C28-C29
54	K1	101	4RF	C10-C11-C12-C13
31	G1	603	CLA	O1A-CGA-O2A-C1
41	d	410	LHG	O10-C23-O8-C6
51	s1	625	LPX	O7-C6-O6-C5
38	C	524	DGA	CAB-CBB-CCB-CDB
38	b	623	DGA	CCA-CDA-CEA-CFA
40	c1	518	DGD	C3A-C4A-C5A-C6A
41	d1	408	LHG	C30-C31-C32-C33
41	g1	624	LHG	C31-C32-C33-C34
41	s1	624	LHG	C30-C31-C32-C33
52	B1	624	3PH	C29-C2A-C2B-C2C
54	k1	101	4RF	C30-C31-C32-C33
34	a	412	SQD	C14-C15-C16-C17
38	b	623	DGA	CEA-CFA-CGA-CHA
41	d1	409	LHG	C11-C12-C13-C14
31	C	512	CLA	C8-C10-C11-C12
31	b1	608	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	c1	506	CLA	O1D-CGD-O2D-CED
40	c	519	DGD	C3B-C4B-C5B-C6B
41	D	410	LHG	C29-C30-C31-C32
41	L	101	LHG	C11-C12-C13-C14
41	n	624	LHG	C26-C27-C28-C29
41	C1	525	LHG	C30-C31-C32-C33
41	L1	101	LHG	C25-C26-C27-C28
41	d1	408	LHG	C13-C14-C15-C16
52	t1	101	3PH	C29-C2A-C2B-C2C
44	D	405	PL9	C37-C38-C39-C40
44	d	405	PL9	C12-C13-C14-C15
31	S	609	CLA	C11-C12-C13-C15
31	S1	602	CLA	C11-C12-C13-C15
31	Y1	614	CLA	C16-C17-C18-C20
31	g1	602	CLA	C16-C17-C18-C19
35	B	622	LMG	C28-C29-C30-C31
35	C	521	LMG	C28-C29-C30-C31
38	B1	625	DGA	CB1-CB2-CB3-CB4
40	c	519	DGD	C1B-C2B-C3B-C4B
41	g	624	LHG	C7-C8-C9-C10
52	B1	624	3PH	C31-C32-C33-C34
31	Y1	614	CLA	O1A-CGA-O2A-C1
31	B	603	CLA	C2B-C3B-CAB-CBB
31	B	605	CLA	C2B-C3B-CAB-CBB
31	C	505	CLA	C2B-C3B-CAB-CBB
31	N	603	CLA	C2B-C3B-CAB-CBB
31	N	611	CLA	C2B-C3B-CAB-CBB
31	N	612	CLA	C2B-C3B-CAB-CBB
31	G	612	CLA	C2B-C3B-CAB-CBB
31	R	608	CLA	C2B-C3B-CAB-CBB
31	R	611	CLA	C2B-C3B-CAB-CBB
31	S	610	CLA	C2B-C3B-CAB-CBB
31	S	613	CLA	C2B-C3B-CAB-CBB
31	Y	603	CLA	C2B-C3B-CAB-CBB
31	b	602	CLA	C2B-C3B-CAB-CBB
31	c	503	CLA	C2B-C3B-CAB-CBB
31	c	505	CLA	C2B-C3B-CAB-CBB
31	n	603	CLA	C2B-C3B-CAB-CBB
31	g	612	CLA	C2B-C3B-CAB-CBB
31	r	611	CLA	C2B-C3B-CAB-CBB
31	r	612	CLA	C2B-C3B-CAB-CBB
31	s	602	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	C1	502	CLA	C2B-C3B-CAB-CBB
31	C1	504	CLA	C2B-C3B-CAB-CBB
31	D1	402	CLA	C2B-C3B-CAB-CBB
31	N1	612	CLA	C2B-C3B-CAB-CBB
31	G1	612	CLA	C2B-C3B-CAB-CBB
31	S1	609	CLA	C2B-C3B-CAB-CBB
31	Y1	612	CLA	C2B-C3B-CAB-CBB
31	Y1	614	CLA	C2B-C3B-CAB-CBB
31	n1	612	CLA	C2B-C3B-CAB-CBB
31	g1	612	CLA	C2B-C3B-CAB-CBB
31	s1	605	CLA	C2B-C3B-CAB-CBB
31	s1	611	CLA	C2B-C3B-CAB-CBB
31	y1	603	CLA	C2B-C3B-CAB-CBB
31	y1	614	CLA	C2B-C3B-CAB-CBB
33	C	514	BCR	C1-C6-C7-C8
33	C	514	BCR	C5-C6-C7-C8
33	C	515	BCR	C23-C24-C25-C30
33	C	516	BCR	C23-C24-C25-C26
33	C	516	BCR	C23-C24-C25-C30
33	D	404	BCR	C1-C6-C7-C8
33	D	404	BCR	C5-C6-C7-C8
33	b	618	BCR	C1-C6-C7-C8
33	b	618	BCR	C5-C6-C7-C8
33	c	514	BCR	C1-C6-C7-C8
33	c	514	BCR	C5-C6-C7-C8
33	A1	411	BCR	C23-C24-C25-C26
33	A1	411	BCR	C23-C24-C25-C30
33	C1	514	BCR	C1-C6-C7-C8
33	C1	514	BCR	C5-C6-C7-C8
33	C1	517	BCR	C23-C24-C25-C30
33	D1	404	BCR	C1-C6-C7-C8
33	D1	404	BCR	C5-C6-C7-C8
33	c1	514	BCR	C1-C6-C7-C8
33	c1	514	BCR	C5-C6-C7-C8
33	d1	404	BCR	C1-C6-C7-C8
37	B1	620	C7Z	C1-C6-C7-C8
37	B1	620	C7Z	C21-C26-C27-C28
37	b1	620	C7Z	C1-C6-C7-C8
46	H	101	RRX	C23-C24-C25-C30
34	M1	101	SQD	C24-C25-C26-C27
35	a	413	LMG	C33-C34-C35-C36
41	Y	624	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
41	d	409	LHG	C28-C29-C30-C31
41	C1	525	LHG	C13-C14-C15-C16
41	Y1	624	LHG	C11-C10-C9-C8
52	S1	626	3PH	C29-C2A-C2B-C2C
41	d1	410	LHG	C8-C7-O7-C5
31	Y	611	CLA	O1D-CGD-O2D-CED
40	c1	518	DGD	C2A-C1A-O1G-C1G
31	B	603	CLA	C10-C11-C12-C13
31	C	503	CLA	C13-C15-C16-C17
31	C	504	CLA	C10-C11-C12-C13
41	D1	410	LHG	C2-C3-O3-P
31	y1	613	CLA	C3-C5-C6-C7
34	B1	626	SQD	C11-C12-C13-C14
35	C1	523	LMG	C32-C33-C34-C35
40	C	520	DGD	C3B-C4B-C5B-C6B
41	D	409	LHG	C29-C30-C31-C32
41	Y	624	LHG	C30-C31-C32-C33
41	D1	408	LHG	C25-C26-C27-C28
54	i1	101	4RF	C07-C08-C09-C10
41	d	409	LHG	C29-C30-C31-C32
41	n1	624	LHG	C33-C34-C35-C36
51	S1	625	LPX	C7-C8-C9-C10
53	A1	414	SPH	C11-C12-C13-C14
54	i1	101	4RF	C27-C28-C29-C30
54	i1	101	4RF	C44-C45-C46-C47
31	N	604	CLA	C2A-CAA-CBA-CGA
31	R	604	CLA	C2A-CAA-CBA-CGA
31	s	604	CLA	C2A-CAA-CBA-CGA
31	S1	613	CLA	C2A-CAA-CBA-CGA
31	b1	607	CLA	C2A-CAA-CBA-CGA
47	g	605	CHL	C2A-CAA-CBA-CGA
47	N1	606	CHL	C2A-CAA-CBA-CGA
47	y1	607	CHL	C2A-CAA-CBA-CGA
31	b	605	CLA	C10-C11-C12-C13
31	c	509	CLA	C13-C15-C16-C17
31	c	512	CLA	C5-C6-C7-C8
38	b	623	DGA	CA4-CA5-CA6-CA7
38	B1	625	DGA	CB5-CB6-CB7-CB8
38	C1	524	DGA	CA4-CA5-CA6-CA7
38	C1	524	DGA	CB7-CB8-CB9-CAB
38	b1	625	DGA	CB7-CB8-CB9-CAB
41	C1	525	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
41	D1	408	LHG	C26-C27-C28-C29
41	d1	409	LHG	C13-C14-C15-C16
52	b1	624	3PH	C2E-C2F-C2G-C2H
54	k1	101	4RF	C34-C35-C36-C37
31	N	614	CLA	O1A-CGA-O2A-C1
41	C	525	LHG	O10-C23-O8-C6
41	C1	525	LHG	O10-C23-O8-C6
41	d1	410	LHG	O10-C23-O8-C6
54	K1	101	4RF	O17-C16-O18-C19
54	i1	101	4RF	O42-C41-O40-C39
44	d	405	PL9	C4-C3-C7-C8
56	R1	626	ERG	C21-C20-C22-C23
56	r1	626	ERG	C21-C20-C22-C23
41	g1	624	LHG	C13-C14-C15-C16
52	S	626	3PH	C37-C38-C39-C3A
54	K1	101	4RF	C27-C28-C29-C30
35	a	413	LMG	O9-C10-O7-C8
38	c1	524	DGA	OB1-CB1-OG2-CG2
41	Y	624	LHG	O9-C7-O7-C5
41	d	410	LHG	O9-C7-O7-C5
31	s	602	CLA	C4-C3-C5-C6
31	s	611	CLA	C4-C3-C5-C6
34	B	621	SQD	C10-C11-C12-C13
40	c1	519	DGD	C3A-C4A-C5A-C6A
41	l	101	LHG	C13-C14-C15-C16
55	R1	625	LMT	C11-C10-C9-C8
44	D	405	PL9	C32-C33-C34-C36
33	c1	515	BCR	C10-C11-C12-C13
49	N	622	XAT	C10-C11-C12-C13
49	N	622	XAT	C30-C31-C32-C33
49	R	621	XAT	C30-C31-C32-C33
49	n	622	XAT	C10-C11-C12-C13
49	r1	621	XAT	C30-C31-C32-C33
50	N	623	NEX	C10-C11-C12-C13
50	R	622	NEX	C30-C31-C32-C33
50	y	623	NEX	C30-C31-C32-C33
50	N1	623	NEX	C10-C11-C12-C13
50	R1	622	NEX	C30-C31-C32-C33
50	r1	622	NEX	C30-C31-C32-C33
50	y1	623	NEX	C10-C11-C12-C13
31	C	503	CLA	C10-C11-C12-C13
31	R1	603	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
47	n	607	CHL	C8-C10-C11-C12
31	c	513	CLA	C2-C3-C5-C6
31	N1	604	CLA	C2-C3-C5-C6
35	C	521	LMG	C15-C16-C17-C18
38	B1	625	DGA	CB3-CB4-CB5-CB6
41	Y	624	LHG	C28-C29-C30-C31
41	l	101	LHG	C33-C34-C35-C36
41	s	624	LHG	C26-C27-C28-C29
41	C1	525	LHG	C24-C25-C26-C27
41	L1	101	LHG	C26-C27-C28-C29
41	Y1	624	LHG	C31-C32-C33-C34
35	J	101	LMG	C28-C29-C30-C31
52	i	101	3PH	C21-C22-C23-C24
31	S	610	CLA	CBA-CGA-O2A-C1
31	c	508	CLA	CBA-CGA-O2A-C1
31	C1	502	CLA	CBA-CGA-O2A-C1
31	C1	508	CLA	CBA-CGA-O2A-C1
52	s1	626	3PH	C32-C31-O31-C3
54	K1	101	4RF	C43-C41-O40-C39
31	C	503	CLA	C11-C12-C13-C14
31	N	604	CLA	C14-C13-C15-C16
31	r1	602	CLA	C6-C7-C8-C9
38	C1	524	DGA	CA6-CA7-CA8-CA9
38	b1	625	DGA	CA6-CA7-CA8-CA9
41	Y	624	LHG	C11-C10-C9-C8
41	L1	101	LHG	C11-C10-C9-C8
41	y1	624	LHG	C28-C29-C30-C31
52	s1	626	3PH	C23-C24-C25-C26
54	I1	102	4RF	C07-C08-C09-C10
31	C	501	CLA	C13-C15-C16-C17
31	N	613	CLA	C5-C6-C7-C8
31	Y	613	CLA	C15-C16-C17-C18
31	B1	604	CLA	C5-C6-C7-C8
31	y1	612	CLA	C13-C15-C16-C17
34	M1	101	SQD	C11-C10-C9-C8
41	c	625	LHG	C13-C14-C15-C16
41	L1	101	LHG	C11-C12-C13-C14
52	B1	624	3PH	C2A-C2B-C2C-C2D
52	t1	101	3PH	C3B-C3C-C3D-C3E
54	K1	101	4RF	C31-C32-C33-C34
40	C	518	DGD	O6E-C1E-O5D-C6D
40	C1	519	DGD	O6D-C1D-O3G-C3G

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Mol	Chain	Res	Type	Atoms
34	A1	412	SQD	C33-C34-C35-C36
34	b1	626	SQD	C34-C35-C36-C37
34	c1	526	SQD	C17-C18-C19-C20
41	d	409	LHG	C11-C12-C13-C14
41	y	624	LHG	C13-C14-C15-C16
41	D1	409	LHG	C11-C12-C13-C14
41	L1	101	LHG	C13-C14-C15-C16
41	N1	624	LHG	C31-C32-C33-C34
52	s	626	3PH	C23-C24-C25-C26
42	C	527	LMK	C2-C3-C4-O2
34	C	526	SQD	C2-C1-O6-C44
34	c	626	SQD	C2-C1-O6-C44
34	a1	412	SQD	C2-C1-O6-C44
34	c1	526	SQD	C2-C1-O6-C44
40	C	519	DGD	C2D-C1D-O3G-C3G
40	c	519	DGD	C2D-C1D-O3G-C3G
40	C1	519	DGD	C2D-C1D-O3G-C3G
31	C	502	CLA	C10-C11-C12-C13
31	S	603	CLA	C5-C6-C7-C8
31	S	603	CLA	C15-C16-C17-C18
31	Y	602	CLA	C8-C10-C11-C12
31	y	614	CLA	C5-C6-C7-C8
31	G1	603	CLA	C5-C6-C7-C8
31	d1	403	CLA	C10-C11-C12-C13
35	A	413	LMG	C30-C31-C32-C33
40	C1	518	DGD	C3A-C4A-C5A-C6A
41	G1	624	LHG	C11-C10-C9-C8
41	c1	525	LHG	C26-C27-C28-C29
41	d1	409	LHG	C28-C29-C30-C31
40	C1	518	DGD	C1B-C2B-C3B-C4B
41	D1	408	LHG	C23-C24-C25-C26
35	c	521	LMG	C16-C17-C18-C19
38	C	524	DGA	CB5-CB6-CB7-CB8
41	d	408	LHG	C13-C14-C15-C16
41	s1	624	LHG	C13-C14-C15-C16
53	y	625	SPH	C7-C8-C9-C10
57	y1	626	PTY	C37-C38-C39-C40
34	A	412	SQD	C24-C25-C26-C27
34	B	621	SQD	C32-C33-C34-C35
34	A1	412	SQD	C31-C32-C33-C34
34	B1	621	SQD	C25-C26-C27-C28
38	c1	524	DGA	CA6-CA7-CA8-CA9

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Mol	Chain	Res	Type	Atoms
41	D	408	LHG	C30-C31-C32-C33
41	D	409	LHG	C11-C12-C13-C14
41	D1	409	LHG	C34-C35-C36-C37
41	N1	624	LHG	C13-C14-C15-C16
41	N1	624	LHG	C27-C28-C29-C30
52	T1	101	3PH	C27-C28-C29-C2A
52	t1	101	3PH	C38-C39-C3A-C3B
31	B	605	CLA	C8-C10-C11-C12
31	C	505	CLA	C3-C5-C6-C7
31	c	509	CLA	CBA-CGA-O2A-C1
31	y	602	CLA	CBA-CGA-O2A-C1
40	C1	519	DGD	C2A-C1A-O1G-C1G
33	B	618	BCR	C9-C10-C11-C12
33	C	516	BCR	C15-C16-C17-C18
33	c	515	BCR	C19-C20-C21-C22
37	b1	620	C7Z	C9-C10-C11-C12
48	G	620	LUT	C29-C30-C31-C32
48	y	621	LUT	C29-C30-C31-C32
48	n1	621	LUT	C9-C10-C11-C12
48	g1	620	LUT	C29-C30-C31-C32
31	B	616	CLA	C16-C17-C18-C20
31	r1	610	CLA	C11-C12-C13-C15
34	c	626	SQD	C28-C29-C30-C31
53	Y	625	SPH	C6-C7-C8-C9
34	A	412	SQD	C8-C7-O47-C45
34	c	626	SQD	C8-C7-O47-C45
34	B1	626	SQD	C8-C7-O47-C45
35	h	102	LMG	C11-C10-O7-C8
35	H1	102	LMG	C11-C10-O7-C8
35	c1	523	LMG	C11-C10-O7-C8
40	C1	519	DGD	C2B-C1B-O2G-C2G
41	D	410	LHG	C8-C7-O7-C5
41	c	625	LHG	C8-C7-O7-C5
41	y	624	LHG	C8-C7-O7-C5
52	i	101	3PH	C22-C21-O21-C2
52	B1	624	3PH	C22-C21-O21-C2
57	y1	627	PTY	C31-C30-O4-C1
41	D1	410	LHG	O10-C23-O8-C6
34	C1	526	SQD	C7-C8-C9-C10
40	c	518	DGD	C1B-C2B-C3B-C4B
34	a	412	SQD	C28-C29-C30-C31
35	D	411	LMG	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
38	b1	625	DGA	CCB-CDB-CEB-CFB
41	D	409	LHG	C28-C29-C30-C31
52	t1	101	3PH	C2A-C2B-C2C-C2D
54	I1	102	4RF	C09-C10-C11-C12
31	A	410	CLA	C8-C10-C11-C12
31	C	501	CLA	C5-C6-C7-C8
31	C	510	CLA	C5-C6-C7-C8
31	D	402	CLA	C15-C16-C17-C18
31	g	602	CLA	C5-C6-C7-C8
31	C1	508	CLA	C8-C10-C11-C12
31	b1	610	CLA	C8-C10-C11-C12
31	c1	506	CLA	C13-C15-C16-C17
31	s1	603	CLA	C8-C10-C11-C12
31	y1	603	CLA	C5-C6-C7-C8
34	B1	626	SQD	O49-C7-O47-C45
35	H1	102	LMG	O9-C10-O7-C8
54	k1	101	4RF	O23-C22-O21-C20
34	b1	626	SQD	C11-C12-C13-C14
35	d1	411	LMG	C19-C20-C21-C22
38	j1	101	DGA	CA4-CA5-CA6-CA7
41	d	408	LHG	C26-C27-C28-C29
41	Y1	624	LHG	C13-C14-C15-C16
41	d1	408	LHG	C29-C30-C31-C32
41	g1	624	LHG	C15-C16-C17-C18
52	s1	626	3PH	C24-C25-C26-C27
53	a1	414	SPH	C6-C7-C8-C9
55	r1	625	LMT	C9-C10-C11-C12
38	c1	524	DGA	CB2-CB3-CB4-CB5
38	j1	101	DGA	CA5-CA6-CA7-CA8
41	N	624	LHG	C26-C27-C28-C29
41	S	624	LHG	C12-C13-C14-C15
41	s	624	LHG	C9-C10-C11-C12
31	S	602	CLA	CBD-CGD-O2D-CED
31	c	508	CLA	C10-C11-C12-C13
31	r	612	CLA	C8-C10-C11-C12
31	B1	617	CLA	C15-C16-C17-C18
31	N1	613	CLA	C15-C16-C17-C18
31	S1	603	CLA	C5-C6-C7-C8
31	s1	611	CLA	C10-C11-C12-C13
33	C	515	BCR	C37-C22-C23-C24
33	b	619	BCR	C11-C12-C13-C35
33	C1	515	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
49	n1	622	XAT	C31-C32-C33-C40
41	D1	409	LHG	C26-C27-C28-C29
52	T1	101	3PH	C22-C23-C24-C25
41	C1	525	LHG	C7-C8-C9-C10
41	g1	624	LHG	C23-C24-C25-C26
38	C1	524	DGA	CA7-CA8-CA9-CAA
41	g1	624	LHG	C28-C29-C30-C31
31	b	615	CLA	C3-C5-C6-C7
31	B1	615	CLA	C3-C5-C6-C7
31	S1	614	CLA	C3-C5-C6-C7
31	b1	615	CLA	C3-C5-C6-C7
33	b	618	BCR	C17-C18-C19-C20
48	Y1	620	LUT	C27-C28-C29-C30
40	c	519	DGD	C5D-C6D-O5D-C1E
34	M1	101	SQD	C13-C14-C15-C16
38	B	625	DGA	CA9-CAA-CBA-CCA
38	B1	625	DGA	CBA-CCA-CDA-CEA
38	j1	101	DGA	CB5-CB6-CB7-CB8
54	k1	101	4RF	C24-C25-C26-C27
31	B1	615	CLA	C13-C15-C16-C17
31	B	612	CLA	C2A-CAA-CBA-CGA
31	r	603	CLA	C2A-CAA-CBA-CGA
32	a1	409	PHO	C2A-CAA-CBA-CGA
47	N	608	CHL	C2A-CAA-CBA-CGA
47	n	607	CHL	C2A-CAA-CBA-CGA
31	C	507	CLA	C16-C17-C18-C19
31	S	613	CLA	C6-C7-C8-C9
31	y	611	CLA	C16-C17-C18-C20
31	B1	602	CLA	C16-C17-C18-C20
31	B1	611	CLA	C16-C17-C18-C19
31	G1	602	CLA	C16-C17-C18-C20
31	S1	603	CLA	C16-C17-C18-C20
31	r1	610	CLA	C11-C12-C13-C14
31	y1	614	CLA	C16-C17-C18-C20
47	S1	608	CHL	C11-C12-C13-C14
34	a	412	SQD	C10-C11-C12-C13
38	c	524	DGA	CDA-CEA-CFA-CGA
38	b1	625	DGA	CDB-CEB-CFB-CGB
41	Y	624	LHG	C13-C14-C15-C16
52	s	626	3PH	C25-C26-C27-C28
52	B1	624	3PH	C3C-C3D-C3E-C3F
31	n1	610	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
35	a	413	LMG	C16-C17-C18-C19
41	D1	408	LHG	C13-C14-C15-C16
42	c1	527	LMK	C17-C18-C19-C20
52	s	626	3PH	C24-C25-C26-C27
54	K1	101	4RF	C29-C30-C31-C32
31	b	607	CLA	C5-C6-C7-C8
31	G1	611	CLA	C5-C6-C7-C8
31	c1	504	CLA	C8-C10-C11-C12
41	N	624	LHG	C16-C17-C18-C19
41	D1	409	LHG	C25-C26-C27-C28
31	c	505	CLA	CBD-CGD-O2D-CED
41	L	101	LHG	C13-C14-C15-C16
41	s	624	LHG	C13-C14-C15-C16
40	c1	518	DGD	O1A-C1A-O1G-C1G
31	G1	603	CLA	C3-C5-C6-C7
31	B	603	CLA	C8-C10-C11-C12
31	a	405	CLA	C10-C11-C12-C13
31	c	510	CLA	C13-C15-C16-C17
31	s	602	CLA	C8-C10-C11-C12
31	b1	614	CLA	C8-C10-C11-C12
31	c1	501	CLA	C13-C15-C16-C17
31	c1	510	CLA	C5-C6-C7-C8
31	g1	610	CLA	C8-C10-C11-C12
38	b1	625	DGA	CA9-CAA-CBA-CCA
38	c1	524	DGA	CAB-CBB-CCB-CDB
41	l	101	LHG	C23-C24-C25-C26
41	D	410	LHG	C24-C25-C26-C27
41	L1	101	LHG	C10-C11-C12-C13
35	h	102	LMG	O6-C5-C6-O5
34	B	621	SQD	C11-C12-C13-C14
34	B1	621	SQD	C26-C27-C28-C29
35	h	102	LMG	C37-C38-C39-C40
41	Y1	624	LHG	C16-C17-C18-C19
41	s1	624	LHG	C31-C32-C33-C34
52	S	626	3PH	C24-C25-C26-C27
52	s1	626	3PH	C25-C26-C27-C28
31	G	603	CLA	C10-C11-C12-C13
31	c	511	CLA	C5-C6-C7-C8
31	y	613	CLA	C15-C16-C17-C18
31	R1	602	CLA	C8-C10-C11-C12
31	c1	508	CLA	C15-C16-C17-C18
31	y1	613	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
45	f	101	HEM	C4B-C3B-CAB-CBB
31	b1	605	CLA	C16-C17-C18-C20
31	c1	501	CLA	C16-C17-C18-C19
31	s1	604	CLA	C6-C7-C8-C9
38	b	623	DGA	CB3-CB4-CB5-CB6
38	B1	625	DGA	CA6-CA7-CA8-CA9
41	D	408	LHG	C28-C29-C30-C31
41	d1	408	LHG	C33-C34-C35-C36
52	S1	626	3PH	C33-C34-C35-C36
40	b1	623	DGD	O6E-C5E-C6E-O5E
44	d	405	PL9	C47-C48-C49-C50
34	A	412	SQD	C14-C15-C16-C17
35	C1	523	LMG	C16-C17-C18-C19
38	C	524	DGA	CA5-CA6-CA7-CA8
41	D1	409	LHG	C28-C29-C30-C31
41	Y1	624	LHG	C28-C29-C30-C31
57	y1	626	PTY	C31-C32-C33-C34
38	b	623	DGA	CB1-CB2-CB3-CB4
40	C	518	DGD	C1B-C2B-C3B-C4B
41	d	409	LHG	C23-C24-C25-C26
41	y1	624	LHG	C23-C24-C25-C26
31	B	606	CLA	C5-C6-C7-C8
31	n	603	CLA	C5-C6-C7-C8
31	C1	503	CLA	C5-C6-C7-C8
31	c1	510	CLA	C13-C15-C16-C17
41	n	624	LHG	C14-C15-C16-C17
41	d1	408	LHG	C26-C27-C28-C29
41	d1	408	LHG	C32-C33-C34-C35
55	r1	625	LMT	C4-C5-C6-C7
40	c1	518	DGD	O6E-C5E-C6E-O5E
34	B1	626	SQD	O47-C45-C46-O48
35	a1	413	LMG	O1-C7-C8-O7
40	c1	519	DGD	O1G-C1G-C2G-O2G
41	d	410	LHG	O7-C5-C6-O8
34	b1	626	SQD	C11-C10-C9-C8
41	s	624	LHG	C31-C32-C33-C34
40	c1	520	DGD	C4E-C5E-C6E-O5E
31	C	508	CLA	CBA-CGA-O2A-C1
34	C	526	SQD	C24-C23-O48-C46
34	B	621	SQD	C13-C14-C15-C16
38	B	625	DGA	CA4-CA5-CA6-CA7
38	B1	625	DGA	CCA-CDA-CEA-CFA

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Mol	Chain	Res	Type	Atoms
41	D	409	LHG	C34-C35-C36-C37
41	c	625	LHG	C28-C29-C30-C31
41	n1	624	LHG	C25-C26-C27-C28
41	n1	624	LHG	C28-C29-C30-C31
41	y1	624	LHG	C33-C34-C35-C36
54	k1	101	4RF	C27-C28-C29-C30
31	C	508	CLA	C10-C11-C12-C13
34	b	621	SQD	C32-C33-C34-C35
41	L	101	LHG	C33-C34-C35-C36
41	l	101	LHG	C28-C29-C30-C31
41	g	624	LHG	C13-C14-C15-C16
41	y	624	LHG	C28-C29-C30-C31
41	C1	525	LHG	C9-C10-C11-C12
41	D1	408	LHG	C11-C12-C13-C14
52	B1	624	3PH	C3D-C3E-C3F-C3G
55	R1	625	LMT	C5-C6-C7-C8
34	A1	412	SQD	C34-C35-C36-C37
35	C	521	LMG	C16-C17-C18-C19
41	y	624	LHG	C16-C17-C18-C19
41	n1	624	LHG	C11-C12-C13-C14
41	y1	624	LHG	C11-C12-C13-C14
53	y	625	SPH	C11-C10-C9-C8
31	A	407	CLA	C2-C1-O2A-CGA
31	r	602	CLA	C2-C1-O2A-CGA
31	s	603	CLA	C2-C1-O2A-CGA
31	s	617	CLA	C2-C1-O2A-CGA
31	y	608	CLA	C2-C1-O2A-CGA
31	r1	604	CLA	C2-C1-O2A-CGA
35	C	521	LMG	O6-C5-C6-O5
40	C1	519	DGD	O6E-C5E-C6E-O5E
31	G	603	CLA	C16-C17-C18-C20
31	S1	604	CLA	C6-C7-C8-C9
31	C1	505	CLA	C15-C16-C17-C18
31	S1	610	CLA	C13-C15-C16-C17
40	C1	519	DGD	C4A-C5A-C6A-C7A
41	N	624	LHG	C31-C32-C33-C34
41	g	624	LHG	C11-C12-C13-C14
41	G1	624	LHG	C28-C29-C30-C31
53	y1	625	SPH	C11-C12-C13-C14
35	c	521	LMG	O6-C5-C6-O5
38	B1	625	DGA	CB9-CAB-CBB-CCB
47	G1	609	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	Y	611	CLA	C3-C5-C6-C7
31	N	613	CLA	C2-C3-C5-C6
35	h	102	LMG	O9-C10-O7-C8
41	D1	408	LHG	O9-C7-O7-C5
51	s1	625	LPX	O1-C3-C4-C5
31	C1	509	CLA	C15-C16-C17-C18
31	r1	612	CLA	C5-C6-C7-C8
35	J	101	LMG	C31-C32-C33-C34
35	b1	622	LMG	C31-C32-C33-C34
38	B	625	DGA	CB9-CAB-CBB-CCB
41	D	408	LHG	C26-C27-C28-C29
31	B	604	CLA	C2A-CAA-CBA-CGA
31	C	501	CLA	C2A-CAA-CBA-CGA
31	G	604	CLA	C2A-CAA-CBA-CGA
31	G	610	CLA	C2A-CAA-CBA-CGA
31	R	613	CLA	C2A-CAA-CBA-CGA
31	Y	610	CLA	C2A-CAA-CBA-CGA
31	b	604	CLA	C2A-CAA-CBA-CGA
31	r	604	CLA	C2A-CAA-CBA-CGA
31	B1	604	CLA	C2A-CAA-CBA-CGA
31	S1	603	CLA	C2A-CAA-CBA-CGA
31	Y1	608	CLA	C2A-CAA-CBA-CGA
31	r1	602	CLA	C2A-CAA-CBA-CGA
47	N	606	CHL	C2A-CAA-CBA-CGA
47	r	607	CHL	C2A-CAA-CBA-CGA
47	g1	607	CHL	C2A-CAA-CBA-CGA
41	D1	409	LHG	C11-C10-C9-C8
41	y1	624	LHG	C34-C35-C36-C37
53	a1	414	SPH	C14-C15-C16-C17
38	J1	101	DGA	CA4-CA5-CA6-CA7
41	n	624	LHG	C28-C29-C30-C31
41	g	624	LHG	C28-C29-C30-C31
53	y1	625	SPH	C6-C7-C8-C9
31	A	405	CLA	C5-C6-C7-C8
31	C	508	CLA	C8-C10-C11-C12
31	C	510	CLA	C15-C16-C17-C18
31	Y	610	CLA	C8-C10-C11-C12
31	C1	512	CLA	C5-C6-C7-C8
31	S1	609	CLA	C10-C11-C12-C13
31	g1	603	CLA	C10-C11-C12-C13
41	S	624	LHG	C9-C10-C11-C12
41	d	409	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
41	C1	525	LHG	C26-C27-C28-C29
41	S1	624	LHG	C29-C30-C31-C32
41	y1	624	LHG	C11-C10-C9-C8
52	b1	624	3PH	C28-C29-C2A-C2B
41	D	409	LHG	C8-C7-O7-C5
57	y1	626	PTY	C11-C8-O7-C6
40	C1	519	DGD	CCB-CDB-CEB-CFB
41	c1	525	LHG	C11-C10-C9-C8
54	i1	101	4RF	C26-C27-C28-C29
31	b	609	CLA	C16-C17-C18-C20
31	b	614	CLA	C16-C17-C18-C19
31	y1	612	CLA	C8-C10-C11-C12
41	N	624	LHG	O1-C1-C2-O2
41	G	630	LHG	O1-C1-C2-O2
41	g	624	LHG	O1-C1-C2-O2
41	d1	408	LHG	O1-C1-C2-O2
31	S	610	CLA	O1A-CGA-O2A-C1
31	c	508	CLA	O1A-CGA-O2A-C1
31	C1	508	CLA	O1A-CGA-O2A-C1
40	C1	520	DGD	O1A-C1A-O1G-C1G
31	b	603	CLA	C3-C5-C6-C7
31	c	507	CLA	C3-C5-C6-C7
31	c	512	CLA	C3-C5-C6-C7
31	A	407	CLA	C1A-C2A-CAA-CBA
31	A	410	CLA	C1A-C2A-CAA-CBA
31	B	602	CLA	C1A-C2A-CAA-CBA
31	B	604	CLA	C1A-C2A-CAA-CBA
31	B	606	CLA	C1A-C2A-CAA-CBA
31	B	607	CLA	C1A-C2A-CAA-CBA
31	C	501	CLA	C1A-C2A-CAA-CBA
31	C	503	CLA	C1A-C2A-CAA-CBA
31	C	511	CLA	C1A-C2A-CAA-CBA
31	N	603	CLA	C1A-C2A-CAA-CBA
31	G	603	CLA	C1A-C2A-CAA-CBA
31	G	610	CLA	C1A-C2A-CAA-CBA
31	G	611	CLA	C1A-C2A-CAA-CBA
31	G	614	CLA	C1A-C2A-CAA-CBA
31	R	608	CLA	C1A-C2A-CAA-CBA
31	R	613	CLA	C1A-C2A-CAA-CBA
31	S	609	CLA	C1A-C2A-CAA-CBA
31	S	610	CLA	C1A-C2A-CAA-CBA
31	Y	602	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
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	a	405	CLA	C1A-C2A-CAA-CBA
31	a	407	CLA	C1A-C2A-CAA-CBA
31	b	602	CLA	C1A-C2A-CAA-CBA
31	b	604	CLA	C1A-C2A-CAA-CBA
31	b	605	CLA	C1A-C2A-CAA-CBA
31	b	606	CLA	C1A-C2A-CAA-CBA
31	b	610	CLA	C1A-C2A-CAA-CBA
31	c	503	CLA	C1A-C2A-CAA-CBA
31	c	504	CLA	C1A-C2A-CAA-CBA
31	c	511	CLA	C1A-C2A-CAA-CBA
31	n	602	CLA	C1A-C2A-CAA-CBA
31	g	603	CLA	C1A-C2A-CAA-CBA
31	g	610	CLA	C1A-C2A-CAA-CBA
31	g	611	CLA	C1A-C2A-CAA-CBA
31	r	613	CLA	C1A-C2A-CAA-CBA
31	s	609	CLA	C1A-C2A-CAA-CBA
31	s	617	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	608	CLA	C1A-C2A-CAA-CBA
31	y	610	CLA	C1A-C2A-CAA-CBA
31	y	611	CLA	C1A-C2A-CAA-CBA
31	A1	405	CLA	C1A-C2A-CAA-CBA
31	B1	604	CLA	C1A-C2A-CAA-CBA
31	B1	607	CLA	C1A-C2A-CAA-CBA
31	C1	501	CLA	C1A-C2A-CAA-CBA
31	C1	503	CLA	C1A-C2A-CAA-CBA
31	C1	507	CLA	C1A-C2A-CAA-CBA
31	C1	511	CLA	C1A-C2A-CAA-CBA
31	N1	602	CLA	C1A-C2A-CAA-CBA
31	N1	603	CLA	C1A-C2A-CAA-CBA
31	G1	603	CLA	C1A-C2A-CAA-CBA
31	G1	610	CLA	C1A-C2A-CAA-CBA
31	G1	611	CLA	C1A-C2A-CAA-CBA
31	G1	614	CLA	C1A-C2A-CAA-CBA
31	R1	602	CLA	C1A-C2A-CAA-CBA
31	R1	609	CLA	C1A-C2A-CAA-CBA
31	R1	610	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	S1	602	CLA	C1A-C2A-CAA-CBA
31	S1	604	CLA	C1A-C2A-CAA-CBA
31	S1	617	CLA	C1A-C2A-CAA-CBA
31	Y1	603	CLA	C1A-C2A-CAA-CBA
31	Y1	608	CLA	C1A-C2A-CAA-CBA
31	Y1	610	CLA	C1A-C2A-CAA-CBA
31	Y1	611	CLA	C1A-C2A-CAA-CBA
31	Y1	614	CLA	C1A-C2A-CAA-CBA
31	a1	405	CLA	C1A-C2A-CAA-CBA
31	a1	410	CLA	C1A-C2A-CAA-CBA
31	b1	604	CLA	C1A-C2A-CAA-CBA
31	b1	606	CLA	C1A-C2A-CAA-CBA
31	b1	607	CLA	C1A-C2A-CAA-CBA
31	b1	610	CLA	C1A-C2A-CAA-CBA
31	c1	503	CLA	C1A-C2A-CAA-CBA
31	c1	507	CLA	C1A-C2A-CAA-CBA
31	c1	512	CLA	C1A-C2A-CAA-CBA
31	n1	602	CLA	C1A-C2A-CAA-CBA
31	n1	603	CLA	C1A-C2A-CAA-CBA
31	g1	603	CLA	C1A-C2A-CAA-CBA
31	g1	610	CLA	C1A-C2A-CAA-CBA
31	g1	611	CLA	C1A-C2A-CAA-CBA
31	r1	602	CLA	C1A-C2A-CAA-CBA
31	r1	609	CLA	C1A-C2A-CAA-CBA
31	r1	610	CLA	C1A-C2A-CAA-CBA
31	s1	602	CLA	C1A-C2A-CAA-CBA
31	s1	603	CLA	C1A-C2A-CAA-CBA
31	s1	604	CLA	C1A-C2A-CAA-CBA
31	s1	609	CLA	C1A-C2A-CAA-CBA
31	s1	617	CLA	C1A-C2A-CAA-CBA
31	y1	603	CLA	C1A-C2A-CAA-CBA
31	y1	611	CLA	C1A-C2A-CAA-CBA
31	y1	614	CLA	C1A-C2A-CAA-CBA
38	B1	625	DGA	CA1-CA2-CA3-CA4
31	B	617	CLA	C8-C10-C11-C12
31	G	603	CLA	C13-C15-C16-C17
31	Y	604	CLA	C10-C11-C12-C13
31	b	606	CLA	C5-C6-C7-C8
31	n	603	CLA	C10-C11-C12-C13
31	s	603	CLA	C5-C6-C7-C8
31	b1	608	CLA	C5-C6-C7-C8
31	b1	615	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
34	c	626	SQD	C13-C14-C15-C16
40	c	518	DGD	C3A-C4A-C5A-C6A
41	d	408	LHG	C11-C12-C13-C14
41	L1	101	LHG	C31-C32-C33-C34
52	s1	626	3PH	C35-C36-C37-C38
53	a1	414	SPH	C11-C12-C13-C14
57	Y1	626	PTY	C39-C40-C41-C42
54	K1	101	4RF	C43-C44-C45-C46
53	A1	414	SPH	C5-C6-C7-C8
35	j	101	LMG	C31-C32-C33-C34
35	c1	521	LMG	C36-C37-C38-C39
41	c	625	LHG	C11-C10-C9-C8
41	c	625	LHG	C24-C25-C26-C27
41	c	625	LHG	C31-C32-C33-C34
52	S	626	3PH	C29-C2A-C2B-C2C
54	i1	101	4RF	C25-C26-C27-C28
31	B	610	CLA	C13-C15-C16-C17
31	C	505	CLA	C10-C11-C12-C13
31	Y1	613	CLA	C8-C10-C11-C12
31	n1	602	CLA	C15-C16-C17-C18
41	D	409	LHG	O6-C4-C5-C6
41	L	101	LHG	O6-C4-C5-C6
41	G	630	LHG	O6-C4-C5-C6
41	S	624	LHG	O6-C4-C5-C6
41	l	101	LHG	O6-C4-C5-C6
41	n	624	LHG	O6-C4-C5-C6
41	g	624	LHG	O6-C4-C5-C6
41	D1	409	LHG	O6-C4-C5-C6
41	N1	624	LHG	O6-C4-C5-C6
41	G1	624	LHG	O6-C4-C5-C6
41	g1	624	LHG	O6-C4-C5-C6
52	S	626	3PH	O11-C1-C2-C3
57	Y1	627	PTY	O14-C5-C6-C1
34	A	412	SQD	O49-C7-O47-C45
34	c	626	SQD	O49-C7-O47-C45
35	c1	523	LMG	O9-C10-O7-C8
41	c	625	LHG	O9-C7-O7-C5
52	i	101	3PH	O22-C21-O21-C2
38	B	625	DGA	CAA-CBA-CCA-CDA
41	n	624	LHG	C31-C32-C33-C34
41	d1	408	LHG	C28-C29-C30-C31
54	i1	101	4RF	C09-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	B	602	CLA	C11-C10-C8-C7
31	B	603	CLA	C6-C7-C8-C10
31	B	608	CLA	C12-C13-C15-C16
31	B	614	CLA	C11-C12-C13-C15
31	C	501	CLA	C11-C12-C13-C15
31	C	506	CLA	C11-C10-C8-C7
31	C	507	CLA	C11-C12-C13-C15
31	C	508	CLA	C11-C10-C8-C7
31	C	513	CLA	C6-C7-C8-C10
31	D	402	CLA	C11-C10-C8-C7
31	D	402	CLA	C11-C12-C13-C15
31	D	403	CLA	C11-C12-C13-C15
31	N	613	CLA	C11-C12-C13-C15
31	G	603	CLA	C11-C12-C13-C15
31	G	613	CLA	C6-C7-C8-C10
31	S	610	CLA	C11-C12-C13-C15
31	S	611	CLA	C6-C7-C8-C10
31	S	611	CLA	C11-C12-C13-C15
31	a	405	CLA	C11-C12-C13-C15
31	b	602	CLA	C11-C10-C8-C7
31	b	603	CLA	C6-C7-C8-C10
31	b	607	CLA	C11-C12-C13-C15
31	b	616	CLA	C11-C12-C13-C15
31	c	502	CLA	C6-C7-C8-C10
31	c	506	CLA	C11-C10-C8-C7
31	c	507	CLA	C11-C10-C8-C7
31	c	510	CLA	C6-C7-C8-C10
31	c	511	CLA	C11-C12-C13-C15
31	c	512	CLA	C6-C7-C8-C10
31	c	513	CLA	C6-C7-C8-C10
31	c	513	CLA	C11-C12-C13-C15
31	n	603	CLA	C6-C7-C8-C10
31	n	603	CLA	C11-C12-C13-C15
31	n	613	CLA	C11-C12-C13-C15
31	g	602	CLA	C6-C7-C8-C10
31	g	603	CLA	C12-C13-C15-C16
31	g	613	CLA	C6-C7-C8-C10
31	g	613	CLA	C11-C10-C8-C7
31	r	603	CLA	C11-C10-C8-C7
31	r	609	CLA	C6-C7-C8-C10
31	s	610	CLA	C11-C10-C8-C7
31	y	602	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
31	B1	604	CLA	C11-C10-C8-C7
31	B1	607	CLA	C11-C10-C8-C7
31	C1	502	CLA	C11-C12-C13-C15
31	C1	509	CLA	C12-C13-C15-C16
31	C1	510	CLA	C12-C13-C15-C16
31	C1	513	CLA	C11-C12-C13-C15
31	D1	402	CLA	C11-C12-C13-C15
31	D1	403	CLA	C11-C12-C13-C15
31	N1	602	CLA	C6-C7-C8-C10
31	N1	610	CLA	C11-C12-C13-C15
31	G1	602	CLA	C6-C7-C8-C10
31	G1	603	CLA	C6-C7-C8-C10
31	G1	610	CLA	C11-C10-C8-C7
31	S1	609	CLA	C6-C7-C8-C10
31	Y1	613	CLA	C11-C12-C13-C15
31	Y1	613	CLA	C12-C13-C15-C16
31	a1	405	CLA	C11-C12-C13-C15
31	a1	406	CLA	C12-C13-C15-C16
31	b1	604	CLA	C11-C12-C13-C15
31	b1	607	CLA	C11-C12-C13-C15
31	c1	507	CLA	C12-C13-C15-C16
31	c1	509	CLA	C6-C7-C8-C10
31	d1	402	CLA	C11-C10-C8-C7
31	n1	610	CLA	C11-C12-C13-C15
31	n1	610	CLA	C12-C13-C15-C16
31	g1	603	CLA	C6-C7-C8-C10
31	g1	610	CLA	C11-C10-C8-C7
31	g1	611	CLA	C6-C7-C8-C10
31	s1	609	CLA	C11-C10-C8-C7
31	y1	602	CLA	C6-C7-C8-C10
31	y1	612	CLA	C11-C10-C8-C7
31	y1	613	CLA	C11-C12-C13-C15
47	Y	607	CHL	C11-C10-C8-C7
47	n	605	CHL	C11-C12-C13-C15
47	N1	607	CHL	C11-C12-C13-C15
47	G1	601	CHL	C12-C13-C15-C16
47	S1	608	CHL	C11-C10-C8-C7
47	Y1	606	CHL	C11-C12-C13-C15
47	Y1	607	CHL	C12-C13-C15-C16
47	Y1	609	CHL	C11-C12-C13-C15
47	Y1	609	CHL	C12-C13-C15-C16
47	n1	607	CHL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
47	y1	609	CHL	C12-C13-C15-C16
41	S	624	LHG	C11-C12-C13-C14
41	l	101	LHG	C31-C32-C33-C34
51	s	625	LPX	C7-C8-C9-C10
54	K1	101	4RF	C32-C33-C34-C35
31	b	608	CLA	C16-C17-C18-C20
31	G1	611	CLA	C16-C17-C18-C20
31	b	612	CLA	C15-C16-C17-C18
31	b	615	CLA	C15-C16-C17-C18
31	A1	410	CLA	C8-C10-C11-C12
31	C1	506	CLA	C15-C16-C17-C18
54	K1	101	4RF	O42-C41-O40-C39
35	a1	413	LMG	C4-C5-C6-O5
31	D	403	CLA	C5-C6-C7-C8
31	B1	611	CLA	C10-C11-C12-C13
31	c1	512	CLA	C5-C6-C7-C8
41	s	624	LHG	C23-C24-C25-C26
41	D1	409	LHG	C23-C24-C25-C26
34	B1	626	SQD	C30-C31-C32-C33
41	s1	624	LHG	C12-C13-C14-C15
52	B1	624	3PH	C3A-C3B-C3C-C3D
54	I1	102	4RF	C51-C52-C53-C54
54	k1	101	4RF	C05-C06-C07-C08
31	b	602	CLA	C4-C3-C5-C6
31	B1	612	CLA	C4-C3-C5-C6
31	b1	612	CLA	C4-C3-C5-C6
32	a	408	PHO	C4-C3-C5-C6
47	y	607	CHL	C4-C3-C5-C6
31	s	611	CLA	C2-C3-C5-C6
31	c1	506	CLA	C2-C3-C5-C6
32	a	408	PHO	C2-C3-C5-C6
44	D	405	PL9	C13-C14-C16-C17
47	y	607	CHL	C2-C3-C5-C6
42	c1	527	LMK	C11-C12-C13-C14
54	k1	101	4RF	C11-C12-C13-C14
31	y	602	CLA	O1A-CGA-O2A-C1
31	R	602	CLA	C5-C6-C7-C8
31	b	603	CLA	C15-C16-C17-C18
31	c	502	CLA	C5-C6-C7-C8
31	s	611	CLA	C10-C11-C12-C13
31	B1	614	CLA	C15-C16-C17-C18
31	C1	505	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	b1	604	CLA	C15-C16-C17-C18
35	w1	201	LMG	C11-C10-O7-C8
31	S	605	CLA	C2A-CAA-CBA-CGA
31	S	610	CLA	C2A-CAA-CBA-CGA
31	c	510	CLA	C2A-CAA-CBA-CGA
31	n	602	CLA	C2A-CAA-CBA-CGA
31	s	610	CLA	C2A-CAA-CBA-CGA
31	C1	505	CLA	C2A-CAA-CBA-CGA
31	N1	602	CLA	C2A-CAA-CBA-CGA
31	Y1	610	CLA	C2A-CAA-CBA-CGA
31	a1	406	CLA	C2A-CAA-CBA-CGA
31	y1	604	CLA	C2A-CAA-CBA-CGA
47	G1	607	CHL	C2A-CAA-CBA-CGA
31	A	405	CLA	C11-C12-C13-C14
31	B	603	CLA	C6-C7-C8-C9
31	B	607	CLA	C6-C7-C8-C9
31	C	506	CLA	C11-C10-C8-C9
31	C	507	CLA	C11-C12-C13-C14
31	C	508	CLA	C11-C10-C8-C9
31	C	512	CLA	C11-C10-C8-C9
31	D	402	CLA	C11-C10-C8-C9
31	D	403	CLA	C14-C13-C15-C16
31	N	613	CLA	C11-C12-C13-C14
31	G	602	CLA	C6-C7-C8-C9
31	G	603	CLA	C11-C12-C13-C14
31	G	613	CLA	C6-C7-C8-C9
31	b	603	CLA	C6-C7-C8-C9
31	c	512	CLA	C14-C13-C15-C16
31	c	513	CLA	C6-C7-C8-C9
31	c	513	CLA	C11-C12-C13-C14
31	n	603	CLA	C6-C7-C8-C9
31	n	613	CLA	C11-C12-C13-C14
31	g	602	CLA	C11-C12-C13-C14
31	g	603	CLA	C11-C12-C13-C14
31	g	613	CLA	C14-C13-C15-C16
31	s	610	CLA	C11-C10-C8-C9
31	y	602	CLA	C6-C7-C8-C9
31	y	610	CLA	C6-C7-C8-C9
31	A1	406	CLA	C14-C13-C15-C16
31	B1	602	CLA	C11-C10-C8-C9
31	B1	604	CLA	C6-C7-C8-C9
31	B1	605	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
31	C1	502	CLA	C11-C12-C13-C14
31	C1	505	CLA	C14-C13-C15-C16
31	C1	509	CLA	C14-C13-C15-C16
31	D1	403	CLA	C11-C12-C13-C14
31	N1	610	CLA	C11-C12-C13-C14
31	G1	602	CLA	C6-C7-C8-C9
31	G1	610	CLA	C11-C12-C13-C14
31	G1	613	CLA	C14-C13-C15-C16
31	S1	609	CLA	C6-C7-C8-C9
31	Y1	602	CLA	C6-C7-C8-C9
31	Y1	602	CLA	C11-C12-C13-C14
31	Y1	613	CLA	C11-C12-C13-C14
31	b1	607	CLA	C11-C12-C13-C14
31	c1	510	CLA	C14-C13-C15-C16
31	d1	402	CLA	C11-C10-C8-C9
31	n1	603	CLA	C14-C13-C15-C16
31	n1	610	CLA	C14-C13-C15-C16
31	g1	603	CLA	C6-C7-C8-C9
31	g1	611	CLA	C6-C7-C8-C9
31	r1	609	CLA	C11-C10-C8-C9
31	y1	610	CLA	C11-C12-C13-C14
31	y1	613	CLA	C11-C10-C8-C9
31	y1	613	CLA	C11-C12-C13-C14
47	N	605	CHL	C11-C10-C8-C9
47	y	606	CHL	C11-C10-C8-C9
47	N1	606	CHL	C11-C10-C8-C9
47	G1	601	CHL	C11-C12-C13-C14
47	G1	607	CHL	C14-C13-C15-C16
47	Y1	606	CHL	C6-C7-C8-C9
47	Y1	606	CHL	C11-C12-C13-C14
47	n1	607	CHL	C11-C12-C13-C14
47	g1	601	CHL	C11-C12-C13-C14
34	b1	626	SQD	C32-C33-C34-C35
41	Y	624	LHG	C9-C10-C11-C12
35	D	411	LMG	O6-C5-C6-O5
35	a	413	LMG	O6-C5-C6-O5
33	a1	411	BCR	C19-C20-C21-C22
48	s1	621	LUT	C29-C30-C31-C32
35	d	411	LMG	C32-C33-C34-C35
41	D	409	LHG	C31-C32-C33-C34
52	S1	626	3PH	C2A-C2B-C2C-C2D
31	D	402	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
31	N	602	CLA	CBA-CGA-O2A-C1
31	b1	617	CLA	CBA-CGA-O2A-C1
41	c	625	LHG	C24-C23-O8-C6
54	k1	101	4RF	C15-C16-O18-C19
40	C1	519	DGD	O1A-C1A-O1G-C1G
52	s1	626	3PH	O32-C31-O31-C3
41	n	624	LHG	C15-C16-C17-C18
40	C1	519	DGD	O1B-C1B-O2G-C2G
41	y	624	LHG	O9-C7-O7-C5
40	C	518	DGD	C2E-C1E-O5D-C6D
31	C	511	CLA	C15-C16-C17-C18
31	y	613	CLA	C8-C10-C11-C12
31	c1	507	CLA	C10-C11-C12-C13
38	c	524	DGA	CB9-CAB-CBB-CCB
52	b1	624	3PH	C32-C33-C34-C35
52	t1	101	3PH	C2E-C2F-C2G-C2H
35	C1	521	LMG	O6-C5-C6-O5
34	A1	412	SQD	O6-C44-C45-C46
35	C	521	LMG	O1-C7-C8-C9
35	a1	413	LMG	C7-C8-C9-O8
35	h1	102	LMG	C7-C8-C9-O8
40	c1	520	DGD	O1G-C1G-C2G-C3G
41	D	410	LHG	C4-C5-C6-O8
41	L	101	LHG	C4-C5-C6-O8
41	g	624	LHG	C4-C5-C6-O8
41	y	624	LHG	C4-C5-C6-O8
41	C1	525	LHG	C4-C5-C6-O8
41	D1	409	LHG	C4-C5-C6-O8
41	d1	410	LHG	C4-C5-C6-O8
42	C	527	LMK	O1-C7-C8-C9
42	c	627	LMK	O1-C7-C8-C9
42	C1	527	LMK	O1-C7-C8-C9
42	c1	527	LMK	O1-C7-C8-C9
52	T1	101	3PH	C1-C2-C3-O31
52	s1	626	3PH	C1-C2-C3-O31
34	c	626	SQD	C18-C19-C20-C21
40	C1	518	DGD	C5B-C6B-C7B-C8B
41	D	408	LHG	C12-C13-C14-C15
41	D	410	LHG	C11-C10-C9-C8
41	d1	408	LHG	C11-C10-C9-C8
31	B1	602	CLA	C3-C5-C6-C7
54	i1	101	4RF	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
31	C	502	CLA	C13-C15-C16-C17
31	C	513	CLA	C10-C11-C12-C13
31	d	402	CLA	C10-C11-C12-C13
31	G1	602	CLA	C10-C11-C12-C13
31	b1	604	CLA	C8-C10-C11-C12
31	y1	612	CLA	C15-C16-C17-C18
35	A	413	LMG	C18-C19-C20-C21
35	c	521	LMG	C29-C30-C31-C32
41	G1	624	LHG	C24-C25-C26-C27
57	y1	626	PTY	C19-C20-C21-C22
31	B	604	CLA	CBA-CGA-O2A-C1
31	S	611	CLA	CBA-CGA-O2A-C1
31	R1	612	CLA	CBA-CGA-O2A-C1
31	c1	501	CLA	CBA-CGA-O2A-C1
32	a	408	PHO	CBA-CGA-O2A-C1
54	I1	102	4RF	C43-C41-O40-C39
40	c1	519	DGD	O6E-C5E-C6E-O5E
31	n	610	CLA	C16-C17-C18-C20
31	S1	604	CLA	C6-C7-C8-C10
31	c1	513	CLA	C16-C17-C18-C20
38	b	623	DGA	CDA-CEA-CFA-CGA
40	C	519	DGD	C9B-CAB-CBB-CCB
41	L	101	LHG	C31-C32-C33-C34
41	d	410	LHG	C11-C10-C9-C8
54	K1	101	4RF	C34-C35-C36-C37
55	R1	625	LMT	C3-C4-C5-C6
31	b	610	CLA	C15-C16-C17-C18
47	Y	606	CHL	C15-C16-C17-C18
38	b1	625	DGA	CB6-CB7-CB8-CB9
41	n	624	LHG	C34-C35-C36-C37
52	t1	101	3PH	C26-C27-C28-C29
57	Y1	626	PTY	C36-C37-C38-C39
57	y1	626	PTY	C11-C12-C13-C14
35	D1	411	LMG	O6-C5-C6-O5
34	B1	626	SQD	C26-C27-C28-C29
52	T1	101	3PH	C29-C2A-C2B-C2C
31	B	612	CLA	O1D-CGD-O2D-CED
32	a1	409	PHO	CHA-CBD-CGD-O1D
32	a1	409	PHO	CHA-CBD-CGD-O2D
47	Y	609	CHL	CHA-CBD-CGD-O1D
47	n	609	CHL	CHA-CBD-CGD-O2D
47	s	607	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
47	s	607	CHL	CHA-CBD-CGD-O2D
47	G1	608	CHL	CHA-CBD-CGD-O1D
47	G1	608	CHL	CHA-CBD-CGD-O2D
47	n1	607	CHL	CHA-CBD-CGD-O1D
47	n1	607	CHL	CHA-CBD-CGD-O2D
50	S	622	NEX	C39-C29-C30-C31
31	r	610	CLA	C10-C11-C12-C13
31	y1	611	CLA	C15-C16-C17-C18
31	R	610	CLA	C3-C5-C6-C7
31	R	612	CLA	C3-C5-C6-C7
35	D	411	LMG	C11-C12-C13-C14
41	C	525	LHG	C13-C14-C15-C16
41	D	410	LHG	C25-C26-C27-C28
54	I1	102	4RF	C26-C27-C28-C29
40	C1	520	DGD	C1B-C2B-C3B-C4B
41	N1	624	LHG	C23-C24-C25-C26
52	T1	101	3PH	C31-C32-C33-C34
52	t1	101	3PH	C31-C32-C33-C34
57	Y1	626	PTY	C30-C31-C32-C33
35	H1	102	LMG	O6-C5-C6-O5
35	h1	102	LMG	O6-C5-C6-O5
31	C1	502	CLA	O1A-CGA-O2A-C1
34	c	626	SQD	C16-C17-C18-C19
34	A1	412	SQD	C11-C12-C13-C14
38	c1	524	DGA	CA5-CA6-CA7-CA8
31	N	613	CLA	C4-C3-C5-C6
31	G	602	CLA	C4-C3-C5-C6
31	c1	506	CLA	C4-C3-C5-C6
44	D	405	PL9	C30-C29-C31-C32
47	Y1	607	CHL	C4-C3-C5-C6
31	C	510	CLA	C2-C3-C5-C6
31	b	602	CLA	C2-C3-C5-C6
31	n	603	CLA	C2-C3-C5-C6
31	B1	612	CLA	C2-C3-C5-C6
31	N1	603	CLA	C2-C3-C5-C6
44	d1	405	PL9	C38-C39-C41-C42
47	Y1	607	CHL	C2-C3-C5-C6
34	b1	626	SQD	C25-C26-C27-C28
31	C	509	CLA	C8-C10-C11-C12
31	N	602	CLA	C13-C15-C16-C17
31	N	603	CLA	C13-C15-C16-C17
31	Y	602	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	b	604	CLA	C13-C15-C16-C17
31	c	502	CLA	C13-C15-C16-C17
31	r	610	CLA	C5-C6-C7-C8
31	S1	611	CLA	C13-C15-C16-C17
31	Y1	602	CLA	C15-C16-C17-C18
32	a	408	PHO	C8-C10-C11-C12
32	A1	409	PHO	C15-C16-C17-C18
47	n	601	CHL	C10-C11-C12-C13
40	B1	623	DGD	O6E-C5E-C6E-O5E
33	C1	514	BCR	C11-C12-C13-C35
37	b	620	C7Z	C7-C8-C9-C19
41	C	525	LHG	C2-C3-O3-P
41	D	410	LHG	O9-C7-O7-C5
41	d1	410	LHG	O9-C7-O7-C5
34	b1	621	SQD	C25-C26-C27-C28
41	D1	408	LHG	C11-C10-C9-C8
31	B	616	CLA	C16-C17-C18-C19
31	Y1	611	CLA	C16-C17-C18-C19
31	s1	604	CLA	C6-C7-C8-C10
34	c	626	SQD	C11-C10-C9-C8
33	C	514	BCR	C11-C12-C13-C14
33	a1	411	BCR	C7-C8-C9-C10
37	b	620	C7Z	C7-C8-C9-C10
49	n1	622	XAT	C27-C28-C29-C30
31	C	508	CLA	O1A-CGA-O2A-C1
31	c	509	CLA	O1A-CGA-O2A-C1
34	C	526	SQD	O10-C23-O48-C46
31	C	513	CLA	C15-C16-C17-C18
31	R	603	CLA	C8-C10-C11-C12
31	b	617	CLA	C8-C10-C11-C12
31	B1	605	CLA	C15-C16-C17-C18
52	T1	101	3PH	C1-O11-P-O12
52	S1	626	3PH	C1-O11-P-O12
41	G	630	LHG	C12-C13-C14-C15
31	C	510	CLA	C2A-CAA-CBA-CGA
31	D	402	CLA	C2A-CAA-CBA-CGA
31	y	602	CLA	C2A-CAA-CBA-CGA
31	R1	604	CLA	C2A-CAA-CBA-CGA
35	c1	521	LMG	O6-C5-C6-O5
40	C	520	DGD	CCB-CDB-CEB-CFB
31	S1	614	CLA	C5-C6-C7-C8
41	D	410	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
41	G	630	LHG	C13-C14-C15-C16
41	l	101	LHG	C35-C36-C37-C38
41	l	101	LHG	C7-C8-C9-C10
41	g	624	LHG	C23-C24-C25-C26
41	n1	624	LHG	C23-C24-C25-C26
31	S	611	CLA	O1A-CGA-O2A-C1
35	d1	411	LMG	C12-C13-C14-C15
38	C1	524	DGA	CB9-CAB-CBB-CCB
38	j1	101	DGA	CB7-CB8-CB9-CAB
31	Y	610	CLA	CBA-CGA-O2A-C1
35	C	521	LMG	C29-C28-O8-C9
54	k1	101	4RF	C43-C41-O40-C39
34	M1	101	SQD	C46-C45-O47-C7
35	B	622	LMG	C9-C8-O7-C10
35	W1	201	LMG	C7-C8-O7-C10
38	b	623	DGA	CG1-CG2-OG2-CB1
40	c	523	DGD	C1G-C2G-O2G-C1B
52	T1	101	3PH	C3-C2-O21-C21
52	t1	101	3PH	C2B-C2C-C2D-C2E
54	I1	102	4RF	C11-C12-C13-C14
54	I1	102	4RF	C44-C45-C46-C47
50	S1	623	NEX	C30-C31-C32-C33
31	n	610	CLA	C13-C15-C16-C17
47	S	608	CHL	C5-C6-C7-C8
47	n	601	CHL	C8-C10-C11-C12
53	a1	414	SPH	C5-C6-C7-C8
38	C1	524	DGA	CB5-CB6-CB7-CB8
41	C	525	LHG	C11-C12-C13-C14
41	D	409	LHG	C26-C27-C28-C29
41	C1	525	LHG	C28-C29-C30-C31
41	y1	624	LHG	C9-C10-C11-C12
54	k1	101	4RF	C47-C48-C49-C50
33	C	514	BCR	C13-C14-C15-C16
33	A1	411	BCR	C19-C20-C21-C22
33	B1	618	BCR	C13-C14-C15-C16
33	C1	514	BCR	C15-C16-C17-C18
48	N	621	LUT	C29-C30-C31-C32
48	N1	620	LUT	C9-C10-C11-C12
48	Y1	621	LUT	C29-C30-C31-C32
49	r	622	XAT	C9-C10-C11-C12
50	R	622	NEX	C33-C34-C35-C15
31	G	603	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
31	b1	605	CLA	C16-C17-C18-C19
34	c1	526	SQD	C24-C25-C26-C27
40	c1	519	DGD	C1A-C2A-C3A-C4A
31	c1	501	CLA	O1A-CGA-O2A-C1
31	r1	609	CLA	C3-C5-C6-C7
31	r1	603	CLA	C10-C11-C12-C13
34	C1	526	SQD	C10-C11-C12-C13
38	b1	625	DGA	CB9-CAB-CBB-CCB
54	I1	102	4RF	C25-C26-C27-C28
55	r1	625	LMT	C4'-C5'-C6'-O6'
41	n	624	LHG	O6-C4-C5-O7
52	s	626	3PH	O11-C1-C2-O21
41	G1	624	LHG	C11-C12-C13-C14
31	c	505	CLA	O1D-CGD-O2D-CED
31	G	610	CLA	CBA-CGA-O2A-C1
31	y	610	CLA	CBA-CGA-O2A-C1
31	s1	609	CLA	CBA-CGA-O2A-C1
38	j1	101	DGA	CA2-CA1-OG1-CG1
31	b1	617	CLA	O1A-CGA-O2A-C1
34	a1	412	SQD	C11-C12-C13-C14
38	b1	625	DGA	CA4-CA5-CA6-CA7
41	d	408	LHG	C30-C31-C32-C33
52	s	626	3PH	C22-C23-C24-C25
38	C	524	DGA	CB2-CB3-CB4-CB5
41	S	624	LHG	C28-C29-C30-C31
41	s	624	LHG	C33-C34-C35-C36
52	B1	624	3PH	C2C-C2D-C2E-C2F
53	a1	414	SPH	C7-C8-C9-C10
54	k1	101	4RF	C03-C04-C05-C06
31	C	510	CLA	C4-C3-C5-C6
31	R	602	CLA	C4-C3-C5-C6
31	N1	603	CLA	C4-C3-C5-C6
31	c1	508	CLA	C4-C3-C5-C6
31	b1	612	CLA	C2-C3-C5-C6
41	Y1	624	LHG	C35-C36-C37-C38
34	A	412	SQD	C25-C26-C27-C28
35	W1	201	LMG	C31-C32-C33-C34
40	C1	519	DGD	C4B-C5B-C6B-C7B
41	n1	624	LHG	C13-C14-C15-C16
52	S	626	3PH	C23-C24-C25-C26
52	S	626	3PH	C3D-C3E-C3F-C3G
52	T1	101	3PH	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
52	T1	101	3PH	C33-C34-C35-C36
31	B	602	CLA	C16-C17-C18-C19
31	Y	613	CLA	C16-C17-C18-C19
31	b	609	CLA	C16-C17-C18-C19
31	B1	607	CLA	C16-C17-C18-C19
31	D1	403	CLA	C16-C17-C18-C20
34	B	621	SQD	C31-C32-C33-C34
34	a	412	SQD	C11-C12-C13-C14
41	D1	408	LHG	C34-C35-C36-C37
41	d1	409	LHG	C10-C11-C12-C13
41	s1	624	LHG	C34-C35-C36-C37
52	i	101	3PH	C27-C28-C29-C2A
54	i1	101	4RF	C49-C50-C51-C52
57	Y1	626	PTY	C35-C36-C37-C38
52	b1	624	3PH	C3F-C3G-C3H-C3I
41	C	525	LHG	C10-C11-C12-C13
52	s1	626	3PH	C29-C2A-C2B-C2C
35	h1	102	LMG	O7-C8-C9-O8
38	C	524	DGA	OG1-CG1-CG2-OG2
38	j1	101	DGA	OG1-CG1-CG2-OG2
41	y	624	LHG	O7-C5-C6-O8
34	M1	101	SQD	C28-C29-C30-C31
38	C1	524	DGA	CA5-CA6-CA7-CA8
38	c1	524	DGA	CBB-CAB-CB9-CB8
38	c1	524	DGA	CDB-CEB-CFB-CGB
52	i	101	3PH	C34-C35-C36-C37
52	i	101	3PH	C3B-C3C-C3D-C3E
41	C	525	LHG	C35-C36-C37-C38
41	C1	525	LHG	C35-C36-C37-C38
52	S	626	3PH	C3F-C3G-C3H-C3I
38	B1	625	DGA	CA8-CA9-CAA-CBA
40	c	523	DGD	CAB-CBB-CCB-CDB
34	a1	412	SQD	C35-C36-C37-C38
41	D1	409	LHG	C35-C36-C37-C38
38	j1	101	DGA	CB4-CB5-CB6-CB7
31	S1	617	CLA	C2A-CAA-CBA-CGA
35	D1	411	LMG	C18-C19-C20-C21
41	d	410	LHG	C31-C32-C33-C34
40	c	519	DGD	O6D-C5D-C6D-O5D
31	C1	510	CLA	C5-C6-C7-C8
31	s1	603	CLA	C10-C11-C12-C13
31	B	607	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
31	B	615	CLA	C2-C1-O2A-CGA
31	C	502	CLA	C2-C1-O2A-CGA
31	a	407	CLA	C2-C1-O2A-CGA
31	C1	511	CLA	C2-C1-O2A-CGA
31	b	608	CLA	C16-C17-C18-C19
31	b	614	CLA	C16-C17-C18-C20
49	N	622	XAT	C26-C27-C28-C29
44	D	405	PL9	C44-C46-C47-C48
44	D1	405	PL9	C14-C16-C17-C18
35	D1	411	LMG	C19-C20-C21-C22
38	B	625	DGA	CB3-CB4-CB5-CB6
41	Y	624	LHG	C31-C32-C33-C34
52	S1	626	3PH	C2D-C2E-C2F-C2G
31	B	604	CLA	O1A-CGA-O2A-C1
31	D	402	CLA	O1A-CGA-O2A-C1
31	n	604	CLA	C5-C6-C7-C8
31	b1	603	CLA	C13-C15-C16-C17
31	g1	602	CLA	C8-C10-C11-C12
34	a1	412	SQD	C13-C14-C15-C16
38	b	623	DGA	CBB-CAB-CB9-CB8
38	B1	625	DGA	CEA-CFA-CGA-CHA
38	b1	625	DGA	CAA-CBA-CCA-CDA
31	s	604	CLA	CBA-CGA-O2A-C1
31	A1	405	CLA	CBA-CGA-O2A-C1
31	B1	612	CLA	CBA-CGA-O2A-C1
31	c1	502	CLA	CBA-CGA-O2A-C1
31	r1	610	CLA	CBA-CGA-O2A-C1
32	A1	408	PHO	CBA-CGA-O2A-C1
38	C1	524	DGA	CA2-CA1-OG1-CG1
41	d1	408	LHG	C24-C23-O8-C6
35	b1	622	LMG	C11-C12-C13-C14
38	B1	625	DGA	CA5-CA6-CA7-CA8
38	b1	625	DGA	CB3-CB4-CB5-CB6
40	C1	520	DGD	CCB-CDB-CEB-CFB
41	d	409	LHG	C33-C34-C35-C36
40	c	520	DGD	C4E-C5E-C6E-O5E
31	n	604	CLA	CBD-CGD-O2D-CED
38	b	623	DGA	CB7-CB8-CB9-CAB
52	i	101	3PH	C38-C39-C3A-C3B
31	C	512	CLA	C13-C15-C16-C17
31	n	602	CLA	C13-C15-C16-C17
31	Y1	614	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	b1	611	CLA	C10-C11-C12-C13
49	g	622	XAT	C14-C15-C35-C34
34	m1	101	SQD	C11-C10-C9-C8
41	N	624	LHG	C11-C12-C13-C14
41	c	625	LHG	C11-C12-C13-C14
57	Y1	626	PTY	C41-C42-C43-C44
41	C	525	LHG	C34-C35-C36-C37
31	b	607	CLA	C13-C15-C16-C17
31	c	501	CLA	C15-C16-C17-C18
31	C1	504	CLA	C15-C16-C17-C18
31	D1	403	CLA	C15-C16-C17-C18
31	Y1	613	CLA	C15-C16-C17-C18
47	r	606	CHL	C2A-CAA-CBA-CGA
31	d	402	CLA	C16-C17-C18-C20
31	C1	510	CLA	C4-C3-C5-C6
31	G1	613	CLA	C4-C3-C5-C6
31	Y1	603	CLA	C4-C3-C5-C6
44	d1	405	PL9	C40-C39-C41-C42
47	y1	609	CHL	C4-C3-C5-C6
41	g	624	LHG	O8-C23-C24-C25
38	b	623	DGA	CAA-CBA-CCA-CDA
51	S1	625	LPX	C14-C15-C16-C17
52	s	626	3PH	C36-C37-C38-C39
31	S	614	CLA	CBA-CGA-O2A-C1
31	G1	610	CLA	CBA-CGA-O2A-C1
31	n1	610	CLA	CBA-CGA-O2A-C1
31	N1	613	CLA	C13-C15-C16-C17
31	c1	507	CLA	C15-C16-C17-C18
31	n1	604	CLA	C15-C16-C17-C18
31	r1	602	CLA	C10-C11-C12-C13
31	y1	613	CLA	C5-C6-C7-C8
41	N	624	LHG	C35-C36-C37-C38
38	B1	625	DGA	CB7-CB8-CB9-CAB
40	c1	519	DGD	C4B-C5B-C6B-C7B
41	G1	624	LHG	C31-C32-C33-C34
52	s1	626	3PH	C2B-C2C-C2D-C2E
52	s1	626	3PH	C34-C35-C36-C37
38	j1	101	DGA	CA7-CA8-CA9-CAA
35	C1	523	LMG	C13-C14-C15-C16
41	N	624	LHG	C30-C31-C32-C33
41	d	409	LHG	C17-C18-C19-C20
41	D1	410	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
41	G1	624	LHG	C33-C34-C35-C36
52	B1	624	3PH	O22-C21-O21-C2
41	D1	409	LHG	O1-C1-C2-O2
31	B	603	CLA	C11-C10-C8-C9
31	B	603	CLA	C14-C13-C15-C16
31	B	608	CLA	C14-C13-C15-C16
31	B	613	CLA	C6-C7-C8-C9
31	B	615	CLA	C11-C12-C13-C14
31	C	501	CLA	C11-C10-C8-C9
31	C	507	CLA	C14-C13-C15-C16
31	C	513	CLA	C6-C7-C8-C9
31	D	402	CLA	C11-C12-C13-C14
31	D	403	CLA	C6-C7-C8-C9
31	D	403	CLA	C11-C12-C13-C14
31	G	603	CLA	C14-C13-C15-C16
31	S	610	CLA	C11-C12-C13-C14
31	S	611	CLA	C6-C7-C8-C9
31	S	611	CLA	C11-C12-C13-C14
31	Y	602	CLA	C6-C7-C8-C9
31	Y	611	CLA	C11-C10-C8-C9
31	a	405	CLA	C11-C12-C13-C14
31	b	602	CLA	C6-C7-C8-C9
31	b	602	CLA	C11-C10-C8-C9
31	c	506	CLA	C11-C10-C8-C9
31	c	507	CLA	C14-C13-C15-C16
31	c	511	CLA	C11-C12-C13-C14
31	c	512	CLA	C6-C7-C8-C9
31	c	512	CLA	C11-C12-C13-C14
31	n	604	CLA	C11-C10-C8-C9
31	g	602	CLA	C6-C7-C8-C9
31	g	603	CLA	C14-C13-C15-C16
31	g	613	CLA	C6-C7-C8-C9
31	g	613	CLA	C11-C10-C8-C9
31	s	603	CLA	C11-C10-C8-C9
31	B1	607	CLA	C11-C10-C8-C9
31	B1	614	CLA	C6-C7-C8-C9
31	C1	504	CLA	C11-C10-C8-C9
31	C1	510	CLA	C14-C13-C15-C16
31	C1	513	CLA	C11-C12-C13-C14
31	D1	402	CLA	C11-C10-C8-C9
31	D1	402	CLA	C11-C12-C13-C14
31	N1	602	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	N1	613	CLA	C11-C12-C13-C14
31	G1	603	CLA	C6-C7-C8-C9
31	G1	610	CLA	C6-C7-C8-C9
31	G1	610	CLA	C11-C10-C8-C9
31	S1	610	CLA	C11-C10-C8-C9
31	Y1	613	CLA	C14-C13-C15-C16
31	a1	405	CLA	C11-C12-C13-C14
31	b1	616	CLA	C11-C12-C13-C14
31	c1	501	CLA	C14-C13-C15-C16
31	c1	503	CLA	C14-C13-C15-C16
31	c1	505	CLA	C14-C13-C15-C16
31	c1	507	CLA	C14-C13-C15-C16
31	c1	509	CLA	C14-C13-C15-C16
31	c1	512	CLA	C11-C10-C8-C9
31	n1	610	CLA	C11-C12-C13-C14
31	g1	610	CLA	C11-C10-C8-C9
31	y1	602	CLA	C6-C7-C8-C9
31	y1	603	CLA	C6-C7-C8-C9
31	y1	612	CLA	C11-C10-C8-C9
47	G	609	CHL	C14-C13-C15-C16
47	Y	601	CHL	C11-C12-C13-C14
47	Y	609	CHL	C14-C13-C15-C16
47	g	601	CHL	C11-C12-C13-C14
47	y	607	CHL	C11-C12-C13-C14
47	N1	605	CHL	C11-C10-C8-C9
47	N1	607	CHL	C11-C10-C8-C9
47	N1	607	CHL	C11-C12-C13-C14
47	G1	609	CHL	C14-C13-C15-C16
47	S1	608	CHL	C11-C10-C8-C9
41	S	624	LHG	C31-C32-C33-C34
54	K1	101	4RF	C05-C06-C07-C08
31	c	513	CLA	C8-C10-C11-C12
31	B1	614	CLA	C13-C15-C16-C17
31	C1	506	CLA	C10-C11-C12-C13
31	C1	512	CLA	C13-C15-C16-C17
31	s1	614	CLA	C5-C6-C7-C8
41	d	410	LHG	C2-C3-O3-P
38	b1	625	DGA	CFB-CGB-CHB-CIB
31	N	602	CLA	O1A-CGA-O2A-C1
31	A	410	CLA	C4B-C3B-CAB-CBB
31	B	602	CLA	C4B-C3B-CAB-CBB
31	B	607	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	B	610	CLA	C4B-C3B-CAB-CBB
31	B	616	CLA	C4B-C3B-CAB-CBB
31	C	501	CLA	C4B-C3B-CAB-CBB
31	C	502	CLA	C4B-C3B-CAB-CBB
31	C	503	CLA	C4B-C3B-CAB-CBB
31	G	604	CLA	C4B-C3B-CAB-CBB
31	R	613	CLA	C4B-C3B-CAB-CBB
31	S	602	CLA	C4B-C3B-CAB-CBB
31	S	605	CLA	C4B-C3B-CAB-CBB
31	S	609	CLA	C4B-C3B-CAB-CBB
31	S	612	CLA	C4B-C3B-CAB-CBB
31	S	614	CLA	C4B-C3B-CAB-CBB
31	b	610	CLA	C4B-C3B-CAB-CBB
31	b	616	CLA	C4B-C3B-CAB-CBB
31	b	617	CLA	C4B-C3B-CAB-CBB
31	c	507	CLA	C4B-C3B-CAB-CBB
31	d	403	CLA	C4B-C3B-CAB-CBB
31	n	614	CLA	C4B-C3B-CAB-CBB
31	g	613	CLA	C4B-C3B-CAB-CBB
31	g	614	CLA	C4B-C3B-CAB-CBB
31	r	609	CLA	C4B-C3B-CAB-CBB
31	r	610	CLA	C4B-C3B-CAB-CBB
31	r	613	CLA	C4B-C3B-CAB-CBB
31	s	603	CLA	C4B-C3B-CAB-CBB
31	s	617	CLA	C4B-C3B-CAB-CBB
31	y	604	CLA	C4B-C3B-CAB-CBB
31	y	611	CLA	C4B-C3B-CAB-CBB
31	B1	605	CLA	C4B-C3B-CAB-CBB
31	B1	608	CLA	C4B-C3B-CAB-CBB
31	B1	613	CLA	C4B-C3B-CAB-CBB
31	B1	617	CLA	C4B-C3B-CAB-CBB
31	C1	507	CLA	C4B-C3B-CAB-CBB
31	D1	402	CLA	C4B-C3B-CAB-CBB
31	N1	613	CLA	C4B-C3B-CAB-CBB
31	N1	614	CLA	C4B-C3B-CAB-CBB
31	G1	610	CLA	C4B-C3B-CAB-CBB
31	R1	602	CLA	C4B-C3B-CAB-CBB
31	R1	608	CLA	C4B-C3B-CAB-CBB
31	R1	612	CLA	C4B-C3B-CAB-CBB
31	S1	610	CLA	C4B-C3B-CAB-CBB
31	S1	614	CLA	C4B-C3B-CAB-CBB
31	Y1	602	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	Y1	603	CLA	C4B-C3B-CAB-CBB
31	Y1	610	CLA	C4B-C3B-CAB-CBB
31	b1	603	CLA	C4B-C3B-CAB-CBB
31	b1	604	CLA	C4B-C3B-CAB-CBB
31	c1	504	CLA	C4B-C3B-CAB-CBB
31	c1	506	CLA	C4B-C3B-CAB-CBB
31	n1	604	CLA	C4B-C3B-CAB-CBB
31	n1	614	CLA	C4B-C3B-CAB-CBB
31	g1	604	CLA	C4B-C3B-CAB-CBB
31	g1	611	CLA	C4B-C3B-CAB-CBB
31	r1	604	CLA	C4B-C3B-CAB-CBB
31	r1	610	CLA	C4B-C3B-CAB-CBB
31	s1	603	CLA	C4B-C3B-CAB-CBB
31	s1	614	CLA	C4B-C3B-CAB-CBB
31	y1	604	CLA	C4B-C3B-CAB-CBB
31	y1	608	CLA	C4B-C3B-CAB-CBB
31	y1	611	CLA	C4B-C3B-CAB-CBB
31	y1	612	CLA	C4B-C3B-CAB-CBB
34	M1	101	SQD	C12-C13-C14-C15
38	c	524	DGA	CB7-CB8-CB9-CAB
41	g1	624	LHG	C11-C12-C13-C14
52	t1	101	3PH	C25-C26-C27-C28
53	A1	414	SPH	C10-C11-C12-C13
34	B	621	SQD	C23-C24-C25-C26
41	N	624	LHG	C11-C10-C9-C8
41	N1	624	LHG	C9-C10-C11-C12
41	G1	624	LHG	C16-C17-C18-C19
31	S	610	CLA	C8-C10-C11-C12
31	c	512	CLA	C13-C15-C16-C17
31	B1	611	CLA	C8-C10-C11-C12
31	S1	609	CLA	C8-C10-C11-C12
31	c1	506	CLA	C8-C10-C11-C12
40	B1	623	DGD	O6D-C5D-C6D-O5D
40	C1	518	DGD	C2G-C1G-O1G-C1A
31	G1	611	CLA	C16-C17-C18-C19
40	c	518	DGD	C6B-C7B-C8B-C9B
34	b1	621	SQD	C24-C23-O48-C46
31	Y	602	CLA	C2A-CAA-CBA-CGA
38	C	524	DGA	CB7-CB8-CB9-CAB
38	c	524	DGA	CB2-CB3-CB4-CB5
52	t1	101	3PH	C3A-C3B-C3C-C3D
53	a1	414	SPH	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	S	602	CLA	O1D-CGD-O2D-CED
34	a	412	SQD	C2-C1-O6-C44
40	B1	623	DGD	C2D-C1D-O3G-C3G
31	s	610	CLA	C15-C16-C17-C18
31	B1	617	CLA	C5-C6-C7-C8
38	C1	524	DGA	CBA-CCA-CDA-CEA
40	C	520	DGD	CAB-CBB-CCB-CDB
41	S	624	LHG	C34-C35-C36-C37
41	Y	624	LHG	C25-C26-C27-C28
41	s	624	LHG	C27-C28-C29-C30
41	y	624	LHG	C11-C12-C13-C14
41	N1	624	LHG	C11-C12-C13-C14
41	d1	410	LHG	C28-C29-C30-C31
42	C	527	LMK	C29-C30-C31-C32
54	K1	101	4RF	C24-C25-C26-C27
41	C	525	LHG	O6-C4-C5-C6
41	D	408	LHG	O6-C4-C5-C6
41	c	625	LHG	O6-C4-C5-C6
41	d	408	LHG	O6-C4-C5-C6
41	d	410	LHG	O6-C4-C5-C6
41	C1	525	LHG	O6-C4-C5-C6
41	L1	101	LHG	O6-C4-C5-C6
41	c1	525	LHG	O6-C4-C5-C6
41	d1	408	LHG	O6-C4-C5-C6
41	d1	409	LHG	O6-C4-C5-C6
52	i	101	3PH	O11-C1-C2-C3
52	B1	624	3PH	O11-C1-C2-C3
34	C1	526	SQD	C26-C27-C28-C29
35	h1	102	LMG	C37-C38-C39-C40
41	L	101	LHG	C25-C26-C27-C28
41	l	101	LHG	C34-C35-C36-C37
34	C	526	SQD	C9-C10-C11-C12
31	B	607	CLA	C6-C7-C8-C10
31	B	613	CLA	C6-C7-C8-C10
31	B	615	CLA	C11-C12-C13-C15
31	C	501	CLA	C11-C10-C8-C7
31	C	505	CLA	C12-C13-C15-C16
31	C	506	CLA	C12-C13-C15-C16
31	C	510	CLA	C11-C10-C8-C7
31	C	512	CLA	C11-C10-C8-C7
31	C	512	CLA	C12-C13-C15-C16
31	C	513	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
31	D	403	CLA	C6-C7-C8-C10
31	G	602	CLA	C6-C7-C8-C10
31	G	602	CLA	C12-C13-C15-C16
31	G	603	CLA	C12-C13-C15-C16
31	G	613	CLA	C11-C10-C8-C7
31	S	611	CLA	C12-C13-C15-C16
31	Y	602	CLA	C6-C7-C8-C10
31	b	604	CLA	C6-C7-C8-C10
31	b	605	CLA	C11-C10-C8-C7
31	b	613	CLA	C11-C10-C8-C7
31	b	617	CLA	C6-C7-C8-C10
31	c	512	CLA	C11-C12-C13-C15
31	c	512	CLA	C12-C13-C15-C16
31	d	402	CLA	C11-C12-C13-C15
31	d	403	CLA	C11-C12-C13-C15
31	n	610	CLA	C6-C7-C8-C10
31	g	603	CLA	C11-C12-C13-C15
31	g	613	CLA	C12-C13-C15-C16
31	s	603	CLA	C11-C10-C8-C7
31	s	609	CLA	C11-C10-C8-C7
31	s	611	CLA	C11-C10-C8-C7
31	y	610	CLA	C6-C7-C8-C10
31	y	614	CLA	C11-C10-C8-C7
31	A1	406	CLA	C12-C13-C15-C16
31	B1	605	CLA	C11-C10-C8-C7
31	B1	608	CLA	C11-C12-C13-C15
31	B1	609	CLA	C11-C12-C13-C15
31	B1	614	CLA	C6-C7-C8-C10
31	B1	616	CLA	C11-C10-C8-C7
31	B1	617	CLA	C6-C7-C8-C10
31	C1	504	CLA	C11-C10-C8-C7
31	C1	505	CLA	C11-C12-C13-C15
31	C1	505	CLA	C12-C13-C15-C16
31	C1	506	CLA	C12-C13-C15-C16
31	C1	507	CLA	C12-C13-C15-C16
31	C1	513	CLA	C11-C10-C8-C7
31	D1	402	CLA	C11-C10-C8-C7
31	N1	610	CLA	C12-C13-C15-C16
31	G1	610	CLA	C6-C7-C8-C10
31	G1	610	CLA	C11-C12-C13-C15
31	G1	613	CLA	C12-C13-C15-C16
31	R1	610	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
31	S1	610	CLA	C11-C10-C8-C7
31	S1	610	CLA	C11-C12-C13-C15
31	S1	611	CLA	C11-C12-C13-C15
31	Y1	602	CLA	C6-C7-C8-C10
31	Y1	602	CLA	C11-C12-C13-C15
31	Y1	603	CLA	C12-C13-C15-C16
31	Y1	610	CLA	C11-C12-C13-C15
31	b1	616	CLA	C11-C12-C13-C15
31	c1	501	CLA	C12-C13-C15-C16
31	c1	503	CLA	C12-C13-C15-C16
31	c1	504	CLA	C11-C10-C8-C7
31	c1	505	CLA	C12-C13-C15-C16
31	c1	509	CLA	C12-C13-C15-C16
31	c1	512	CLA	C11-C10-C8-C7
31	n1	603	CLA	C12-C13-C15-C16
31	g1	602	CLA	C6-C7-C8-C10
31	g1	603	CLA	C12-C13-C15-C16
31	r1	608	CLA	C6-C7-C8-C10
31	r1	609	CLA	C11-C10-C8-C7
31	y1	610	CLA	C11-C12-C13-C15
31	y1	613	CLA	C11-C10-C8-C7
32	A	409	PHO	C6-C7-C8-C10
47	N	605	CHL	C11-C10-C8-C7
47	N	606	CHL	C11-C10-C8-C7
47	Y	609	CHL	C12-C13-C15-C16
47	n	606	CHL	C11-C12-C13-C15
47	g	601	CHL	C11-C12-C13-C15
47	y	606	CHL	C11-C10-C8-C7
47	N1	601	CHL	C12-C13-C15-C16
47	N1	605	CHL	C11-C10-C8-C7
47	N1	606	CHL	C11-C10-C8-C7
47	N1	606	CHL	C11-C12-C13-C15
47	N1	607	CHL	C11-C10-C8-C7
47	Y1	606	CHL	C6-C7-C8-C10
47	n1	601	CHL	C12-C13-C15-C16
47	n1	605	CHL	C12-C13-C15-C16
47	g1	601	CHL	C6-C7-C8-C10
31	c	512	CLA	C15-C16-C17-C18
31	C1	507	CLA	C15-C16-C17-C18
47	G	601	CHL	C10-C11-C12-C13
54	k1	101	4RF	O17-C16-O18-C19
40	C	523	DGD	CDA-CEA-CFA-CGA

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Mol	Chain	Res	Type	Atoms
44	D1	405	PL9	C47-C48-C49-C50
54	k1	101	4RF	C35-C36-C37-C38
31	B1	603	CLA	C13-C15-C16-C17
31	c1	505	CLA	C13-C15-C16-C17
31	c1	513	CLA	C16-C17-C18-C19
41	Y1	624	LHG	C33-C34-C35-C36
41	g1	624	LHG	C16-C17-C18-C19
31	R1	612	CLA	O1A-CGA-O2A-C1
35	C	521	LMG	O10-C28-O8-C9
41	C	525	LHG	C30-C31-C32-C33
52	s	626	3PH	C3D-C3E-C3F-C3G
31	N	604	CLA	C3A-C2A-CAA-CBA
31	N	613	CLA	C3A-C2A-CAA-CBA
31	R	604	CLA	C3A-C2A-CAA-CBA
31	c	506	CLA	C3A-C2A-CAA-CBA
31	n	613	CLA	C3A-C2A-CAA-CBA
31	B1	602	CLA	C3A-C2A-CAA-CBA
31	B1	610	CLA	C3A-C2A-CAA-CBA
31	N1	614	CLA	C3A-C2A-CAA-CBA
31	S1	605	CLA	C3A-C2A-CAA-CBA
31	Y1	604	CLA	C4-C3-C5-C6
31	c1	505	CLA	C3A-C2A-CAA-CBA
31	c1	510	CLA	C4-C3-C5-C6
31	y1	603	CLA	C4-C3-C5-C6
32	a	409	PHO	C3A-C2A-CAA-CBA
32	a1	408	PHO	C4-C3-C5-C6
44	D	405	PL9	C15-C14-C16-C17
47	g	606	CHL	C3A-C2A-CAA-CBA
47	G1	607	CHL	C4-C3-C5-C6
47	n1	601	CHL	C3A-C2A-CAA-CBA
31	N	613	CLA	C15-C16-C17-C18
31	b1	612	CLA	C15-C16-C17-C18
56	r1	626	ERG	C22-C23-C24-C28
41	D	408	LHG	C11-C12-C13-C14
54	k1	101	4RF	C44-C45-C46-C47
35	c1	521	LMG	O7-C10-C11-C12
31	s	602	CLA	C2-C3-C5-C6
31	Y1	603	CLA	C2-C3-C5-C6
31	c1	510	CLA	C2-C3-C5-C6
35	D	411	LMG	C28-C29-C30-C31
41	y1	624	LHG	C26-C27-C28-C29
35	j	101	LMG	O6-C1-O1-C7

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Mol	Chain	Res	Type	Atoms
52	i	101	3PH	C3E-C3F-C3G-C3H
41	c	625	LHG	O10-C23-O8-C6
54	I1	102	4RF	O42-C41-O40-C39
31	c	503	CLA	C8-C10-C11-C12
38	C	524	DGA	CBB-CAB-CB9-CB8
31	b	607	CLA	CBA-CGA-O2A-C1
41	D1	408	LHG	C24-C23-O8-C6
34	A	412	SQD	C30-C31-C32-C33
35	a	413	LMG	C32-C33-C34-C35
52	t1	101	3PH	C2D-C2E-C2F-C2G
33	C	515	BCR	C19-C20-C21-C22
33	b	619	BCR	C9-C10-C11-C12
33	D1	404	BCR	C9-C10-C11-C12
33	d1	404	BCR	C13-C14-C15-C16
37	B	620	C7Z	C29-C30-C31-C32
37	b1	620	C7Z	C33-C34-C35-C15
46	h1	101	RRX	C19-C20-C21-C22
48	R	620	LUT	C13-C14-C15-C35
48	R	620	LUT	C33-C34-C35-C15
48	g	621	LUT	C29-C30-C31-C32
48	R1	620	LUT	C33-C34-C35-C15
48	n1	620	LUT	C9-C10-C11-C12
49	y	622	XAT	C29-C30-C31-C32
31	B1	617	CLA	C3-C5-C6-C7
31	R1	608	CLA	C3-C5-C6-C7
31	B1	612	CLA	C13-C15-C16-C17
33	c	514	BCR	C37-C22-C23-C24
48	n	621	LUT	C31-C32-C33-C40
48	s1	620	LUT	C31-C32-C33-C40
38	C1	524	DGA	CB4-CB5-CB6-CB7
41	d	409	LHG	C13-C14-C15-C16
41	n	624	LHG	C25-C26-C27-C28
38	B	625	DGA	CFA-CGA-CHA-CIA
54	k1	101	4RF	O42-C41-O40-C39
41	c1	525	LHG	C25-C26-C27-C28
31	C	510	CLA	C13-C15-C16-C17
49	y	622	XAT	C11-C12-C13-C14
49	y1	622	XAT	C27-C28-C29-C30
38	c1	524	DGA	CBB-CCB-CDB-CEB
41	D1	410	LHG	C31-C32-C33-C34
34	B	621	SQD	C7-C8-C9-C10
54	I1	102	4RF	C41-C43-C44-C45

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Mol	Chain	Res	Type	Atoms
57	Y1	626	PTY	C8-C11-C12-C13
35	d	411	LMG	C4-C5-C6-O5
41	Y1	624	LHG	C30-C31-C32-C33
41	s1	624	LHG	C1-C2-C3-O3
52	T1	101	3PH	C3F-C3G-C3H-C3I
31	b1	605	CLA	O1D-CGD-O2D-CED
40	c1	519	DGD	C2A-C1A-O1G-C1G
41	s	624	LHG	C28-C29-C30-C31
41	D1	408	LHG	C24-C25-C26-C27
52	T1	101	3PH	C34-C35-C36-C37
31	D1	403	CLA	C10-C11-C12-C13
34	B1	626	SQD	O6-C44-C45-C46
34	B1	626	SQD	C44-C45-C46-O48
34	m1	101	SQD	C44-C45-C46-O48
35	A	413	LMG	C7-C8-C9-O8
35	a	413	LMG	O1-C7-C8-C9
35	b	622	LMG	C7-C8-C9-O8
35	c	521	LMG	O1-C7-C8-C9
35	a1	413	LMG	O1-C7-C8-C9
38	C	524	DGA	OG1-CG1-CG2-CG3
40	c	523	DGD	O1G-C1G-C2G-C3G
40	b1	623	DGD	O1G-C1G-C2G-C3G
41	G	630	LHG	C4-C5-C6-O8
41	d	410	LHG	C4-C5-C6-O8
41	l	101	LHG	C4-C5-C6-O8
41	D1	410	LHG	C4-C5-C6-O8
41	L1	101	LHG	C4-C5-C6-O8
41	G1	624	LHG	C4-C5-C6-O8
41	d1	409	LHG	C4-C5-C6-O8
41	s1	624	LHG	C4-C5-C6-O8
54	i1	101	4RF	C19-C20-C39-O40
54	k1	101	4RF	O18-C19-C20-C39
57	y1	627	PTY	O4-C1-C6-C5
38	C	524	DGA	CA8-CA9-CAA-CBA
52	B1	624	3PH	C38-C39-C3A-C3B
31	c	513	CLA	C3-C5-C6-C7
40	c	520	DGD	O6E-C5E-C6E-O5E
35	C	521	LMG	C11-C12-C13-C14
40	c1	518	DGD	C3B-C4B-C5B-C6B
41	L	101	LHG	C28-C29-C30-C31
41	S	624	LHG	C14-C15-C16-C17
41	d1	410	LHG	C30-C31-C32-C33

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Mol	Chain	Res	Type	Atoms
41	g1	624	LHG	C11-C10-C9-C8
54	I1	102	4RF	C49-C50-C51-C52
41	n	624	LHG	C23-C24-C25-C26
41	d1	410	LHG	C7-C8-C9-C10
41	c1	525	LHG	C35-C36-C37-C38
31	B	610	CLA	C16-C17-C18-C20
31	b	608	CLA	C13-C15-C16-C17
41	n	624	LHG	C11-C12-C13-C14
41	y1	624	LHG	C30-C31-C32-C33
42	C1	527	LMK	C11-C12-C13-C14
54	k1	101	4RF	C12-C13-C14-C15
31	Y	610	CLA	O1A-CGA-O2A-C1
31	r1	610	CLA	O1A-CGA-O2A-C1
32	a	408	PHO	O1A-CGA-O2A-C1
41	L	101	LHG	C35-C36-C37-C38
38	C	524	DGA	CB3-CB4-CB5-CB6
40	c	519	DGD	C6B-C7B-C8B-C9B
54	K1	101	4RF	C52-C53-C54-C55
38	c	524	DGA	CG1-CG2-CG3-OXT
38	c1	524	DGA	CG1-CG2-CG3-OXT
38	j1	101	DGA	CG1-CG2-CG3-OXT
47	G	607	CHL	C1A-C2A-CAA-CBA
47	g	607	CHL	C1A-C2A-CAA-CBA
47	y	605	CHL	C1A-C2A-CAA-CBA
47	N1	607	CHL	C1A-C2A-CAA-CBA
47	g1	607	CHL	C1A-C2A-CAA-CBA
41	n1	624	LHG	C35-C36-C37-C38
34	C1	526	SQD	C33-C34-C35-C36
35	w1	201	LMG	C36-C37-C38-C39
41	D	409	LHG	C30-C31-C32-C33
41	d	408	LHG	C11-C10-C9-C8
41	D1	409	LHG	C31-C32-C33-C34
31	C1	512	CLA	C4-C3-C5-C6
44	d	405	PL9	C15-C14-C16-C17
47	Y	607	CHL	C4-C3-C5-C6
47	n1	605	CHL	C4-C3-C5-C6
41	S	624	LHG	C11-C10-C9-C8
41	c	625	LHG	C33-C34-C35-C36
35	w1	201	LMG	O7-C10-C11-C12
31	G1	613	CLA	C2-C3-C5-C6
31	y1	603	CLA	C2-C3-C5-C6
32	a1	408	PHO	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
47	G1	607	CHL	C2-C3-C5-C6
31	r	610	CLA	C3-C5-C6-C7
31	a1	410	CLA	C3-C5-C6-C7
40	c1	518	DGD	C2A-C3A-C4A-C5A
41	G1	624	LHG	C35-C36-C37-C38
34	a1	412	SQD	C24-C25-C26-C27
34	B	621	SQD	C30-C31-C32-C33
41	d1	410	LHG	C11-C10-C9-C8
31	N	604	CLA	C16-C17-C18-C19
31	n	610	CLA	C16-C17-C18-C19
31	r	603	CLA	C11-C12-C13-C15
41	D	408	LHG	O6-C4-C5-O7
41	D	409	LHG	O6-C4-C5-O7
41	L	101	LHG	O6-C4-C5-O7
41	c	625	LHG	O6-C4-C5-O7
41	d	409	LHG	O6-C4-C5-O7
41	s	624	LHG	O6-C4-C5-O7
41	d1	409	LHG	O6-C4-C5-O7
41	n1	624	LHG	O6-C4-C5-O7
41	g1	624	LHG	O6-C4-C5-O7
52	S	626	3PH	O11-C1-C2-O21
52	t1	101	3PH	O11-C1-C2-O21
57	y1	627	PTY	O14-C5-C6-O7
41	S1	624	LHG	C31-C32-C33-C34
52	S	626	3PH	C27-C28-C29-C2A
47	s1	606	CHL	C2A-CAA-CBA-CGA
41	g1	624	LHG	C35-C36-C37-C38
31	C	503	CLA	C2B-C3B-CAB-CBB
31	S	605	CLA	C2B-C3B-CAB-CBB
31	d	403	CLA	C2B-C3B-CAB-CBB
31	R1	612	CLA	C2B-C3B-CAB-CBB
31	c1	504	CLA	C2B-C3B-CAB-CBB
31	s1	603	CLA	C2B-C3B-CAB-CBB
33	A	411	BCR	C23-C24-C25-C30
33	D	404	BCR	C23-C24-C25-C30
33	a	411	BCR	C23-C24-C25-C30
33	c	514	BCR	C23-C24-C25-C30
33	c	516	BCR	C1-C6-C7-C8
33	C1	514	BCR	C23-C24-C25-C30
33	C1	516	BCR	C23-C24-C25-C30
33	a1	411	BCR	C23-C24-C25-C30
33	c1	514	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
33	c1	515	BCR	C23-C24-C25-C30
33	c1	516	BCR	C1-C6-C7-C8
37	B	620	C7Z	C1-C6-C7-C8
37	b1	620	C7Z	C21-C26-C27-C28
48	N1	620	LUT	C1-C6-C7-C8
42	c	627	LMK	C29-C30-C31-C32
31	S	602	CLA	C5-C6-C7-C8
31	y	602	CLA	C13-C15-C16-C17
32	a	408	PHO	C15-C16-C17-C18
41	D	410	LHG	C2-C3-O3-P
41	s	624	LHG	C2-C3-O3-P
31	A	410	CLA	C3-C5-C6-C7
38	C	524	DGA	CB9-CAB-CBB-CCB
38	b1	625	DGA	CBB-CAB-CB9-CB8
40	C1	519	DGD	C2A-C3A-C4A-C5A
53	y	625	SPH	O1-C1-C2-N2
41	D	409	LHG	C25-C26-C27-C28
31	n	603	CLA	C13-C15-C16-C17
31	Y1	612	CLA	C8-C10-C11-C12
35	D1	411	LMG	C32-C33-C34-C35
41	c	625	LHG	C9-C10-C11-C12
41	y	624	LHG	C32-C33-C34-C35
33	C	516	BCR	C9-C10-C11-C12
57	y1	627	PTY	O30-C30-O4-C1
34	b1	626	SQD	C12-C13-C14-C15
57	Y1	626	PTY	C11-C12-C13-C14
31	Y1	610	CLA	C16-C17-C18-C20
31	Y1	611	CLA	C16-C17-C18-C20
31	b1	605	CLA	CAA-CBA-CGA-O2A
34	m1	101	SQD	O47-C7-C8-C9
41	n	624	LHG	O8-C23-C24-C25
35	H	102	LMG	C28-C29-C30-C31
31	b	602	CLA	C8-C10-C11-C12
31	c	509	CLA	C10-C11-C12-C13
31	s	610	CLA	C8-C10-C11-C12
34	b	621	SQD	O47-C45-C46-O48
34	B1	626	SQD	O6-C44-C45-O47
34	a1	412	SQD	O47-C45-C46-O48
35	A	413	LMG	O7-C8-C9-O8
35	C	521	LMG	O1-C7-C8-O7
35	H	102	LMG	O7-C8-C9-O8
35	a	413	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
35	h	102	LMG	O7-C8-C9-O8
35	w1	201	LMG	O7-C8-C9-O8
40	C	519	DGD	O1G-C1G-C2G-O2G
41	C	525	LHG	O7-C5-C6-O8
41	C1	525	LHG	O7-C5-C6-O8
41	Y1	624	LHG	O7-C5-C6-O8
42	C	527	LMK	O1-C7-C8-O7
52	i	101	3PH	O21-C2-C3-O31
52	T1	101	3PH	O21-C2-C3-O31
54	K1	101	4RF	O21-C20-C39-O40
57	y1	627	PTY	O4-C1-C6-O7
41	d	409	LHG	C34-C35-C36-C37
44	D	405	PL9	C4-C3-C7-C8
44	d1	405	PL9	C4-C3-C7-C8
41	c	625	LHG	C35-C36-C37-C38
31	C	513	CLA	C3-C5-C6-C7
40	c	520	DGD	C2A-C3A-C4A-C5A
31	c1	508	CLA	C10-C11-C12-C13
31	A	406	CLA	O1D-CGD-O2D-CED
52	B1	624	3PH	C2F-C2G-C2H-C2I
35	c	521	LMG	C28-C29-C30-C31
40	C1	519	DGD	C1A-C2A-C3A-C4A
31	G	610	CLA	O1A-CGA-O2A-C1
31	y	610	CLA	O1A-CGA-O2A-C1
31	B	609	CLA	C4-C3-C5-C6
31	n	613	CLA	C4-C3-C5-C6
31	N1	613	CLA	C4-C3-C5-C6
47	Y1	609	CHL	C4-C3-C5-C6
34	c1	526	SQD	C32-C33-C34-C35
41	d	408	LHG	C34-C35-C36-C37
41	n	624	LHG	C30-C31-C32-C33
53	Y	625	SPH	C10-C11-C12-C13
50	g	623	NEX	C30-C31-C32-C33
31	b	608	CLA	C10-C11-C12-C13
31	n	602	CLA	C15-C16-C17-C18
31	G1	602	CLA	C5-C6-C7-C8
31	c1	507	CLA	C13-C15-C16-C17
31	y1	614	CLA	C13-C15-C16-C17
31	N1	613	CLA	C2-C3-C5-C6
31	Y1	604	CLA	C2-C3-C5-C6
47	n1	605	CHL	C2-C3-C5-C6
47	y1	609	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
34	A1	412	SQD	C9-C10-C11-C12
38	C1	524	DGA	CAA-CBA-CCA-CDA
31	r1	612	CLA	C2-C1-O2A-CGA
42	C1	527	LMK	C1-C2-C3-C4
42	c1	527	LMK	O8-C28-C29-C30
31	D1	403	CLA	C16-C17-C18-C19
38	J1	101	DGA	CB2-CB3-CB4-CB5
41	n1	624	LHG	C14-C15-C16-C17
52	B1	624	3PH	C2B-C2C-C2D-C2E
53	y	625	SPH	C10-C11-C12-C13
31	y	612	CLA	C13-C15-C16-C17
31	b1	615	CLA	C15-C16-C17-C18
34	b	621	SQD	C7-C8-C9-C10
57	y1	626	PTY	C23-C24-C25-C26
31	s1	609	CLA	O1A-CGA-O2A-C1
31	B	602	CLA	C11-C10-C8-C9
31	B	606	CLA	C6-C7-C8-C9
31	B	609	CLA	C11-C12-C13-C14
31	C	506	CLA	C14-C13-C15-C16
31	C	510	CLA	C11-C10-C8-C9
31	C	512	CLA	C14-C13-C15-C16
31	C	513	CLA	C11-C12-C13-C14
31	G	603	CLA	C6-C7-C8-C9
31	G	613	CLA	C11-C10-C8-C9
31	S	611	CLA	C14-C13-C15-C16
31	Y	614	CLA	C11-C10-C8-C9
31	b	604	CLA	C6-C7-C8-C9
31	b	608	CLA	C11-C12-C13-C14
31	b	616	CLA	C11-C12-C13-C14
31	c	509	CLA	C6-C7-C8-C9
31	d	402	CLA	C11-C12-C13-C14
31	d	403	CLA	C11-C12-C13-C14
31	n	603	CLA	C11-C12-C13-C14
31	s	611	CLA	C11-C10-C8-C9
31	B1	608	CLA	C11-C12-C13-C14
31	B1	609	CLA	C11-C12-C13-C14
31	B1	617	CLA	C6-C7-C8-C9
31	c1	504	CLA	C11-C10-C8-C9
31	c1	511	CLA	C11-C10-C8-C9
31	r1	608	CLA	C6-C7-C8-C9
47	N	607	CHL	C11-C10-C8-C9
47	G1	601	CHL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
47	Y1	609	CHL	C14-C13-C15-C16
47	g1	601	CHL	C6-C7-C8-C9
47	y1	609	CHL	C14-C13-C15-C16
41	g	624	LHG	C9-C10-C11-C12
34	C1	526	SQD	C19-C20-C21-C22
41	N1	624	LHG	C35-C36-C37-C38
41	y1	624	LHG	C35-C36-C37-C38
31	c	505	CLA	C5-C6-C7-C8
31	n	602	CLA	C10-C11-C12-C13
35	j	101	LMG	C11-C12-C13-C14
40	C	519	DGD	C9A-CAA-CBA-CCA
41	S1	624	LHG	C30-C31-C32-C33
34	M1	101	SQD	O5-C1-O6-C44
34	c1	526	SQD	O5-C1-O6-C44
53	y	625	SPH	O1-C1-C2-C3
41	n	624	LHG	C35-C36-C37-C38
35	a1	413	LMG	C30-C31-C32-C33
41	G	630	LHG	C10-C11-C12-C13
31	b1	613	CLA	C8-C10-C11-C12
40	C	520	DGD	C4E-C5E-C6E-O5E
49	N1	622	XAT	C14-C15-C35-C34
40	C1	520	DGD	O6D-C5D-C6D-O5D
35	c1	521	LMG	C21-C22-C23-C24
38	b	623	DGA	CA8-CA9-CAA-CBA
41	C	525	LHG	C12-C13-C14-C15
52	b1	624	3PH	C34-C35-C36-C37
31	B	602	CLA	C16-C17-C18-C20
31	Y	613	CLA	C16-C17-C18-C20
31	B1	607	CLA	C16-C17-C18-C20
42	c	627	LMK	C2-C3-C4-O2
40	c	519	DGD	C5A-C6A-C7A-C8A
53	Y1	625	SPH	C9-C10-C11-C12
54	I1	102	4RF	C32-C33-C34-C35
40	b1	623	DGD	C2D-C1D-O3G-C3G
41	D	409	LHG	C33-C34-C35-C36
38	j1	101	DGA	OG2-CG2-CG3-OXT
31	r1	612	CLA	C8-C10-C11-C12
47	g	601	CHL	C10-C11-C12-C13
35	D1	411	LMG	C33-C34-C35-C36
41	c1	525	LHG	C30-C31-C32-C33
41	s1	624	LHG	C33-C34-C35-C36
31	C	511	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	s1	603	CLA	C13-C15-C16-C17
41	d	410	LHG	O1-C1-C2-O2
41	n1	624	LHG	O1-C1-C2-O2
31	a	406	CLA	C3-C5-C6-C7
31	b	613	CLA	C3-C5-C6-C7
31	g	613	CLA	C3-C5-C6-C7
31	B	602	CLA	C4-C3-C5-C6
53	Y1	625	SPH	C6-C7-C8-C9
33	b	619	BCR	C13-C14-C15-C16
33	c	515	BCR	C9-C10-C11-C12
48	r	620	LUT	C9-C10-C11-C12
31	A1	405	CLA	CAA-CBA-CGA-O2A
31	C1	510	CLA	C2-C3-C5-C6
31	d	402	CLA	C16-C17-C18-C19
31	n1	613	CLA	C16-C17-C18-C19
55	R1	625	LMT	C4'-C5'-C6'-O6'
40	c	523	DGD	C7B-C8B-C9B-CAB
34	A1	412	SQD	C30-C31-C32-C33
41	d1	410	LHG	C33-C34-C35-C36
41	D1	409	LHG	C33-C34-C35-C36
41	n1	624	LHG	C9-C10-C11-C12
52	i	101	3PH	C39-C3A-C3B-C3C
31	C	509	CLA	C15-C16-C17-C18
31	G	602	CLA	C5-C6-C7-C8
31	C1	513	CLA	C15-C16-C17-C18
41	D	409	LHG	O9-C7-O7-C5
41	S	624	LHG	C1-C2-C3-O3
41	n1	624	LHG	C1-C2-C3-O3
41	C	525	LHG	C31-C32-C33-C34
41	G1	624	LHG	C9-C10-C11-C12
54	k1	101	4RF	C10-C11-C12-C13
50	N	623	NEX	C20-C13-C14-C15
50	n	623	NEX	C11-C10-C9-C19
50	r	623	NEX	C40-C33-C34-C35
50	n1	623	NEX	C20-C13-C14-C15
50	s1	623	NEX	C40-C33-C34-C35
31	c	501	CLA	C3-C5-C6-C7
31	B1	607	CLA	C3-C5-C6-C7
35	C1	521	LMG	O7-C10-C11-C12
32	A1	409	PHO	CBA-CGA-O2A-C1
31	n	602	CLA	C8-C10-C11-C12
31	s	609	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	y1	611	CLA	C10-C11-C12-C13
53	Y	625	SPH	C14-C15-C16-C17
55	r1	625	LMT	C5-C6-C7-C8
41	D	410	LHG	O6-C4-C5-C6
41	d	409	LHG	O6-C4-C5-C6
41	n1	624	LHG	O6-C4-C5-C6
52	s	626	3PH	O11-C1-C2-C3
57	y1	627	PTY	O14-C5-C6-C1
31	S1	603	CLA	C16-C17-C18-C19
38	b1	625	DGA	CB5-CB6-CB7-CB8
52	B1	624	3PH	C3B-C3C-C3D-C3E
34	b1	621	SQD	O10-C23-O48-C46
31	A	406	CLA	C10-C11-C12-C13
31	D	403	CLA	C10-C11-C12-C13
33	c1	517	BCR	C37-C22-C23-C24
41	d1	410	LHG	C2-C3-O3-P
48	G1	620	LUT	C27-C28-C29-C39
40	c1	520	DGD	C5A-C6A-C7A-C8A
41	G1	624	LHG	C34-C35-C36-C37
41	d1	408	LHG	C24-C25-C26-C27
31	A	406	CLA	C11-C10-C8-C7
31	B	609	CLA	C11-C12-C13-C15
31	C	502	CLA	C11-C12-C13-C15
31	C	503	CLA	C11-C10-C8-C7
31	C	507	CLA	C11-C10-C8-C7
31	C	510	CLA	C6-C7-C8-C10
31	C	513	CLA	C11-C12-C13-C15
31	N	602	CLA	C11-C10-C8-C7
31	N	604	CLA	C6-C7-C8-C10
31	G	613	CLA	C12-C13-C15-C16
31	S	603	CLA	C11-C10-C8-C7
31	Y	614	CLA	C11-C10-C8-C7
31	b	608	CLA	C11-C12-C13-C15
31	b	615	CLA	C11-C12-C13-C15
31	c	501	CLA	C11-C10-C8-C7
31	c	508	CLA	C12-C13-C15-C16
31	c	512	CLA	C11-C10-C8-C7
31	c	513	CLA	C11-C10-C8-C7
31	n	613	CLA	C12-C13-C15-C16
31	y	612	CLA	C11-C12-C13-C15
31	B1	604	CLA	C6-C7-C8-C10
31	B1	608	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
31	B1	616	CLA	C11-C12-C13-C15
31	C1	511	CLA	C11-C12-C13-C15
31	D1	402	CLA	C6-C7-C8-C10
31	D1	403	CLA	C6-C7-C8-C10
31	N1	613	CLA	C11-C12-C13-C15
31	Y1	612	CLA	C11-C10-C8-C7
31	Y1	614	CLA	C11-C10-C8-C7
31	n1	602	CLA	C11-C10-C8-C7
31	n1	613	CLA	C11-C10-C8-C7
31	g1	602	CLA	C12-C13-C15-C16
31	y1	602	CLA	C12-C13-C15-C16
32	a	409	PHO	C6-C7-C8-C10
47	N	605	CHL	C12-C13-C15-C16
47	N	607	CHL	C11-C10-C8-C7
47	y	601	CHL	C11-C10-C8-C7
47	N1	605	CHL	C11-C12-C13-C15
47	G1	601	CHL	C6-C7-C8-C10
47	G1	607	CHL	C11-C10-C8-C7
47	G1	609	CHL	C11-C12-C13-C15
47	Y1	607	CHL	C11-C10-C8-C7
47	n1	606	CHL	C11-C12-C13-C15
41	S1	624	LHG	C23-C24-C25-C26
38	B	625	DGA	CA6-CA7-CA8-CA9
41	d	409	LHG	C24-C25-C26-C27
41	g1	624	LHG	C9-C10-C11-C12
31	C	510	CLA	C8-C10-C11-C12
31	b1	609	CLA	C13-C15-C16-C17
33	b	619	BCR	C11-C12-C13-C14
33	c	515	BCR	C7-C8-C9-C10
33	B1	618	BCR	C21-C22-C23-C24
33	C1	514	BCR	C17-C18-C19-C20
33	C1	517	BCR	C7-C8-C9-C10
33	c1	517	BCR	C21-C22-C23-C24
48	s1	620	LUT	C31-C32-C33-C34
49	Y	622	XAT	C27-C28-C29-C30
50	s	623	NEX	C11-C12-C13-C14
31	N	604	CLA	CBA-CGA-O2A-C1
31	B1	605	CLA	CBA-CGA-O2A-C1
34	B	621	SQD	C16-C17-C18-C19
34	a1	412	SQD	C28-C29-C30-C31
35	w1	201	LMG	C37-C38-C39-C40
40	c1	519	DGD	CCB-CDB-CEB-CFB

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Mol	Chain	Res	Type	Atoms
31	b	607	CLA	O1A-CGA-O2A-C1
31	A1	405	CLA	O1A-CGA-O2A-C1
32	A1	408	PHO	O1A-CGA-O2A-C1
38	j1	101	DGA	OA1-CA1-OG1-CG1
34	A	412	SQD	C45-C44-O6-C1
34	A1	412	SQD	C45-C44-O6-C1
34	C1	526	SQD	C5-C6-S-O8
35	j	101	LMG	C8-C7-O1-C1
35	W1	201	LMG	C8-C7-O1-C1
35	w1	201	LMG	C8-C7-O1-C1
40	C1	519	DGD	C5D-C6D-O5D-C1E
40	c1	519	DGD	C5D-C6D-O5D-C1E
42	c	627	LMK	C8-C9-O8-C28
31	D	403	CLA	C13-C15-C16-C17
31	c	510	CLA	C8-C10-C11-C12
31	n	610	CLA	C8-C10-C11-C12
31	y	611	CLA	C5-C6-C7-C8
31	R	608	CLA	C2A-CAA-CBA-CGA
31	B	610	CLA	C16-C17-C18-C19
40	c1	519	DGD	C2B-C1B-O2G-C2G
35	w1	201	LMG	O9-C10-O7-C8
41	c1	525	LHG	O9-C7-O7-C5
57	y1	626	PTY	O10-C8-O7-C6
41	N1	624	LHG	C24-C25-C26-C27
31	C1	509	CLA	C4-C3-C5-C6
47	N	609	CHL	C4-C3-C5-C6
31	S	614	CLA	O1A-CGA-O2A-C1
31	s	604	CLA	O1A-CGA-O2A-C1
31	G1	610	CLA	O1A-CGA-O2A-C1
31	n1	610	CLA	O1A-CGA-O2A-C1
38	C1	524	DGA	OA1-CA1-OG1-CG1
41	d1	408	LHG	O10-C23-O8-C6
31	n	613	CLA	C2-C3-C5-C6
31	Y1	613	CLA	C13-C15-C16-C17
31	b1	606	CLA	C10-C11-C12-C13
41	C1	525	LHG	C34-C35-C36-C37
41	D1	409	LHG	C30-C31-C32-C33
54	i1	101	4RF	C51-C52-C53-C54
41	d	410	LHG	O1-C1-C2-C3
34	c	626	SQD	C15-C16-C17-C18
31	n1	602	CLA	C8-C10-C11-C12
34	B1	621	SQD	C46-C45-O47-C7

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Mol	Chain	Res	Type	Atoms
34	b1	621	SQD	C46-C45-O47-C7
34	m1	101	SQD	C46-C45-O47-C7
38	B	625	DGA	CG1-CG2-OG2-CB1
38	B1	625	DGA	CG1-CG2-OG2-CB1
40	C	523	DGD	C1G-C2G-O2G-C1B
35	H	102	LMG	C19-C20-C21-C22
31	B1	612	CLA	O1A-CGA-O2A-C1
31	c1	502	CLA	O1A-CGA-O2A-C1
31	g1	613	CLA	C13-C15-C16-C17
33	a1	411	BCR	C9-C10-C11-C12
57	Y1	626	PTY	C20-C21-C22-C23
31	b	615	CLA	C16-C17-C18-C19
47	S1	608	CHL	C11-C12-C13-C15
34	a	412	SQD	C34-C35-C36-C37
31	r1	602	CLA	C3-C5-C6-C7
31	r1	608	CLA	C5-C6-C7-C8
52	S	626	3PH	C2E-C2F-C2G-C2H
54	I1	102	4RF	C12-C13-C14-C15
40	c	520	DGD	CCB-CDB-CEB-CFB
41	L	101	LHG	C34-C35-C36-C37
44	d1	405	PL9	C47-C48-C49-C50
31	c	505	CLA	C15-C16-C17-C18
40	c1	519	DGD	O1B-C1B-O2G-C2G
41	C	525	LHG	O6-C4-C5-O7
41	G	630	LHG	O6-C4-C5-O7
41	d	408	LHG	O6-C4-C5-O7
41	C1	525	LHG	O6-C4-C5-O7
41	L1	101	LHG	O6-C4-C5-O7
41	d1	408	LHG	O6-C4-C5-O7
52	i	101	3PH	O11-C1-C2-O21
57	y1	626	PTY	O14-C5-C6-O7
35	W1	201	LMG	O6-C1-O1-C7
34	A	412	SQD	C44-C45-C46-O48
34	C1	526	SQD	O6-C44-C45-C46
34	b1	626	SQD	O6-C44-C45-C46
35	H	102	LMG	C7-C8-C9-O8
35	h	102	LMG	C7-C8-C9-O8
35	w1	201	LMG	O1-C7-C8-C9
40	c1	519	DGD	O1G-C1G-C2G-C3G
41	S	624	LHG	C4-C5-C6-O8
41	Y	624	LHG	C4-C5-C6-O8
41	c	625	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
41	s	624	LHG	C4-C5-C6-O8
41	n1	624	LHG	C4-C5-C6-O8
52	s	626	3PH	C1-C2-C3-O31
54	K1	101	4RF	C19-C20-C39-O40
54	i1	101	4RF	O18-C19-C20-C39
57	Y1	627	PTY	O4-C1-C6-C5
57	y1	626	PTY	O4-C1-C6-C5
40	c1	519	DGD	C1B-C2B-C3B-C4B
31	D1	403	CLA	C5-C6-C7-C8
31	S1	602	CLA	C5-C6-C7-C8
47	n	609	CHL	C8-C10-C11-C12
45	F	101	HEM	C4B-C3B-CAB-CBB
45	F	101	HEM	C4C-C3C-CAC-CBC
45	f	101	HEM	C4C-C3C-CAC-CBC
31	b	613	CLA	C16-C17-C18-C19
31	r	603	CLA	C11-C12-C13-C14
35	A1	413	LMG	C34-C35-C36-C37
41	g1	624	LHG	C26-C27-C28-C29
51	s1	625	LPX	C9-C10-C11-C12
31	c	503	CLA	C5-C6-C7-C8
31	d	403	CLA	C8-C10-C11-C12
31	y	604	CLA	C13-C15-C16-C17
40	c	519	DGD	C4D-C5D-C6D-O5D
31	C	506	CLA	C4-C3-C5-C6
31	r	609	CLA	C4-C3-C5-C6
31	n1	604	CLA	C4-C3-C5-C6
31	y1	611	CLA	C4-C3-C5-C6
31	C	506	CLA	C2A-CAA-CBA-CGA
31	G	602	CLA	C2A-CAA-CBA-CGA
31	g1	610	CLA	C2A-CAA-CBA-CGA
35	H	102	LMG	O7-C10-C11-C12
31	B	602	CLA	C2-C3-C5-C6
31	n1	610	CLA	C2-C3-C5-C6
47	Y1	609	CHL	C2-C3-C5-C6
34	b1	621	SQD	C13-C14-C15-C16
40	C1	520	DGD	C3B-C4B-C5B-C6B
50	S	622	NEX	C7-C8-C9-C19
50	s	623	NEX	C7-C8-C9-C19
50	N1	623	NEX	C7-C8-C9-C19
51	S	625	LPX	C2-C1-O2-P1
53	Y	625	SPH	N2-C2-C3-O3
53	A1	414	SPH	N2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
57	Y1	626	PTY	C2-C3-O11-P1
31	B	617	CLA	C10-C11-C12-C13
47	G1	601	CHL	C5-C6-C7-C8
40	c1	519	DGD	O1A-C1A-O1G-C1G
31	b1	604	CLA	C3-C5-C6-C7
34	C1	526	SQD	C9-C10-C11-C12
41	d	410	LHG	C30-C31-C32-C33
52	b1	624	3PH	C22-C23-C24-C25
34	C1	526	SQD	O6-C44-C45-O47
34	a1	412	SQD	O6-C44-C45-O47
34	b1	626	SQD	O6-C44-C45-O47
34	c1	526	SQD	O6-C44-C45-O47
35	b	622	LMG	O7-C8-C9-O8
35	B1	622	LMG	O1-C7-C8-O7
35	C1	521	LMG	O7-C8-C9-O8
40	C	523	DGD	O1G-C1G-C2G-O2G
41	D	410	LHG	O7-C5-C6-O8
41	S	624	LHG	O7-C5-C6-O8
41	n	624	LHG	O7-C5-C6-O8
41	L1	101	LHG	O7-C5-C6-O8
41	c1	525	LHG	O7-C5-C6-O8
41	s1	624	LHG	O7-C5-C6-O8
52	s1	626	3PH	O21-C2-C3-O31
54	I1	102	4RF	O18-C19-C20-O21
57	Y1	627	PTY	O4-C1-C6-O7
41	g	624	LHG	C35-C36-C37-C38
31	B	604	CLA	C15-C16-C17-C18
31	B1	606	CLA	C13-C15-C16-C17
31	C	506	CLA	C6-C7-C8-C9
31	N	604	CLA	C6-C7-C8-C9
31	G	613	CLA	C14-C13-C15-C16
31	c	506	CLA	C11-C12-C13-C14
31	c	508	CLA	C14-C13-C15-C16
31	n	613	CLA	C14-C13-C15-C16
31	g	602	CLA	C11-C10-C8-C9
31	y	613	CLA	C11-C10-C8-C9
31	y	614	CLA	C11-C10-C8-C9
31	B1	610	CLA	C6-C7-C8-C9
31	S1	610	CLA	C11-C12-C13-C14
31	Y1	614	CLA	C11-C10-C8-C9
31	b1	603	CLA	C6-C7-C8-C9
31	b1	604	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
31	g1	602	CLA	C6-C7-C8-C9
31	g1	602	CLA	C14-C13-C15-C16
32	A1	408	PHO	C6-C7-C8-C9
47	n	605	CHL	C14-C13-C15-C16
47	y	609	CHL	C11-C12-C13-C14
47	N1	601	CHL	C14-C13-C15-C16
47	n1	601	CHL	C14-C13-C15-C16
47	y1	607	CHL	C6-C7-C8-C9
47	y1	607	CHL	C14-C13-C15-C16
31	b1	617	CLA	C16-C17-C18-C20
34	b1	626	SQD	C29-C30-C31-C32
40	c	520	DGD	C3B-C4B-C5B-C6B
40	c1	518	DGD	O6D-C5D-C6D-O5D
31	R	609	CLA	CAA-CBA-CGA-O2A
47	n	607	CHL	CAA-CBA-CGA-O2A
41	G	630	LHG	C11-C10-C9-C8
41	D1	409	LHG	C13-C14-C15-C16
52	s	626	3PH	C26-C27-C28-C29
41	D1	408	LHG	O10-C23-O8-C6
38	c	524	DGA	CA6-CA7-CA8-CA9
52	B1	624	3PH	C2E-C2F-C2G-C2H
31	G	610	CLA	C15-C16-C17-C18
31	y	612	CLA	C8-C10-C11-C12
42	c1	527	LMK	C11-C10-O7-C8
34	c1	526	SQD	C7-C8-C9-C10
54	i1	101	4RF	C13-C14-C15-C16
31	R	612	CLA	C5-C6-C7-C8
32	A1	409	PHO	O1A-CGA-O2A-C1
38	C	524	DGA	CBB-CCB-CDB-CEB
41	G	630	LHG	C16-C17-C18-C19
41	S1	624	LHG	C13-C14-C15-C16
41	Y1	624	LHG	C9-C10-C11-C12
31	b	616	CLA	C2-C1-O2A-CGA
31	c	503	CLA	C2-C1-O2A-CGA
31	n	614	CLA	C2-C1-O2A-CGA
31	r	604	CLA	C2-C1-O2A-CGA
31	r	608	CLA	C2-C1-O2A-CGA
31	C1	504	CLA	C2-C1-O2A-CGA
31	S1	611	CLA	C2-C1-O2A-CGA
31	Y1	611	CLA	C2-C1-O2A-CGA
31	b1	605	CLA	C2-C1-O2A-CGA
31	n1	613	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
31	n1	614	CLA	C2-C1-O2A-CGA
31	s1	610	CLA	C2-C1-O2A-CGA
31	s1	611	CLA	C2-C1-O2A-CGA
33	D1	404	BCR	C13-C14-C15-C16
48	r1	620	LUT	C29-C30-C31-C32
49	r	622	XAT	C33-C34-C35-C15
31	B	605	CLA	C16-C17-C18-C19
31	B	612	CLA	C16-C17-C18-C19
31	b	605	CLA	C5-C6-C7-C8
41	s1	624	LHG	C2-C3-O3-P
38	C1	524	DGA	CAB-CBB-CCB-CDB
41	D	409	LHG	C16-C17-C18-C19
40	c	519	DGD	C9A-CAA-CBA-CCA
41	S1	624	LHG	C35-C36-C37-C38
40	C1	518	DGD	C3B-C4B-C5B-C6B
51	S	625	LPX	C14-C15-C16-C17
53	A1	414	SPH	C15-C16-C17-C18
35	j	101	LMG	C30-C31-C32-C33
31	B	610	CLA	C4-C3-C5-C6
31	b	605	CLA	C4-C3-C5-C6
31	b	614	CLA	C4-C3-C5-C6
31	r	603	CLA	C4-C3-C5-C6
31	s1	603	CLA	C4-C3-C5-C6
31	A	406	CLA	C3-C5-C6-C7
41	L	101	LHG	C29-C30-C31-C32
31	S	614	CLA	C5-C6-C7-C8
41	y	624	LHG	C35-C36-C37-C38
35	B1	622	LMG	C14-C15-C16-C17
53	y	625	SPH	C11-C12-C13-C14
41	g1	624	LHG	C24-C25-C26-C27
31	C	502	CLA	C16-C17-C18-C19
31	c	505	CLA	C16-C17-C18-C20
31	r	612	CLA	C5-C6-C7-C8
38	C1	524	DGA	CB3-CB4-CB5-CB6
52	i	101	3PH	C24-C25-C26-C27
52	B1	624	3PH	C25-C26-C27-C28
31	C1	505	CLA	O1D-CGD-O2D-CED
35	B1	622	LMG	C10-C11-C12-C13
31	N	604	CLA	O1A-CGA-O2A-C1
31	s	610	CLA	O1A-CGA-O2A-C1
31	B1	605	CLA	O1A-CGA-O2A-C1
34	c1	526	SQD	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
40	C	520	DGD	O6E-C5E-C6E-O5E
34	B	621	SQD	C4-C5-C6-S
34	C	526	SQD	C4-C5-C6-S
34	c	626	SQD	C4-C5-C6-S
47	G1	609	CHL	C4C-C3C-CAC-CBC
34	c	626	SQD	C7-C8-C9-C10
34	b1	626	SQD	C9-C10-C11-C12
40	B1	623	DGD	C2A-C1A-O1G-C1G
40	C1	520	DGD	C2B-C1B-O2G-C2G
54	I1	102	4RF	C27-C28-C29-C30
53	Y1	625	SPH	C15-C16-C17-C18
54	K1	101	4RF	C01-C02-C03-C04
31	b1	616	CLA	C8-C10-C11-C12
41	C	525	LHG	O1-C1-C2-O2
31	B	604	CLA	C3-C5-C6-C7
31	c	508	CLA	C3-C5-C6-C7
35	c	521	LMG	C33-C34-C35-C36
40	c	520	DGD	C2B-C3B-C4B-C5B
33	C1	514	BCR	C37-C22-C23-C24
37	B1	620	C7Z	C11-C12-C13-C20
31	B	611	CLA	C4B-C3B-CAB-CBB
31	N	602	CLA	C1A-C2A-CAA-CBA
31	N	611	CLA	C1A-C2A-CAA-CBA
31	R	604	CLA	C1A-C2A-CAA-CBA
31	Y	614	CLA	C4B-C3B-CAB-CBB
31	g	603	CLA	C4B-C3B-CAB-CBB
31	r	603	CLA	C1A-C2A-CAA-CBA
31	r	608	CLA	C4B-C3B-CAB-CBB
31	r	611	CLA	C1A-C2A-CAA-CBA
31	s	609	CLA	C4B-C3B-CAB-CBB
31	s	611	CLA	C4B-C3B-CAB-CBB
31	y	614	CLA	C4B-C3B-CAB-CBB
31	B1	602	CLA	C4B-C3B-CAB-CBB
31	B1	605	CLA	C1A-C2A-CAA-CBA
31	D1	402	CLA	C1A-C2A-CAA-CBA
31	D1	403	CLA	C1A-C2A-CAA-CBA
31	N1	603	CLA	C4B-C3B-CAB-CBB
31	G1	603	CLA	C4B-C3B-CAB-CBB
31	G1	604	CLA	C1A-C2A-CAA-CBA
31	S1	603	CLA	C4B-C3B-CAB-CBB
31	S1	611	CLA	C4B-C3B-CAB-CBB
31	Y1	604	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
31	b1	602	CLA	C4B-C3B-CAB-CBB
31	b1	605	CLA	C1A-C2A-CAA-CBA
31	b1	616	CLA	C4B-C3B-CAB-CBB
31	n1	603	CLA	C4B-C3B-CAB-CBB
31	g1	603	CLA	C4B-C3B-CAB-CBB
31	g1	614	CLA	C1A-C2A-CAA-CBA
31	r1	603	CLA	C4B-C3B-CAB-CBB
31	r1	608	CLA	C4B-C3B-CAB-CBB
31	y1	608	CLA	C1A-C2A-CAA-CBA
34	A1	412	SQD	C24-C23-O48-C46
38	C	524	DGA	CA2-CA1-OG1-CG1
38	J1	101	DGA	CA2-CA3-CA4-CA5
41	S	624	LHG	C10-C11-C12-C13
31	n	602	CLA	C4-C3-C5-C6
47	n	609	CHL	C4-C3-C5-C6
34	C	526	SQD	O5-C1-O6-C44
41	L	101	LHG	O7-C7-C8-C9
41	n1	624	LHG	O8-C23-C24-C25
41	N1	624	LHG	C18-C19-C20-C21
31	G	602	CLA	C2-C3-C5-C6
48	G1	620	LUT	C27-C28-C29-C30
49	n1	622	XAT	C31-C32-C33-C34
50	g	623	NEX	C13-C14-C15-C35
34	B1	626	SQD	C24-C25-C26-C27
41	d1	409	LHG	C33-C34-C35-C36
31	n	613	CLA	C16-C17-C18-C19
38	B1	625	DGA	CFA-CGA-CHA-CIA
54	k1	101	4RF	C01-C02-C03-C04
35	D	411	LMG	C19-C20-C21-C22
54	k1	101	4RF	C26-C27-C28-C29
31	r1	603	CLA	C2A-CAA-CBA-CGA
47	R1	607	CHL	C2A-CAA-CBA-CGA
41	D	410	LHG	C30-C31-C32-C33
52	S1	626	3PH	C2C-C2D-C2E-C2F
31	c	511	CLA	C10-C11-C12-C13
34	b	621	SQD	C17-C18-C19-C20
38	B1	625	DGA	CA2-CA3-CA4-CA5
35	a1	413	LMG	O9-C10-O7-C8
34	b1	626	SQD	C28-C29-C30-C31
38	c	524	DGA	CA4-CA5-CA6-CA7
40	c	520	DGD	C6B-C7B-C8B-C9B
41	D	408	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
41	d	408	LHG	C24-C25-C26-C27
41	Y1	624	LHG	C11-C12-C13-C14
31	R	603	CLA	C3-C5-C6-C7
31	N	610	CLA	C11-C12-C13-C15
31	R	608	CLA	C6-C7-C8-C10
31	Y	604	CLA	C6-C7-C8-C10
31	Y	610	CLA	C6-C7-C8-C10
31	a	405	CLA	C6-C7-C8-C10
31	b	605	CLA	C11-C12-C13-C15
31	c	508	CLA	C11-C10-C8-C7
31	d	402	CLA	C6-C7-C8-C10
31	n	603	CLA	C12-C13-C15-C16
31	y	611	CLA	C12-C13-C15-C16
31	B1	602	CLA	C12-C13-C15-C16
31	B1	613	CLA	C11-C10-C8-C7
31	C1	501	CLA	C11-C12-C13-C15
31	C1	507	CLA	C6-C7-C8-C10
31	C1	512	CLA	C11-C10-C8-C7
31	N1	613	CLA	C12-C13-C15-C16
31	G1	602	CLA	C12-C13-C15-C16
31	R1	612	CLA	C6-C7-C8-C10
31	Y1	604	CLA	C6-C7-C8-C10
31	b1	602	CLA	C11-C10-C8-C7
31	b1	603	CLA	C6-C7-C8-C10
31	b1	613	CLA	C11-C10-C8-C7
31	c1	510	CLA	C12-C13-C15-C16
31	c1	513	CLA	C11-C10-C8-C7
31	d1	402	CLA	C6-C7-C8-C10
31	n1	603	CLA	C11-C10-C8-C7
31	g1	610	CLA	C12-C13-C15-C16
31	s1	610	CLA	C6-C7-C8-C10
31	s1	611	CLA	C11-C12-C13-C15
31	y1	604	CLA	C6-C7-C8-C10
31	y1	613	CLA	C12-C13-C15-C16
32	A1	409	PHO	C6-C7-C8-C10
32	a1	409	PHO	C6-C7-C8-C10
47	N	606	CHL	C11-C12-C13-C15
47	N	609	CHL	C11-C10-C8-C7
47	Y	601	CHL	C11-C10-C8-C7
47	n	606	CHL	C11-C10-C8-C7
47	n	609	CHL	C11-C10-C8-C7
47	g	609	CHL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
47	G1	607	CHL	C11-C12-C13-C15
47	n1	601	CHL	C11-C12-C13-C15
47	g1	609	CHL	C11-C12-C13-C15
41	D	409	LHG	C24-C25-C26-C27
31	c	508	CLA	C16-C17-C18-C20
31	r	609	CLA	C10-C11-C12-C13
31	b1	615	CLA	C5-C6-C7-C8
40	C	520	DGD	C7B-C8B-C9B-CAB
41	d1	409	LHG	C24-C23-O8-C6
35	W1	201	LMG	C29-C30-C31-C32
41	C1	525	LHG	C14-C15-C16-C17
41	d1	410	LHG	C25-C26-C27-C28
54	k1	101	4RF	C45-C46-C47-C48
41	d	409	LHG	C19-C20-C21-C22
38	C1	524	DGA	CB6-CB7-CB8-CB9
52	s	626	3PH	C3E-C3F-C3G-C3H
34	b1	621	SQD	C11-C10-C9-C8
38	C1	524	DGA	CDA-CEA-CFA-CGA
41	d1	409	LHG	C30-C31-C32-C33
40	B1	623	DGD	O1A-C1A-O1G-C1G
41	S	624	LHG	C2-C3-O3-P
54	I1	102	4RF	C46-C47-C48-C49
31	s	604	CLA	C4-C3-C5-C6
41	C1	525	LHG	C25-C26-C27-C28
31	C	506	CLA	C2-C3-C5-C6
31	r	609	CLA	C2-C3-C5-C6
31	y1	611	CLA	C2-C3-C5-C6
31	C1	501	CLA	C8-C10-C11-C12
40	C1	520	DGD	O1B-C1B-O2G-C2G
31	y	613	CLA	O1A-CGA-O2A-C1
42	c1	527	LMK	O7-C10-C11-C12
41	d	410	LHG	O6-C4-C5-O7
41	g	624	LHG	O6-C4-C5-O7
41	G1	624	LHG	O6-C4-C5-O7
41	c1	525	LHG	O6-C4-C5-O7
52	B1	624	3PH	O11-C1-C2-O21
57	Y1	627	PTY	O14-C5-C6-O7
38	J1	101	DGA	CBB-CAB-CB9-CB8
34	b1	621	SQD	C24-C25-C26-C27
47	N1	606	CHL	C3-C5-C6-C7
41	D	409	LHG	C17-C18-C19-C20
41	c1	525	LHG	C8-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
41	y1	624	LHG	C8-C7-O7-C5
31	y	613	CLA	C2A-CAA-CBA-CGA
31	b1	614	CLA	C2A-CAA-CBA-CGA
31	c1	501	CLA	C2A-CAA-CBA-CGA
32	a1	408	PHO	C2A-CAA-CBA-CGA
47	r1	607	CHL	C2A-CAA-CBA-CGA
31	A	406	CLA	C11-C10-C8-C9
31	C	502	CLA	C11-C12-C13-C14
31	C	503	CLA	C11-C10-C8-C9
31	C	505	CLA	C14-C13-C15-C16
31	C	510	CLA	C6-C7-C8-C9
31	N	602	CLA	C11-C10-C8-C9
31	S	603	CLA	C11-C10-C8-C9
31	b	615	CLA	C11-C12-C13-C14
31	c	510	CLA	C6-C7-C8-C9
31	c	512	CLA	C11-C10-C8-C9
31	n	610	CLA	C6-C7-C8-C9
31	y	612	CLA	C11-C12-C13-C14
31	B1	608	CLA	C14-C13-C15-C16
31	B1	616	CLA	C11-C12-C13-C14
31	D1	403	CLA	C6-C7-C8-C9
31	S1	611	CLA	C11-C12-C13-C14
31	Y1	610	CLA	C11-C12-C13-C14
31	Y1	612	CLA	C11-C10-C8-C9
31	n1	602	CLA	C11-C10-C8-C9
31	n1	603	CLA	C11-C10-C8-C9
31	n1	613	CLA	C11-C10-C8-C9
31	y1	602	CLA	C14-C13-C15-C16
47	N	606	CHL	C11-C10-C8-C9
47	G	609	CHL	C11-C12-C13-C14
47	N1	606	CHL	C11-C12-C13-C14
47	Y1	607	CHL	C11-C10-C8-C9
31	S	610	CLA	C13-C15-C16-C17
31	A1	410	CLA	C10-C11-C12-C13
40	C1	518	DGD	C4A-C5A-C6A-C7A
41	D1	408	LHG	C10-C11-C12-C13
52	T1	101	3PH	C3D-C3E-C3F-C3G
33	D	404	BCR	C9-C10-C11-C12
33	a	411	BCR	C9-C10-C11-C12
33	a	411	BCR	C13-C14-C15-C16
33	a	411	BCR	C15-C16-C17-C18
33	c1	515	BCR	C19-C20-C21-C22

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Mol	Chain	Res	Type	Atoms
37	B1	620	C7Z	C13-C14-C15-C35
48	S	620	LUT	C29-C30-C31-C32
48	Y	620	LUT	C29-C30-C31-C32
48	G1	620	LUT	C33-C34-C35-C15
48	S1	621	LUT	C29-C30-C31-C32
48	s1	620	LUT	C29-C30-C31-C32
50	G	623	NEX	C9-C10-C11-C12
31	Y	611	CLA	C16-C17-C18-C19
31	B1	615	CLA	C16-C17-C18-C19
38	b	623	DGA	CFB-CGB-CHB-CIB
31	n	604	CLA	O1D-CGD-O2D-CED
31	d	403	CLA	C13-C15-C16-C17
31	n	603	CLA	C8-C10-C11-C12
35	c1	521	LMG	C29-C30-C31-C32
31	N	611	CLA	C1-C2-C3-C4
31	G	604	CLA	C1-C2-C3-C4
31	G	614	CLA	C1-C2-C3-C4
31	n	611	CLA	C1-C2-C3-C4
31	g	604	CLA	C1-C2-C3-C4
31	g	614	CLA	C1-C2-C3-C4
31	N1	611	CLA	C1-C2-C3-C4
31	G1	604	CLA	C1-C2-C3-C4
31	G1	614	CLA	C1-C2-C3-C4
31	n1	611	CLA	C1-C2-C3-C4
31	g1	604	CLA	C1-C2-C3-C4
31	g1	614	CLA	C1-C2-C3-C4
34	M1	101	SQD	O5-C5-C6-S
47	N	608	CHL	C1-C2-C3-C4
47	G	606	CHL	C1-C2-C3-C4
47	G	607	CHL	C1-C2-C3-C4
47	n	608	CHL	C1-C2-C3-C4
47	g	606	CHL	C1-C2-C3-C4
47	g	607	CHL	C1-C2-C3-C4
47	r	607	CHL	C1-C2-C3-C4
47	N1	608	CHL	C1-C2-C3-C4
47	G1	606	CHL	C1-C2-C3-C4
47	R1	607	CHL	C1-C2-C3-C4
47	n1	608	CHL	C1-C2-C3-C4
47	g1	606	CHL	C1-C2-C3-C4
47	r1	607	CHL	C1-C2-C3-C4
48	G	621	LUT	C21-C26-C27-C28
50	R	622	NEX	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
50	S	622	NEX	C7-C8-C9-C10
50	s	623	NEX	C7-C8-C9-C10
50	N1	623	NEX	C7-C8-C9-C10
50	y1	623	NEX	C7-C8-C9-C10
41	D1	408	LHG	C31-C32-C33-C34
41	D1	410	LHG	C10-C11-C12-C13
40	C	518	DGD	C5B-C6B-C7B-C8B
41	N	624	LHG	C34-C35-C36-C37
41	L1	101	LHG	C12-C13-C14-C15
41	D1	409	LHG	C9-C10-C11-C12
35	b1	622	LMG	C4-C5-C6-O5
38	C	524	DGA	OA1-CA1-OG1-CG1
34	A1	412	SQD	O6-C44-C45-O47
34	m1	101	SQD	O47-C45-C46-O48
35	c	521	LMG	O1-C7-C8-O7
35	B1	622	LMG	O7-C8-C9-O8
35	C1	523	LMG	O1-C7-C8-O7
35	a1	413	LMG	O7-C8-C9-O8
40	c	523	DGD	O1G-C1G-C2G-O2G
40	b1	623	DGD	O1G-C1G-C2G-O2G
40	c1	520	DGD	O1G-C1G-C2G-O2G
41	L	101	LHG	O7-C5-C6-O8
41	c	625	LHG	O7-C5-C6-O8
41	d	408	LHG	O7-C5-C6-O8
41	l	101	LHG	O7-C5-C6-O8
41	s	624	LHG	O7-C5-C6-O8
41	d1	409	LHG	O7-C5-C6-O8
42	c	627	LMK	O1-C7-C8-O7
42	C1	527	LMK	O1-C7-C8-O7
54	K1	101	4RF	O18-C19-C20-O21
54	k1	101	4RF	O18-C19-C20-O21
57	y1	626	PTY	O4-C1-C6-O7
35	A1	413	LMG	C12-C13-C14-C15
41	d	410	LHG	C28-C29-C30-C31
41	D	410	LHG	C1-C2-C3-O3
31	N	603	CLA	C8-C10-C11-C12
31	c1	505	CLA	C15-C16-C17-C18
34	c1	526	SQD	C11-C10-C9-C8
34	B	621	SQD	C44-C45-C46-O48
34	b	621	SQD	C44-C45-C46-O48
34	c1	526	SQD	O6-C44-C45-C46
35	J	101	LMG	C7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
35	j	101	LMG	C7-C8-C9-O8
35	B1	622	LMG	O1-C7-C8-C9
35	C1	521	LMG	C7-C8-C9-O8
35	w1	201	LMG	C7-C8-C9-O8
38	C1	524	DGA	OG1-CG1-CG2-CG3
40	C	523	DGD	O1G-C1G-C2G-C3G
41	N1	624	LHG	C4-C5-C6-O8
41	c1	525	LHG	C4-C5-C6-O8
41	g1	624	LHG	C4-C5-C6-O8
31	c	506	CLA	C4-C3-C5-C6
44	D1	405	PL9	C40-C39-C41-C42
54	I1	102	4RF	C10-C11-C12-C13
31	B1	604	CLA	C13-C15-C16-C17
47	g1	601	CHL	C5-C6-C7-C8
31	R	602	CLA	C2-C3-C5-C6
31	r	603	CLA	C2-C3-C5-C6
31	C1	509	CLA	C2-C3-C5-C6
47	N	609	CHL	C2-C3-C5-C6
47	Y	607	CHL	C2-C3-C5-C6
47	N1	608	CHL	CBD-CGD-O2D-CED
53	y	625	SPH	C6-C7-C8-C9
31	b	606	CLA	CAD-CBD-CGD-O2D
31	b	613	CLA	CAD-CBD-CGD-O2D
31	c	503	CLA	CAD-CBD-CGD-O2D
31	c	504	CLA	CAD-CBD-CGD-O2D
31	C1	503	CLA	CAD-CBD-CGD-O2D
31	N1	604	CLA	CAD-CBD-CGD-O2D
31	n1	604	CLA	CAD-CBD-CGD-O2D
31	g1	604	CLA	CAD-CBD-CGD-O2D
47	s	607	CHL	C1A-C2A-CAA-CBA
47	n1	601	CHL	CAD-CBD-CGD-O2D
34	c	626	SQD	C9-C10-C11-C12
38	c	524	DGA	CA8-CA9-CAA-CBA
31	B	607	CLA	CBA-CGA-O2A-C1
31	y	613	CLA	CBA-CGA-O2A-C1
31	d1	402	CLA	CBA-CGA-O2A-C1
31	a	405	CLA	C8-C10-C11-C12
31	a	410	CLA	C5-C6-C7-C8
31	c	513	CLA	C15-C16-C17-C18
40	C	518	DGD	C2B-C3B-C4B-C5B
35	w1	201	LMG	C28-C29-C30-C31
41	S	624	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
31	N	604	CLA	C16-C17-C18-C20
31	Y1	610	CLA	C16-C17-C18-C19
31	a1	410	CLA	C11-C12-C13-C15
31	a	405	CLA	C2A-CAA-CBA-CGA
31	c	506	CLA	C2A-CAA-CBA-CGA
31	G1	610	CLA	C2A-CAA-CBA-CGA
38	B	625	DGA	CBB-CAB-CB9-CB8
38	J1	101	DGA	CB6-CB7-CB8-CB9
31	B	607	CLA	O1A-CGA-O2A-C1
31	A1	410	CLA	O1A-CGA-O2A-C1
31	d1	402	CLA	O1A-CGA-O2A-C1
41	d1	408	LHG	C34-C35-C36-C37
41	s	624	LHG	C34-C35-C36-C37
52	T1	101	3PH	C3A-C3B-C3C-C3D
41	D	408	LHG	C31-C32-C33-C34
41	d	409	LHG	C31-C32-C33-C34
53	A1	414	SPH	C13-C14-C15-C16
31	B	610	CLA	CAD-CBD-CGD-O1D
31	C	504	CLA	CAD-CBD-CGD-O1D
31	N	603	CLA	CHA-CBD-CGD-O1D
31	G	603	CLA	CHA-CBD-CGD-O1D
31	G	603	CLA	CHA-CBD-CGD-O2D
31	S	613	CLA	CHA-CBD-CGD-O1D
31	S	613	CLA	CHA-CBD-CGD-O2D
31	Y	603	CLA	CHA-CBD-CGD-O1D
31	b	605	CLA	CAD-CBD-CGD-O1D
31	b	606	CLA	CAD-CBD-CGD-O1D
31	b	610	CLA	CAD-CBD-CGD-O1D
31	b	613	CLA	CAD-CBD-CGD-O1D
31	c	503	CLA	CAD-CBD-CGD-O1D
31	c	504	CLA	CAD-CBD-CGD-O1D
31	c	509	CLA	CHA-CBD-CGD-O1D
31	c	509	CLA	CHA-CBD-CGD-O2D
31	r	604	CLA	CHA-CBD-CGD-O1D
31	r	604	CLA	CHA-CBD-CGD-O2D
31	B1	608	CLA	CAD-CBD-CGD-O1D
31	B1	611	CLA	CHA-CBD-CGD-O1D
31	B1	611	CLA	CHA-CBD-CGD-O2D
31	C1	502	CLA	CAD-CBD-CGD-O1D
31	C1	503	CLA	CAD-CBD-CGD-O1D
31	N1	604	CLA	CAD-CBD-CGD-O1D
31	Y1	604	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
31	Y1	604	CLA	CHA-CBD-CGD-O2D
31	b1	605	CLA	CAD-CBD-CGD-O1D
31	c1	512	CLA	CHA-CBD-CGD-O1D
31	c1	512	CLA	CHA-CBD-CGD-O2D
31	n1	602	CLA	CHA-CBD-CGD-O2D
31	n1	603	CLA	CHA-CBD-CGD-O1D
31	n1	603	CLA	CHA-CBD-CGD-O2D
31	n1	604	CLA	CAD-CBD-CGD-O1D
31	g1	602	CLA	CHA-CBD-CGD-O1D
31	g1	602	CLA	CHA-CBD-CGD-O2D
31	g1	603	CLA	CHA-CBD-CGD-O1D
31	g1	603	CLA	CHA-CBD-CGD-O2D
31	g1	604	CLA	CAD-CBD-CGD-O1D
31	y1	602	CLA	CHA-CBD-CGD-O1D
31	y1	602	CLA	CHA-CBD-CGD-O2D
32	A	409	PHO	CHA-CBD-CGD-O1D
32	A	409	PHO	CHA-CBD-CGD-O2D
32	a	409	PHO	CHA-CBD-CGD-O2D
32	A1	408	PHO	CHA-CBD-CGD-O1D
32	A1	408	PHO	CHA-CBD-CGD-O2D
33	A	411	BCR	C19-C20-C21-C22
33	c	516	BCR	C13-C14-C15-C16
33	B1	619	BCR	C13-C14-C15-C16
33	C1	514	BCR	C19-C20-C21-C22
33	c1	514	BCR	C13-C14-C15-C16
37	B1	620	C7Z	C33-C34-C35-C15
37	B1	620	C7Z	C29-C30-C31-C32
41	D	409	LHG	C3-O3-P-O5
41	D	409	LHG	C4-O6-P-O5
41	N	624	LHG	C3-O3-P-O5
41	G	630	LHG	C3-O3-P-O5
41	S	624	LHG	C3-O3-P-O6
41	S	624	LHG	C4-O6-P-O5
41	Y	624	LHG	C3-O3-P-O5
41	d	409	LHG	C3-O3-P-O5
41	d	409	LHG	C4-O6-P-O5
41	d	410	LHG	C4-O6-P-O4
41	l	101	LHG	C3-O3-P-O5
41	n	624	LHG	C3-O3-P-O5
41	g	624	LHG	C3-O3-P-O5
41	s	624	LHG	C4-O6-P-O5
41	y	624	LHG	C3-O3-P-O5

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Mol	Chain	Res	Type	Atoms
41	y	624	LHG	C4-O6-P-O4
41	D1	408	LHG	C3-O3-P-O5
41	D1	408	LHG	C4-O6-P-O4
41	L1	101	LHG	C3-O3-P-O5
41	L1	101	LHG	C4-O6-P-O5
41	N1	624	LHG	C3-O3-P-O5
41	N1	624	LHG	C4-O6-P-O4
41	Y1	624	LHG	C3-O3-P-O5
41	d1	408	LHG	C3-O3-P-O6
41	d1	409	LHG	C3-O3-P-O6
41	d1	410	LHG	C3-O3-P-O4
42	C	527	LMK	C7-C8-O7-C10
42	C	527	LMK	C9-C8-O7-C10
42	C1	527	LMK	C9-C8-O7-C10
47	N	606	CHL	CHA-CBD-CGD-O1D
47	N	606	CHL	CHA-CBD-CGD-O2D
47	S	601	CHL	CAD-CBD-CGD-O1D
47	S	608	CHL	CHA-CBD-CGD-O2D
47	Y	609	CHL	CHA-CBD-CGD-O2D
47	n	606	CHL	CHA-CBD-CGD-O2D
47	n	609	CHL	CHA-CBD-CGD-O1D
47	s	601	CHL	CAD-CBD-CGD-O1D
47	y	607	CHL	CHA-CBD-CGD-O1D
47	y	607	CHL	CHA-CBD-CGD-O2D
47	N1	606	CHL	CHA-CBD-CGD-O1D
47	N1	606	CHL	CHA-CBD-CGD-O2D
47	Y1	607	CHL	CHA-CBD-CGD-O2D
47	n1	601	CHL	CAD-CBD-CGD-O1D
47	g1	609	CHL	CHA-CBD-CGD-O1D
47	g1	609	CHL	CHA-CBD-CGD-O2D
47	r1	606	CHL	CHA-CBD-CGD-O1D
47	r1	606	CHL	CHA-CBD-CGD-O2D
47	y1	606	CHL	CHA-CBD-CGD-O1D
47	y1	606	CHL	CHA-CBD-CGD-O2D
48	N	620	LUT	C9-C10-C11-C12
48	G	621	LUT	C29-C30-C31-C32
48	S	621	LUT	C25-C26-C27-C28
48	g	620	LUT	C29-C30-C31-C32
48	G1	621	LUT	C9-C10-C11-C12
48	Y1	620	LUT	C29-C30-C31-C32
48	r1	620	LUT	C25-C26-C27-C28
48	y1	621	LUT	C33-C34-C35-C15

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Mol	Chain	Res	Type	Atoms
50	s	623	NEX	C39-C29-C30-C31
50	y	623	NEX	C29-C30-C31-C32
50	Y1	623	NEX	C39-C29-C30-C31
50	y1	623	NEX	C29-C30-C31-C32
51	S	625	LPX	C1-O2-P1-O4
51	s	625	LPX	C1-O2-P1-O4
57	y1	626	PTY	N1-C2-C3-O11
34	b1	626	SQD	C19-C20-C21-C22
31	D1	402	CLA	C3-C5-C6-C7
34	M1	101	SQD	C26-C27-C28-C29
40	C1	519	DGD	C1B-C2B-C3B-C4B
54	i1	101	4RF	C01-C02-C03-C04
31	c1	513	CLA	O1A-CGA-O2A-C1
41	N	624	LHG	C24-C25-C26-C27
52	T1	101	3PH	C32-C33-C34-C35
31	R1	610	CLA	C8-C10-C11-C12
31	Y1	603	CLA	C15-C16-C17-C18
31	B	617	CLA	C4-C3-C5-C6
44	D	405	PL9	C35-C34-C36-C37
31	B	602	CLA	C2B-C3B-CAB-CBB
31	B	609	CLA	C2B-C3B-CAB-CBB
31	B	611	CLA	C2B-C3B-CAB-CBB
31	C	501	CLA	C2B-C3B-CAB-CBB
31	N	610	CLA	C2B-C3B-CAB-CBB
31	N	614	CLA	C2B-C3B-CAB-CBB
31	G	610	CLA	C2B-C3B-CAB-CBB
31	G	611	CLA	C2B-C3B-CAB-CBB
31	R	603	CLA	C2B-C3B-CAB-CBB
31	S	604	CLA	C2B-C3B-CAB-CBB
31	S	612	CLA	C2B-C3B-CAB-CBB
31	Y	604	CLA	C2B-C3B-CAB-CBB
31	Y	608	CLA	C2B-C3B-CAB-CBB
31	Y	612	CLA	C2B-C3B-CAB-CBB
31	Y	614	CLA	C2B-C3B-CAB-CBB
31	a	407	CLA	C2B-C3B-CAB-CBB
31	b	603	CLA	C2B-C3B-CAB-CBB
31	b	604	CLA	C2B-C3B-CAB-CBB
31	b	606	CLA	C2B-C3B-CAB-CBB
31	b	607	CLA	C2B-C3B-CAB-CBB
31	c	511	CLA	C2B-C3B-CAB-CBB
31	c	513	CLA	C2B-C3B-CAB-CBB
31	g	611	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	r	603	CLA	C2B-C3B-CAB-CBB
31	r	608	CLA	C2B-C3B-CAB-CBB
31	s	605	CLA	C2B-C3B-CAB-CBB
31	s	609	CLA	C2B-C3B-CAB-CBB
31	s	610	CLA	C2B-C3B-CAB-CBB
31	s	611	CLA	C2B-C3B-CAB-CBB
31	s	613	CLA	C2B-C3B-CAB-CBB
31	y	602	CLA	C2B-C3B-CAB-CBB
31	y	608	CLA	C2B-C3B-CAB-CBB
31	y	612	CLA	C2B-C3B-CAB-CBB
31	B1	602	CLA	C2B-C3B-CAB-CBB
31	B1	603	CLA	C2B-C3B-CAB-CBB
31	B1	604	CLA	C2B-C3B-CAB-CBB
31	B1	606	CLA	C2B-C3B-CAB-CBB
31	D1	403	CLA	C2B-C3B-CAB-CBB
31	N1	603	CLA	C2B-C3B-CAB-CBB
31	N1	610	CLA	C2B-C3B-CAB-CBB
31	N1	614	CLA	C2B-C3B-CAB-CBB
31	G1	603	CLA	C2B-C3B-CAB-CBB
31	G1	611	CLA	C2B-C3B-CAB-CBB
31	G1	613	CLA	C2B-C3B-CAB-CBB
31	G1	614	CLA	C2B-C3B-CAB-CBB
31	R1	604	CLA	C2B-C3B-CAB-CBB
31	S1	603	CLA	C2B-C3B-CAB-CBB
31	S1	605	CLA	C2B-C3B-CAB-CBB
31	S1	611	CLA	C2B-C3B-CAB-CBB
31	S1	613	CLA	C2B-C3B-CAB-CBB
31	S1	617	CLA	C2B-C3B-CAB-CBB
31	Y1	603	CLA	C2B-C3B-CAB-CBB
31	Y1	608	CLA	C2B-C3B-CAB-CBB
31	Y1	611	CLA	C2B-C3B-CAB-CBB
31	b1	602	CLA	C2B-C3B-CAB-CBB
31	b1	610	CLA	C2B-C3B-CAB-CBB
31	b1	613	CLA	C2B-C3B-CAB-CBB
31	n1	603	CLA	C2B-C3B-CAB-CBB
31	n1	613	CLA	C2B-C3B-CAB-CBB
31	g1	603	CLA	C2B-C3B-CAB-CBB
31	g1	614	CLA	C2B-C3B-CAB-CBB
31	r1	603	CLA	C2B-C3B-CAB-CBB
31	r1	608	CLA	C2B-C3B-CAB-CBB
31	r1	609	CLA	C2B-C3B-CAB-CBB
31	r1	612	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	s1	604	CLA	C2B-C3B-CAB-CBB
31	s1	610	CLA	C2B-C3B-CAB-CBB
31	s1	613	CLA	C2B-C3B-CAB-CBB
33	B	618	BCR	C23-C24-C25-C30
33	c	517	BCR	C23-C24-C25-C30
33	d	404	BCR	C1-C6-C7-C8
33	c1	516	BCR	C5-C6-C7-C8
34	B1	626	SQD	C10-C11-C12-C13
54	k1	101	4RF	C28-C29-C30-C31
31	c1	508	CLA	C2-C3-C5-C6
31	C1	511	CLA	C8-C10-C11-C12
33	C	516	BCR	C11-C12-C13-C35
33	A1	411	BCR	C7-C8-C9-C34
41	D	409	LHG	C2-C3-O3-P
41	L1	101	LHG	C2-C3-O3-P
41	S1	624	LHG	C2-C3-O3-P
41	d1	408	LHG	C2-C3-O3-P
41	d1	409	LHG	C2-C3-O3-P
52	s	626	3PH	C2-C1-O11-P
41	s	624	LHG	C11-C10-C9-C8
52	s1	626	3PH	C2C-C2D-C2E-C2F
41	d	410	LHG	C33-C34-C35-C36
31	n	613	CLA	C10-C11-C12-C13
40	C	523	DGD	C9B-CAB-CBB-CCB
31	C1	509	CLA	C16-C17-C18-C19
31	n1	613	CLA	C16-C17-C18-C20
47	n	607	CHL	C16-C17-C18-C20
38	B	625	DGA	CB1-CB2-CB3-CB4
31	S1	614	CLA	CAA-CBA-CGA-O2A
35	A1	413	LMG	O7-C10-C11-C12
40	c1	518	DGD	C4D-C5D-C6D-O5D
34	b	621	SQD	C27-C28-C29-C30
41	y	624	LHG	C15-C16-C17-C18
41	D1	409	LHG	C24-C25-C26-C27
31	A1	410	CLA	C2A-CAA-CBA-CGA
31	C1	501	CLA	C2A-CAA-CBA-CGA
34	B1	626	SQD	C29-C30-C31-C32
40	c	518	DGD	C5A-C6A-C7A-C8A
31	c1	510	CLA	C3-C5-C6-C7
31	b	603	CLA	C5-C6-C7-C8
34	A1	412	SQD	O10-C23-O48-C46
34	B1	621	SQD	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
35	h	102	LMG	C15-C16-C17-C18
35	A1	413	LMG	C36-C37-C38-C39
41	y1	624	LHG	O9-C7-O7-C5
31	N	610	CLA	C8-C10-C11-C12
31	b	612	CLA	C5-C6-C7-C8
31	g1	602	CLA	C15-C16-C17-C18
35	b1	622	LMG	C21-C22-C23-C24
41	Y	624	LHG	C24-C25-C26-C27
41	n1	624	LHG	C29-C30-C31-C32
51	S	625	LPX	C11-C10-C9-C8
35	B1	622	LMG	C9-C8-O7-C10
35	b1	622	LMG	C9-C8-O7-C10
38	b1	625	DGA	CG1-CG2-OG2-CB1
40	B1	623	DGD	C3G-C2G-O2G-C1B
41	N	624	LHG	C6-C5-O7-C7
52	S1	626	3PH	C1-C2-O21-C21
41	D	408	LHG	C9-C10-C11-C12
41	N	624	LHG	C28-C29-C30-C31
33	D	404	BCR	C18-C19-C20-C21
33	d	404	BCR	C18-C19-C20-C21
31	b1	614	CLA	C13-C15-C16-C17
41	C	525	LHG	C14-C15-C16-C17
41	D	410	LHG	C33-C34-C35-C36
52	i	101	3PH	C22-C23-C24-C25
34	B1	621	SQD	C28-C29-C30-C31
54	K1	101	4RF	C11-C12-C13-C14
48	g	620	LUT	C33-C34-C35-C15
50	G	623	NEX	C13-C14-C15-C35
31	Y	603	CLA	C16-C17-C18-C20
31	B1	605	CLA	C16-C17-C18-C20
31	b1	617	CLA	C16-C17-C18-C19
31	c	510	CLA	C15-C16-C17-C18
41	N	624	LHG	O6-C4-C5-C6
57	y1	626	PTY	O14-C5-C6-C1
31	c1	513	CLA	CBA-CGA-O2A-C1
31	b	610	CLA	C13-C15-C16-C17
31	Y	602	CLA	C11-C10-C8-C9
31	b	605	CLA	C11-C10-C8-C9
31	b	612	CLA	C6-C7-C8-C9
31	b	613	CLA	C11-C10-C8-C9
31	y	604	CLA	C14-C13-C15-C16
31	C1	505	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	C1	506	CLA	C14-C13-C15-C16
31	C1	507	CLA	C14-C13-C15-C16
31	C1	513	CLA	C6-C7-C8-C9
31	N1	610	CLA	C14-C13-C15-C16
31	Y1	603	CLA	C14-C13-C15-C16
31	b1	602	CLA	C11-C10-C8-C9
31	c1	507	CLA	C11-C10-C8-C9
31	n1	602	CLA	C14-C13-C15-C16
31	g1	603	CLA	C14-C13-C15-C16
31	y1	614	CLA	C11-C12-C13-C14
47	N	609	CHL	C11-C10-C8-C9
47	n	609	CHL	C11-C10-C8-C9
47	y1	606	CHL	C11-C10-C8-C9
35	J	101	LMG	C16-C17-C18-C19
31	B	612	CLA	C11-C12-C13-C15
31	Y	604	CLA	C12-C13-C15-C16
31	y	604	CLA	C12-C13-C15-C16
31	b1	605	CLA	C6-C7-C8-C10
31	n1	602	CLA	C11-C12-C13-C15
31	n1	602	CLA	C12-C13-C15-C16
31	r1	602	CLA	C11-C10-C8-C7
47	g1	601	CHL	C12-C13-C15-C16
40	c	523	DGD	C3A-C4A-C5A-C6A
50	S	622	NEX	C28-C29-C30-C31
50	s	623	NEX	C28-C29-C30-C31
50	Y1	623	NEX	C28-C29-C30-C31
50	n1	623	NEX	C28-C29-C30-C31
41	L1	101	LHG	C34-C35-C36-C37
41	d1	408	LHG	C1-C2-C3-O3
32	A1	409	PHO	O1D-CGD-O2D-CED
41	l	101	LHG	O6-C4-C5-O7
41	D1	409	LHG	O6-C4-C5-O7
41	N1	624	LHG	O6-C4-C5-O7
41	D	408	LHG	C34-C35-C36-C37
41	c	625	LHG	C10-C11-C12-C13
51	s	625	LPX	C11-C10-C9-C8
40	c	519	DGD	O6D-C1D-O3G-C3G
31	b	615	CLA	C16-C17-C18-C20
47	N	607	CHL	C8-C10-C11-C12
38	c	524	DGA	CB3-CB4-CB5-CB6
54	K1	101	4RF	C33-C34-C35-C36
35	h1	102	LMG	O7-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
35	H	102	LMG	C15-C16-C17-C18
41	D	409	LHG	C19-C20-C21-C22
42	c1	527	LMK	C2-C3-C4-O2
40	c1	518	DGD	C2E-C1E-O5D-C6D
31	c	510	CLA	C4-C3-C5-C6
31	s1	610	CLA	C4-C3-C5-C6
44	d	405	PL9	C20-C19-C21-C22
41	Y1	624	LHG	C32-C33-C34-C35
52	b1	624	3PH	C33-C34-C35-C36
34	B1	626	SQD	C7-C8-C9-C10
47	G1	609	CHL	C2-C3-C5-C6
34	C	526	SQD	C12-C13-C14-C15
41	Y	624	LHG	C27-C28-C29-C30
52	b1	624	3PH	C39-C3A-C3B-C3C
31	c	505	CLA	C16-C17-C18-C19
40	C	520	DGD	C5A-C6A-C7A-C8A
41	L1	101	LHG	C33-C34-C35-C36
54	I1	102	4RF	C52-C53-C54-C55
57	y1	626	PTY	C17-C18-C19-C20
35	h1	102	LMG	O9-C10-O7-C8
31	B	606	CLA	C10-C11-C12-C13
41	c1	525	LHG	C2-C3-O3-P
38	C1	524	DGA	CA3-CA4-CA5-CA6
41	c	625	LHG	C25-C26-C27-C28
52	T1	101	3PH	C25-C26-C27-C28
34	c	626	SQD	O47-C45-C46-O48
41	D1	409	LHG	O7-C5-C6-O8
31	s	602	CLA	C5-C6-C7-C8
31	S1	613	CLA	C5-C6-C7-C8
38	c1	524	DGA	CFA-CGA-CHA-CIA
31	Y	608	CLA	CBA-CGA-O2A-C1
48	R1	620	LUT	C9-C10-C11-C12
35	d1	411	LMG	C18-C19-C20-C21
52	B1	624	3PH	C39-C3A-C3B-C3C
31	B	605	CLA	C16-C17-C18-C20
31	B	612	CLA	C5-C6-C7-C8
35	h1	102	LMG	C11-C10-O7-C8
38	C1	524	DGA	CB2-CB1-OG2-CG2
41	L	101	LHG	C19-C20-C21-C22
31	d	402	CLA	CAA-CBA-CGA-O2A
31	r	609	CLA	CAA-CBA-CGA-O2A
35	d1	411	LMG	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
41	Y	624	LHG	C29-C30-C31-C32
42	c1	527	LMK	C13-C14-C15-C27
31	S1	609	CLA	C2A-CAA-CBA-CGA
31	C1	508	CLA	C5-C6-C7-C8
31	b1	605	CLA	C13-C15-C16-C17
31	c1	508	CLA	C8-C10-C11-C12
34	M1	101	SQD	C25-C26-C27-C28
41	N1	624	LHG	C14-C15-C16-C17
31	b1	615	CLA	CBA-CGA-O2A-C1
41	d1	409	LHG	C35-C36-C37-C38
31	B	616	CLA	C2-C1-O2A-CGA
31	G	603	CLA	C2-C1-O2A-CGA
31	a	405	CLA	C2-C1-O2A-CGA
31	c	507	CLA	C2-C1-O2A-CGA
31	n	611	CLA	C2-C1-O2A-CGA
31	N1	614	CLA	C2-C1-O2A-CGA
31	b1	607	CLA	C2-C1-O2A-CGA
31	n1	610	CLA	C2-C1-O2A-CGA
31	g	610	CLA	C4-C3-C5-C6
31	C1	506	CLA	C4-C3-C5-C6
47	y	606	CHL	C4-C3-C5-C6
31	B	609	CLA	C16-C17-C18-C20
41	d	409	LHG	C35-C36-C37-C38
31	N	613	CLA	CAA-CBA-CGA-O2A
31	N1	613	CLA	CAA-CBA-CGA-O2A
31	B	609	CLA	C2-C3-C5-C6
35	a	413	LMG	C7-C8-C9-O8
44	D	405	PL9	C29-C31-C32-C33
54	K1	101	4RF	O18-C19-C20-C39
35	H1	102	LMG	C10-C11-C12-C13
47	N	605	CHL	C3-C5-C6-C7
47	S1	608	CHL	CAA-CBA-CGA-O2A
54	I1	102	4RF	C14-C15-C16-O18
35	H1	102	LMG	C11-C12-C13-C14
41	s	624	LHG	C10-C11-C12-C13
41	d	409	LHG	C8-C7-O7-C5
31	A	405	CLA	C10-C11-C12-C13
31	r1	603	CLA	C3-C5-C6-C7
33	C1	515	BCR	C17-C18-C19-C20
31	A1	410	CLA	CBA-CGA-O2A-C1
31	C1	505	CLA	CBD-CGD-O2D-CED
38	c1	524	DGA	CA2-CA3-CA4-CA5

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Mol	Chain	Res	Type	Atoms
41	y	624	LHG	C34-C35-C36-C37
31	Y	608	CLA	O1A-CGA-O2A-C1
31	R	609	CLA	C10-C11-C12-C13
31	B1	610	CLA	C8-C10-C11-C12
52	T1	101	3PH	C37-C38-C39-C3A
31	B	607	CLA	C2A-CAA-CBA-CGA
31	C	502	CLA	C2A-CAA-CBA-CGA
31	g	602	CLA	C2A-CAA-CBA-CGA
31	s1	613	CLA	C2A-CAA-CBA-CGA
33	B	618	BCR	C13-C14-C15-C16
33	B	619	BCR	C13-C14-C15-C16
33	c	514	BCR	C19-C20-C21-C22
33	b1	618	BCR	C19-C20-C21-C22
33	c1	514	BCR	C19-C20-C21-C22
33	c1	517	BCR	C19-C20-C21-C22
48	Y	620	LUT	C33-C34-C35-C15
49	R	621	XAT	C33-C34-C35-C15
31	y	602	CLA	C16-C17-C18-C19
31	b1	608	CLA	C16-C17-C18-C20
34	a1	412	SQD	C9-C10-C11-C12
31	y1	613	CLA	C4-C3-C5-C6
47	N1	609	CHL	C4-C3-C5-C6
31	Y	604	CLA	C15-C16-C17-C18
31	Y1	603	CLA	C10-C11-C12-C13
34	C1	526	SQD	C17-C18-C19-C20
44	D	405	PL9	C47-C48-C49-C51
34	C1	526	SQD	C30-C31-C32-C33
42	c1	527	LMK	O9-C10-C11-C12
31	Y	612	CLA	C13-C15-C16-C17
56	R1	626	ERG	C22-C23-C24-C28
34	C1	526	SQD	C27-C28-C29-C30
35	B	622	LMG	C21-C22-C23-C24
32	A1	409	PHO	CBD-CGD-O2D-CED
47	n	607	CHL	C16-C17-C18-C19
41	Y	624	LHG	C16-C17-C18-C19
52	T1	101	3PH	C2D-C2E-C2F-C2G
40	C	523	DGD	C1A-C2A-C3A-C4A
31	R	608	CLA	C6-C7-C8-C9
31	Y	604	CLA	C14-C13-C15-C16
31	Y	610	CLA	C11-C12-C13-C14
31	a	405	CLA	C6-C7-C8-C9
31	n	603	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
31	s	609	CLA	C11-C10-C8-C9
31	y	611	CLA	C14-C13-C15-C16
31	B1	613	CLA	C11-C10-C8-C9
31	B1	617	CLA	C11-C12-C13-C14
31	C1	501	CLA	C11-C12-C13-C14
31	C1	507	CLA	C6-C7-C8-C9
31	C1	508	CLA	C11-C12-C13-C14
31	R1	610	CLA	C11-C10-C8-C9
31	b1	610	CLA	C6-C7-C8-C9
31	b1	613	CLA	C11-C10-C8-C9
31	c1	513	CLA	C6-C7-C8-C9
31	s1	611	CLA	C14-C13-C15-C16
31	y1	602	CLA	C11-C12-C13-C14
31	y1	613	CLA	C14-C13-C15-C16
32	A1	409	PHO	C6-C7-C8-C9
47	N	605	CHL	C14-C13-C15-C16
47	n	606	CHL	C11-C10-C8-C9
47	N1	605	CHL	C11-C12-C13-C14
47	G1	609	CHL	C11-C12-C13-C14
31	s	610	CLA	CBA-CGA-O2A-C1
31	S1	610	CLA	C8-C10-C11-C12
41	d	409	LHG	C2-C3-O3-P
38	B1	625	DGA	CFB-CGB-CHB-CIB
31	b	608	CLA	C4B-C3B-CAB-CBB
31	c	506	CLA	C4B-C3B-CAB-CBB
31	s	604	CLA	C4B-C3B-CAB-CBB
31	s	612	CLA	C4B-C3B-CAB-CBB
31	B1	615	CLA	C4B-C3B-CAB-CBB
31	C1	510	CLA	C4B-C3B-CAB-CBB
31	S1	602	CLA	C4B-C3B-CAB-CBB
31	b1	607	CLA	C4B-C3B-CAB-CBB
31	g1	602	CLA	C4B-C3B-CAB-CBB
31	s1	609	CLA	C4B-C3B-CAB-CBB
31	y1	613	CLA	C4B-C3B-CAB-CBB
51	s1	625	LPX	C7-C8-C9-C10
35	h	102	LMG	C16-C17-C18-C19
38	c1	524	DGA	CB3-CB4-CB5-CB6
31	c	506	CLA	C15-C16-C17-C18
34	b1	626	SQD	C13-C14-C15-C16
52	b1	624	3PH	C27-C28-C29-C2A
31	c1	512	CLA	C16-C17-C18-C19
31	B	612	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
31	y	610	CLA	C15-C16-C17-C18
41	d1	409	LHG	O10-C23-O8-C6
31	N1	612	CLA	C2A-CAA-CBA-CGA
47	y1	606	CHL	C2A-CAA-CBA-CGA
34	a1	412	SQD	C25-C26-C27-C28
31	R	603	CLA	C4-C3-C5-C6
31	b	610	CLA	C4-C3-C5-C6
31	s	614	CLA	C4-C3-C5-C6
47	Y	609	CHL	C4-C3-C5-C6
34	B1	626	SQD	C14-C15-C16-C17
31	n	602	CLA	C2-C3-C5-C6
31	C1	506	CLA	C2-C3-C5-C6
52	s1	626	3PH	O11-C1-C2-O21
47	N	608	CHL	O2A-C1-C2-C3
47	n1	608	CHL	O2A-C1-C2-C3
34	b1	621	SQD	C12-C13-C14-C15
31	b1	615	CLA	O1A-CGA-O2A-C1
33	c	517	BCR	C19-C20-C21-C22
48	g1	621	LUT	C13-C14-C15-C35
31	b	612	CLA	C13-C15-C16-C17
31	c	504	CLA	C15-C16-C17-C18
31	D1	402	CLA	CBA-CGA-O2A-C1
40	C	518	DGD	C6A-C7A-C8A-C9A
41	g1	624	LHG	C25-C26-C27-C28
52	s	626	3PH	C2C-C2D-C2E-C2F
54	k1	101	4RF	C02-C03-C04-C05
31	B	604	CLA	C6-C7-C8-C10
31	R	603	CLA	C11-C10-C8-C7
31	Y	604	CLA	C11-C10-C8-C7
31	Y	613	CLA	C11-C12-C13-C15
31	y	604	CLA	C11-C12-C13-C15
31	C1	513	CLA	C6-C7-C8-C10
31	D1	403	CLA	C11-C10-C8-C7
31	R1	610	CLA	C6-C7-C8-C10
31	b1	610	CLA	C11-C12-C13-C15
31	b1	617	CLA	C6-C7-C8-C10
31	c1	513	CLA	C6-C7-C8-C10
31	n1	613	CLA	C12-C13-C15-C16
47	G	609	CHL	C11-C12-C13-C15
47	G1	601	CHL	C11-C12-C13-C15
47	Y1	606	CHL	C12-C13-C15-C16
47	n1	606	CHL	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
47	y1	609	CHL	C11-C12-C13-C15
31	A1	405	CLA	C15-C16-C17-C18
31	y1	602	CLA	C8-C10-C11-C12
41	g	624	LHG	C12-C13-C14-C15
51	s1	625	LPX	C12-C13-C14-C15
35	h	102	LMG	C19-C20-C21-C22
41	D1	409	LHG	C32-C33-C34-C35
41	L1	101	LHG	C17-C18-C19-C20
31	b	610	CLA	CBA-CGA-O2A-C1
38	C1	524	DGA	OB1-CB1-OG2-CG2
31	B	609	CLA	C13-C15-C16-C17
31	b1	607	CLA	C15-C16-C17-C18
47	N	607	CHL	CAA-CBA-CGA-O2A
41	c1	525	LHG	C24-C25-C26-C27
31	n	613	CLA	C16-C17-C18-C20
31	a1	410	CLA	C11-C12-C13-C14
52	t1	101	3PH	C32-C33-C34-C35
41	g	624	LHG	O10-C23-C24-C25
31	Y	603	CLA	C10-C11-C12-C13
31	D1	402	CLA	O1A-CGA-O2A-C1
35	H1	102	LMG	C12-C13-C14-C15
54	I1	102	4RF	C47-C48-C49-C50
31	C	506	CLA	C3A-C2A-CAA-CBA
31	C	512	CLA	C3A-C2A-CAA-CBA
31	b	612	CLA	C3A-C2A-CAA-CBA
31	b	613	CLA	C3A-C2A-CAA-CBA
31	y1	613	CLA	C3A-C2A-CAA-CBA
47	S	608	CHL	C3A-C2A-CAA-CBA
47	Y	609	CHL	C3A-C2A-CAA-CBA
47	n	608	CHL	C3A-C2A-CAA-CBA
47	y	601	CHL	C3A-C2A-CAA-CBA
47	g1	601	CHL	C4-C3-C5-C6
34	b1	626	SQD	C10-C11-C12-C13
40	C	519	DGD	C5B-C6B-C7B-C8B
41	c	625	LHG	C16-C17-C18-C19
31	c	506	CLA	C2-C3-C5-C6
31	s	604	CLA	C2-C3-C5-C6
47	n	609	CHL	C2-C3-C5-C6
51	S1	625	LPX	C12-C13-C14-C15
41	n	624	LHG	C11-C10-C9-C8
35	d	411	LMG	C11-C12-C13-C14
41	S1	624	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
33	D	404	BCR	C20-C21-C22-C37
33	d	404	BCR	C20-C21-C22-C37
50	N	623	NEX	C39-C29-C30-C31
50	G1	623	NEX	C39-C29-C30-C31
50	S1	623	NEX	C39-C29-C30-C31
50	Y1	623	NEX	C40-C33-C34-C35
50	n1	623	NEX	C39-C29-C30-C31
54	I1	102	4RF	C24-C25-C26-C27
31	C	512	CLA	C5-C6-C7-C8
31	c1	504	CLA	C15-C16-C17-C18
31	g1	610	CLA	C15-C16-C17-C18
41	L	101	LHG	O9-C7-O7-C5
41	d1	408	LHG	O9-C7-O7-C5
47	r1	607	CHL	C2C-C3C-CAC-CBC
51	S1	625	LPX	C11-C12-C13-C14
54	K1	101	4RF	C09-C10-C11-C12
31	c	501	CLA	C2-C1-O2A-CGA
31	c	513	CLA	C2-C1-O2A-CGA
31	s	609	CLA	C2-C1-O2A-CGA
31	y	602	CLA	C2-C1-O2A-CGA
31	G1	614	CLA	C2-C1-O2A-CGA
33	d	404	BCR	C9-C10-C11-C12
33	c1	516	BCR	C13-C14-C15-C16
37	B	620	C7Z	C33-C34-C35-C15
48	G1	620	LUT	C9-C10-C11-C12
48	y1	620	LUT	C29-C30-C31-C32
50	N	623	NEX	C33-C34-C35-C15
50	g1	623	NEX	C29-C30-C31-C32
41	C	525	LHG	C33-C34-C35-C36
41	N1	624	LHG	C30-C31-C32-C33
52	s	626	3PH	C33-C34-C35-C36
31	C	509	CLA	C5-C6-C7-C8
31	y	610	CLA	C5-C6-C7-C8
31	y	613	CLA	C13-C15-C16-C17
37	B	620	C7Z	C11-C12-C13-C20
41	D1	409	LHG	C2-C3-O3-P
48	g	620	LUT	C27-C28-C29-C39
49	R	621	XAT	C31-C32-C33-C40
51	S	625	LPX	C4-C3-O1-P1
34	C1	526	SQD	C28-C29-C30-C31
52	T1	101	3PH	C2A-C2B-C2C-C2D
53	y	625	SPH	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
40	C	518	DGD	CAB-CBB-CCB-CDB
33	C	515	BCR	C21-C22-C23-C24
33	c	514	BCR	C21-C22-C23-C24
37	B1	620	C7Z	C11-C12-C13-C14
44	d1	405	PL9	C15-C14-C16-C17
44	d1	405	PL9	C30-C29-C31-C32
44	d1	405	PL9	C13-C14-C16-C17
41	d	409	LHG	O9-C7-O7-C5
35	d1	411	LMG	C21-C22-C23-C24
47	y	607	CHL	C10-C11-C12-C13
44	d	405	PL9	C2-C3-C7-C8
34	a1	412	SQD	O6-C44-C45-C46
35	D1	411	LMG	C7-C8-C9-O8
38	b	623	DGA	OG1-CG1-CG2-CG3
40	C	519	DGD	O1G-C1G-C2G-C3G
41	Y1	624	LHG	C4-C5-C6-O8
57	Y1	626	PTY	C31-C32-C33-C34
31	B	604	CLA	C6-C7-C8-C9
31	G	602	CLA	C11-C10-C8-C9
31	G	610	CLA	C11-C12-C13-C14
31	Y	613	CLA	C11-C12-C13-C14
31	b	603	CLA	C11-C10-C8-C9
31	c	508	CLA	C11-C10-C8-C9
31	c	509	CLA	C11-C10-C8-C9
31	y	604	CLA	C11-C12-C13-C14
31	B1	604	CLA	C14-C13-C15-C16
31	B1	615	CLA	C6-C7-C8-C9
31	C1	511	CLA	C14-C13-C15-C16
31	a1	406	CLA	C6-C7-C8-C9
31	b1	602	CLA	C11-C12-C13-C14
31	b1	617	CLA	C6-C7-C8-C9
31	b1	617	CLA	C11-C10-C8-C9
31	c1	510	CLA	C11-C12-C13-C14
31	c1	513	CLA	C11-C12-C13-C14
31	g1	602	CLA	C11-C10-C8-C9
31	g1	603	CLA	C11-C12-C13-C14
31	g1	611	CLA	C11-C12-C13-C14
32	A	408	PHO	C11-C10-C8-C9
47	n	607	CHL	C14-C13-C15-C16
47	G1	609	CHL	C11-C10-C8-C9
39	b	624	GOL	C1-C2-C3-O3
41	n1	624	LHG	O1-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
31	b	602	CLA	C16-C17-C18-C20
35	c1	523	LMG	C13-C14-C15-C16
41	d	409	LHG	C30-C31-C32-C33
41	N1	624	LHG	C29-C30-C31-C32
53	A1	414	SPH	C7-C8-C9-C10
31	C	506	CLA	C15-C16-C17-C18
31	G	613	CLA	C15-C16-C17-C18
34	b1	621	SQD	C14-C15-C16-C17
34	B1	621	SQD	C13-C14-C15-C16
34	B1	626	SQD	C32-C33-C34-C35
41	l	101	LHG	C12-C13-C14-C15
41	n1	624	LHG	C16-C17-C18-C19
52	i	101	3PH	C3C-C3D-C3E-C3F
53	Y1	625	SPH	C13-C14-C15-C16
47	g1	607	CHL	CAA-CBA-CGA-O2A
35	b	622	LMG	C9-C8-O7-C10
40	b1	623	DGD	C1G-C2G-O2G-C1B
47	N	609	CHL	C8-C10-C11-C12
40	C1	519	DGD	C3A-C4A-C5A-C6A
47	N	609	CHL	C1A-C2A-CAA-CBA
47	G	609	CHL	C1A-C2A-CAA-CBA
47	g	609	CHL	C1A-C2A-CAA-CBA
47	N1	609	CHL	C1A-C2A-CAA-CBA
47	G1	607	CHL	C1A-C2A-CAA-CBA
47	n1	607	CHL	C1A-C2A-CAA-CBA
47	g1	609	CHL	C1A-C2A-CAA-CBA
47	y1	609	CHL	C1A-C2A-CAA-CBA
38	c1	524	DGA	CAA-CBA-CCA-CDA
48	n1	620	LUT	C29-C30-C31-C32
35	h1	102	LMG	C12-C13-C14-C15
31	y	602	CLA	C4-C3-C5-C6
47	G1	601	CHL	C4-C3-C5-C6
52	B1	624	3PH	C21-C22-C23-C24
52	b1	624	3PH	C21-C22-C23-C24
31	C1	509	CLA	C16-C17-C18-C20
41	d	409	LHG	C27-C28-C29-C30
31	c	510	CLA	C2-C3-C5-C6
47	g1	601	CHL	C2-C3-C5-C6
38	C	524	DGA	CDA-CEA-CFA-CGA
41	N1	624	LHG	C19-C20-C21-C22
41	Y	624	LHG	O1-C1-C2-O2
41	Y1	624	LHG	O1-C1-C2-O2

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Mol	Chain	Res	Type	Atoms
41	c1	525	LHG	O1-C1-C2-O2
31	s1	614	CLA	O1A-CGA-O2A-C1
41	g	624	LHG	C16-C17-C18-C19
41	N1	624	LHG	C17-C18-C19-C20
41	Y	624	LHG	C19-C20-C21-C22
47	S	601	CHL	CAA-CBA-CGA-O2A
38	b	623	DGA	CFA-CGA-CHA-CIA
31	c	502	CLA	C2A-CAA-CBA-CGA
47	N	607	CHL	C2A-CAA-CBA-CGA
34	c1	526	SQD	C25-C26-C27-C28
35	b	622	LMG	C11-C12-C13-C14
41	D	410	LHG	C26-C27-C28-C29
41	c1	525	LHG	C16-C17-C18-C19
31	b	610	CLA	O1A-CGA-O2A-C1
31	B	605	CLA	C1A-C2A-CAA-CBA
31	C	512	CLA	C1A-C2A-CAA-CBA
31	D	403	CLA	C1A-C2A-CAA-CBA
31	N	612	CLA	C1A-C2A-CAA-CBA
31	R	609	CLA	C1A-C2A-CAA-CBA
31	Y	611	CLA	C1A-C2A-CAA-CBA
31	c	506	CLA	C1A-C2A-CAA-CBA
31	n	613	CLA	C1A-C2A-CAA-CBA
31	B1	610	CLA	C1A-C2A-CAA-CBA
31	C1	502	CLA	C1A-C2A-CAA-CBA
31	Y1	602	CLA	C1A-C2A-CAA-CBA
31	c1	502	CLA	C1A-C2A-CAA-CBA
31	d1	403	CLA	C1A-C2A-CAA-CBA
31	y1	604	CLA	C1A-C2A-CAA-CBA
31	y1	610	CLA	C1A-C2A-CAA-CBA
33	D	404	BCR	C20-C21-C22-C23
33	d	404	BCR	C20-C21-C22-C23
50	r	623	NEX	C32-C33-C34-C35
50	y	623	NEX	C28-C29-C30-C31
50	G1	623	NEX	C28-C29-C30-C31
50	S1	623	NEX	C28-C29-C30-C31
41	D1	410	LHG	C25-C26-C27-C28
41	D1	410	LHG	C29-C30-C31-C32
31	C	505	CLA	C16-C17-C18-C20
31	b	613	CLA	C16-C17-C18-C20
41	l	101	LHG	O9-C7-O7-C5
41	D1	410	LHG	C9-C10-C11-C12
31	D	402	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
53	y	625	SPH	C9-C10-C11-C12
38	c	524	DGA	CA2-CA3-CA4-CA5
38	c1	524	DGA	CB5-CB6-CB7-CB8
31	D1	402	CLA	C5-C6-C7-C8
31	B	607	CLA	C2B-C3B-CAB-CBB
31	B	610	CLA	C2B-C3B-CAB-CBB
31	B	616	CLA	C2B-C3B-CAB-CBB
31	C	502	CLA	C2B-C3B-CAB-CBB
31	C	510	CLA	C2B-C3B-CAB-CBB
31	G	604	CLA	C2B-C3B-CAB-CBB
31	R	613	CLA	C2B-C3B-CAB-CBB
31	S	609	CLA	C2B-C3B-CAB-CBB
31	Y	611	CLA	C2B-C3B-CAB-CBB
31	b	608	CLA	C2B-C3B-CAB-CBB
31	b	617	CLA	C2B-C3B-CAB-CBB
31	c	506	CLA	C2B-C3B-CAB-CBB
31	g	603	CLA	C2B-C3B-CAB-CBB
31	g	613	CLA	C2B-C3B-CAB-CBB
31	r	609	CLA	C2B-C3B-CAB-CBB
31	r	610	CLA	C2B-C3B-CAB-CBB
31	s	604	CLA	C2B-C3B-CAB-CBB
31	s	612	CLA	C2B-C3B-CAB-CBB
31	y	604	CLA	C2B-C3B-CAB-CBB
31	y	611	CLA	C2B-C3B-CAB-CBB
31	y	614	CLA	C2B-C3B-CAB-CBB
31	B1	605	CLA	C2B-C3B-CAB-CBB
31	B1	617	CLA	C2B-C3B-CAB-CBB
31	C1	507	CLA	C2B-C3B-CAB-CBB
31	C1	510	CLA	C2B-C3B-CAB-CBB
31	N1	604	CLA	C2B-C3B-CAB-CBB
31	N1	613	CLA	C2B-C3B-CAB-CBB
31	S1	602	CLA	C2B-C3B-CAB-CBB
31	S1	610	CLA	C2B-C3B-CAB-CBB
31	S1	614	CLA	C2B-C3B-CAB-CBB
31	Y1	610	CLA	C2B-C3B-CAB-CBB
31	a1	407	CLA	C2B-C3B-CAB-CBB
31	b1	603	CLA	C2B-C3B-CAB-CBB
31	b1	604	CLA	C2B-C3B-CAB-CBB
31	b1	607	CLA	C2B-C3B-CAB-CBB
31	b1	616	CLA	C2B-C3B-CAB-CBB
31	c1	513	CLA	C2B-C3B-CAB-CBB
31	n1	604	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	n1	614	CLA	C2B-C3B-CAB-CBB
31	g1	602	CLA	C2B-C3B-CAB-CBB
31	g1	610	CLA	C2B-C3B-CAB-CBB
31	g1	611	CLA	C2B-C3B-CAB-CBB
31	r1	610	CLA	C2B-C3B-CAB-CBB
31	s1	609	CLA	C2B-C3B-CAB-CBB
31	y1	604	CLA	C2B-C3B-CAB-CBB
31	y1	612	CLA	C2B-C3B-CAB-CBB
31	y1	613	CLA	C2B-C3B-CAB-CBB
33	A	411	BCR	C23-C24-C25-C26
33	C	515	BCR	C23-C24-C25-C26
33	C	517	BCR	C23-C24-C25-C26
33	C	517	BCR	C23-C24-C25-C30
33	D	404	BCR	C23-C24-C25-C26
33	a	411	BCR	C23-C24-C25-C26
33	c	514	BCR	C23-C24-C25-C26
33	c	516	BCR	C5-C6-C7-C8
33	c	517	BCR	C23-C24-C25-C26
33	d	404	BCR	C5-C6-C7-C8
33	d	404	BCR	C23-C24-C25-C30
33	C1	514	BCR	C23-C24-C25-C26
33	C1	515	BCR	C23-C24-C25-C30
33	C1	516	BCR	C23-C24-C25-C26
33	a1	411	BCR	C23-C24-C25-C26
33	c1	514	BCR	C23-C24-C25-C26
33	c1	515	BCR	C23-C24-C25-C26
33	d1	404	BCR	C5-C6-C7-C8
37	b1	620	C7Z	C25-C26-C27-C28
46	H	101	RRX	C23-C24-C25-C26
48	R	620	LUT	C1-C6-C7-C8
48	Y	620	LUT	C1-C6-C7-C8
48	n	620	LUT	C1-C6-C7-C8
48	N1	620	LUT	C5-C6-C7-C8
48	N1	621	LUT	C1-C6-C7-C8
48	G1	621	LUT	C1-C6-C7-C8
47	S	601	CHL	CAA-CBA-CGA-O1A
42	c1	527	LMK	C28-C29-C30-C31
34	a	412	SQD	C35-C36-C37-C38
31	C1	510	CLA	C8-C10-C11-C12
41	l	101	LHG	C2-C3-O3-P
41	D1	408	LHG	C2-C3-O3-P
35	b	622	LMG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
51	s	625	LPX	C16-C17-C18-C19
52	S	626	3PH	C38-C39-C3A-C3B
54	I1	102	4RF	C04-C05-C06-C07
47	N	601	CHL	C3-C5-C6-C7
31	a1	405	CLA	C8-C10-C11-C12
31	B	616	CLA	C4-C3-C5-C6
31	c	504	CLA	C4-C3-C5-C6
31	r	608	CLA	C4-C3-C5-C6
34	C	526	SQD	C31-C32-C33-C34
38	B	625	DGA	CB2-CB3-CB4-CB5
31	R	603	CLA	C2-C3-C5-C6
31	C1	512	CLA	C2-C3-C5-C6
31	y1	613	CLA	C2-C3-C5-C6
47	n	608	CHL	O2A-C1-C2-C3
47	r	607	CHL	O2A-C1-C2-C3
47	R1	607	CHL	O2A-C1-C2-C3
31	n1	604	CLA	C10-C11-C12-C13
38	b	623	DGA	CBB-CCB-CDB-CEB
31	B	605	CLA	C11-C12-C13-C15
31	C	508	CLA	C12-C13-C15-C16
31	R	609	CLA	C11-C10-C8-C7
31	R	610	CLA	C6-C7-C8-C10
31	Y	610	CLA	C11-C12-C13-C15
31	b	607	CLA	C12-C13-C15-C16
31	b	611	CLA	C11-C10-C8-C7
31	d	402	CLA	C11-C10-C8-C7
31	y	611	CLA	C11-C10-C8-C7
31	B1	617	CLA	C11-C12-C13-C15
31	C1	506	CLA	C11-C10-C8-C7
31	C1	508	CLA	C11-C12-C13-C15
31	C1	510	CLA	C11-C12-C13-C15
31	N1	603	CLA	C11-C10-C8-C7
31	Y1	602	CLA	C12-C13-C15-C16
31	Y1	604	CLA	C11-C10-C8-C7
31	b1	608	CLA	C11-C12-C13-C15
31	g1	603	CLA	C11-C12-C13-C15
31	y1	602	CLA	C11-C12-C13-C15
47	g1	601	CHL	C11-C12-C13-C15
47	y1	607	CHL	C11-C10-C8-C7
41	d	408	LHG	C31-C32-C33-C34
31	c	503	CLA	C16-C17-C18-C19
31	B1	615	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
47	s	608	CHL	C11-C12-C13-C14
31	A	406	CLA	C2A-CAA-CBA-CGA
31	S1	611	CLA	C2A-CAA-CBA-CGA
31	s1	611	CLA	C2A-CAA-CBA-CGA
31	R	610	CLA	C10-C11-C12-C13
31	Y	603	CLA	C5-C6-C7-C8
31	b1	603	CLA	C5-C6-C7-C8
34	A	412	SQD	O47-C45-C46-O48
38	B	625	DGA	CA2-CA3-CA4-CA5
51	S	625	LPX	C12-C13-C14-C15
41	d	408	LHG	C10-C11-C12-C13
47	Y	607	CHL	C13-C15-C16-C17
41	n	624	LHG	C16-C17-C18-C19
41	G1	624	LHG	C14-C15-C16-C17
52	s	626	3PH	C34-C35-C36-C37
54	I1	102	4RF	C53-C54-C55-C56
31	B	610	CLA	C3-C5-C6-C7
31	b1	613	CLA	C3-C5-C6-C7
32	A	408	PHO	C8-C10-C11-C12
31	Y	611	CLA	C16-C17-C18-C20
35	B	622	LMG	C29-C30-C31-C32
54	I1	102	4RF	C29-C30-C31-C32
41	d	410	LHG	C1-C2-C3-O3
47	R	606	CHL	C2A-CAA-CBA-CGA
31	A	405	CLA	C8-C10-C11-C12
31	c1	513	CLA	C15-C16-C17-C18
33	D	404	BCR	C11-C12-C13-C35
33	A1	411	BCR	C11-C12-C13-C35
33	B1	618	BCR	C7-C8-C9-C34
31	s	612	CLA	CAA-CBA-CGA-O2A
31	b	617	CLA	C4-C3-C5-C6
31	c	502	CLA	C4-C3-C5-C6
31	c	511	CLA	C4-C3-C5-C6
31	R1	609	CLA	C4-C3-C5-C6
47	N	605	CHL	C4-C3-C5-C6
47	s1	608	CHL	CAA-CBA-CGA-O2A
31	Y1	614	CLA	C15-C16-C17-C18
31	s1	611	CLA	C5-C6-C7-C8
31	b	614	CLA	C2-C3-C5-C6
31	s	614	CLA	C2-C3-C5-C6
31	A1	406	CLA	C2-C3-C5-C6
31	n1	604	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
31	s1	603	CLA	C2-C3-C5-C6
47	Y	609	CHL	C2-C3-C5-C6
47	y	606	CHL	C2-C3-C5-C6
47	N1	609	CHL	C2-C3-C5-C6
38	B	625	DGA	CCA-CDA-CEA-CFA
41	c1	525	LHG	C12-C13-C14-C15
40	c	523	DGD	O6D-C5D-C6D-O5D
41	d1	410	LHG	C34-C35-C36-C37
51	S1	625	LPX	C6-C7-C8-C9
31	y1	602	CLA	C2-C1-O2A-CGA
31	b1	609	CLA	C8-C10-C11-C12
31	N1	612	CLA	CAA-CBA-CGA-O2A
31	S1	612	CLA	CAA-CBA-CGA-O2A
41	C	525	LHG	C28-C29-C30-C31
47	S1	608	CHL	C10-C11-C12-C13
38	C	524	DGA	CA9-CAA-CBA-CCA
35	a1	413	LMG	C11-C10-O7-C8
41	g1	624	LHG	C34-C35-C36-C37
31	B	602	CLA	C6-C7-C8-C9
31	N	613	CLA	C14-C13-C15-C16
31	b	606	CLA	C11-C12-C13-C14
31	n	602	CLA	C11-C10-C8-C9
31	y	602	CLA	C11-C12-C13-C14
31	B1	613	CLA	C14-C13-C15-C16
31	g1	613	CLA	C14-C13-C15-C16
47	n1	605	CHL	C11-C10-C8-C9
35	C	521	LMG	C39-C40-C41-C42
41	s1	624	LHG	C25-C26-C27-C28
54	i1	101	4RF	C06-C07-C08-C09
38	c	524	DGA	CBB-CAB-CB9-CB8
40	B1	623	DGD	C4A-C5A-C6A-C7A
41	c	625	LHG	C30-C31-C32-C33
41	d1	410	LHG	C31-C32-C33-C34
35	A	413	LMG	C29-C30-C31-C32
31	b	616	CLA	C13-C15-C16-C17
31	S1	609	CLA	C5-C6-C7-C8
38	C1	524	DGA	CFA-CGA-CHA-CIA
31	B1	616	CLA	C16-C17-C18-C20
34	C	526	SQD	C13-C14-C15-C16
34	a1	412	SQD	C16-C17-C18-C19
35	w1	201	LMG	O6-C1-O1-C7
53	Y	625	SPH	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	s	609	CLA	C4-C3-C5-C6
31	A1	406	CLA	C4-C3-C5-C6
31	S1	610	CLA	C4-C3-C5-C6
31	b1	602	CLA	C4-C3-C5-C6
31	y1	614	CLA	C4-C3-C5-C6
32	a1	409	PHO	C4-C3-C5-C6
44	d	405	PL9	C45-C44-C46-C47
47	y	609	CHL	C4-C3-C5-C6
47	n1	609	CHL	C4-C3-C5-C6
47	g1	607	CHL	C4-C3-C5-C6
31	s1	612	CLA	CAA-CBA-CGA-O2A
41	D	410	LHG	C5-C4-O6-P
49	n1	622	XAT	C14-C15-C35-C34
31	G1	612	CLA	C2A-CAA-CBA-CGA
31	B	610	CLA	C2-C3-C5-C6
31	b	605	CLA	C2-C3-C5-C6
34	A	412	SQD	C11-C12-C13-C14
34	B1	626	SQD	C9-C10-C11-C12
41	g1	624	LHG	C29-C30-C31-C32
31	G	610	CLA	C5-C6-C7-C8
31	y	611	CLA	C13-C15-C16-C17
31	G1	603	CLA	C10-C11-C12-C13
31	C	502	CLA	C16-C17-C18-C20
31	Y	603	CLA	C16-C17-C18-C19
31	C1	510	CLA	C16-C17-C18-C20
31	N1	610	CLA	C16-C17-C18-C20
35	B	622	LMG	C19-C20-C21-C22
41	D	409	LHG	C32-C33-C34-C35
47	R	607	CHL	O2A-C1-C2-C3
47	g	606	CHL	O2A-C1-C2-C3
31	a1	405	CLA	C5-C6-C7-C8
54	I1	102	4RF	C03-C04-C05-C06
34	c	626	SQD	C44-C45-C46-O48
35	C1	523	LMG	O1-C7-C8-C9
38	J1	101	DGA	OG2-CG2-CG3-OXT
38	c1	524	DGA	OG2-CG2-CG3-OXT
35	b1	622	LMG	C16-C17-C18-C19
35	h1	102	LMG	O10-C28-O8-C9
31	s1	614	CLA	CBA-CGA-O2A-C1
31	S	602	CLA	C2A-CAA-CBA-CGA
31	a	406	CLA	C2A-CAA-CBA-CGA
31	r	608	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
31	r	613	CLA	C2A-CAA-CBA-CGA
31	s	613	CLA	C2A-CAA-CBA-CGA
31	B1	607	CLA	C2A-CAA-CBA-CGA
31	c1	510	CLA	C2A-CAA-CBA-CGA
31	s1	605	CLA	C2A-CAA-CBA-CGA
31	B	609	CLA	C16-C17-C18-C19
31	B1	605	CLA	C16-C17-C18-C19
42	C1	527	LMK	O9-C10-C11-C12
34	M1	101	SQD	C10-C11-C12-C13
34	A	412	SQD	O47-C7-C8-C9
41	G	630	LHG	C33-C34-C35-C36
41	S	624	LHG	C33-C34-C35-C36
41	G1	624	LHG	C15-C16-C17-C18
31	b1	612	CLA	C8-C10-C11-C12
35	a	413	LMG	C31-C32-C33-C34
41	G	630	LHG	C11-C12-C13-C14
41	Y1	624	LHG	O6-C4-C5-O7
52	b1	624	3PH	O11-C1-C2-O21
31	c1	505	CLA	C4-C3-C5-C6
44	D1	405	PL9	C45-C44-C46-C47
44	d1	405	PL9	C45-C44-C46-C47
50	r1	622	NEX	C33-C34-C35-C15
31	c	513	CLA	CAA-CBA-CGA-O2A
34	M1	101	SQD	O47-C7-C8-C9
34	b1	621	SQD	O47-C7-C8-C9
41	d	410	LHG	C27-C28-C29-C30
38	B	625	DGA	CBA-CCA-CDA-CEA
41	d1	408	LHG	C8-C7-O7-C5
54	K1	101	4RF	C48-C49-C50-C51
31	B	606	CLA	C4B-C3B-CAB-CBB
31	C	504	CLA	C4B-C3B-CAB-CBB
31	C	510	CLA	C4B-C3B-CAB-CBB
31	c	512	CLA	C4B-C3B-CAB-CBB
31	n	613	CLA	C4B-C3B-CAB-CBB
31	B1	609	CLA	C4B-C3B-CAB-CBB
31	C1	505	CLA	C4B-C3B-CAB-CBB
31	C1	506	CLA	C4B-C3B-CAB-CBB
31	N1	604	CLA	C4B-C3B-CAB-CBB
31	R1	609	CLA	C4B-C3B-CAB-CBB
31	a1	407	CLA	C4B-C3B-CAB-CBB
31	b1	617	CLA	C4B-C3B-CAB-CBB
31	c1	507	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	c1	513	CLA	C4B-C3B-CAB-CBB
31	g1	610	CLA	C4B-C3B-CAB-CBB
31	g1	613	CLA	C4B-C3B-CAB-CBB
31	r1	602	CLA	C4B-C3B-CAB-CBB
31	n	602	CLA	O1A-CGA-O2A-C1
31	n1	613	CLA	O1A-CGA-O2A-C1
47	R1	606	CHL	C2A-CAA-CBA-CGA
35	a	413	LMG	C30-C31-C32-C33
51	s	625	LPX	C12-C13-C14-C15
31	b1	605	CLA	CAA-CBA-CGA-O1A
35	B1	622	LMG	C11-C12-C13-C14
31	r	609	CLA	C8-C10-C11-C12
35	h1	102	LMG	C16-C17-C18-C19
31	b	612	CLA	C16-C17-C18-C19
31	y	602	CLA	C16-C17-C18-C20
35	w1	201	LMG	O9-C10-C11-C12
34	C1	526	SQD	O49-C7-O47-C45
35	B1	622	LMG	C33-C34-C35-C36
54	k1	101	4RF	C07-C08-C09-C10
32	a	408	PHO	CHA-CBD-CGD-O1D
32	a	409	PHO	CHA-CBD-CGD-O1D
47	G	606	CHL	CHA-CBD-CGD-O2D
47	S	608	CHL	CHA-CBD-CGD-O1D
47	Y1	607	CHL	CHA-CBD-CGD-O1D
47	s1	601	CHL	CHA-CBD-CGD-O1D
47	s1	601	CHL	CHA-CBD-CGD-O2D
47	s1	607	CHL	CHA-CBD-CGD-O1D
47	s1	607	CHL	CHA-CBD-CGD-O2D
50	N	623	NEX	C40-C33-C34-C35
50	n	623	NEX	C39-C29-C30-C31
50	y	623	NEX	C39-C29-C30-C31
31	S1	611	CLA	O1A-CGA-O2A-C1
31	B1	613	CLA	C8-C10-C11-C12
31	c1	511	CLA	C5-C6-C7-C8
31	R	612	CLA	CAA-CBA-CGA-O2A
41	G1	624	LHG	O8-C23-C24-C25
31	N1	612	CLA	CAA-CBA-CGA-O1A
47	y	605	CHL	CAA-CBA-CGA-O2A
35	c1	523	LMG	C28-C29-C30-C31
35	B1	622	LMG	C13-C14-C15-C16
38	B	625	DGA	CA7-CA8-CA9-CAA
41	D1	410	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
41	c1	525	LHG	C34-C35-C36-C37
41	s	624	LHG	O6-C4-C5-C6
41	Y1	624	LHG	O6-C4-C5-C6
52	b1	624	3PH	O11-C1-C2-C3
52	t1	101	3PH	O11-C1-C2-C3
31	C1	513	CLA	C4-C3-C5-C6
34	B	621	SQD	O47-C45-C46-O48
34	C	526	SQD	O6-C44-C45-O47
34	a	412	SQD	O6-C44-C45-O47
35	c	521	LMG	O7-C8-C9-O8
40	c	519	DGD	O1G-C1G-C2G-O2G
41	y1	624	LHG	O7-C5-C6-O8
31	B1	615	CLA	C15-C16-C17-C18
41	L	101	LHG	C8-C7-O7-C5
31	S	614	CLA	CAA-CBA-CGA-O2A
41	N1	624	LHG	O8-C23-C24-C25
44	D1	405	PL9	C12-C11-C9-C8
47	n1	609	CHL	C2-C3-C5-C6
31	R1	609	CLA	C3-C5-C6-C7
40	c1	518	DGD	O6E-C1E-O5D-C6D
31	S	603	CLA	C13-C15-C16-C17
31	a	406	CLA	C5-C6-C7-C8
31	a	406	CLA	C15-C16-C17-C18
31	C1	509	CLA	C13-C15-C16-C17
31	y1	604	CLA	C13-C15-C16-C17
52	B1	624	3PH	C2-C1-O11-P
34	a	412	SQD	C26-C27-C28-C29
31	B	607	CLA	C11-C10-C8-C7
31	G	610	CLA	C11-C12-C13-C15
31	c	506	CLA	C6-C7-C8-C10
31	s	610	CLA	C6-C7-C8-C10
31	B1	605	CLA	C12-C13-C15-C16
31	S1	603	CLA	C11-C12-C13-C15
31	b1	607	CLA	C12-C13-C15-C16
31	c1	507	CLA	C6-C7-C8-C10
31	c1	513	CLA	C11-C12-C13-C15
31	g1	610	CLA	C11-C12-C13-C15
47	n1	605	CHL	C11-C10-C8-C7
54	i1	101	4RF	C03-C04-C05-C06
47	y	605	CHL	CAA-CBA-CGA-O1A
35	a	413	LMG	C13-C14-C15-C16
38	j1	101	DGA	CB3-CB4-CB5-CB6

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Mol	Chain	Res	Type	Atoms
48	N1	621	LUT	C9-C10-C11-C12
35	D1	411	LMG	C10-C11-C12-C13
31	S1	612	CLA	CAA-CBA-CGA-O1A
35	c1	521	LMG	O9-C10-C11-C12
31	B	606	CLA	C11-C12-C13-C14
31	C	512	CLA	C11-C12-C13-C14
31	Y	602	CLA	C11-C12-C13-C14
31	b	611	CLA	C11-C12-C13-C14
31	c	505	CLA	C11-C10-C8-C9
31	n	604	CLA	C6-C7-C8-C9
31	s	603	CLA	C6-C7-C8-C9
31	s	611	CLA	C6-C7-C8-C9
31	y	613	CLA	C11-C12-C13-C14
31	B1	607	CLA	C11-C12-C13-C14
31	B1	611	CLA	C11-C10-C8-C9
31	C1	512	CLA	C14-C13-C15-C16
31	D1	403	CLA	C11-C10-C8-C9
31	N1	604	CLA	C6-C7-C8-C9
31	b1	613	CLA	C14-C13-C15-C16
31	n1	610	CLA	C6-C7-C8-C9
47	N	607	CHL	C11-C12-C13-C14
47	N	609	CHL	C14-C13-C15-C16
47	y1	606	CHL	C6-C7-C8-C9
40	C	518	DGD	O6D-C5D-C6D-O5D
35	c1	523	LMG	C30-C31-C32-C33
41	d	408	LHG	C14-C15-C16-C17
35	a1	413	LMG	C8-C7-O1-C1
40	C1	519	DGD	C2G-C3G-O3G-C1D
40	c1	518	DGD	C5D-C6D-O5D-C1E
52	s1	626	3PH	C1-O11-P-O12
41	L1	101	LHG	C30-C31-C32-C33
54	k1	101	4RF	C13-C14-C15-C16
31	s	612	CLA	CAA-CBA-CGA-O1A
31	C	512	CLA	C2A-CAA-CBA-CGA
31	B	604	CLA	C2-C1-O2A-CGA
31	S	604	CLA	C2-C1-O2A-CGA
31	B1	607	CLA	C2-C1-O2A-CGA
31	C1	501	CLA	C2-C1-O2A-CGA
31	Y1	602	CLA	C2-C1-O2A-CGA
31	Y1	610	CLA	C2-C1-O2A-CGA
31	y1	613	CLA	C2-C1-O2A-CGA
47	Y	606	CHL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
47	g	601	CHL	C2-C1-O2A-CGA
47	r	607	CHL	C2-C1-O2A-CGA
47	R1	607	CHL	C2-C1-O2A-CGA
34	A	412	SQD	C11-C10-C9-C8
31	c	502	CLA	C16-C17-C18-C20
31	g1	613	CLA	C16-C17-C18-C19
31	Y1	602	CLA	C5-C6-C7-C8
31	s1	602	CLA	C5-C6-C7-C8
41	N1	624	LHG	C24-C23-O8-C6
53	a1	414	SPH	C9-C10-C11-C12
54	k1	101	4RF	C33-C34-C35-C36
31	B	613	CLA	C3A-C2A-CAA-CBA
31	R	610	CLA	C3A-C2A-CAA-CBA
31	c	501	CLA	C3A-C2A-CAA-CBA
31	c	513	CLA	C3A-C2A-CAA-CBA
31	n	610	CLA	C3A-C2A-CAA-CBA
31	n	614	CLA	C3A-C2A-CAA-CBA
31	s	605	CLA	C3A-C2A-CAA-CBA
31	s	612	CLA	C3A-C2A-CAA-CBA
47	N	608	CHL	C3A-C2A-CAA-CBA
47	G1	601	CHL	C3A-C2A-CAA-CBA
47	G1	607	CHL	C3A-C2A-CAA-CBA
47	n1	607	CHL	C3A-C2A-CAA-CBA
52	S1	626	3PH	C3B-C3C-C3D-C3E
31	c	502	CLA	C2-C3-C5-C6
41	g	624	LHG	C10-C11-C12-C13
38	C1	524	DGA	CEB-CFB-CGB-CHB
31	y	604	CLA	C5-C6-C7-C8
47	s	601	CHL	CAA-CBA-CGA-O2A
40	C1	518	DGD	C9B-CAB-CBB-CCB
52	S1	626	3PH	C39-C3A-C3B-C3C
31	g1	611	CLA	C16-C17-C18-C20
35	h1	102	LMG	C29-C28-O8-C9
41	L	101	LHG	C26-C27-C28-C29
31	d1	402	CLA	CAA-CBA-CGA-O2A
35	H1	102	LMG	O7-C10-C11-C12
38	C1	524	DGA	CFB-CGB-CHB-CIB
41	G	630	LHG	C34-C35-C36-C37
35	b	622	LMG	C7-C8-O7-C10
42	c	627	LMK	C1-C2-C3-N4
57	Y1	626	PTY	C19-C20-C21-C22
53	Y	625	SPH	C4-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
53	a1	414	SPH	C4-C5-C6-C7
33	C1	517	BCR	C10-C11-C12-C13
33	c1	516	BCR	C10-C11-C12-C13
50	n	623	NEX	C30-C31-C32-C33
34	B	621	SQD	C11-C10-C9-C8
47	S	606	CHL	C2A-CAA-CBA-CGA
47	g	601	CHL	C5-C6-C7-C8
48	G	621	LUT	C9-C10-C11-C12
41	s1	624	LHG	C10-C11-C12-C13
31	s1	612	CLA	CAA-CBA-CGA-O1A
31	Y	602	CLA	C15-C16-C17-C18
47	n	607	CHL	C10-C11-C12-C13
41	D1	408	LHG	O2-C2-C3-O3
41	D	408	LHG	C10-C11-C12-C13
31	g	610	CLA	C2-C3-C5-C6
31	B	617	CLA	C15-C16-C17-C18
31	c	509	CLA	C5-C6-C7-C8
31	b1	602	CLA	C15-C16-C17-C18
49	r	622	XAT	O24-C26-C27-C28
49	y1	622	XAT	O24-C26-C27-C28
50	N	623	NEX	C12-C13-C14-C15
50	N	623	NEX	C28-C29-C30-C31
50	n	623	NEX	C28-C29-C30-C31
50	y1	623	NEX	O24-C26-C27-C28
31	n1	612	CLA	CAA-CBA-CGA-O2A
47	s	601	CHL	CAA-CBA-CGA-O1A
31	G	602	CLA	C10-C11-C12-C13
41	S1	624	LHG	C5-C4-O6-P
35	c1	523	LMG	C11-C12-C13-C14
40	c1	520	DGD	C4A-C5A-C6A-C7A
41	d1	409	LHG	C9-C10-C11-C12
31	n1	611	CLA	O2A-C1-C2-C3
47	g1	606	CHL	O2A-C1-C2-C3
41	d	409	LHG	C25-C26-C27-C28
41	C	525	LHG	C9-C10-C11-C12
41	d1	409	LHG	C31-C32-C33-C34
40	C1	518	DGD	O1G-C1G-C2G-C3G
52	i	101	3PH	C1-C2-C3-O31
52	t1	101	3PH	C1-C2-C3-O31
31	c1	512	CLA	C13-C15-C16-C17
41	d1	410	LHG	C24-C25-C26-C27
41	d	410	LHG	C34-C35-C36-C37

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Mol	Chain	Res	Type	Atoms
53	A1	414	SPH	C11-C10-C9-C8
47	s1	601	CHL	CAA-CBA-CGA-O1A
47	s1	601	CHL	CAA-CBA-CGA-O2A
35	B	622	LMG	C14-C15-C16-C17
35	J	101	LMG	C32-C33-C34-C35
35	j	101	LMG	C12-C13-C14-C15
40	c1	519	DGD	C2A-C3A-C4A-C5A
38	c1	524	DGA	CA1-CA2-CA3-CA4
52	s	626	3PH	C28-C29-C2A-C2B
31	B1	609	CLA	CBA-CGA-O2A-C1
54	k1	101	4RF	C09-C10-C11-C12
31	y	604	CLA	C4-C3-C5-C6
31	S1	614	CLA	C2A-CAA-CBA-CGA
31	n1	611	CLA	C2A-CAA-CBA-CGA
31	g1	611	CLA	C2A-CAA-CBA-CGA
47	N1	608	CHL	C2A-CAA-CBA-CGA
31	c1	505	CLA	CAA-CBA-CGA-O2A
41	g1	624	LHG	O8-C23-C24-C25
33	b1	618	BCR	C13-C14-C15-C16
48	N	621	LUT	C33-C34-C35-C15
49	r1	621	XAT	C29-C30-C31-C32
54	K1	101	4RF	C46-C47-C48-C49
31	b1	608	CLA	C16-C17-C18-C19
44	D1	405	PL9	C2-C3-C7-C8
52	s	626	3PH	C32-C33-C34-C35
31	R	610	CLA	C5-C6-C7-C8
31	C1	503	CLA	C15-C16-C17-C18
52	B1	624	3PH	C22-C23-C24-C25
31	n	602	CLA	CBA-CGA-O2A-C1
52	b1	624	3PH	C3D-C3E-C3F-C3G
31	s	611	CLA	CAA-CBA-CGA-O2A
31	y1	613	CLA	CAA-CBA-CGA-O2A
38	B1	625	DGA	OG2-CB1-CB2-CB3
41	n1	624	LHG	O7-C7-C8-C9
35	d1	411	LMG	C22-C23-C24-C25
35	B	622	LMG	C18-C19-C20-C21
41	Y	624	LHG	C33-C34-C35-C36
53	Y1	625	SPH	C10-C11-C12-C13
47	S1	608	CHL	C3-C5-C6-C7
34	A1	412	SQD	C10-C11-C12-C13
38	c1	524	DGA	CA3-CA4-CA5-CA6
40	c	519	DGD	C7B-C8B-C9B-CAB

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Mol	Chain	Res	Type	Atoms
52	t1	101	3PH	O21-C2-C3-O31
31	C1	501	CLA	O1A-CGA-O2A-C1
31	g1	603	CLA	C5-C6-C7-C8
31	C	503	CLA	C14-C13-C15-C16
31	N	610	CLA	C11-C12-C13-C14
31	b	605	CLA	C11-C12-C13-C14
31	b	616	CLA	C6-C7-C8-C9
31	y	602	CLA	C14-C13-C15-C16
31	B1	602	CLA	C14-C13-C15-C16
31	C1	512	CLA	C11-C10-C8-C9
31	N1	613	CLA	C14-C13-C15-C16
31	G1	602	CLA	C14-C13-C15-C16
31	S1	611	CLA	C6-C7-C8-C9
31	Y1	613	CLA	C6-C7-C8-C9
31	g1	610	CLA	C14-C13-C15-C16
47	y	607	CHL	C6-C7-C8-C9
31	b1	611	CLA	C16-C17-C18-C20
31	y	613	CLA	CAA-CBA-CGA-O2A
31	S1	610	CLA	CAA-CBA-CGA-O2A
57	y1	626	PTY	O4-C30-C31-C32
31	B	607	CLA	C15-C16-C17-C18
47	y	607	CHL	C13-C15-C16-C17
31	A1	405	CLA	CAA-CBA-CGA-O1A
41	n	624	LHG	O10-C23-C24-C25
41	Y	624	LHG	O6-C4-C5-C6
41	d1	410	LHG	O6-C4-C5-C6
52	s1	626	3PH	O11-C1-C2-C3
33	C1	514	BCR	C11-C12-C13-C14
42	c	627	LMK	C11-C10-O7-C8
41	L1	101	LHG	C29-C30-C31-C32
38	b	623	DGA	OG2-CB1-CB2-CB3
38	c	524	DGA	OG1-CA1-CA2-CA3
38	b1	625	DGA	OG2-CB1-CB2-CB3
34	A1	412	SQD	C26-C27-C28-C29
41	l	101	LHG	C29-C30-C31-C32
34	b1	626	SQD	C35-C36-C37-C38
34	m1	101	SQD	C28-C29-C30-C31
41	n	624	LHG	C19-C20-C21-C22
31	B	602	CLA	C6-C7-C8-C10
31	B	606	CLA	C11-C12-C13-C15
31	B	610	CLA	C6-C7-C8-C10
31	B	613	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
31	B	616	CLA	C6-C7-C8-C10
31	C	506	CLA	C11-C12-C13-C15
31	C	512	CLA	C11-C12-C13-C15
31	N	602	CLA	C12-C13-C15-C16
31	N	613	CLA	C12-C13-C15-C16
31	R	608	CLA	C11-C10-C8-C7
31	Y	602	CLA	C12-C13-C15-C16
31	b	606	CLA	C11-C12-C13-C15
31	b	613	CLA	C6-C7-C8-C10
31	c	505	CLA	C11-C10-C8-C7
31	c	507	CLA	C6-C7-C8-C10
31	n	602	CLA	C11-C10-C8-C7
31	n	604	CLA	C6-C7-C8-C10
31	r	610	CLA	C11-C10-C8-C7
31	y	602	CLA	C11-C12-C13-C15
31	B1	611	CLA	C11-C10-C8-C7
31	B1	613	CLA	C12-C13-C15-C16
31	B1	615	CLA	C6-C7-C8-C10
31	C1	512	CLA	C12-C13-C15-C16
31	N1	604	CLA	C6-C7-C8-C10
31	R1	602	CLA	C6-C7-C8-C10
31	S1	602	CLA	C6-C7-C8-C10
31	S1	602	CLA	C11-C10-C8-C7
31	Y1	603	CLA	C11-C10-C8-C7
31	b1	605	CLA	C12-C13-C15-C16
31	b1	613	CLA	C12-C13-C15-C16
31	b1	614	CLA	C6-C7-C8-C10
31	c1	511	CLA	C6-C7-C8-C10
31	n1	610	CLA	C6-C7-C8-C10
31	g1	610	CLA	C6-C7-C8-C10
31	g1	613	CLA	C12-C13-C15-C16
31	y1	603	CLA	C11-C10-C8-C7
32	a	408	PHO	C11-C12-C13-C15
47	n	605	CHL	C11-C10-C8-C7
47	y	609	CHL	C11-C12-C13-C15
47	y1	606	CHL	C6-C7-C8-C10
41	d	410	LHG	C29-C30-C31-C32
31	B1	609	CLA	O1A-CGA-O2A-C1
31	C	508	CLA	C3-C5-C6-C7
31	s	609	CLA	C3-C5-C6-C7
31	A	410	CLA	C2B-C3B-CAB-CBB
31	B	606	CLA	C2B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	C	504	CLA	C2B-C3B-CAB-CBB
31	N	613	CLA	C2B-C3B-CAB-CBB
31	S	602	CLA	C2B-C3B-CAB-CBB
31	S	614	CLA	C2B-C3B-CAB-CBB
31	b	610	CLA	C2B-C3B-CAB-CBB
31	b	616	CLA	C2B-C3B-CAB-CBB
31	c	507	CLA	C2B-C3B-CAB-CBB
31	n	614	CLA	C2B-C3B-CAB-CBB
31	g	614	CLA	C2B-C3B-CAB-CBB
31	r	613	CLA	C2B-C3B-CAB-CBB
31	s	603	CLA	C2B-C3B-CAB-CBB
31	s	617	CLA	C2B-C3B-CAB-CBB
31	y	613	CLA	C2B-C3B-CAB-CBB
31	B1	608	CLA	C2B-C3B-CAB-CBB
31	B1	609	CLA	C2B-C3B-CAB-CBB
31	B1	613	CLA	C2B-C3B-CAB-CBB
31	B1	615	CLA	C2B-C3B-CAB-CBB
31	C1	505	CLA	C2B-C3B-CAB-CBB
31	C1	506	CLA	C2B-C3B-CAB-CBB
31	G1	610	CLA	C2B-C3B-CAB-CBB
31	R1	602	CLA	C2B-C3B-CAB-CBB
31	R1	608	CLA	C2B-C3B-CAB-CBB
31	Y1	602	CLA	C2B-C3B-CAB-CBB
31	b1	617	CLA	C2B-C3B-CAB-CBB
31	c1	502	CLA	C2B-C3B-CAB-CBB
31	c1	506	CLA	C2B-C3B-CAB-CBB
31	c1	507	CLA	C2B-C3B-CAB-CBB
31	n1	602	CLA	C2B-C3B-CAB-CBB
31	g1	604	CLA	C2B-C3B-CAB-CBB
31	g1	613	CLA	C2B-C3B-CAB-CBB
31	r1	602	CLA	C2B-C3B-CAB-CBB
31	r1	604	CLA	C2B-C3B-CAB-CBB
31	s1	614	CLA	C2B-C3B-CAB-CBB
31	s1	617	CLA	C2B-C3B-CAB-CBB
31	y1	608	CLA	C2B-C3B-CAB-CBB
31	y1	611	CLA	C2B-C3B-CAB-CBB
33	B	618	BCR	C23-C24-C25-C26
33	c	515	BCR	C23-C24-C25-C30
33	d	404	BCR	C23-C24-C25-C26
37	B	620	C7Z	C21-C26-C27-C28
37	B1	620	C7Z	C25-C26-C27-C28
48	R	620	LUT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
48	Y	620	LUT	C5-C6-C7-C8
48	n	620	LUT	C5-C6-C7-C8
48	r	620	LUT	C1-C6-C7-C8
48	r	620	LUT	C5-C6-C7-C8
48	N1	621	LUT	C5-C6-C7-C8
48	G1	621	LUT	C5-C6-C7-C8
48	S1	620	LUT	C5-C6-C7-C8
48	y1	621	LUT	C1-C6-C7-C8
48	y1	621	LUT	C5-C6-C7-C8
38	b	623	DGA	CCB-CDB-CEB-CFB
34	C1	526	SQD	C8-C7-O47-C45
40	C1	520	DGD	O2G-C1B-C2B-C3B
35	A1	413	LMG	C4-C5-C6-O5
35	D	411	LMG	C14-C15-C16-C17
35	H	102	LMG	C16-C17-C18-C19
40	B1	623	DGD	C3A-C4A-C5A-C6A
41	n1	624	LHG	C30-C31-C32-C33
51	S	625	LPX	C7-C8-C9-C10
31	B	610	CLA	C2-C1-O2A-CGA
31	Y	604	CLA	C2-C1-O2A-CGA
31	c	512	CLA	C2-C1-O2A-CGA
31	b1	602	CLA	C2-C1-O2A-CGA
31	s1	609	CLA	C2-C1-O2A-CGA
32	A	409	PHO	C2-C1-O2A-CGA
31	N	611	CLA	O2A-C1-C2-C3
34	b	621	SQD	C29-C30-C31-C32
38	c	524	DGA	CEA-CFA-CGA-CHA
52	s	626	3PH	C38-C39-C3A-C3B
49	R	621	XAT	C26-C27-C28-C29
49	G1	622	XAT	C26-C27-C28-C29
41	d1	408	LHG	C35-C36-C37-C38
40	c	519	DGD	CCB-CDB-CEB-CFB
31	S1	602	CLA	C3-C5-C6-C7
44	d	405	PL9	C24-C26-C27-C28
34	c1	526	SQD	O47-C7-C8-C9
35	J	101	LMG	O7-C10-C11-C12
41	N	624	LHG	O8-C23-C24-C25
47	n1	605	CHL	CAA-CBA-CGA-O2A
31	c	501	CLA	C13-C15-C16-C17
42	c1	527	LMK	C10-C11-C12-C13
41	n1	624	LHG	C31-C32-C33-C34
47	g1	605	CHL	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
31	b1	603	CLA	C3-C5-C6-C7
31	A	405	CLA	CAA-CBA-CGA-O2A
31	b	603	CLA	CAA-CBA-CGA-O2A
31	n	613	CLA	CAA-CBA-CGA-O2A
31	r1	612	CLA	CAA-CBA-CGA-O2A
41	D1	409	LHG	O7-C7-C8-C9
51	s1	625	LPX	O6-C6-C7-C8
31	s1	610	CLA	C2-C3-C5-C6
44	D	405	PL9	C28-C29-C31-C32
31	b1	609	CLA	C10-C11-C12-C13
31	n1	613	CLA	C8-C10-C11-C12
41	D	410	LHG	O2-C2-C3-O3
31	B	613	CLA	C2A-CAA-CBA-CGA
31	b	603	CLA	C2A-CAA-CBA-CGA
41	l	101	LHG	C8-C7-O7-C5
41	L1	101	LHG	C9-C10-C11-C12
41	n1	624	LHG	C11-C10-C9-C8
31	B	616	CLA	C13-C15-C16-C17
31	Y1	612	CLA	C15-C16-C17-C18
35	W1	201	LMG	O7-C10-C11-C12
41	d	410	LHG	O8-C23-C24-C25
52	s1	626	3PH	C22-C23-C24-C25
31	c1	512	CLA	C16-C17-C18-C20
41	d1	409	LHG	C26-C27-C28-C29
31	b1	616	CLA	C10-C11-C12-C13
31	g1	613	CLA	C10-C11-C12-C13
31	B	602	CLA	CAA-CBA-CGA-O2A
31	Y	613	CLA	CAA-CBA-CGA-O2A
31	b	608	CLA	CAA-CBA-CGA-O2A
31	B1	603	CLA	CAA-CBA-CGA-O2A
31	B1	615	CLA	CAA-CBA-CGA-O2A
32	A1	409	PHO	CAA-CBA-CGA-O2A
35	j	101	LMG	O7-C10-C11-C12
38	C1	524	DGA	OG2-CB1-CB2-CB3
54	I1	102	4RF	O40-C41-C43-C44
31	d1	402	CLA	C3-C5-C6-C7
34	b	621	SQD	C4-C5-C6-S
34	C1	526	SQD	C4-C5-C6-S
34	b1	621	SQD	C4-C5-C6-S
34	c1	526	SQD	C4-C5-C6-S
34	m1	101	SQD	C4-C5-C6-S
35	A1	413	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
35	C1	521	LMG	C12-C13-C14-C15
35	b1	622	LMG	C14-C15-C16-C17
31	b1	607	CLA	C4-C3-C5-C6
31	c1	513	CLA	C4-C3-C5-C6
44	D1	405	PL9	C12-C11-C9-C10
41	s1	624	LHG	C7-C8-C9-C10
41	L	101	LHG	C17-C18-C19-C20
31	G	614	CLA	CAA-CBA-CGA-O2A
31	r	610	CLA	CAA-CBA-CGA-O2A
31	R1	604	CLA	CAA-CBA-CGA-O2A
38	b1	625	DGA	OG1-CA1-CA2-CA3
52	B1	624	3PH	O31-C31-C32-C33
31	b	610	CLA	C2-C3-C5-C6
41	d1	409	LHG	C29-C30-C31-C32
40	c	520	DGD	O6D-C5D-C6D-O5D
31	r1	608	CLA	C2A-CAA-CBA-CGA
47	G	606	CHL	C2A-CAA-CBA-CGA
47	Y	609	CHL	C2A-CAA-CBA-CGA
35	C1	523	LMG	C31-C32-C33-C34
52	s	626	3PH	C2E-C2F-C2G-C2H
31	n1	612	CLA	CAA-CBA-CGA-O1A
31	Y	613	CLA	C10-C11-C12-C13
31	B	608	CLA	CAA-CBA-CGA-O2A
31	Y1	613	CLA	CAA-CBA-CGA-O2A
31	g1	603	CLA	CAA-CBA-CGA-O2A
35	W1	201	LMG	O8-C28-C29-C30
41	D	408	LHG	O7-C7-C8-C9
40	C1	519	DGD	C2B-C3B-C4B-C5B
35	C1	521	LMG	O9-C10-C11-C12
31	Y	610	CLA	C10-C11-C12-C13
40	c1	520	DGD	O6D-C5D-C6D-O5D
34	a1	412	SQD	C14-C15-C16-C17
35	C	521	LMG	C30-C31-C32-C33
38	b	623	DGA	CB4-CB5-CB6-CB7
40	c1	520	DGD	C3A-C4A-C5A-C6A
31	B	607	CLA	C11-C10-C8-C9
31	B	607	CLA	C14-C13-C15-C16
31	B	613	CLA	C11-C12-C13-C14
31	R	609	CLA	C11-C10-C8-C9
31	c	501	CLA	C6-C7-C8-C9
31	B1	605	CLA	C14-C13-C15-C16
31	N1	603	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
47	Y	609	CHL	C11-C12-C13-C14
47	n	606	CHL	C11-C12-C13-C14
47	G1	607	CHL	C11-C12-C13-C14
47	n1	605	CHL	C14-C13-C15-C16
47	g1	607	CHL	C11-C10-C8-C9
47	s1	608	CHL	C11-C10-C8-C9
47	y1	607	CHL	C11-C10-C8-C9
40	c	518	DGD	CCB-CDB-CEB-CFB
52	s	626	3PH	C3C-C3D-C3E-C3F
41	L	101	LHG	C2-C3-O3-P
41	N1	624	LHG	C2-C3-O3-P
52	T1	101	3PH	C2-C1-O11-P
31	c	503	CLA	CAA-CBA-CGA-O2A
31	C1	503	CLA	CAA-CBA-CGA-O2A
31	c1	503	CLA	CAA-CBA-CGA-O2A
35	c	521	LMG	O7-C10-C11-C12
41	y	624	LHG	O8-C23-C24-C25
41	S1	624	LHG	O8-C23-C24-C25
34	C1	526	SQD	O10-C23-O48-C46
35	h	102	LMG	O10-C28-O8-C9
41	n	624	LHG	C4-C5-C6-O8
54	I1	102	4RF	O18-C19-C20-C39
40	C	518	DGD	C4D-C5D-C6D-O5D
34	a1	412	SQD	C15-C16-C17-C18
31	Y	613	CLA	C13-C15-C16-C17
31	b1	609	CLA	C5-C6-C7-C8
31	c1	512	CLA	C15-C16-C17-C18
31	B	617	CLA	C1A-C2A-CAA-CBA
31	N	604	CLA	C1A-C2A-CAA-CBA
31	N	604	CLA	C4B-C3B-CAB-CBB
31	N	613	CLA	C4B-C3B-CAB-CBB
31	S	617	CLA	C4B-C3B-CAB-CBB
31	Y	608	CLA	C1A-C2A-CAA-CBA
31	b	616	CLA	C1A-C2A-CAA-CBA
31	c	510	CLA	C4B-C3B-CAB-CBB
31	d	402	CLA	C4B-C3B-CAB-CBB
31	g	610	CLA	C4B-C3B-CAB-CBB
31	s	612	CLA	C1A-C2A-CAA-CBA
31	s	614	CLA	C1A-C2A-CAA-CBA
31	y	613	CLA	C4B-C3B-CAB-CBB
31	R1	603	CLA	C1A-C2A-CAA-CBA
31	c1	502	CLA	C4B-C3B-CAB-CBB

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Mol	Chain	Res	Type	Atoms
31	n1	602	CLA	C4B-C3B-CAB-CBB
31	s1	602	CLA	C4B-C3B-CAB-CBB
31	s1	614	CLA	C1A-C2A-CAA-CBA
31	s1	617	CLA	C4B-C3B-CAB-CBB
31	y1	602	CLA	C1A-C2A-CAA-CBA
38	B	625	DGA	CDB-CEB-CFB-CGB
41	s	624	LHG	C24-C25-C26-C27
41	d1	409	LHG	C15-C16-C17-C18
31	S1	611	CLA	CBA-CGA-O2A-C1
31	Y	603	CLA	C4-C3-C5-C6
31	n	610	CLA	C4-C3-C5-C6
31	s	610	CLA	C4-C3-C5-C6
31	n1	613	CLA	C4-C3-C5-C6
55	R1	625	LMT	C9-C10-C11-C12
31	B	609	CLA	CAA-CBA-CGA-O2A
31	B	612	CLA	CAA-CBA-CGA-O2A
31	N	604	CLA	CAA-CBA-CGA-O2A
31	B1	608	CLA	CAA-CBA-CGA-O2A
31	C1	512	CLA	CAA-CBA-CGA-O2A
34	a1	412	SQD	O47-C7-C8-C9
35	d	411	LMG	O7-C10-C11-C12
41	Y	624	LHG	O8-C23-C24-C25
52	s1	626	3PH	O21-C21-C22-C23
31	B	616	CLA	C2-C3-C5-C6
31	c	504	CLA	C2-C3-C5-C6
31	y	602	CLA	C2-C3-C5-C6
35	H1	102	LMG	O7-C8-C9-O8
40	C	519	DGD	O2G-C2G-C3G-O3G
34	a	412	SQD	C32-C33-C34-C35
33	C	516	BCR	C11-C12-C13-C14
33	A1	411	BCR	C11-C12-C13-C14
33	B1	618	BCR	C7-C8-C9-C10
48	g	620	LUT	C27-C28-C29-C30
49	R	621	XAT	C31-C32-C33-C34
33	c1	514	BCR	C15-C16-C17-C18
48	n	621	LUT	C9-C10-C11-C12
41	N1	624	LHG	O10-C23-O8-C6
38	b1	625	DGA	CA7-CA8-CA9-CAA
35	C1	523	LMG	C11-C12-C13-C14
34	C1	526	SQD	C24-C23-O48-C46
31	R	610	CLA	CAA-CBA-CGA-O2A
31	s	614	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	C1	505	CLA	CAA-CBA-CGA-O2A
31	G1	603	CLA	CAA-CBA-CGA-O2A
31	b1	610	CLA	CAA-CBA-CGA-O2A
31	b1	613	CLA	CAA-CBA-CGA-O2A
38	C	524	DGA	OG1-CA1-CA2-CA3
40	C1	518	DGD	O1G-C1A-C2A-C3A
41	D	410	LHG	O8-C23-C24-C25
41	N1	624	LHG	O7-C7-C8-C9
41	y1	624	LHG	O8-C23-C24-C25
52	S1	626	3PH	O21-C21-C22-C23
38	C	524	DGA	CEA-CFA-CGA-CHA
41	n1	624	LHG	C18-C19-C20-C21
41	n1	624	LHG	C19-C20-C21-C22
31	G1	602	CLA	C2A-CAA-CBA-CGA
35	b	622	LMG	C21-C22-C23-C24
40	C	519	DGD	C5A-C6A-C7A-C8A
42	C1	527	LMK	C2-C3-C4-O3
47	n	609	CHL	C2C-C3C-CAC-CBC
35	c	521	LMG	C32-C33-C34-C35
34	B1	626	SQD	C28-C29-C30-C31
34	m1	101	SQD	C10-C11-C12-C13
31	B	612	CLA	C16-C17-C18-C20
31	C	503	CLA	CAA-CBA-CGA-O2A
31	b1	608	CLA	CAA-CBA-CGA-O2A
31	c1	508	CLA	CAA-CBA-CGA-O2A
35	c1	523	LMG	O7-C10-C11-C12
47	G1	607	CHL	CAA-CBA-CGA-O2A
41	D	408	LHG	C27-C28-C29-C30
34	B	621	SQD	C17-C18-C19-C20
31	Y	604	CLA	C13-C15-C16-C17
31	C1	510	CLA	C13-C15-C16-C17
31	B	604	CLA	C4-C3-C5-C6
31	B1	610	CLA	C2-C1-O2A-CGA
31	B1	612	CLA	C2-C1-O2A-CGA
31	b1	606	CLA	C2-C1-O2A-CGA
31	c1	505	CLA	C2-C1-O2A-CGA
31	c1	513	CLA	C2-C1-O2A-CGA
47	G	609	CHL	C2-C1-O2A-CGA
47	N1	609	CHL	C2-C1-O2A-CGA
47	g1	601	CHL	C2-C1-O2A-CGA
31	b1	615	CLA	CAA-CBA-CGA-O2A
31	B	607	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
31	B	613	CLA	C12-C13-C15-C16
31	B	616	CLA	C12-C13-C15-C16
31	S	611	CLA	C11-C10-C8-C7
31	Y	603	CLA	C11-C12-C13-C15
31	b	604	CLA	C12-C13-C15-C16
31	b	613	CLA	C11-C12-C13-C15
31	c	505	CLA	C12-C13-C15-C16
31	s	611	CLA	C6-C7-C8-C10
31	s	611	CLA	C12-C13-C15-C16
31	y	602	CLA	C11-C10-C8-C7
31	y	613	CLA	C11-C12-C13-C15
31	Y1	602	CLA	C11-C10-C8-C7
31	Y1	603	CLA	C6-C7-C8-C10
31	a1	406	CLA	C11-C10-C8-C7
31	b1	605	CLA	C11-C10-C8-C7
31	b1	613	CLA	C11-C12-C13-C15
31	b1	615	CLA	C11-C12-C13-C15
31	b1	617	CLA	C12-C13-C15-C16
31	c1	506	CLA	C11-C10-C8-C7
31	c1	507	CLA	C11-C12-C13-C15
31	c1	512	CLA	C11-C12-C13-C15
31	r1	608	CLA	C11-C10-C8-C7
31	r1	612	CLA	C6-C7-C8-C10
32	a1	408	PHO	C6-C7-C8-C10
47	N1	606	CHL	C12-C13-C15-C16
47	g1	607	CHL	C11-C10-C8-C7
47	y1	607	CHL	C12-C13-C15-C16
31	n1	613	CLA	CBA-CGA-O2A-C1
31	c	511	CLA	C2-C3-C5-C6
31	b1	603	CLA	C8-C10-C11-C12
34	C1	526	SQD	C12-C13-C14-C15
53	y	625	SPH	C13-C14-C15-C16
54	k1	101	4RF	C08-C09-C10-C11
52	S1	626	3PH	C3F-C3G-C3H-C3I
47	G	609	CHL	C2C-C3C-CAC-CBC
35	a1	413	LMG	C33-C34-C35-C36
52	S1	626	3PH	C28-C29-C2A-C2B
40	B1	623	DGD	C1G-C2G-O2G-C1B
40	b1	623	DGD	C3G-C2G-O2G-C1B
47	S1	606	CHL	C2A-CAA-CBA-CGA
31	s1	614	CLA	CAA-CBA-CGA-O2A
40	c1	518	DGD	C4A-C5A-C6A-C7A

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Mol	Chain	Res	Type	Atoms
41	y	624	LHG	C9-C10-C11-C12
53	Y	625	SPH	C12-C13-C14-C15
57	y1	626	PTY	C21-C22-C23-C24
31	B	611	CLA	C8-C10-C11-C12
41	G	630	LHG	C35-C36-C37-C38
41	s	624	LHG	C35-C36-C37-C38
33	b1	619	BCR	C9-C10-C11-C12
46	h	101	RRX	C13-C14-C15-C16
48	N1	621	LUT	C29-C30-C31-C32
31	s1	603	CLA	C2A-CAA-CBA-CGA
31	s1	610	CLA	C2A-CAA-CBA-CGA
56	r1	626	ERG	C22-C23-C24-C25
31	g1	614	CLA	O2A-C1-C2-C3
35	b	622	LMG	C15-C16-C17-C18
31	B1	615	CLA	C8-C10-C11-C12
31	c1	511	CLA	C13-C15-C16-C17
41	n1	624	LHG	C24-C25-C26-C27
31	B	603	CLA	CAA-CBA-CGA-O2A
52	s	626	3PH	O21-C21-C22-C23
41	D	409	LHG	C35-C36-C37-C38
41	d	408	LHG	C35-C36-C37-C38
31	y1	613	CLA	CAA-CBA-CGA-O1A
34	B1	626	SQD	C27-C28-C29-C30
34	b	621	SQD	C11-C10-C9-C8
41	N1	624	LHG	C16-C17-C18-C19
31	C	511	CLA	C4-C3-C5-C6
31	b	607	CLA	C3A-C2A-CAA-CBA
31	R1	604	CLA	CAA-CBA-CGA-O1A
35	J	101	LMG	O9-C10-C11-C12
35	j	101	LMG	O9-C10-C11-C12
31	g	613	CLA	C5-C6-C7-C8
31	y	613	CLA	C16-C17-C18-C19
40	C	520	DGD	O6D-C5D-C6D-O5D
41	g	624	LHG	C27-C28-C29-C30
31	S	617	CLA	CAA-CBA-CGA-O2A
31	b	602	CLA	CAA-CBA-CGA-O2A
31	b	612	CLA	CAA-CBA-CGA-O2A
31	n	604	CLA	CAA-CBA-CGA-O2A
31	n	611	CLA	CAA-CBA-CGA-O2A
31	g1	613	CLA	CAA-CBA-CGA-O2A
40	c1	518	DGD	O1G-C1A-C2A-C3A
41	d1	408	LHG	O7-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
31	r	608	CLA	C2-C3-C5-C6
31	n1	613	CLA	C2-C3-C5-C6
50	n	623	NEX	C11-C10-C9-C8
50	n1	623	NEX	C12-C13-C14-C15
31	r1	609	CLA	C10-C11-C12-C13
31	r	610	CLA	CAA-CBA-CGA-O1A
31	S1	610	CLA	CAA-CBA-CGA-O1A
34	C	526	SQD	C11-C12-C13-C14
38	C1	524	DGA	CA8-CA9-CAA-CBA
31	s	609	CLA	C8-C10-C11-C12
35	H1	102	LMG	O6-C1-O1-C7
31	g	614	CLA	CAA-CBA-CGA-O2A
31	G1	614	CLA	CAA-CBA-CGA-O2A
31	b1	609	CLA	CAA-CBA-CGA-O2A
47	g1	605	CHL	CAA-CBA-CGA-O2A
53	y	625	SPH	C4-C5-C6-C7
31	r1	612	CLA	CAA-CBA-CGA-O1A
34	m1	101	SQD	O49-C7-C8-C9
38	c	524	DGA	OA1-CA1-CA2-CA3
38	B1	625	DGA	OB1-CB1-CB2-CB3
38	b1	625	DGA	OB1-CB1-CB2-CB3
54	I1	102	4RF	O42-C41-C43-C44
38	b1	625	DGA	CA2-CA3-CA4-CA5
41	G	630	LHG	C32-C33-C34-C35
41	D1	408	LHG	C35-C36-C37-C38
31	B	610	CLA	C6-C7-C8-C9
31	B	614	CLA	C11-C12-C13-C14
31	C	508	CLA	C14-C13-C15-C16
31	R	608	CLA	C11-C10-C8-C9
31	R	610	CLA	C6-C7-C8-C9
31	Y	604	CLA	C6-C7-C8-C9
31	Y	610	CLA	C6-C7-C8-C9
31	b	604	CLA	C11-C12-C13-C14
31	b	607	CLA	C11-C12-C13-C14
31	c	507	CLA	C11-C12-C13-C14
31	d	402	CLA	C11-C10-C8-C9
31	s	610	CLA	C6-C7-C8-C9
31	y	611	CLA	C11-C10-C8-C9
31	C1	510	CLA	C6-C7-C8-C9
31	G1	611	CLA	C6-C7-C8-C9
31	S1	602	CLA	C6-C7-C8-C9
31	Y1	602	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
31	b1	604	CLA	C6-C7-C8-C9
31	b1	605	CLA	C14-C13-C15-C16
31	c1	507	CLA	C6-C7-C8-C9
31	n1	602	CLA	C11-C12-C13-C14
31	s1	610	CLA	C6-C7-C8-C9
31	s1	611	CLA	C11-C12-C13-C14
47	y	609	CHL	C14-C13-C15-C16
47	n1	606	CHL	C11-C10-C8-C9
41	n	624	LHG	C33-C34-C35-C36
31	A	405	CLA	CAA-CBA-CGA-O1A
31	B	602	CLA	CAA-CBA-CGA-O1A
31	y	613	CLA	CAA-CBA-CGA-O1A
32	A1	409	PHO	CAA-CBA-CGA-O1A
35	H	102	LMG	O9-C10-C11-C12
31	B	610	CLA	C5-C6-C7-C8
31	S	610	CLA	C10-C11-C12-C13
34	A	412	SQD	C10-C11-C12-C13
41	d	410	LHG	O2-C2-C3-O3
34	A	412	SQD	C27-C28-C29-C30
31	C	513	CLA	C13-C15-C16-C17
31	N1	610	CLA	C8-C10-C11-C12
31	R	609	CLA	CAA-CBA-CGA-O1A
31	R	610	CLA	CAA-CBA-CGA-O1A
31	B1	615	CLA	CAA-CBA-CGA-O1A
40	C1	520	DGD	O1B-C1B-C2B-C3B
41	D	408	LHG	O9-C7-C8-C9
41	L	101	LHG	O9-C7-C8-C9
41	d	410	LHG	O10-C23-C24-C25
47	g1	608	CHL	C2A-CAA-CBA-CGA
57	Y1	626	PTY	C15-C16-C17-C18
35	C1	523	LMG	O7-C10-C11-C12
44	D	405	PL9	C18-C19-C21-C22
47	G1	601	CHL	C2-C3-C5-C6
31	y1	603	CLA	C8-C10-C11-C12
34	b	621	SQD	O5-C5-C6-S
34	B1	621	SQD	O5-C5-C6-S
34	C1	526	SQD	O5-C5-C6-S
34	c1	526	SQD	O5-C5-C6-S
42	c	627	LMK	O10-C28-O8-C9
48	g	621	LUT	C21-C26-C27-C28
31	C1	512	CLA	CAA-CBA-CGA-O1A
34	c1	526	SQD	O49-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
51	s1	625	LPX	O7-C6-C7-C8
57	y1	626	PTY	O30-C30-C31-C32
57	y1	626	PTY	C24-C25-C26-C27
31	B1	607	CLA	C13-C15-C16-C17
40	c	523	DGD	C4D-C5D-C6D-O5D
40	C	519	DGD	CDB-CEB-CFB-CGB
47	R	607	CHL	CAA-CBA-CGA-O2A
47	n	607	CHL	C15-C16-C17-C18
37	B	620	C7Z	C11-C12-C13-C14
48	g	621	LUT	C27-C28-C29-C30
31	c1	505	CLA	CAA-CBA-CGA-O1A
31	g1	603	CLA	CAA-CBA-CGA-O1A
41	y	624	LHG	O10-C23-C24-C25
41	D1	409	LHG	O9-C7-C8-C9
41	n1	624	LHG	O10-C23-C24-C25
47	n1	605	CHL	CAA-CBA-CGA-O1A
42	C	527	LMK	C30-C31-C32-C33
31	b	609	CLA	C10-C11-C12-C13
35	d	411	LMG	C8-C7-O1-C1
35	A1	413	LMG	C8-C7-O1-C1
38	C1	524	DGA	OG1-CG1-CG2-OG2
52	b1	624	3PH	C3E-C3F-C3G-C3H
31	c	503	CLA	CAA-CBA-CGA-O1A
31	B1	603	CLA	CAA-CBA-CGA-O1A
31	c1	503	CLA	CAA-CBA-CGA-O1A
34	a1	412	SQD	O49-C7-C8-C9
35	c	521	LMG	O9-C10-C11-C12
35	d	411	LMG	O9-C10-C11-C12
35	c1	523	LMG	O9-C10-C11-C12
38	b	623	DGA	OB1-CB1-CB2-CB3
38	C1	524	DGA	OB1-CB1-CB2-CB3
41	n1	624	LHG	O9-C7-C8-C9
31	B	607	CLA	CAA-CBA-CGA-O2A
31	g	613	CLA	CAA-CBA-CGA-O2A
31	b1	602	CLA	CAA-CBA-CGA-O2A
40	c1	518	DGD	O2G-C1B-C2B-C3B
31	G	610	CLA	C8-C10-C11-C12
31	b1	611	CLA	C5-C6-C7-C8
31	G1	603	CLA	C2A-CAA-CBA-CGA
35	A	413	LMG	C34-C35-C36-C37
35	D1	411	LMG	C11-C12-C13-C14
31	b	602	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
31	c1	502	CLA	C16-C17-C18-C19
31	s1	610	CLA	C16-C17-C18-C19
31	N1	610	CLA	C5-C6-C7-C8
31	c1	505	CLA	C8-C10-C11-C12
31	B	603	CLA	CAA-CBA-CGA-O1A
31	B	608	CLA	CAA-CBA-CGA-O1A
31	Y	613	CLA	CAA-CBA-CGA-O1A
31	C1	503	CLA	CAA-CBA-CGA-O1A
38	b1	625	DGA	OA1-CA1-CA2-CA3
41	S1	624	LHG	O10-C23-C24-C25
41	y1	624	LHG	O10-C23-C24-C25
41	S1	624	LHG	C33-C34-C35-C36
31	B	608	CLA	C15-C16-C17-C18
31	B1	602	CLA	C8-C10-C11-C12
31	Y1	604	CLA	C10-C11-C12-C13
32	a	409	PHO	C10-C11-C12-C13
31	b	610	CLA	CAA-CBA-CGA-O2A
31	A1	406	CLA	CAA-CBA-CGA-O2A
34	B1	621	SQD	O47-C7-C8-C9
38	B	625	DGA	OG2-CB1-CB2-CB3
41	G	630	LHG	O8-C23-C24-C25
31	y1	614	CLA	C2-C3-C5-C6
47	N	605	CHL	C15-C16-C17-C18
33	B1	619	BCR	C9-C10-C11-C12
31	B1	608	CLA	CAA-CBA-CGA-O1A
31	G1	603	CLA	CAA-CBA-CGA-O1A
31	Y1	613	CLA	CAA-CBA-CGA-O1A
31	b1	615	CLA	CAA-CBA-CGA-O1A
35	W1	201	LMG	O9-C10-C11-C12
34	m1	101	SQD	C23-C24-C25-C26
31	A	410	CLA	CAD-CBD-CGD-O2D
31	C	504	CLA	CAD-CBD-CGD-O2D
31	N	603	CLA	CAD-CBD-CGD-O2D
31	y	614	CLA	CAD-CBD-CGD-O2D
31	B1	613	CLA	CAD-CBD-CGD-O2D
31	c1	511	CLA	CAD-CBD-CGD-O2D
31	n1	602	CLA	CAD-CBD-CGD-O2D
47	S	607	CHL	C1A-C2A-CAA-CBA
47	S1	606	CHL	CAD-CBD-CGD-O2D
47	g1	606	CHL	CAD-CBD-CGD-O2D
47	g1	609	CHL	CAD-CBD-CGD-O2D
31	R	608	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
31	C	513	CLA	CAA-CBA-CGA-O2A
31	b	617	CLA	CAA-CBA-CGA-O2A
31	B1	607	CLA	CAA-CBA-CGA-O2A
41	D1	408	LHG	O8-C23-C24-C25
47	g1	606	CHL	CAA-CBA-CGA-O2A
47	G	609	CHL	C3-C5-C6-C7
31	N	604	CLA	CAA-CBA-CGA-O1A
31	s	614	CLA	CAA-CBA-CGA-O1A
31	b1	608	CLA	CAA-CBA-CGA-O1A
31	b1	610	CLA	CAA-CBA-CGA-O1A
35	W1	201	LMG	O10-C28-C29-C30
41	Y	624	LHG	O10-C23-C24-C25
52	B1	624	3PH	O32-C31-C32-C33
31	d	402	CLA	C5-C6-C7-C8
31	s	613	CLA	C5-C6-C7-C8
31	b1	617	CLA	C13-C15-C16-C17
38	c	524	DGA	OA1-CA1-OG1-CG1
35	A	413	LMG	C11-C12-C13-C14
38	B1	625	DGA	CCB-CDB-CEB-CFB
32	a	408	PHO	C10-C11-C12-C13
31	S	610	CLA	C2-C1-O2A-CGA
31	S	613	CLA	C2-C1-O2A-CGA
31	d1	403	CLA	C2-C1-O2A-CGA
31	g1	614	CLA	C2-C1-O2A-CGA
31	s1	604	CLA	C2-C1-O2A-CGA
47	N	609	CHL	C2-C1-O2A-CGA
47	n	607	CHL	C2-C1-O2A-CGA
47	n	608	CHL	C2-C1-O2A-CGA
47	G1	606	CHL	C2-C1-O2A-CGA
31	G	614	CLA	CAA-CBA-CGA-O1A
31	b	603	CLA	CAA-CBA-CGA-O1A
31	c1	508	CLA	CAA-CBA-CGA-O1A
38	C	524	DGA	OA1-CA1-CA2-CA3
41	D	410	LHG	O10-C23-C24-C25
31	B	605	CLA	CAA-CBA-CGA-O2A
31	D	402	CLA	CAA-CBA-CGA-O2A
31	C1	513	CLA	CAA-CBA-CGA-O2A
31	c1	502	CLA	CAA-CBA-CGA-O2A
35	C	521	LMG	O7-C10-C11-C12
35	h	102	LMG	O7-C10-C11-C12
32	a1	409	PHO	C1A-C2A-CAA-CBA
31	C	505	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
31	c1	511	CLA	C16-C17-C18-C20
35	b1	622	LMG	C19-C20-C21-C22
41	y	624	LHG	C31-C32-C33-C34
31	C	509	CLA	C2A-CAA-CBA-CGA
32	A	409	PHO	C2A-CAA-CBA-CGA
41	N	624	LHG	C29-C30-C31-C32
31	g	611	CLA	CAA-CBA-CGA-O2A
40	c	518	DGD	C2B-C3B-C4B-C5B
31	B	612	CLA	CAA-CBA-CGA-O1A
31	b	608	CLA	CAA-CBA-CGA-O1A
31	r	602	CLA	C5-C6-C7-C8
54	i1	101	4RF	C22-C24-C25-C26
31	C	505	CLA	CAA-CBA-CGA-O2A
31	n	603	CLA	CAA-CBA-CGA-O2A
31	g	604	CLA	CAA-CBA-CGA-O2A
31	s	610	CLA	CAA-CBA-CGA-O2A
31	D1	402	CLA	CAA-CBA-CGA-O2A
31	c1	512	CLA	CAA-CBA-CGA-O2A
38	C	524	DGA	OG2-CB1-CB2-CB3
41	d	408	LHG	O8-C23-C24-C25
41	c1	525	LHG	O7-C7-C8-C9
47	r1	607	CHL	CAA-CBA-CGA-O2A
47	y1	606	CHL	CAA-CBA-CGA-O2A
52	s1	626	3PH	C32-C33-C34-C35
31	y	613	CLA	C10-C11-C12-C13
47	g	608	CHL	CBD-CGD-O2D-CED
41	D1	410	LHG	C8-C7-O7-C5
31	B	609	CLA	CAA-CBA-CGA-O1A
31	C	503	CLA	CAA-CBA-CGA-O1A
31	b	612	CLA	CAA-CBA-CGA-O1A
31	C1	505	CLA	CAA-CBA-CGA-O1A
41	N1	624	LHG	O9-C7-C8-C9
52	s1	626	3PH	O22-C21-C22-C23
34	C1	526	SQD	C23-C24-C25-C26
54	i1	101	4RF	C35-C36-C37-C38
44	D	405	PL9	C2-C3-C7-C8
44	d1	405	PL9	C2-C3-C7-C8
31	A	406	CLA	C8-C10-C11-C12
52	t1	101	3PH	C28-C29-C2A-C2B
34	B1	626	SQD	C11-C10-C9-C8
31	B	610	CLA	CAA-CBA-CGA-O2A
31	G	613	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
31	S	611	CLA	CAA-CBA-CGA-O2A
31	g	603	CLA	CAA-CBA-CGA-O2A
31	r	612	CLA	CAA-CBA-CGA-O2A
31	s	603	CLA	CAA-CBA-CGA-O2A
31	B1	609	CLA	CAA-CBA-CGA-O2A
31	a1	405	CLA	CAA-CBA-CGA-O2A
31	s1	617	CLA	CAA-CBA-CGA-O2A
35	d1	411	LMG	O7-C10-C11-C12
38	B1	625	DGA	OG1-CA1-CA2-CA3
40	C	523	DGD	O1G-C1A-C2A-C3A
47	y	606	CHL	CAA-CBA-CGA-O2A
54	K1	101	4RF	O40-C41-C43-C44
54	i1	101	4RF	C46-C47-C48-C49
31	n	611	CLA	CAA-CBA-CGA-O1A
31	s	610	CLA	CAA-CBA-CGA-O1A
31	b1	613	CLA	CAA-CBA-CGA-O1A
35	C1	523	LMG	O9-C10-C11-C12
40	C1	518	DGD	O1A-C1A-C2A-C3A
41	d1	408	LHG	O9-C7-C8-C9
38	c	524	DGA	CAB-CBB-CCB-CDB
41	N1	624	LHG	C15-C16-C17-C18

All (1) ring outliers are listed below:

Mol	Chain	Res	Type	Atoms
50	n1	623	NEX	C1-C2-C3-C4-C5-C6

637 monomers are involved in 2147 short contacts:

Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	s	620	LUT	8	0
31	c	508	CLA	8	0
31	g	613	CLA	5	0
47	g1	607	CHL	3	0
33	C1	514	BCR	9	0
47	s1	601	CHL	1	0
31	c	507	CLA	4	0
47	n1	609	CHL	3	0
31	D1	403	CLA	1	0
52	t1	101	3PH	4	0
31	A	406	CLA	6	0
33	D1	404	BCR	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	A	413	LMG	12	0
31	Y	612	CLA	4	0
47	G	605	CHL	2	0
48	s	621	LUT	6	0
31	y1	612	CLA	6	0
48	N	621	LUT	3	0
48	r1	620	LUT	6	0
35	h	102	LMG	6	0
35	C1	521	LMG	9	0
32	A	408	PHO	6	0
33	c	517	BCR	6	0
31	R1	610	CLA	3	0
31	c1	511	CLA	9	0
31	a1	405	CLA	7	0
31	C	509	CLA	4	0
31	Y1	610	CLA	2	0
45	F1	101	HEM	1	0
41	D	408	LHG	3	0
47	y	601	CHL	5	0
47	y1	606	CHL	1	0
31	r	608	CLA	3	0
35	b	622	LMG	5	0
31	b	605	CLA	6	0
31	c	510	CLA	3	0
47	R1	607	CHL	1	0
31	y1	613	CLA	5	0
31	b1	616	CLA	8	0
31	G1	602	CLA	6	0
38	B	625	DGA	4	0
31	b1	606	CLA	4	0
44	D1	405	PL9	8	0
31	r	604	CLA	1	0
46	H1	101	RRX	5	0
31	b	608	CLA	6	0
39	b	625	GOL	1	0
31	g1	603	CLA	2	0
31	s	604	CLA	2	0
34	A1	412	SQD	2	0
31	y	611	CLA	1	0
31	b1	610	CLA	10	0
31	B1	605	CLA	8	0
31	n1	613	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	b1	602	CLA	7	0
31	S	614	CLA	2	0
40	C	518	DGD	6	0
31	S1	605	CLA	2	0
47	Y1	606	CHL	4	0
31	g1	611	CLA	3	0
50	g1	623	NEX	1	0
31	B	617	CLA	4	0
31	R1	608	CLA	3	0
31	B1	603	CLA	7	0
31	Y1	608	CLA	1	0
34	A	412	SQD	4	0
31	S1	603	CLA	3	0
56	r1	626	ERG	5	0
48	n1	620	LUT	4	0
31	R1	604	CLA	2	0
33	a	411	BCR	4	0
35	B	622	LMG	3	0
31	A	407	CLA	2	0
31	b1	615	CLA	8	0
47	Y1	601	CHL	3	0
40	C	520	DGD	5	0
31	B1	614	CLA	3	0
41	G	630	LHG	6	0
31	b	602	CLA	2	0
31	b	615	CLA	2	0
31	Y	613	CLA	3	0
31	b1	612	CLA	4	0
48	n1	621	LUT	8	0
47	n1	606	CHL	1	0
38	b1	625	DGA	5	0
31	s1	603	CLA	5	0
31	b	613	CLA	2	0
33	d1	404	BCR	5	0
31	g	603	CLA	4	0
41	n1	624	LHG	4	0
31	A1	406	CLA	7	0
33	b1	619	BCR	2	0
44	d1	405	PL9	6	0
31	G1	614	CLA	1	0
55	r1	625	LMT	3	0
47	y1	601	CHL	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	b	606	CLA	5	0
35	c1	523	LMG	10	0
31	C1	504	CLA	8	0
31	r1	612	CLA	3	0
49	G	622	XAT	7	0
41	d	410	LHG	5	0
31	B	609	CLA	4	0
31	C	506	CLA	4	0
31	b	610	CLA	9	0
31	g	604	CLA	1	0
47	y1	607	CHL	6	0
54	i1	101	4RF	5	0
31	b	612	CLA	8	0
31	B1	606	CLA	4	0
31	B1	608	CLA	5	0
31	C	510	CLA	4	0
47	r1	606	CHL	2	0
48	g1	621	LUT	5	0
31	Y1	613	CLA	8	0
31	r1	609	CLA	7	0
31	B	607	CLA	5	0
40	C	519	DGD	8	0
31	n	602	CLA	4	0
41	D1	409	LHG	6	0
47	N1	605	CHL	2	0
31	b	614	CLA	3	0
52	S1	626	3PH	2	0
31	c	504	CLA	3	0
31	S1	610	CLA	4	0
41	d1	409	LHG	3	0
45	f	101	HEM	5	0
47	g1	608	CHL	3	0
31	s	603	CLA	1	0
31	Y1	602	CLA	13	0
45	F	101	HEM	2	0
47	s	608	CHL	5	0
49	r	622	XAT	6	0
50	R1	622	NEX	4	0
47	g1	609	CHL	3	0
49	G1	622	XAT	8	0
31	s1	611	CLA	5	0
31	c1	507	CLA	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	G1	601	CHL	3	0
54	I1	102	4RF	3	0
31	C1	506	CLA	7	0
31	G	602	CLA	9	0
31	a1	407	CLA	4	0
41	n	624	LHG	7	0
32	a1	408	PHO	7	0
49	g1	622	XAT	8	0
31	y	612	CLA	4	0
31	B1	616	CLA	5	0
41	D1	408	LHG	2	0
35	W1	201	LMG	4	0
48	S1	621	LUT	6	0
31	N1	611	CLA	1	0
50	s1	623	NEX	1	0
31	D1	402	CLA	10	0
47	Y1	609	CHL	2	0
34	b1	626	SQD	9	0
31	c1	512	CLA	5	0
31	C1	509	CLA	3	0
47	S	607	CHL	2	0
33	B1	619	BCR	3	0
31	c	512	CLA	1	0
31	y	602	CLA	20	0
51	s	625	LPX	1	0
47	R	606	CHL	2	0
31	r	612	CLA	1	0
47	G1	606	CHL	2	0
41	G1	624	LHG	3	0
31	b	607	CLA	2	0
31	Y	603	CLA	7	0
31	y	613	CLA	7	0
31	n	604	CLA	4	0
31	y1	603	CLA	4	0
57	Y1	627	PTY	1	0
31	C1	501	CLA	7	0
47	S1	607	CHL	2	0
31	G1	604	CLA	2	0
47	g	609	CHL	4	0
47	s	601	CHL	2	0
47	s	606	CHL	2	0
31	c	502	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	Y	610	CLA	4	0
33	c1	517	BCR	5	0
31	c	505	CLA	5	0
31	B1	612	CLA	4	0
31	s1	610	CLA	6	0
31	N1	614	CLA	1	0
31	n1	603	CLA	5	0
31	g1	610	CLA	2	0
35	H	102	LMG	4	0
49	g	622	XAT	6	0
31	b	609	CLA	9	0
31	Y1	612	CLA	3	0
40	c	523	DGD	6	0
48	r	620	LUT	3	0
31	y	608	CLA	2	0
40	c	519	DGD	8	0
40	b1	623	DGD	1	0
35	D	411	LMG	3	0
48	S	620	LUT	3	0
31	b	604	CLA	3	0
31	c1	505	CLA	9	0
49	r1	621	XAT	4	0
47	N	608	CHL	3	0
31	y	614	CLA	2	0
35	D1	411	LMG	3	0
47	y	606	CHL	2	0
31	b1	607	CLA	5	0
50	N	623	NEX	2	0
31	d1	402	CLA	6	0
34	a	412	SQD	4	0
31	C	505	CLA	7	0
31	R	611	CLA	1	0
31	S	617	CLA	1	0
48	S1	620	LUT	5	0
57	y1	626	PTY	5	0
31	c	509	CLA	6	0
31	y1	614	CLA	7	0
31	c	503	CLA	1	0
42	C1	527	LMK	1	0
47	N	606	CHL	3	0
35	w1	201	LMG	3	0
31	G	614	CLA	1	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	N1	602	CLA	5	0
31	N1	613	CLA	2	0
49	y1	622	XAT	9	0
54	K1	101	4RF	6	0
31	S	613	CLA	4	0
47	n1	608	CHL	1	0
50	S1	623	NEX	4	0
54	k1	101	4RF	3	0
57	Y1	626	PTY	6	0
47	S	601	CHL	3	0
31	s	617	CLA	2	0
34	c	626	SQD	2	0
31	s	611	CLA	4	0
31	N1	610	CLA	8	0
47	r	607	CHL	2	0
31	B1	615	CLA	7	0
49	N1	622	XAT	8	0
41	C	525	LHG	1	0
46	h1	101	RRX	9	0
48	R1	620	LUT	6	0
33	C	515	BCR	3	0
40	c1	518	DGD	7	0
31	B1	613	CLA	10	0
47	s1	607	CHL	3	0
31	B	605	CLA	8	0
31	y1	602	CLA	13	0
31	B	616	CLA	2	0
31	g1	612	CLA	1	0
33	A	411	BCR	2	0
48	S	621	LUT	6	0
31	r	609	CLA	3	0
35	H1	102	LMG	5	0
41	Y	624	LHG	4	0
41	S	624	LHG	8	0
31	G1	613	CLA	5	0
31	s1	609	CLA	3	0
47	N	609	CHL	2	0
48	R	620	LUT	5	0
31	Y	602	CLA	8	0
31	B	608	CLA	6	0
31	s1	602	CLA	4	0
31	y1	610	CLA	9	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
49	n1	622	XAT	8	0
31	C	511	CLA	6	0
40	C1	518	DGD	10	0
31	s	614	CLA	2	0
31	a	410	CLA	5	0
31	Y	604	CLA	4	0
31	s1	604	CLA	4	0
47	n	605	CHL	4	0
41	d1	410	LHG	6	0
47	N1	609	CHL	3	0
52	B1	624	3PH	10	0
33	B1	618	BCR	6	0
47	s	607	CHL	1	0
48	G1	620	LUT	2	0
31	a	406	CLA	5	0
47	N	607	CHL	5	0
31	C	507	CLA	6	0
47	g	601	CHL	4	0
31	A1	410	CLA	5	0
38	J1	101	DGA	2	0
31	r1	610	CLA	6	0
35	C	521	LMG	7	0
48	G1	621	LUT	5	0
31	S	605	CLA	2	0
31	s	605	CLA	1	0
34	B1	626	SQD	2	0
47	r1	607	CHL	2	0
47	s1	608	CHL	5	0
49	N	622	XAT	5	0
31	c	513	CLA	7	0
31	Y	614	CLA	2	0
35	d1	411	LMG	2	0
47	g	608	CHL	5	0
31	r	603	CLA	1	0
31	S	603	CLA	1	0
35	A1	413	LMG	7	0
31	B1	617	CLA	2	0
31	n1	614	CLA	1	0
47	g1	606	CHL	2	0
31	B1	611	CLA	6	0
31	C1	502	CLA	1	0
31	b1	604	CLA	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	R	607	CHL	2	0
31	c1	513	CLA	10	0
31	A	405	CLA	11	0
31	R	612	CLA	5	0
31	b1	609	CLA	9	0
31	r1	608	CLA	5	0
41	C1	525	LHG	9	0
31	C1	505	CLA	9	0
48	G	620	LUT	6	0
31	B1	609	CLA	7	0
32	a	408	PHO	4	0
47	n	606	CHL	3	0
31	c	501	CLA	5	0
31	R1	603	CLA	4	0
31	Y1	603	CLA	2	0
47	G	606	CHL	1	0
35	a1	413	LMG	7	0
35	b1	622	LMG	6	0
47	n1	607	CHL	4	0
31	Y	611	CLA	1	0
31	D	403	CLA	1	0
31	s	609	CLA	4	0
44	D	405	PL9	6	0
50	N1	623	NEX	4	0
38	j1	101	DGA	3	0
31	B	615	CLA	3	0
47	S	608	CHL	7	0
41	L	101	LHG	3	0
47	y1	609	CHL	3	0
48	n	620	LUT	5	0
33	c	514	BCR	4	0
48	n	621	LUT	6	0
31	g1	602	CLA	6	0
31	G	613	CLA	2	0
35	J	101	LMG	2	0
31	S	610	CLA	2	0
31	y1	604	CLA	3	0
33	b	618	BCR	4	0
34	c1	526	SQD	5	0
33	C1	515	BCR	6	0
31	y1	611	CLA	7	0
47	S1	608	CHL	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
48	y1	620	LUT	5	0
47	y1	605	CHL	4	0
41	L1	101	LHG	9	0
48	N1	620	LUT	4	0
34	C	526	SQD	2	0
47	n1	601	CHL	5	0
31	C1	507	CLA	10	0
47	g1	605	CHL	2	0
32	a1	409	PHO	3	0
31	S1	602	CLA	4	0
50	y1	623	NEX	1	0
41	d	408	LHG	2	0
31	b	617	CLA	4	0
47	G1	605	CHL	2	0
34	B	621	SQD	3	0
31	R	604	CLA	1	0
31	y	610	CLA	6	0
41	c	625	LHG	4	0
48	y	620	LUT	5	0
48	N1	621	LUT	7	0
49	y	622	XAT	5	0
31	d	402	CLA	5	0
35	c1	521	LMG	7	0
31	C	508	CLA	3	0
50	r1	622	NEX	1	0
31	S1	609	CLA	2	0
31	B	612	CLA	9	0
41	s1	624	LHG	3	0
31	a1	406	CLA	4	0
31	c	506	CLA	7	0
31	G1	603	CLA	7	0
41	g	624	LHG	7	0
50	Y1	623	NEX	2	0
33	c	515	BCR	5	0
47	n1	605	CHL	5	0
47	G1	608	CHL	2	0
35	a	413	LMG	6	0
38	b	623	DGA	3	0
52	T1	101	3PH	1	0
31	B	613	CLA	6	0
48	s1	621	LUT	7	0
32	A1	408	PHO	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	c1	502	CLA	4	0
31	B	602	CLA	2	0
31	S	602	CLA	2	0
47	G	601	CHL	6	0
31	G1	610	CLA	1	0
47	G	609	CHL	3	0
52	s1	626	3PH	3	0
33	c1	515	BCR	7	0
33	b	619	BCR	1	0
31	g	611	CLA	2	0
31	C	502	CLA	5	0
31	c1	508	CLA	9	0
31	b	603	CLA	3	0
34	m1	101	SQD	3	0
33	C	517	BCR	7	0
31	S1	612	CLA	1	0
47	n	601	CHL	7	0
32	A1	409	PHO	4	0
49	Y1	622	XAT	9	0
31	s1	605	CLA	2	0
31	B	611	CLA	3	0
31	S	611	CLA	3	0
31	B1	610	CLA	4	0
31	C1	512	CLA	7	0
40	C	523	DGD	5	0
47	Y	605	CHL	3	0
31	b	611	CLA	7	0
34	B1	621	SQD	4	0
31	A	410	CLA	8	0
31	C	512	CLA	5	0
31	n	603	CLA	9	0
52	i	101	3PH	1	0
49	n	622	XAT	5	0
31	c1	510	CLA	5	0
31	g1	614	CLA	1	0
31	N	603	CLA	4	0
31	r	610	CLA	3	0
31	G	603	CLA	4	0
33	B	618	BCR	4	0
31	N	604	CLA	3	0
31	a	405	CLA	4	0
41	N1	624	LHG	4	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
47	Y	601	CHL	2	0
46	h	101	RRX	3	0
35	h1	102	LMG	3	0
31	N1	603	CLA	2	0
31	b1	613	CLA	7	0
34	M1	101	SQD	6	0
47	G1	607	CHL	4	0
50	S	622	NEX	2	0
41	S1	624	LHG	6	0
31	B	610	CLA	5	0
47	r	606	CHL	1	0
31	n1	611	CLA	1	0
40	C1	519	DGD	8	0
31	y	603	CLA	10	0
31	g	610	CLA	1	0
31	G	604	CLA	6	0
31	S1	604	CLA	4	0
33	c1	516	BCR	7	0
31	d1	403	CLA	2	0
31	R	603	CLA	1	0
47	y	609	CHL	3	0
50	s	623	NEX	2	0
34	b	621	SQD	2	0
56	R1	626	ERG	8	0
40	C1	520	DGD	6	0
50	G	623	NEX	3	0
49	R1	621	XAT	3	0
31	a1	410	CLA	5	0
31	S1	614	CLA	1	0
33	C	516	BCR	4	0
32	A	409	PHO	2	0
41	y1	624	LHG	7	0
47	G1	609	CHL	3	0
31	b1	614	CLA	3	0
51	S	625	LPX	2	0
33	a1	411	BCR	4	0
31	n	610	CLA	3	0
47	G	608	CHL	4	0
31	B	614	CLA	1	0
31	D	402	CLA	6	0
33	b1	618	BCR	3	0
33	d	404	BCR	5	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	j	101	LMG	5	0
41	D	409	LHG	6	0
47	Y	606	CHL	2	0
31	c1	504	CLA	7	0
39	b	624	GOL	1	0
31	g1	604	CLA	4	0
31	r	602	CLA	3	0
47	n	607	CHL	6	0
31	C	503	CLA	4	0
47	N1	608	CHL	4	0
31	G1	611	CLA	3	0
34	C1	526	SQD	2	0
48	Y	620	LUT	4	0
46	H	101	RRX	26	0
50	n	623	NEX	3	0
47	y	605	CHL	2	0
48	y	621	LUT	6	0
38	c1	524	DGA	3	0
33	A1	411	BCR	4	0
41	Y1	624	LHG	7	0
31	S	604	CLA	3	0
31	R1	612	CLA	2	0
31	g	602	CLA	9	0
38	C	524	DGA	2	0
47	N1	601	CHL	4	0
31	s	610	CLA	3	0
38	B1	625	DGA	5	0
31	C1	508	CLA	8	0
47	R1	606	CHL	3	0
31	n	613	CLA	7	0
31	Y1	614	CLA	7	0
40	c1	519	DGD	11	0
31	B1	602	CLA	4	0
31	R1	609	CLA	3	0
47	N	605	CHL	7	0
31	N	613	CLA	5	0
31	b1	617	CLA	2	0
47	n	609	CHL	8	0
35	c	521	LMG	3	0
52	b1	624	3PH	6	0
48	G	621	LUT	10	0
31	s	613	CLA	3	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
31	R	610	CLA	3	0
31	b1	608	CLA	11	0
40	c1	520	DGD	8	0
47	y	607	CHL	2	0
35	d	411	LMG	4	0
31	y	604	CLA	2	0
31	d	403	CLA	3	0
31	Y1	604	CLA	3	0
33	C1	517	BCR	5	0
31	B	604	CLA	4	0
48	N	620	LUT	3	0
41	l	101	LHG	9	0
31	c1	501	CLA	4	0
33	B	619	BCR	2	0
41	d	409	LHG	3	0
31	S	609	CLA	4	0
31	c1	506	CLA	7	0
31	C	513	CLA	6	0
31	B	603	CLA	9	0
41	c1	525	LHG	9	0
31	C	501	CLA	6	0
38	C1	524	DGA	4	0
40	c	520	DGD	5	0
31	n1	610	CLA	5	0
31	r1	603	CLA	7	0
53	y	625	SPH	4	0
31	R	608	CLA	2	0
31	r1	602	CLA	2	0
31	Y	608	CLA	2	0
31	A1	405	CLA	3	0
47	g	605	CHL	2	0
28	A1	401	OEX	1	0
31	C1	511	CLA	3	0
31	c1	503	CLA	5	0
31	y1	608	CLA	2	0
31	B1	604	CLA	8	0
31	C1	510	CLA	5	0
31	b1	605	CLA	4	0
47	N	601	CHL	3	0
49	Y	622	XAT	3	0
41	s	624	LHG	7	0
31	A1	407	CLA	2	0

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Mol	Chain	Res	Type	Clashes	Symm-Clashes
35	B1	622	LMG	9	0
31	G	610	CLA	1	0
31	S1	611	CLA	6	0
31	s	612	CLA	2	0
31	N	610	CLA	5	0
33	c1	514	BCR	12	0
47	Y	609	CHL	6	0
31	B	606	CLA	7	0
31	b	616	CLA	6	0
33	C1	516	BCR	6	0
33	C	514	BCR	6	0
52	S	626	3PH	3	0
31	N1	604	CLA	5	0
53	A1	414	SPH	5	0
48	y1	621	LUT	6	0
52	s	626	3PH	1	0
31	s	602	CLA	3	0
44	d	405	PL9	4	0
31	c1	509	CLA	5	0
41	y	624	LHG	7	0
41	D	410	LHG	1	0
47	n	608	CHL	2	0
31	s1	612	CLA	1	0
48	Y	621	LUT	6	0
41	g1	624	LHG	5	0
31	R	602	CLA	3	0
31	g1	613	CLA	7	0
47	N1	607	CHL	1	0
49	R	621	XAT	3	0
31	C1	503	CLA	3	0
32	a	409	PHO	5	0
47	s1	606	CHL	2	0
50	R	622	NEX	3	0
40	B1	623	DGD	5	0
47	g	606	CHL	1	0
31	s1	613	CLA	1	0
28	a	401	OEX	1	0
48	g1	620	LUT	5	0
47	S	606	CHL	3	0
48	g	620	LUT	4	0
31	N	611	CLA	2	0
31	b1	611	CLA	6	0

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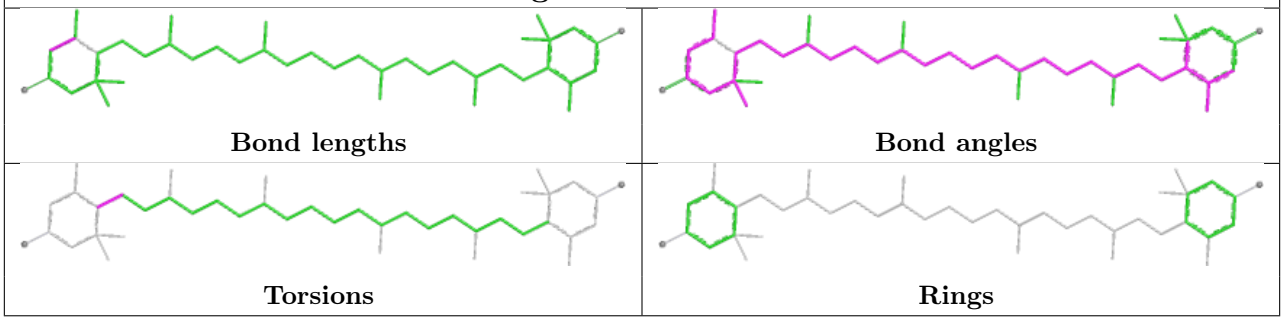
Mol	Chain	Res	Type	Clashes	Symm-Clashes
34	a1	412	SQD	7	0
31	n1	602	CLA	4	0
53	Y1	625	SPH	3	0
48	s1	620	LUT	2	0
31	c	511	CLA	6	0
34	b1	621	SQD	5	0
31	C	504	CLA	5	0
31	n1	604	CLA	1	0
33	D	404	BCR	1	0
48	g	621	LUT	10	0
53	a1	414	SPH	5	0
47	S1	606	CHL	3	0
53	y1	625	SPH	7	0
41	D1	410	LHG	3	0
31	S1	613	CLA	3	0
41	d1	408	LHG	2	0
31	R	609	CLA	3	0
48	Y1	620	LUT	7	0
31	Y1	611	CLA	1	0
47	S1	601	CHL	1	0
33	c	516	BCR	5	0
51	s1	625	LPX	2	0
53	Y	625	SPH	3	0
31	C1	513	CLA	7	0
31	N1	612	CLA	1	0
31	B1	607	CLA	4	0
31	S	612	CLA	2	0
47	Y1	607	CHL	5	0
47	g1	601	CHL	7	0
31	N	602	CLA	4	0
31	b1	603	CLA	6	0
47	Y1	605	CHL	1	0
40	c	518	DGD	6	0
47	Y	607	CHL	5	0
48	Y1	621	LUT	8	0
35	C1	523	LMG	5	0
47	N1	606	CHL	4	0

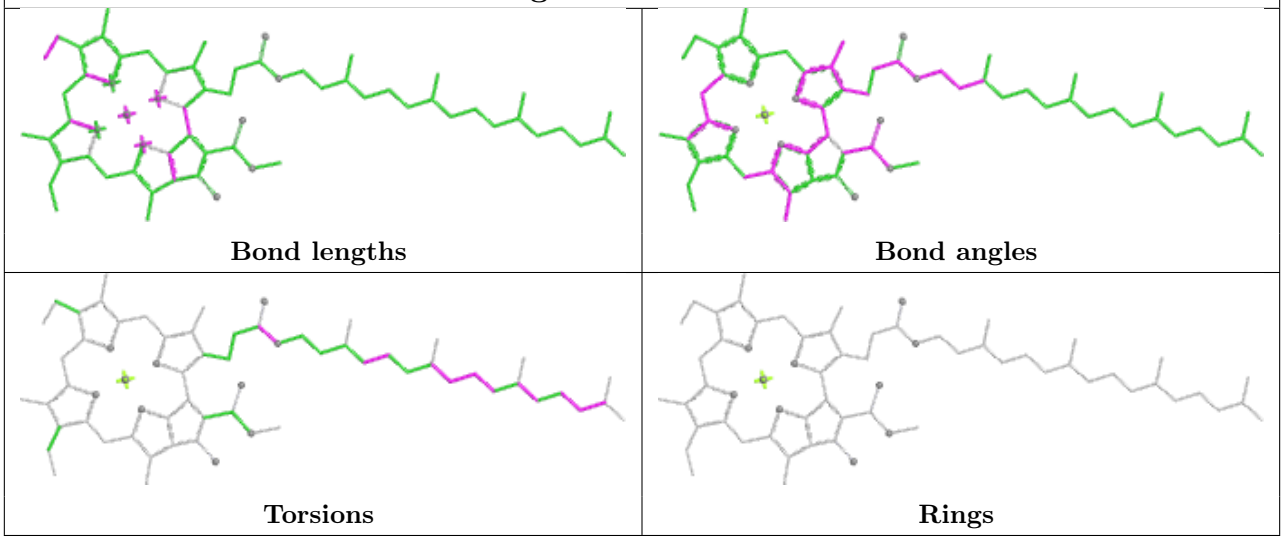
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included. 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 LUT s 620



Ligand CLA c 508



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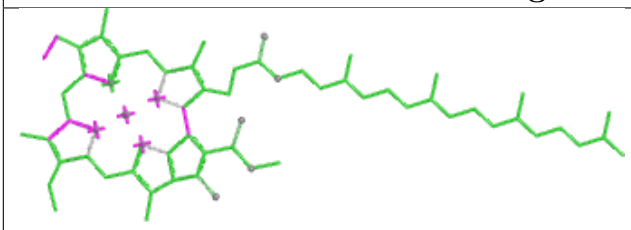
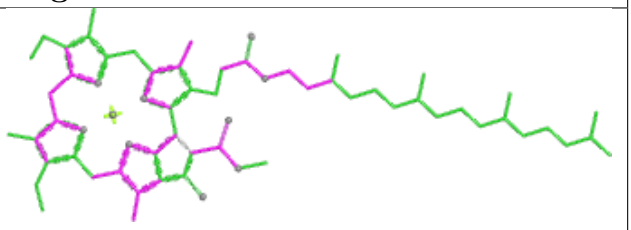
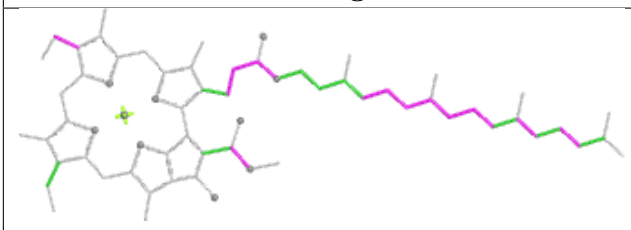


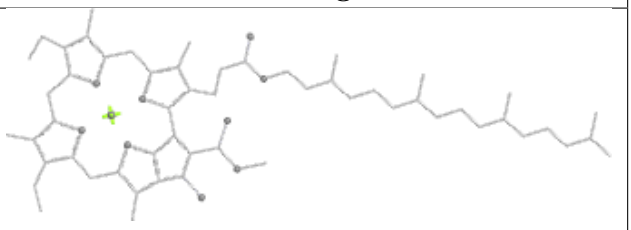
Bond lengths



Bond angles

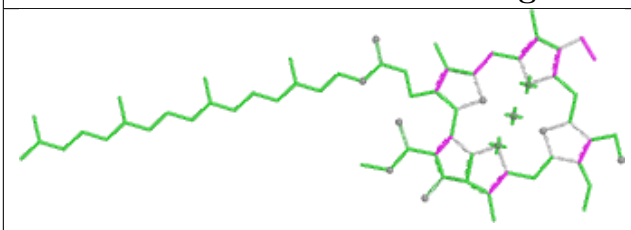


Torsions



Rings

Ligand CHL g1 607



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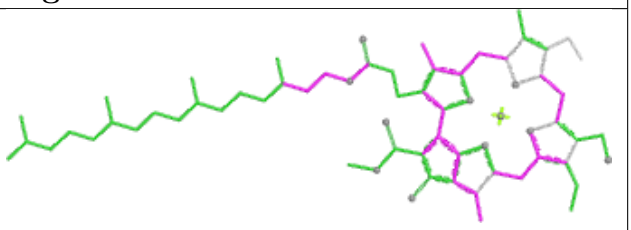
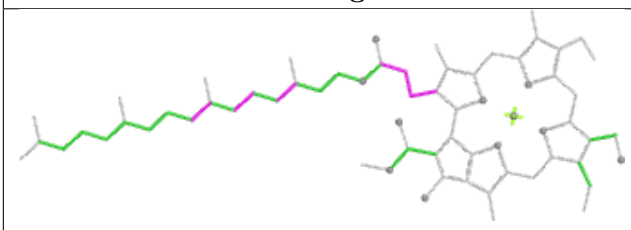
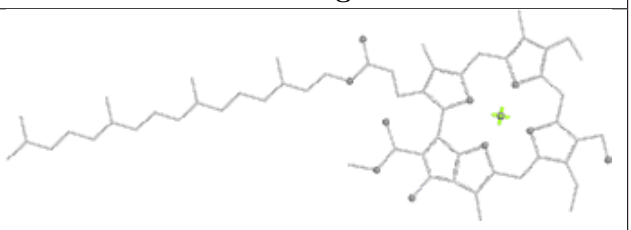


Bond angles

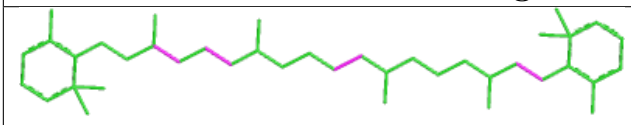


Torsions

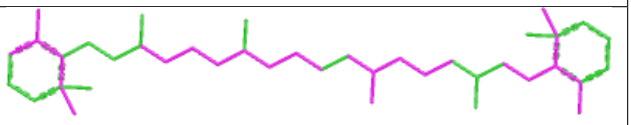


Rings

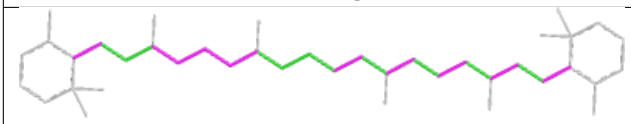
Ligand BCR C1 514



Bond lengths



Bond angles



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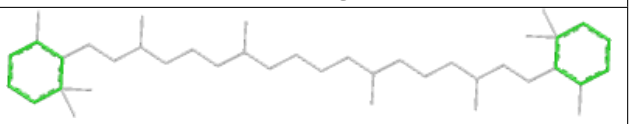
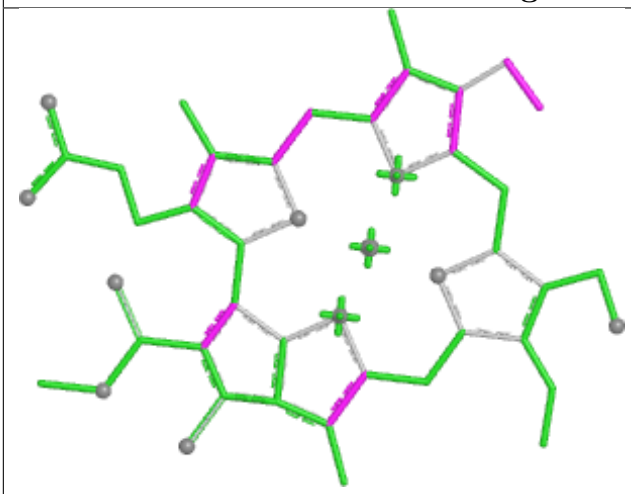


Rings

Ligand CHL s1 601



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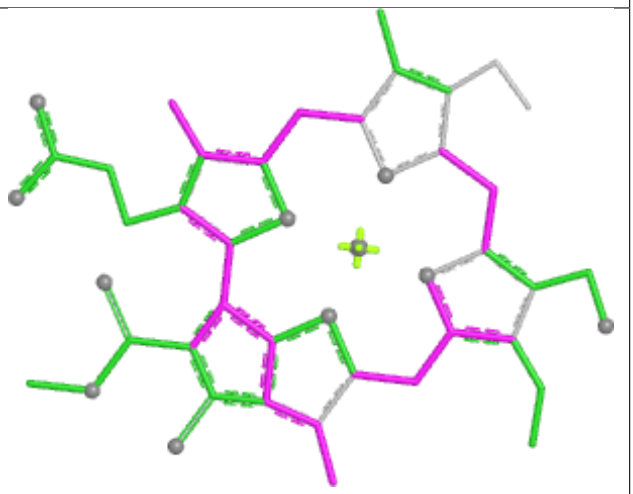
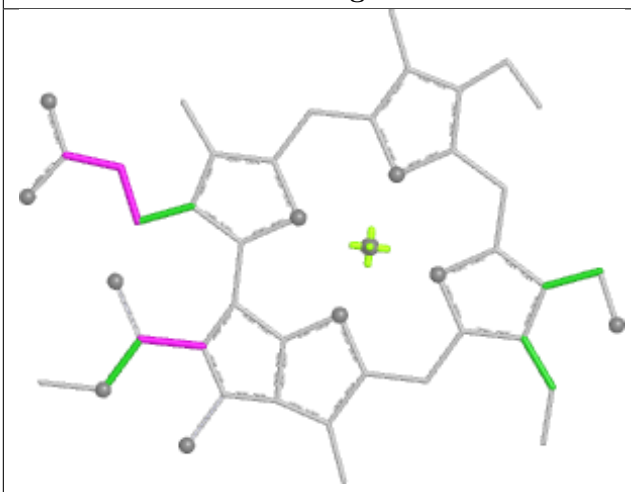
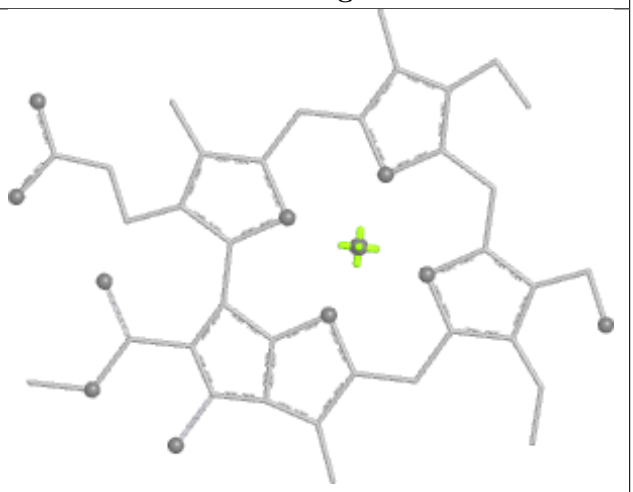


Bond angles

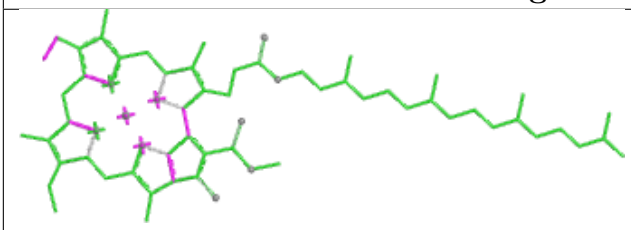


Torsions



Rings

Ligand CLA c 507



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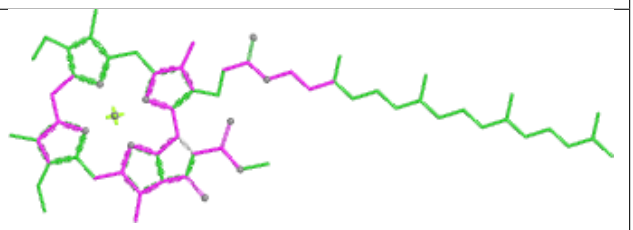

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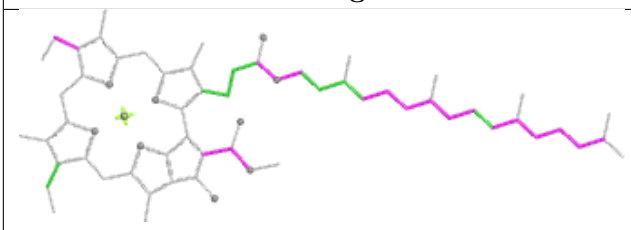

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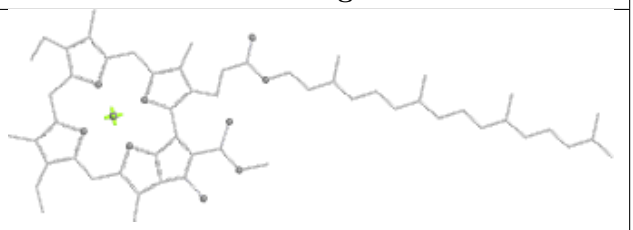
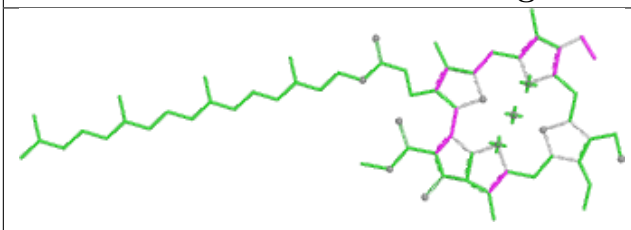


Rings

Ligand CHL n1 609



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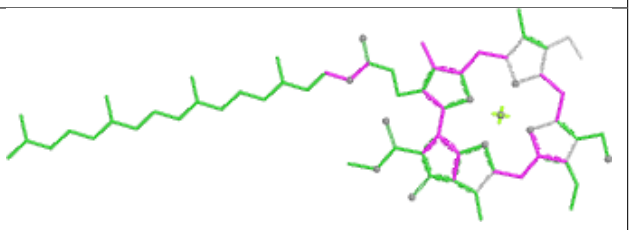

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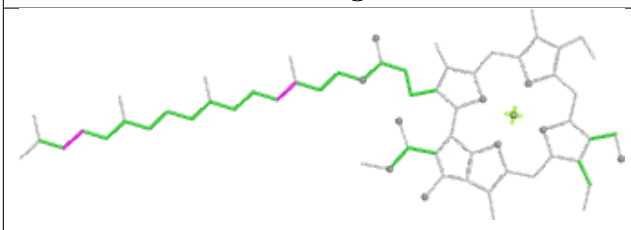

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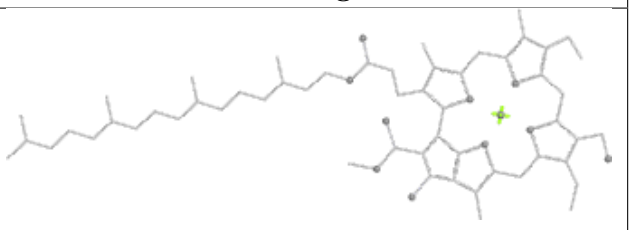
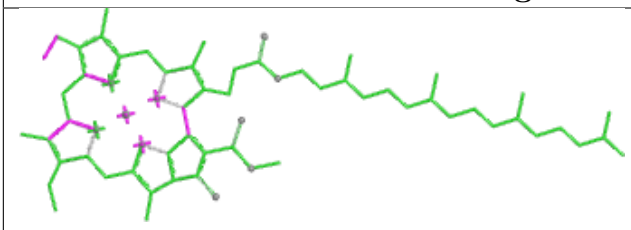


Rings

Ligand CLA D1 403



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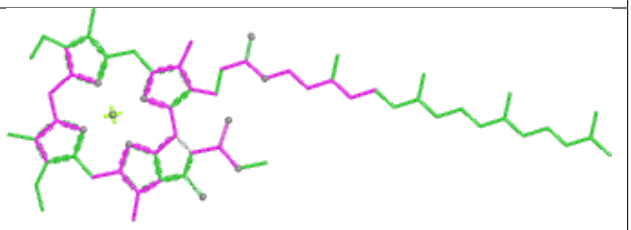
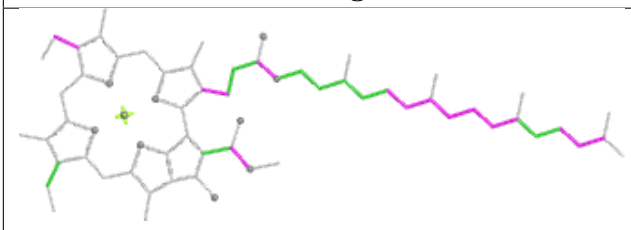
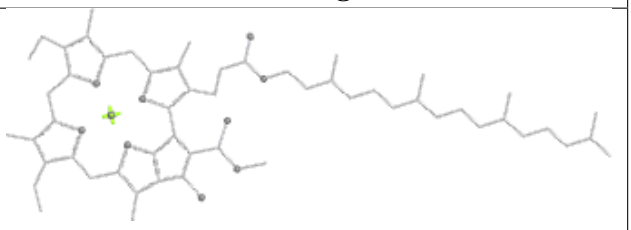


Bond angles

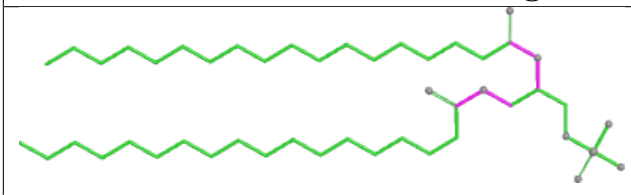


Torsions



Rings

Ligand 3PH t1 101



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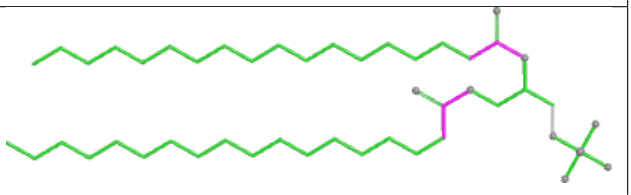
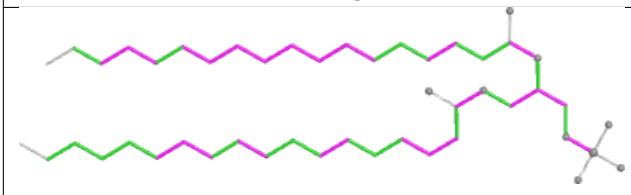
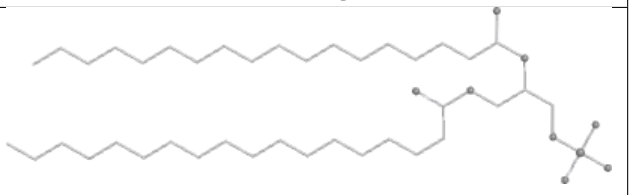


Bond angles

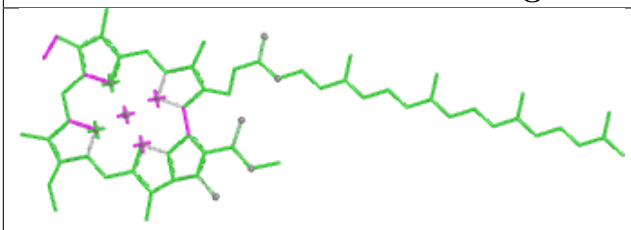


Torsions



Rings

Ligand CLA A 406



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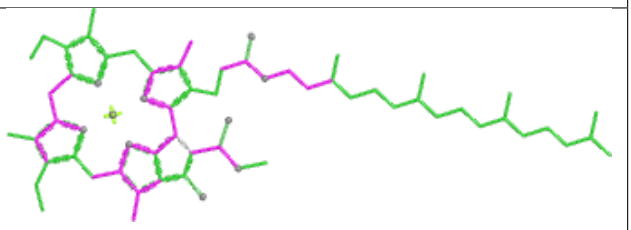
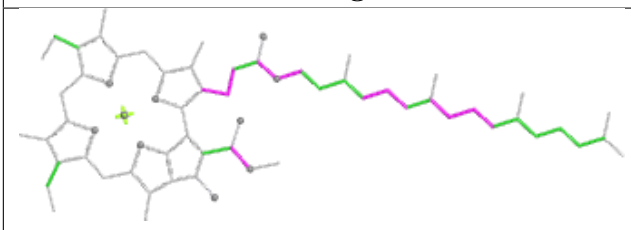


Bond angles



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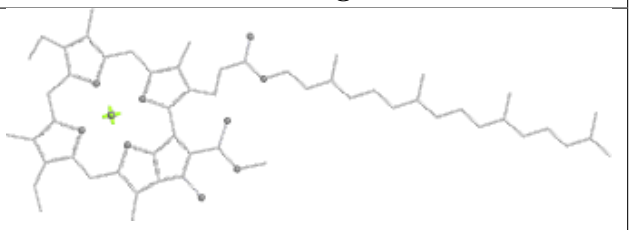
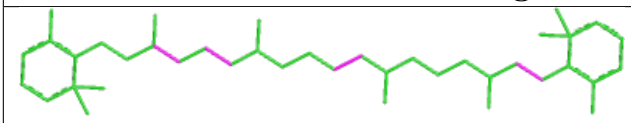


Rings

Ligand BCR D1 404



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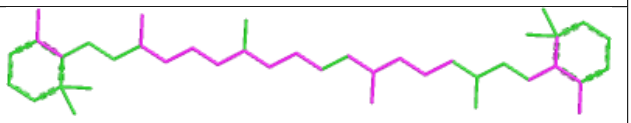
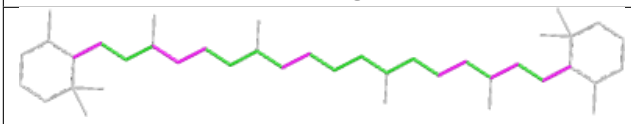
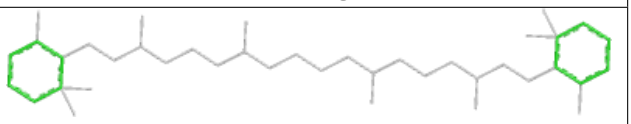


Bond angles

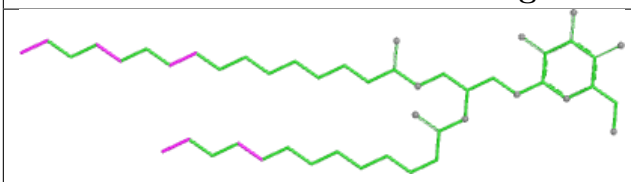


Torsions



Rings

Ligand LMG A 413



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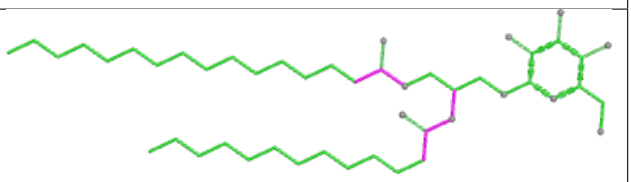
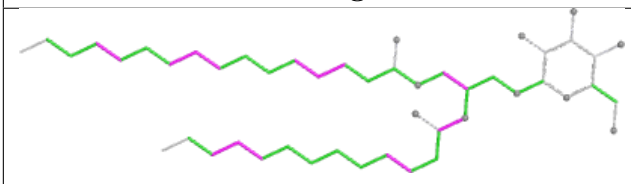
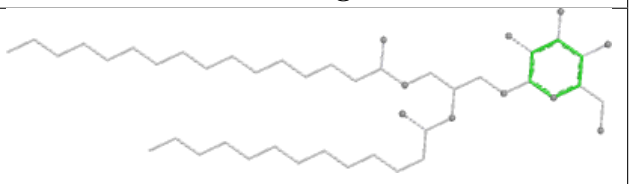


Bond angles

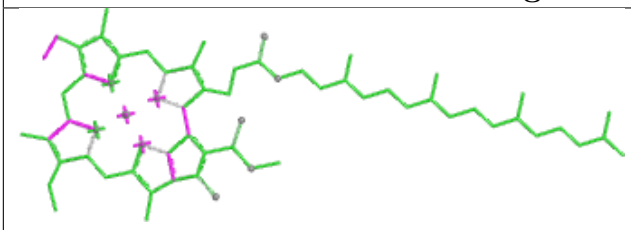


Torsions



Rings

Ligand CLA Y 612



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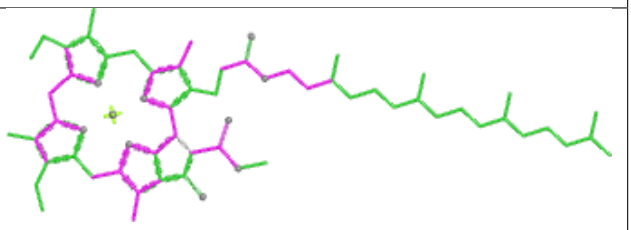
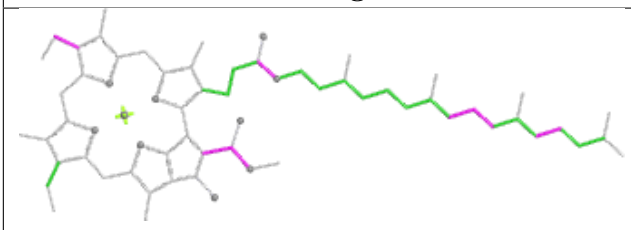
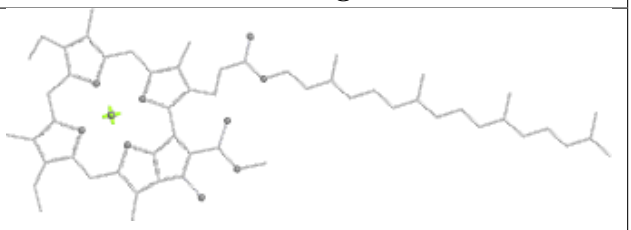


Bond angles

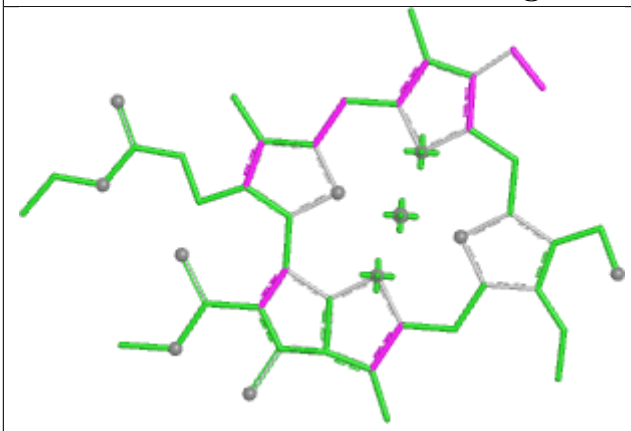


Torsions



Rings

Ligand CHL G 605



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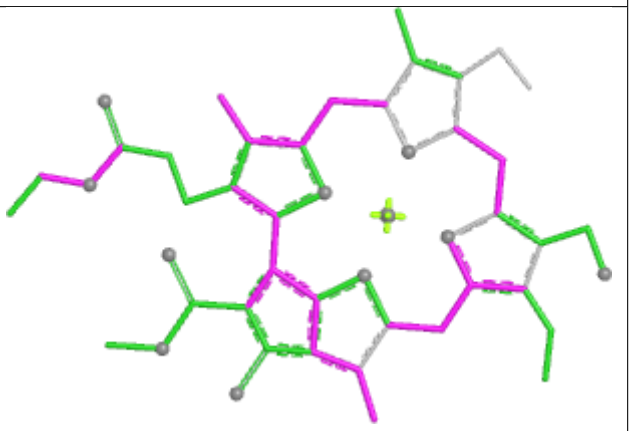
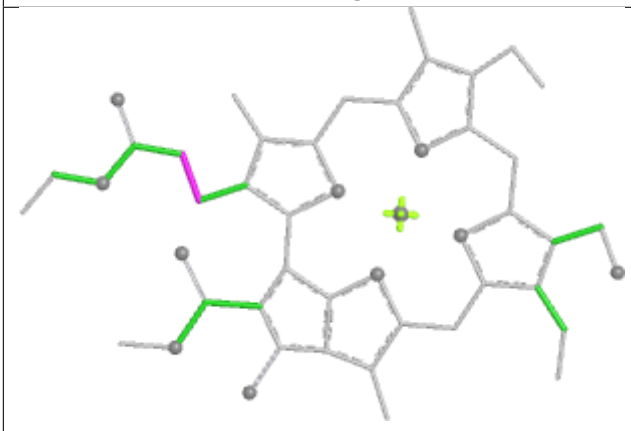


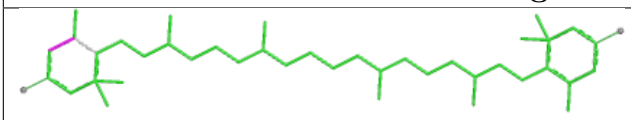
Bond angles

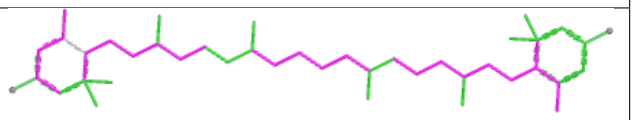


Torsions

Rings

Ligand LUT s 621


Bond lengths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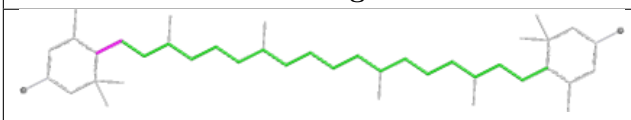
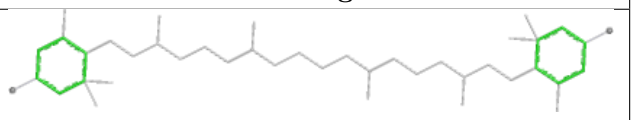
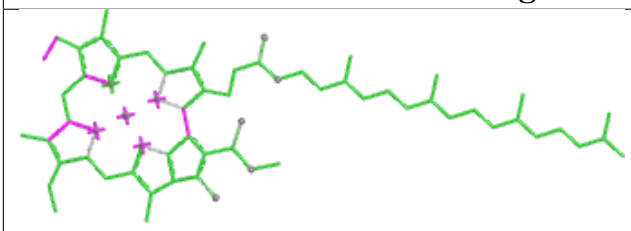

Torsions


Rings

Ligand CLA y1 612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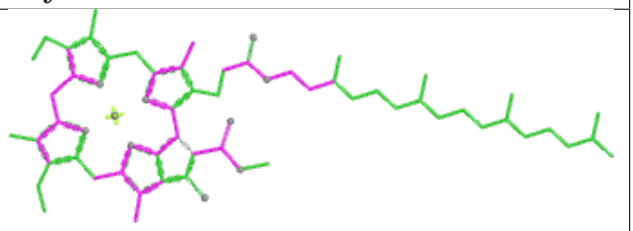
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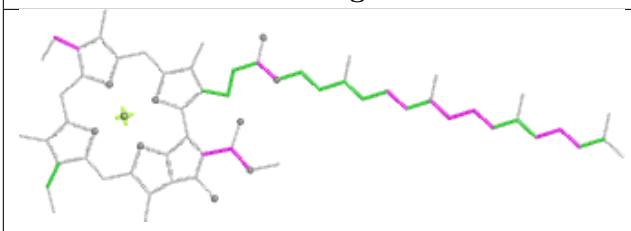
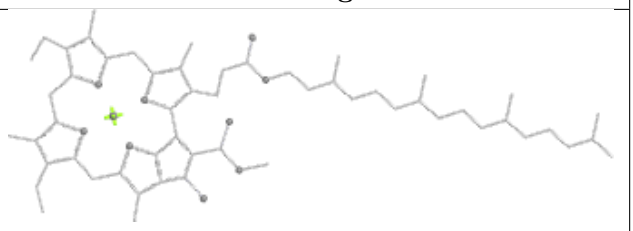
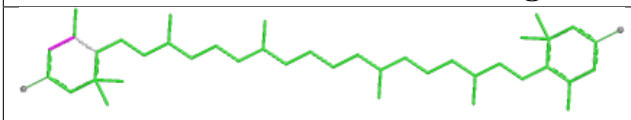

Torsions


Rings

Ligand LUT N 621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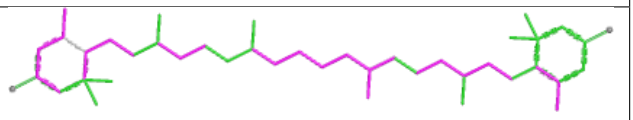
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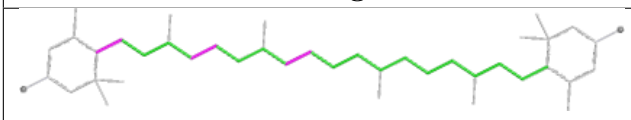
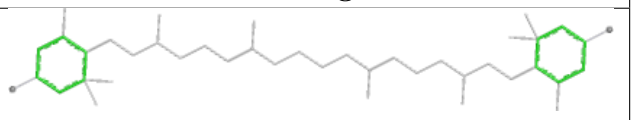

Torsions


Rings

Ligand LUT r1 620

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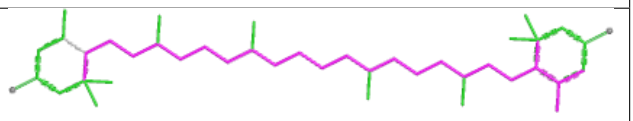
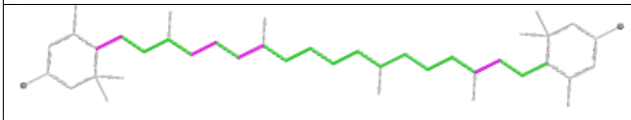
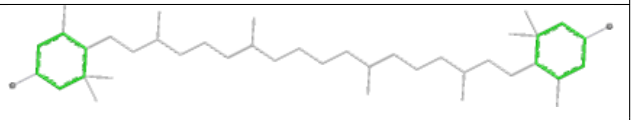
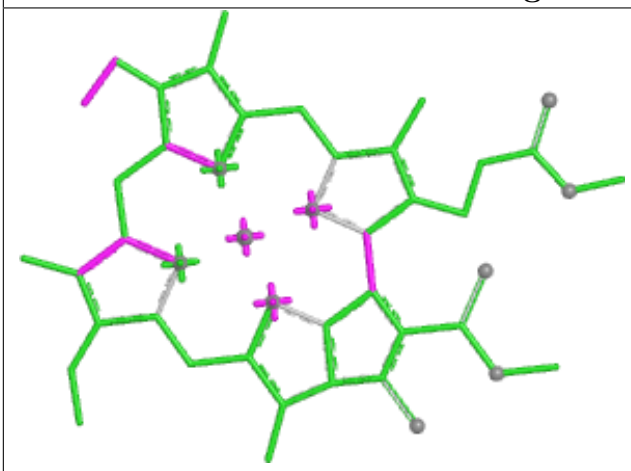

Bond angles

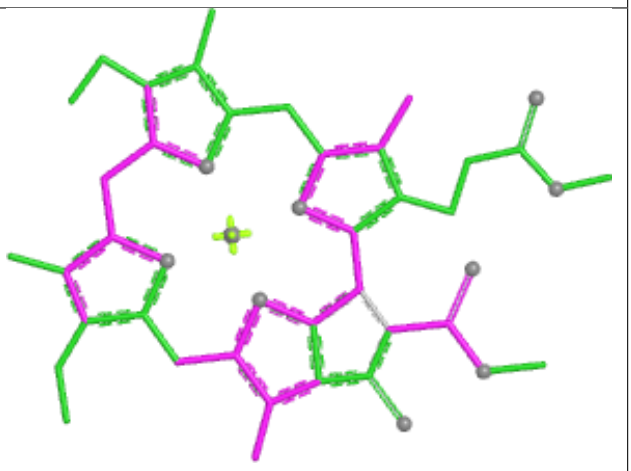

Torsions


Rings

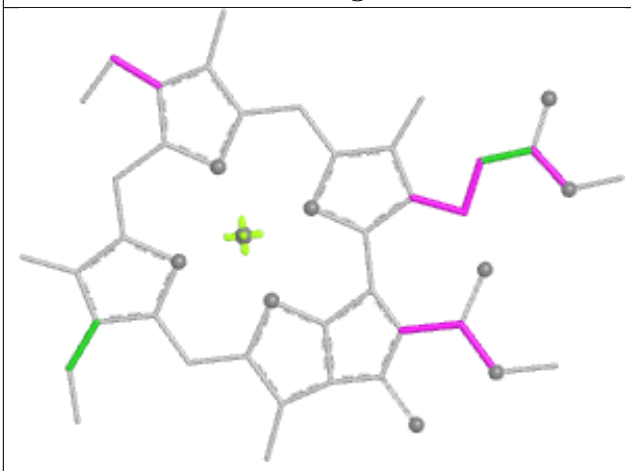
Ligand CLA R 613



Bond lengths



Bond angles



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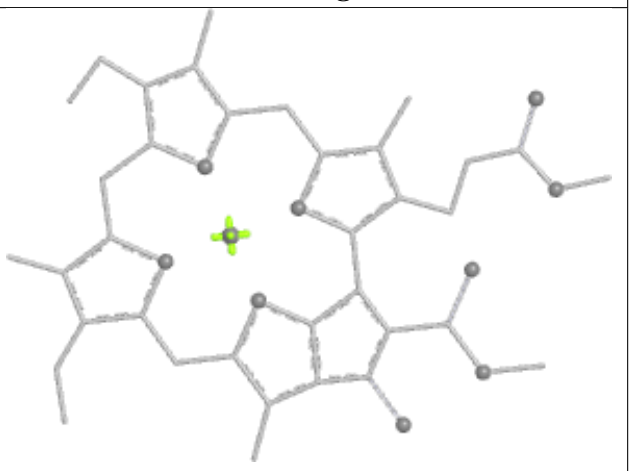
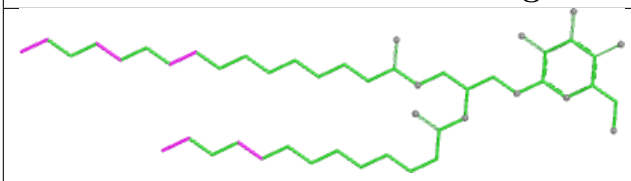


Rings

Ligand LMG h 102



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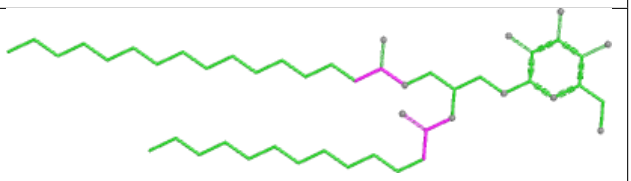
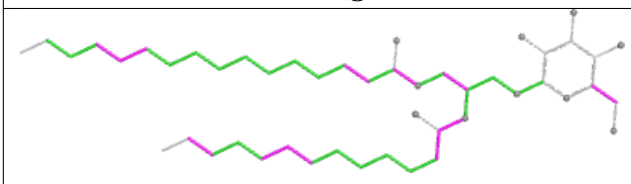


Bond angles



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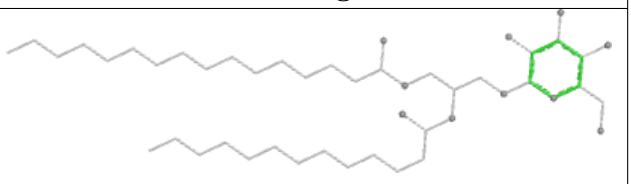
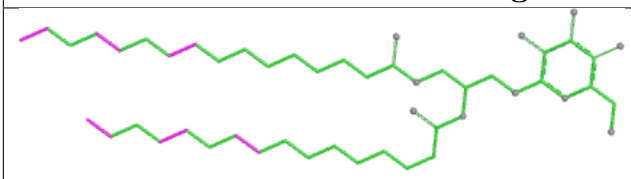


Rings

Ligand LMG C1 521



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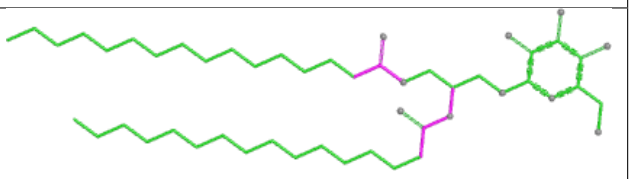
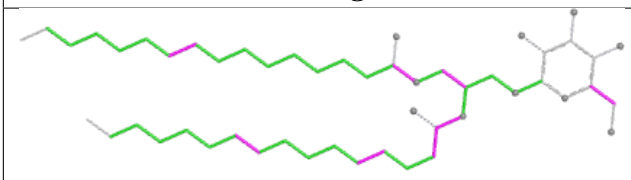


Bond angles



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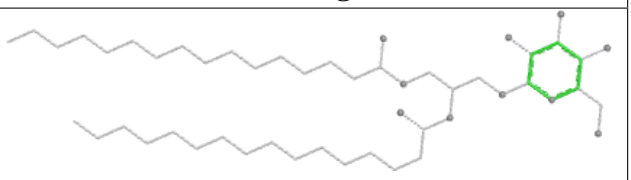
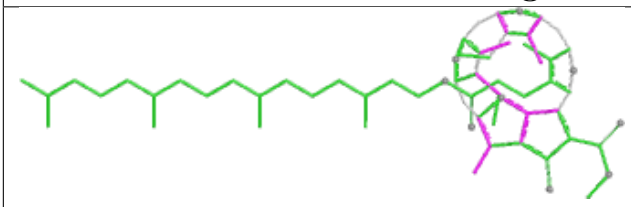


Rings

Ligand PHO A 408



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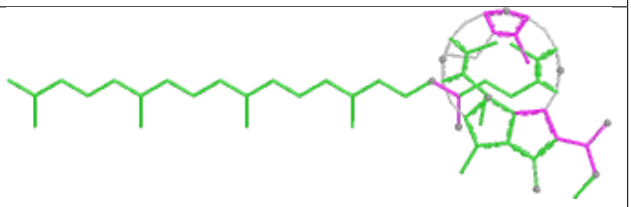
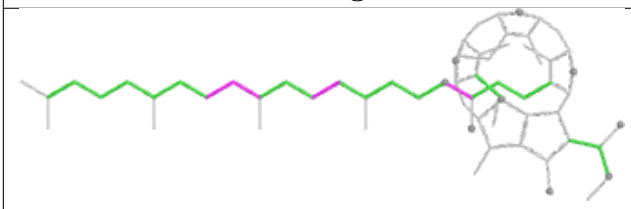


Bond angles



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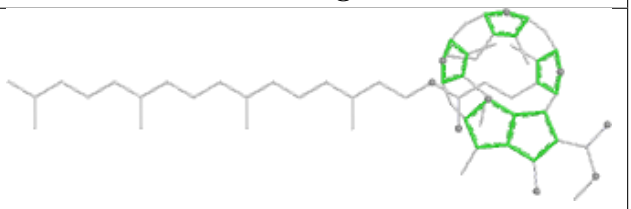
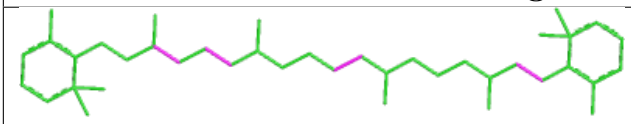


Rings

Ligand BCR c 517



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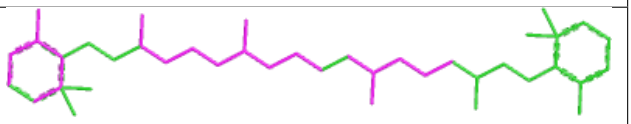
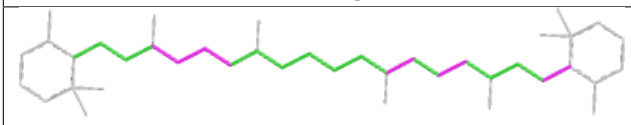
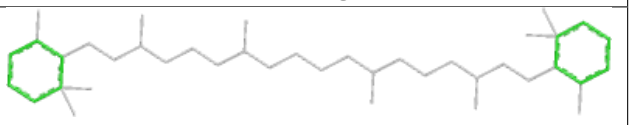


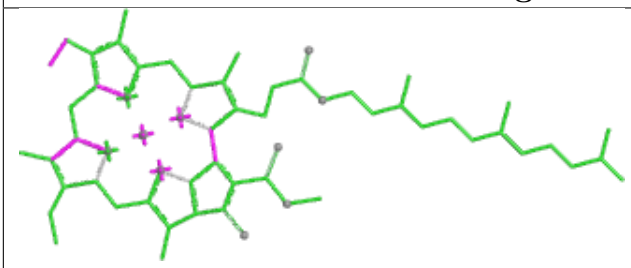
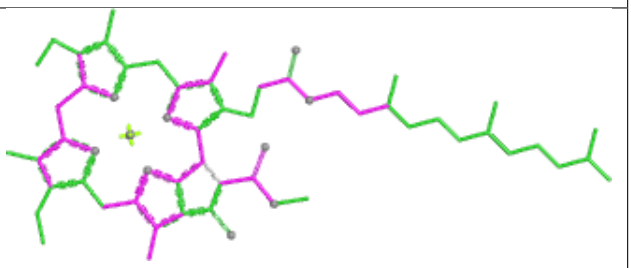
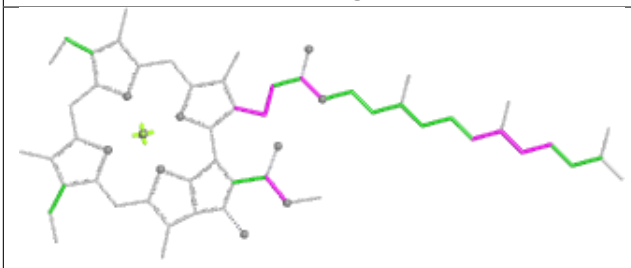
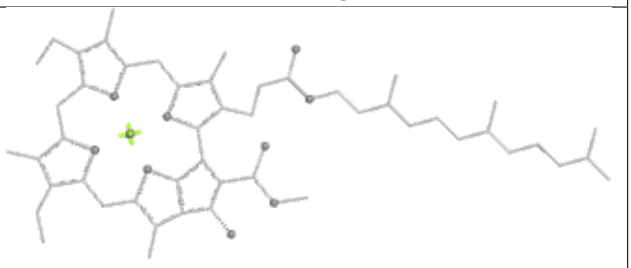
Bond angles

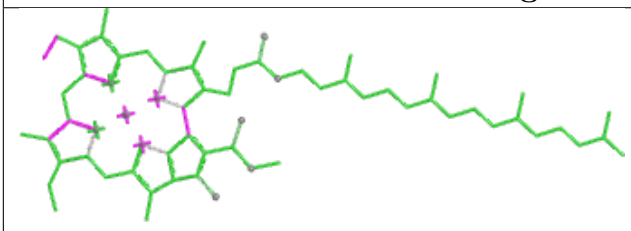
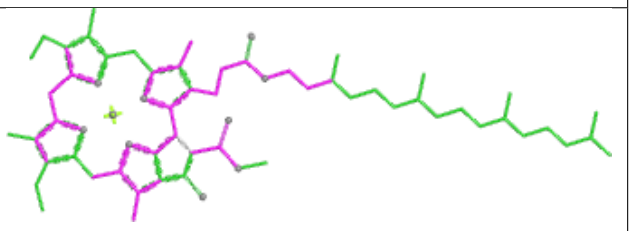
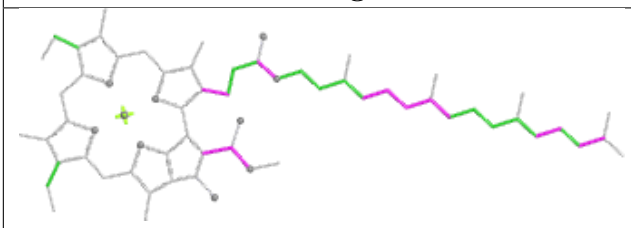
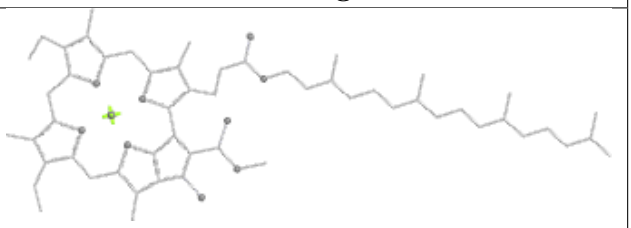


Torsions

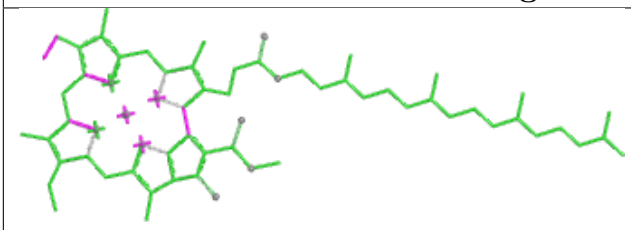


Rings

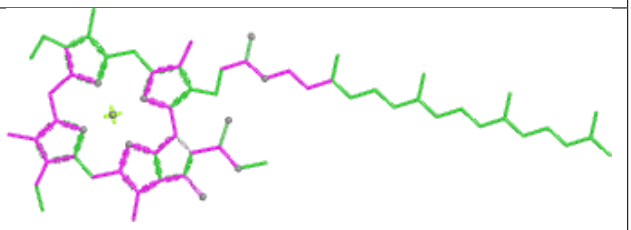
Ligand CLA R1 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA c1 511	
	
Bond lengths	Bond angles
	
Torsions	Rings

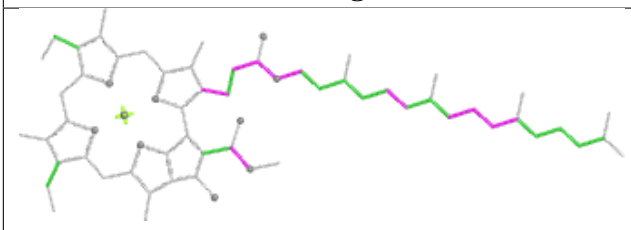
Ligand CLA a1 405



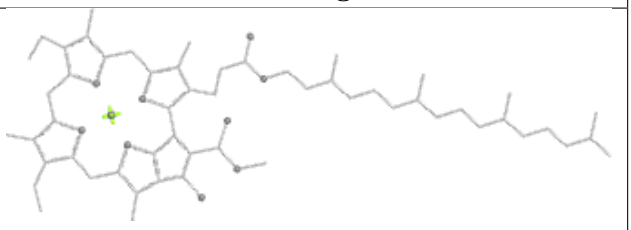
Bond lengths



Bond angles

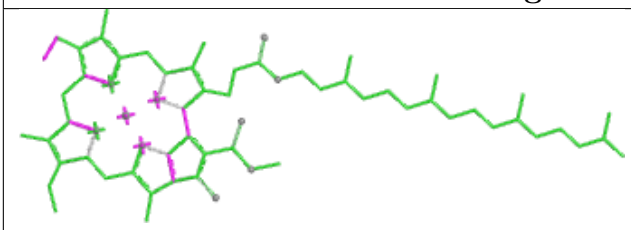


Torsions

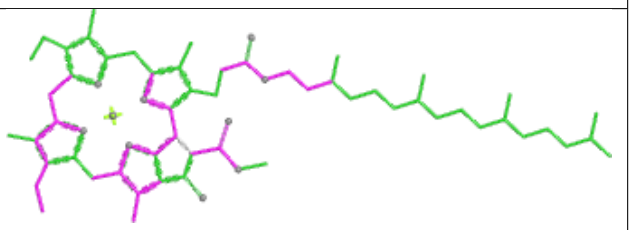


Rings

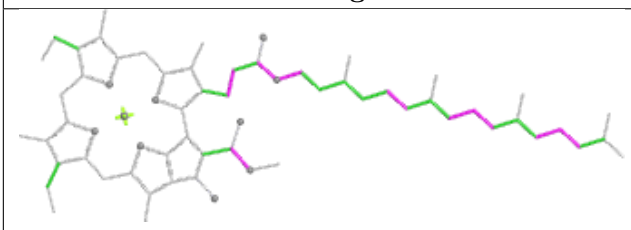
Ligand CLA C 509



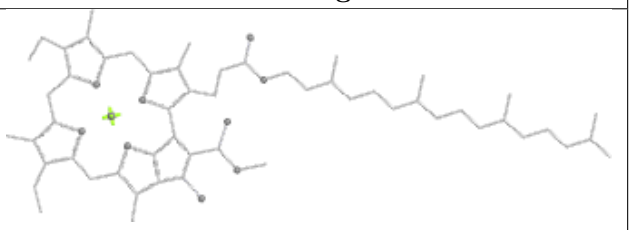
Bond lengths



Bond angles

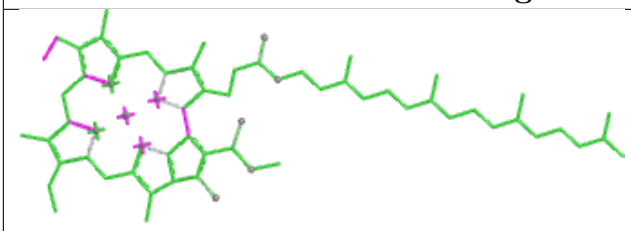


Torsions



Rings

Ligand CLA Y1 610



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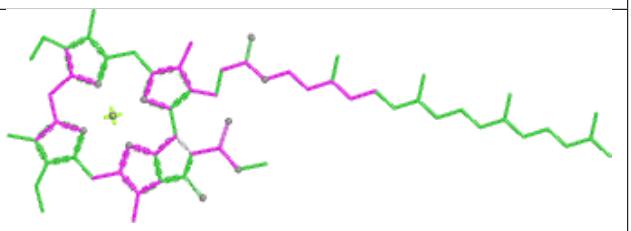
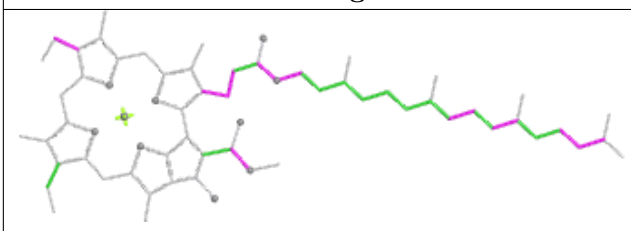
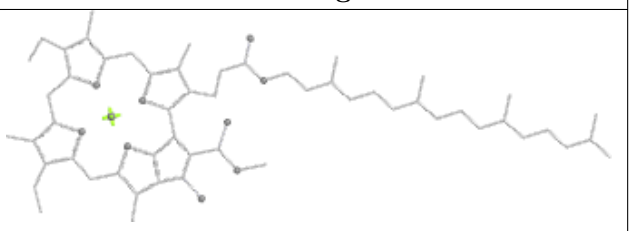


Bond angles

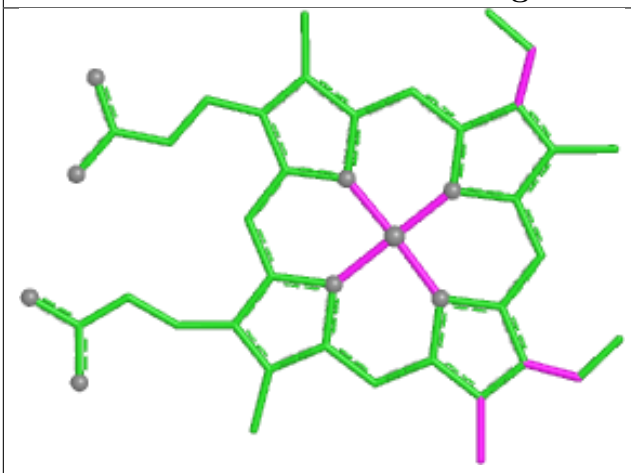


Torsions

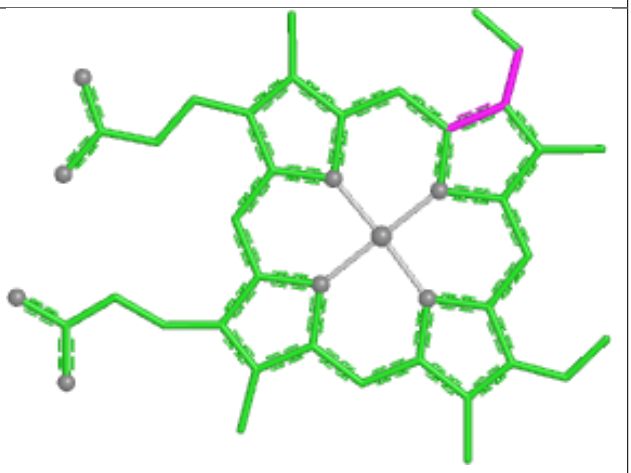


Rings

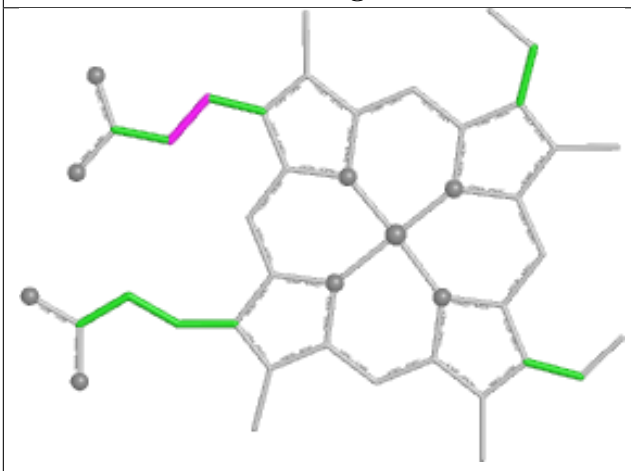
Ligand HEM F1 101



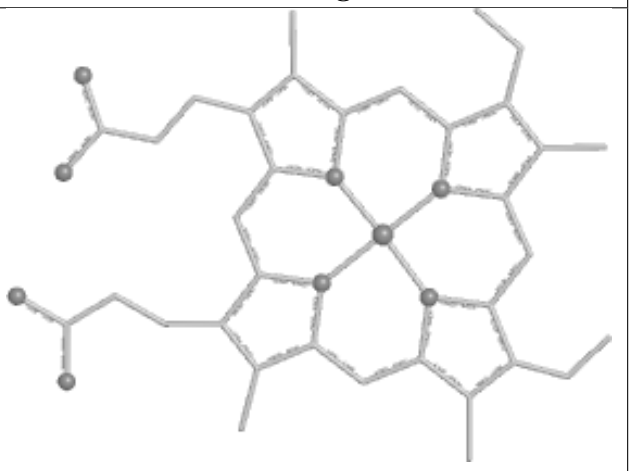
Bond lengths



Bond angles

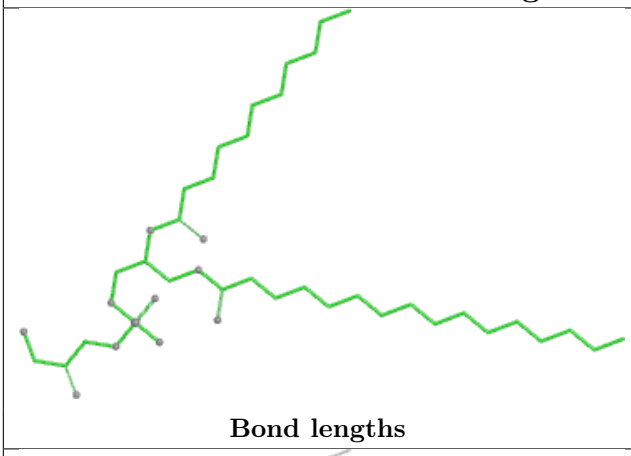


Torsions



Rings

Ligand LHG D 408



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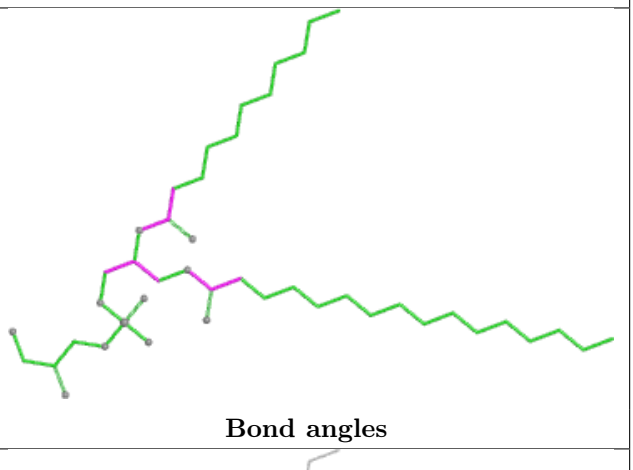
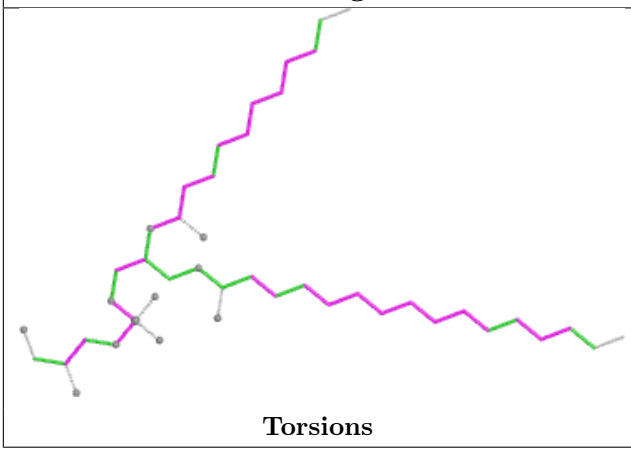


Bond angles



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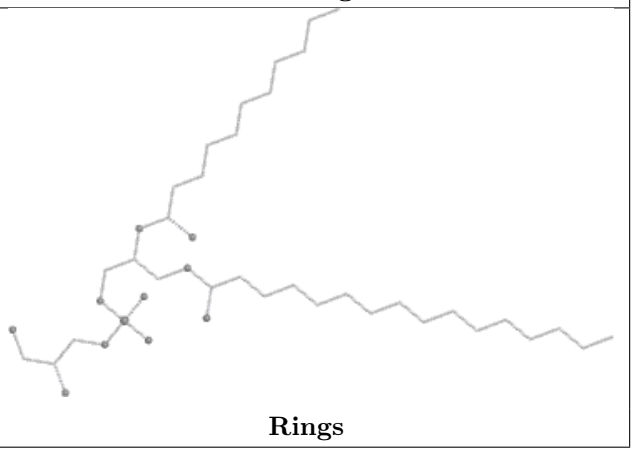
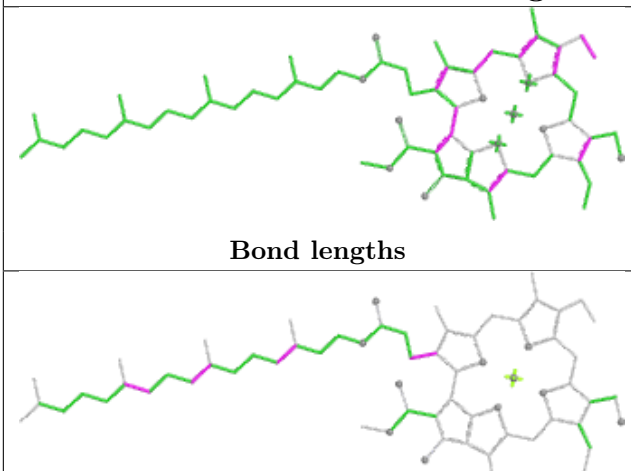


Rings

Ligand CHL y 601



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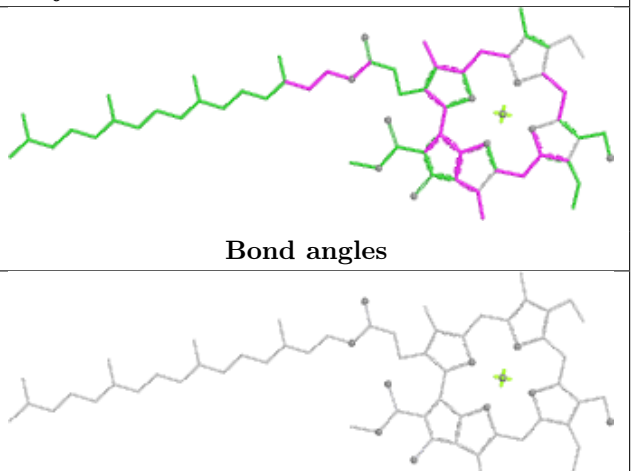
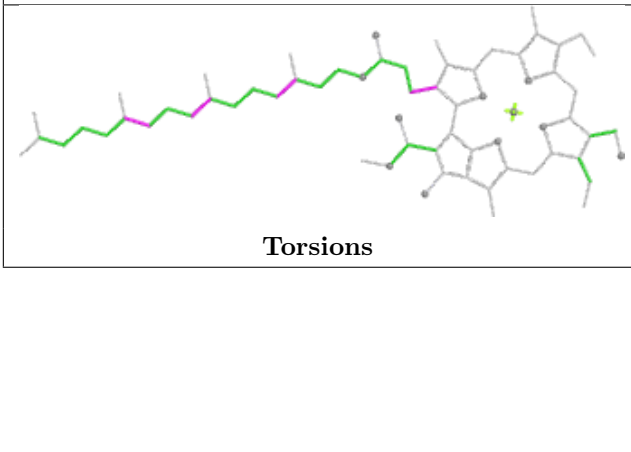


Bond angles



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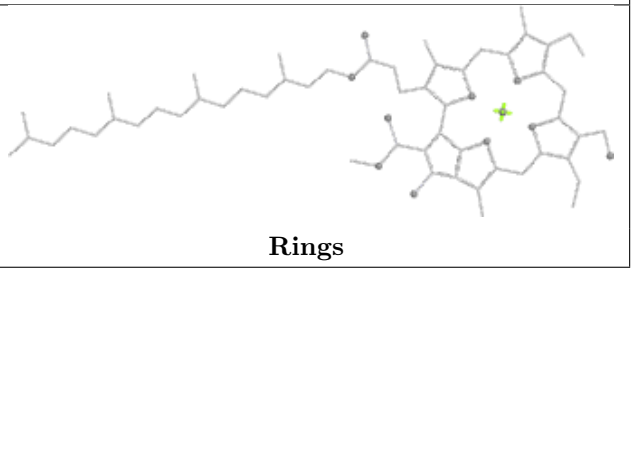
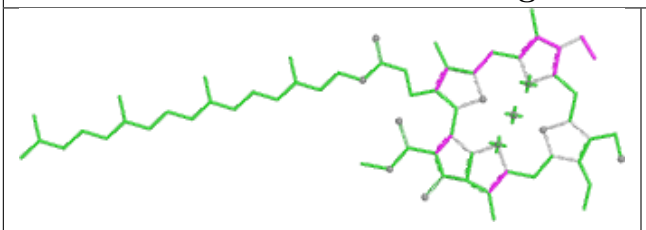


Rings

Ligand CHL y1 606



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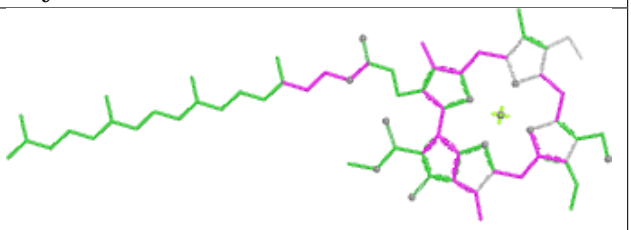
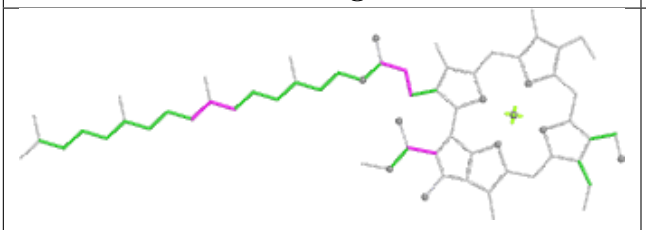


Bond angles



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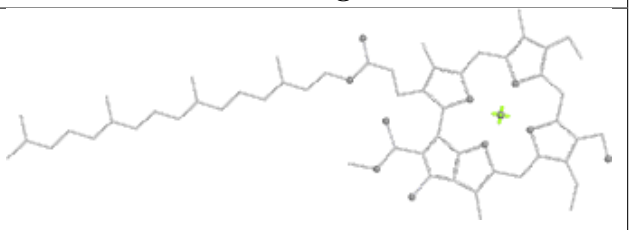
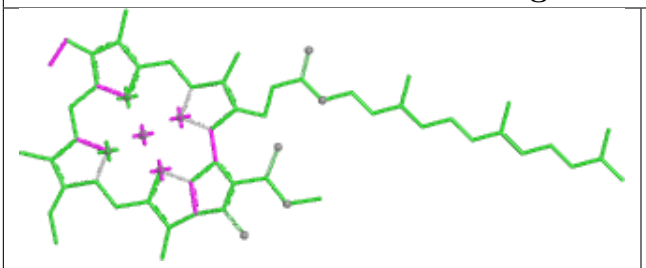


Rings

Ligand CLA r 608



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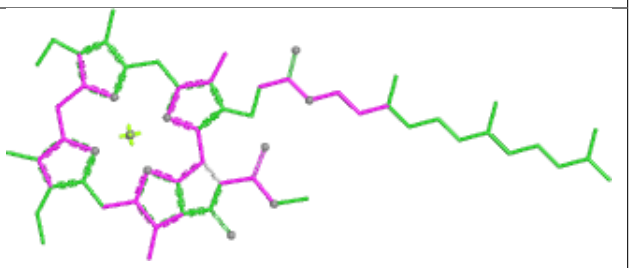
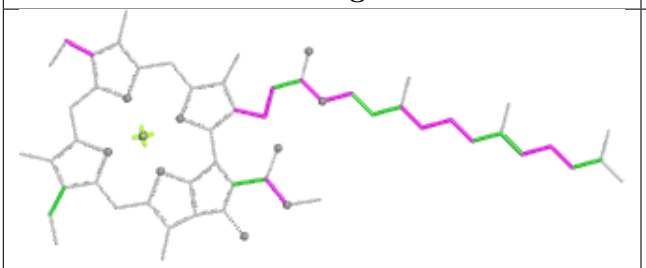


Bond angles



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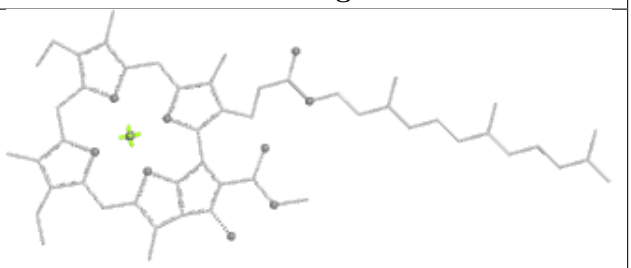
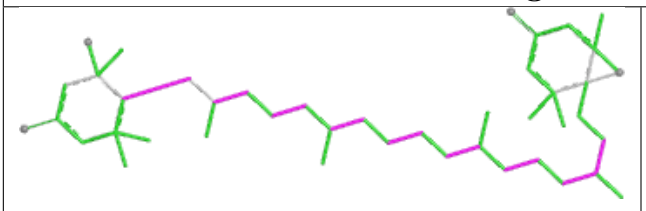


Rings

Ligand NEX y 623



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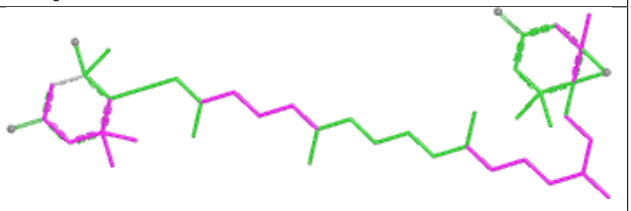
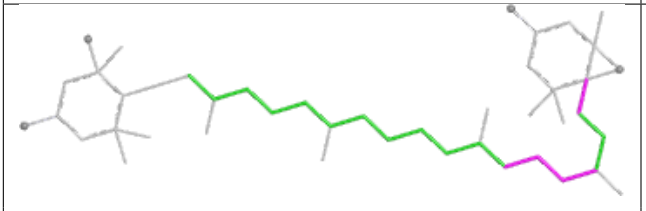
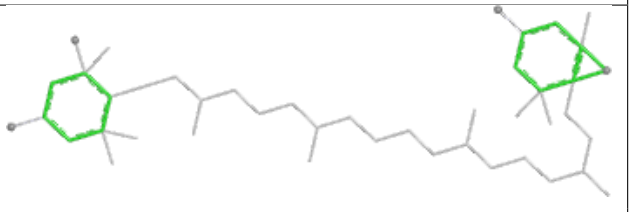


Bond angles

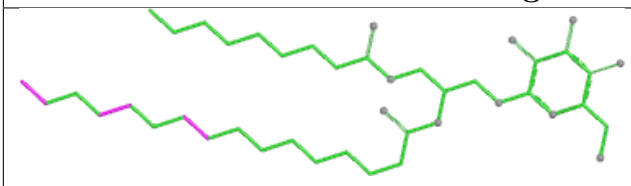


Torsions



Rings

Ligand LMG b 622



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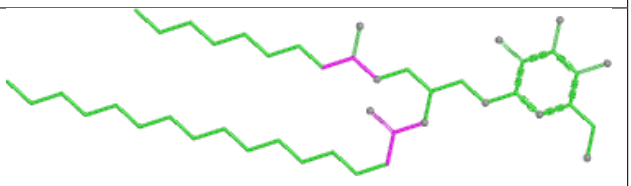
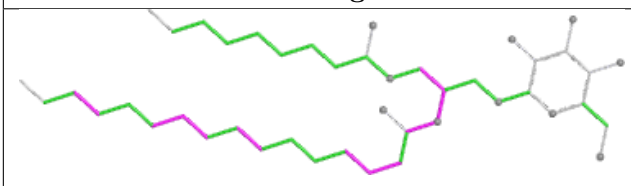
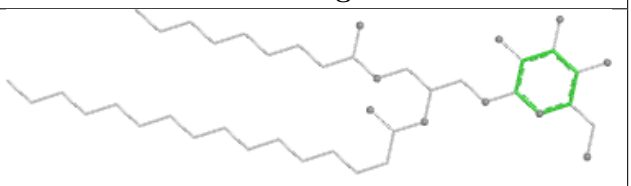


Bond angles

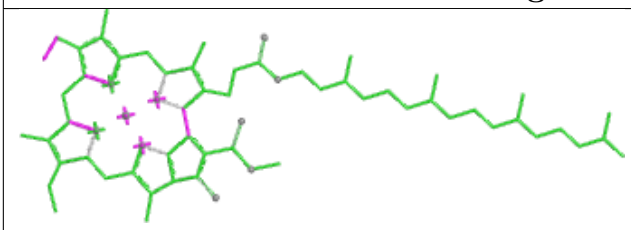


Torsions



Rings

Ligand CLA b 605



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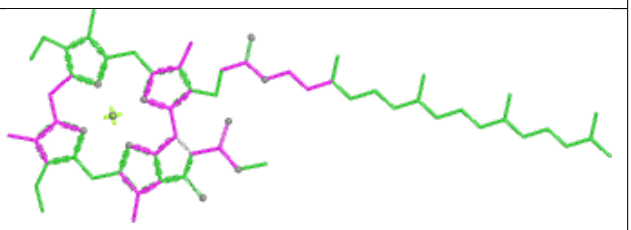
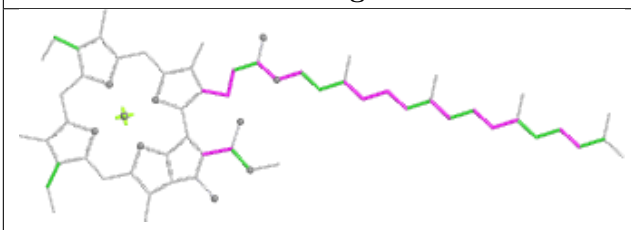


Bond angles



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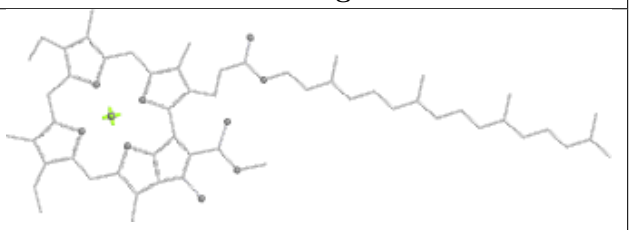
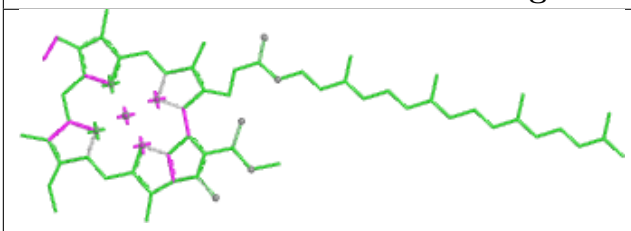


Rings

Ligand CLA c 510



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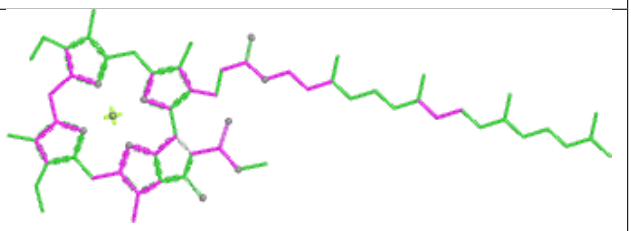
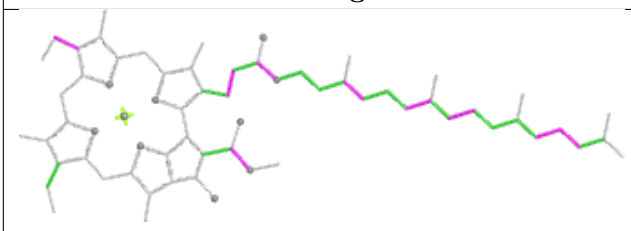
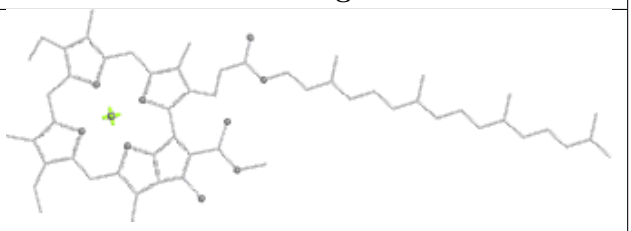


Bond angles

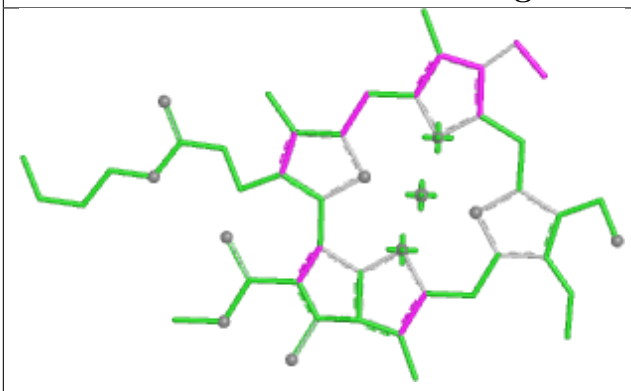


Torsions



Rings

Ligand CHL R1 607



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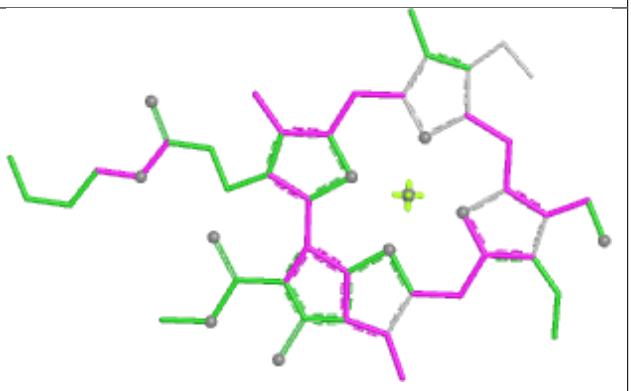
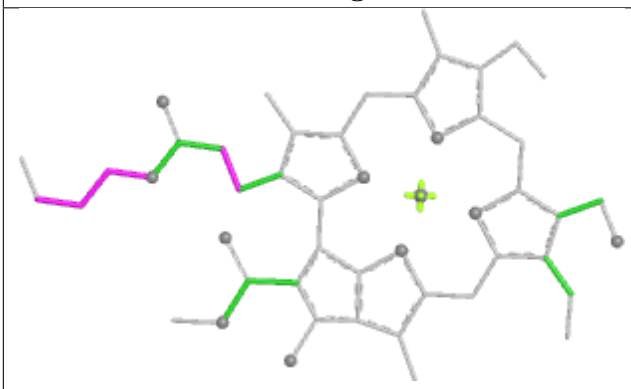
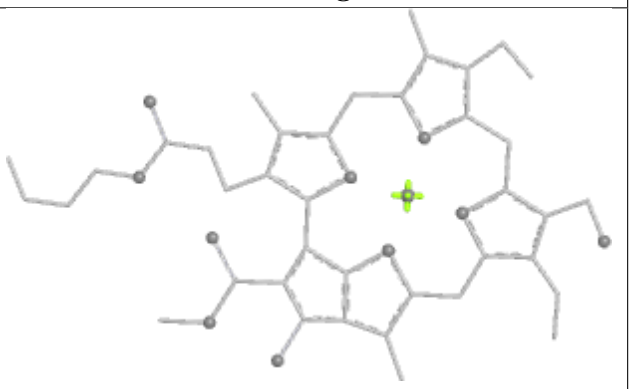


Bond angles

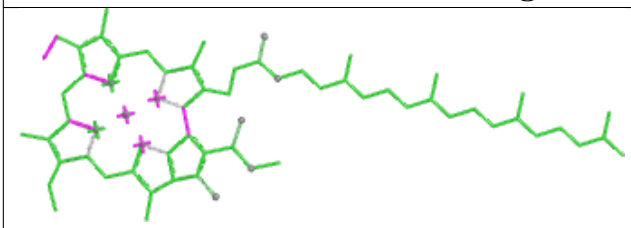


Torsions



Rings

Ligand CLA y1 613



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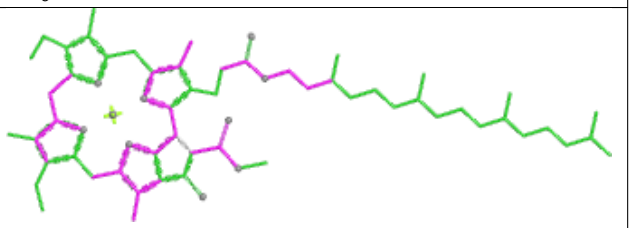

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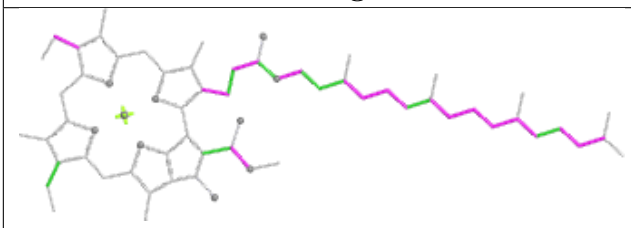

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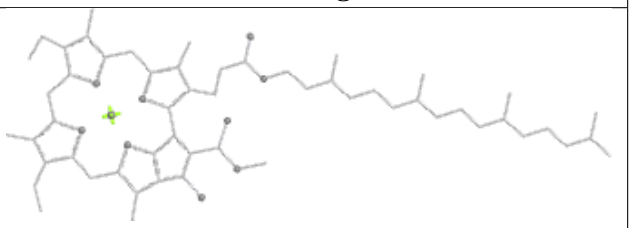
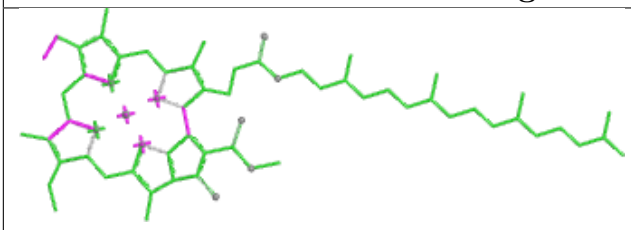


Rings

Ligand CLA b1 616



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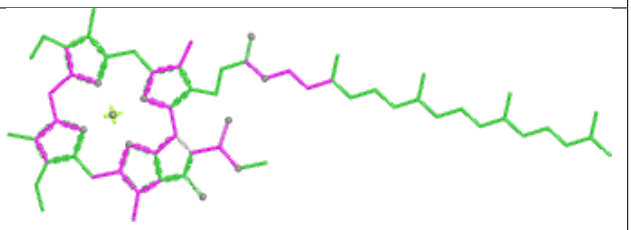
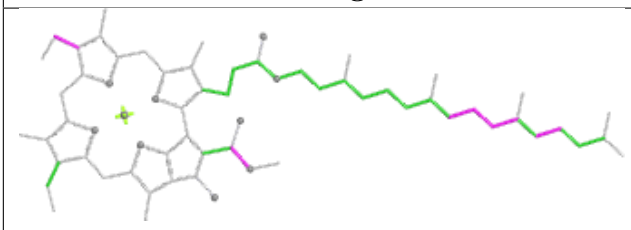


Bond angles



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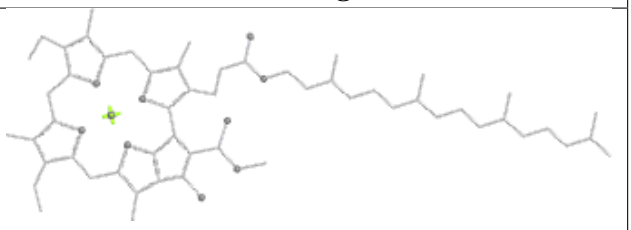
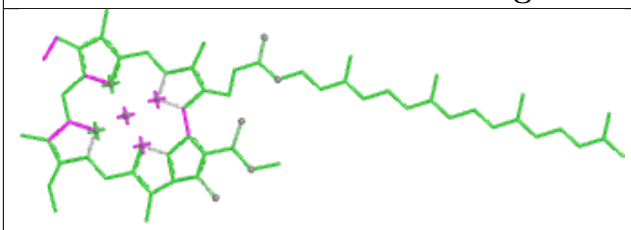
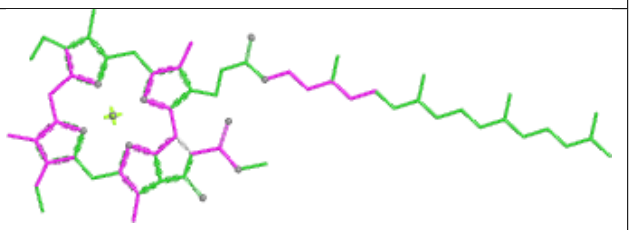


Rings

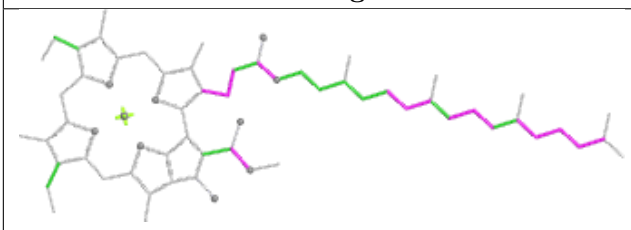
Ligand CLA G1 602



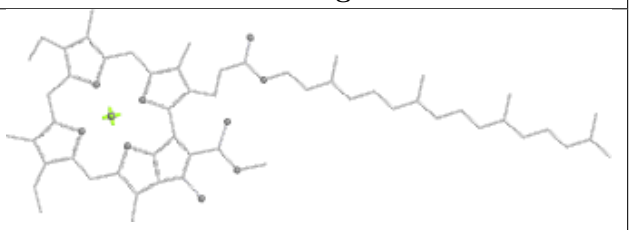
Bond lengths



Bond angles

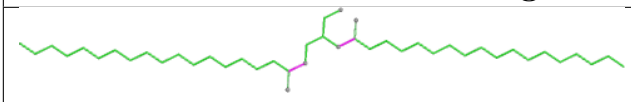


Torsions

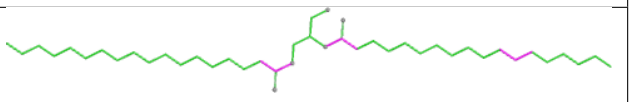


Rings

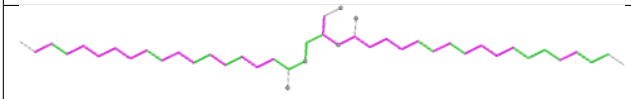
Ligand DGA B 625



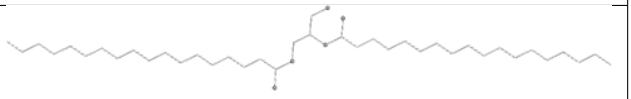
Bond lengths



Bond angles

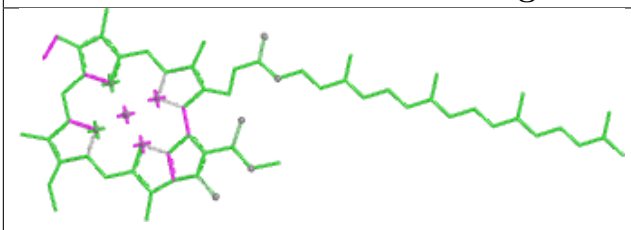


Torsions

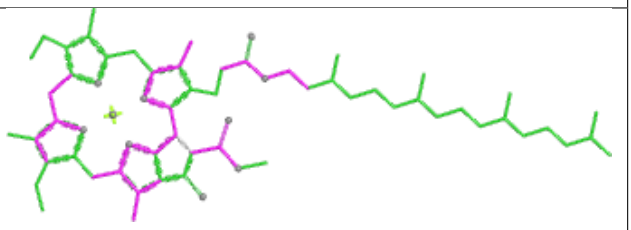


Rings

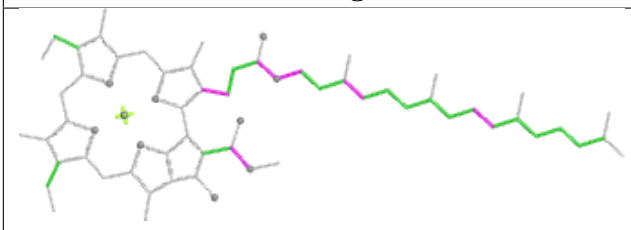
Ligand CLA b1 606



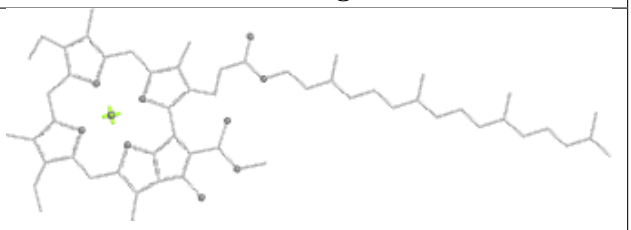
Bond lengths



Bond angles

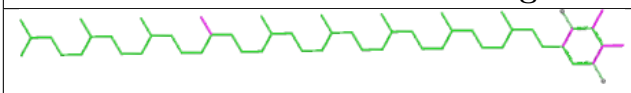


Torsions



Rings

Ligand PL9 D1 405



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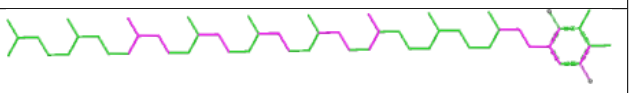

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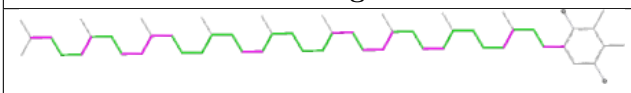

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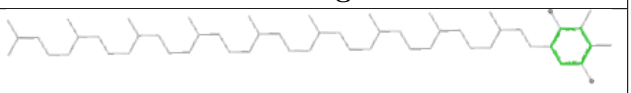
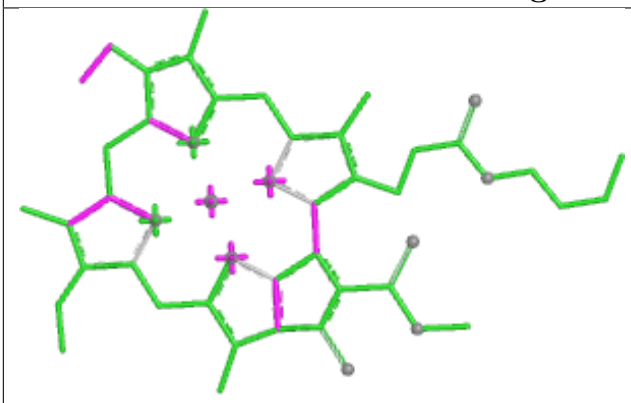


Rings

Ligand CLA r 604



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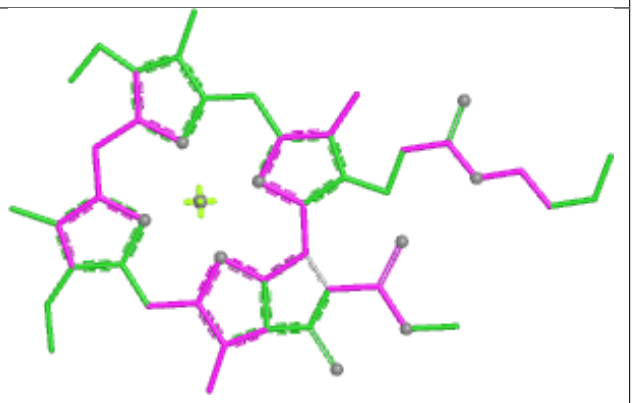

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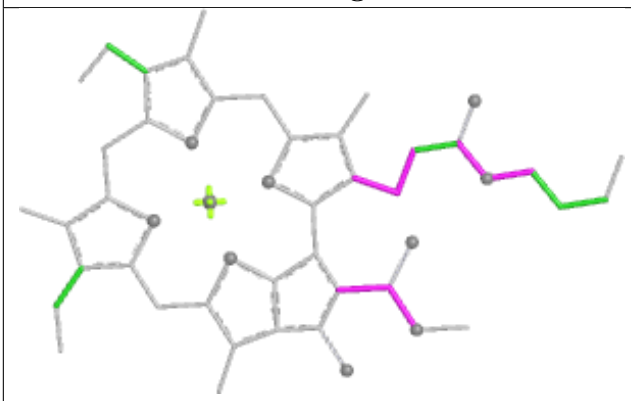

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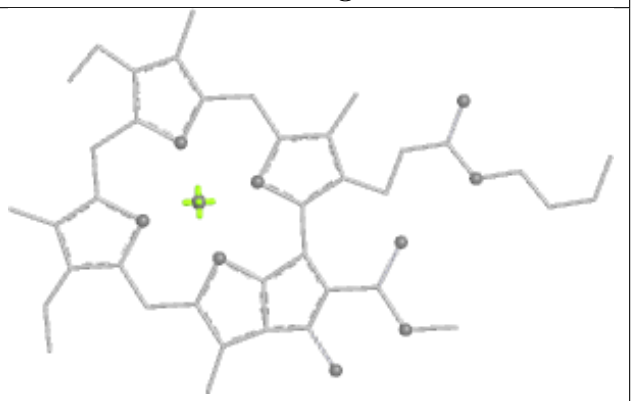
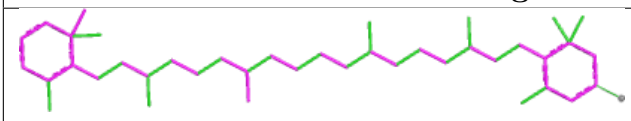


Rings

Ligand RRX H1 101



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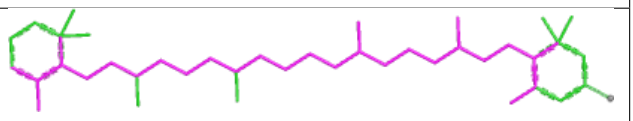

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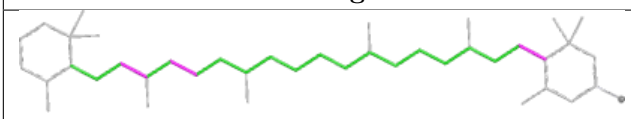

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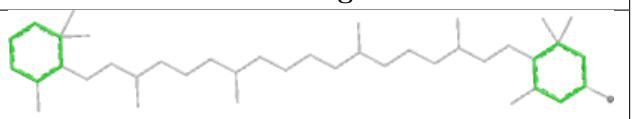
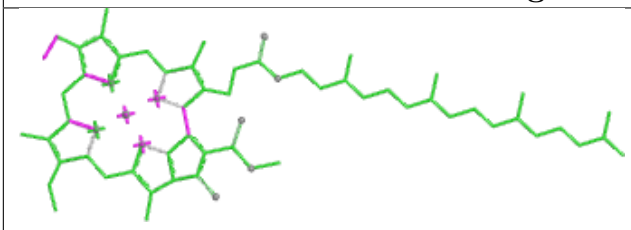


Rings

Ligand CLA b 608



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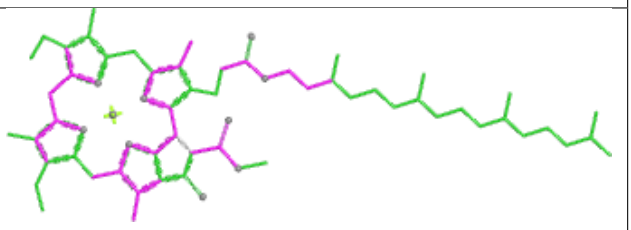

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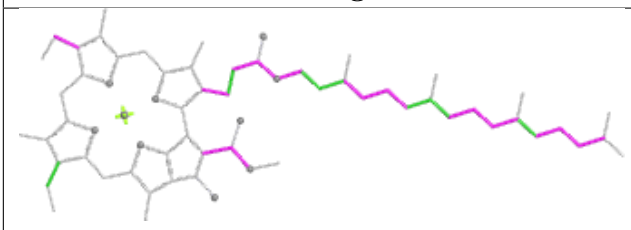

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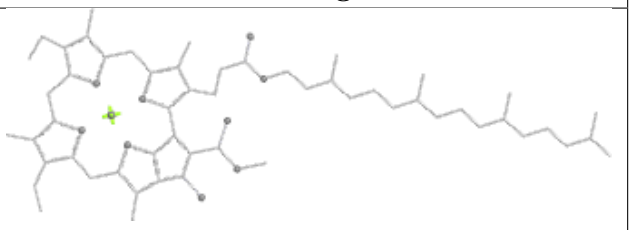
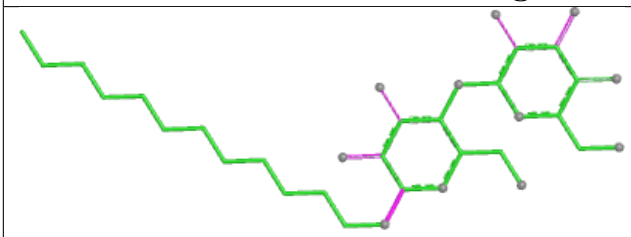


Rings

Ligand LMT R1 625



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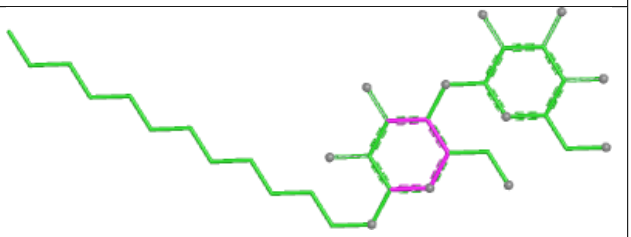

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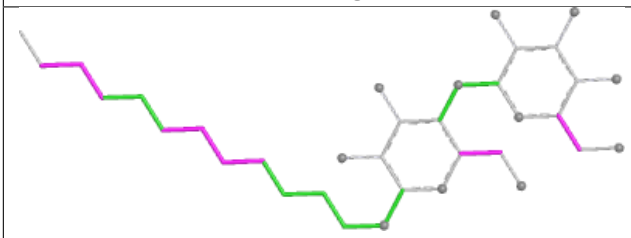

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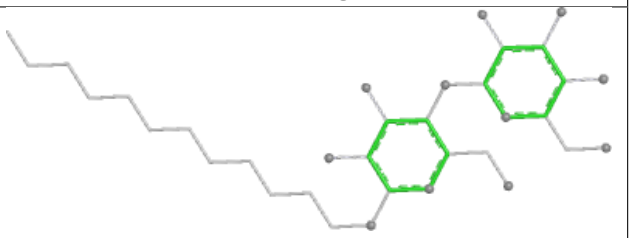
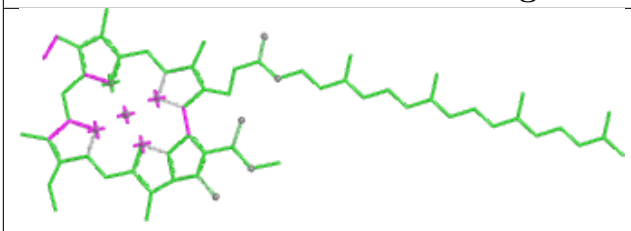


Rings

Ligand CLA g1 603



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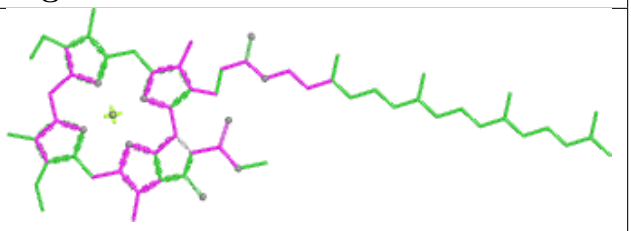

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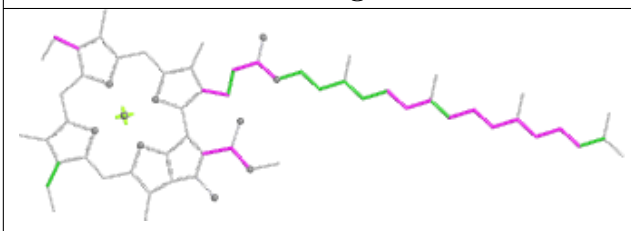

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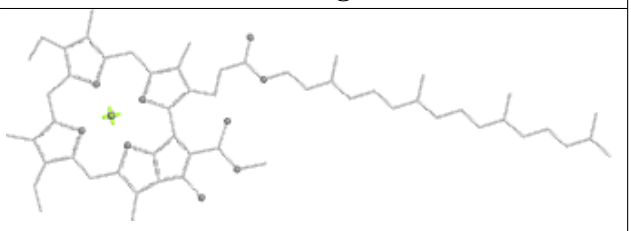
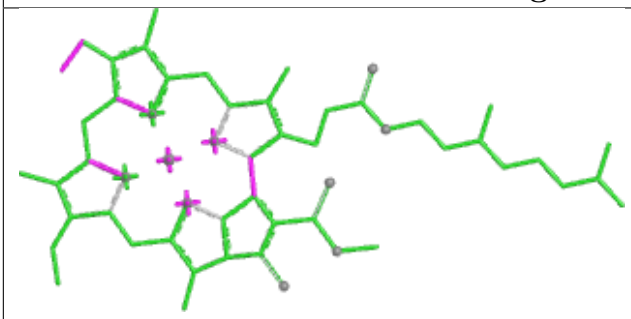


Rings

Ligand CLA s 604



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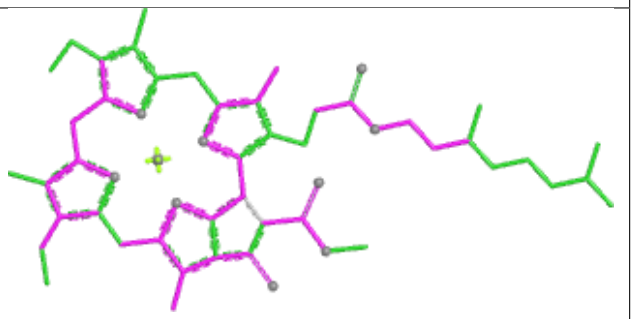

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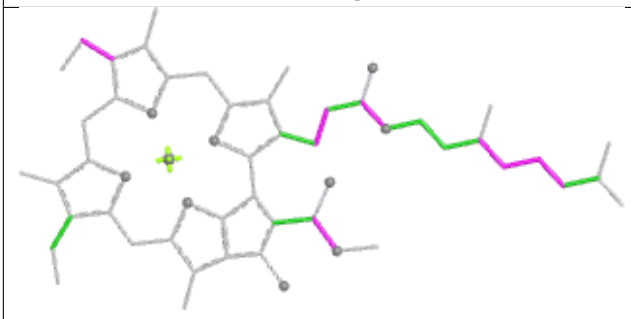

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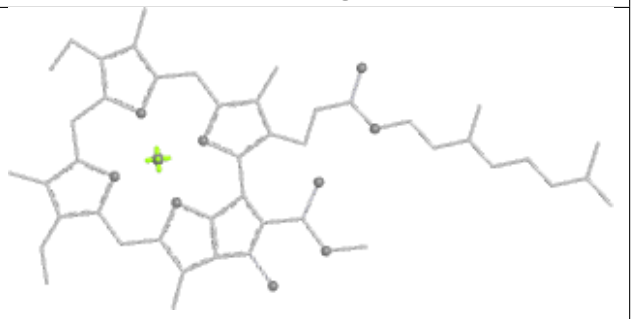
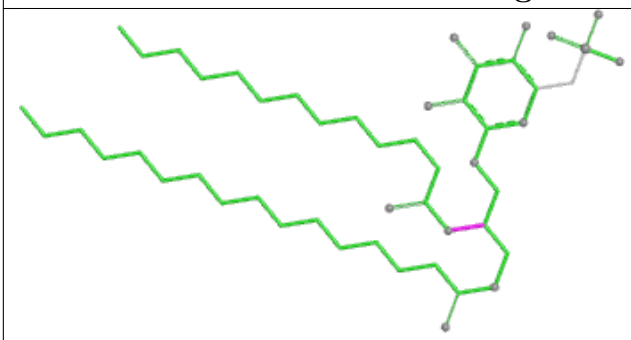


Rings

Ligand SQD A1 412



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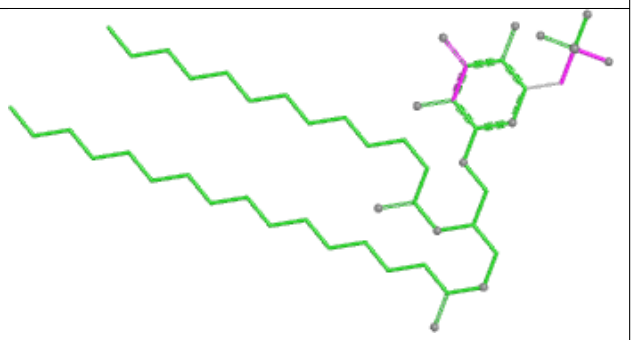

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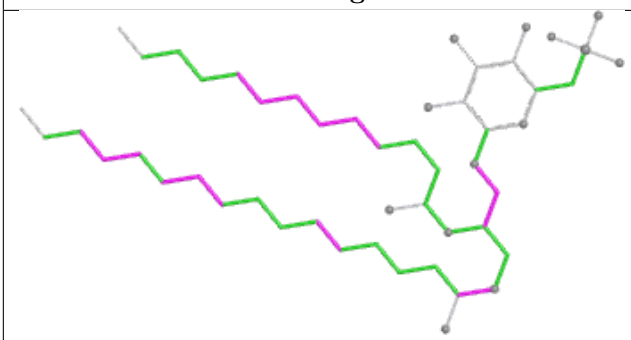

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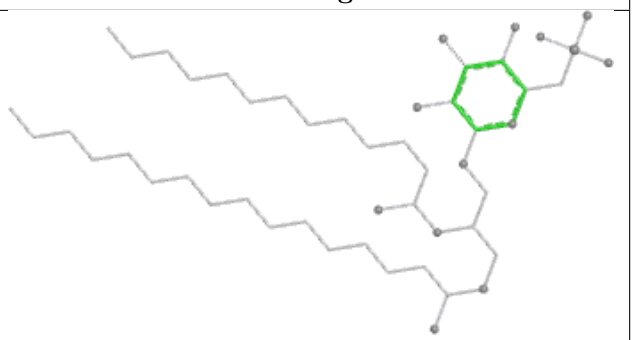
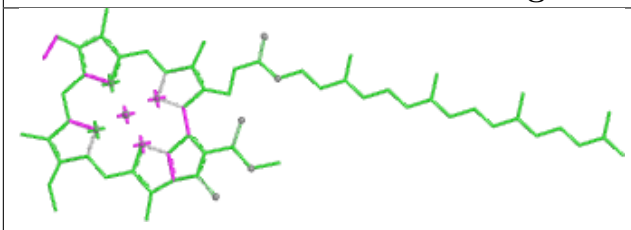


Rings

Ligand CLA y 611



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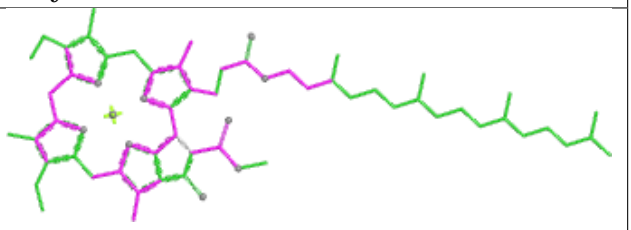

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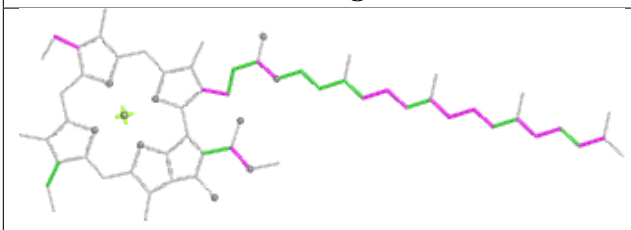

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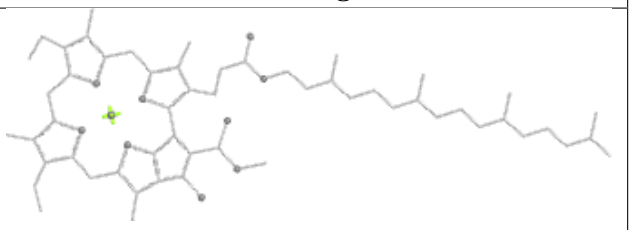
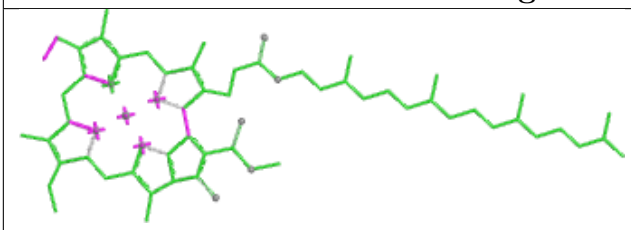


Rings

Ligand CLA b1 610



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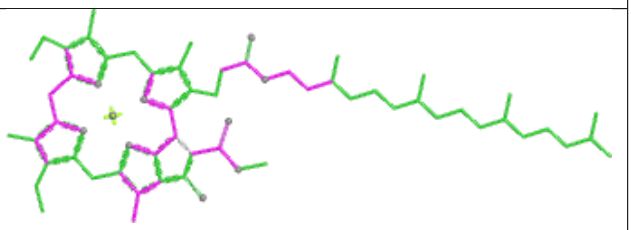

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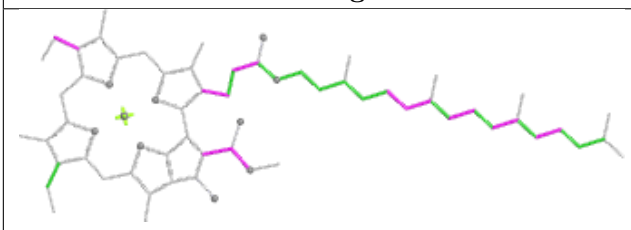

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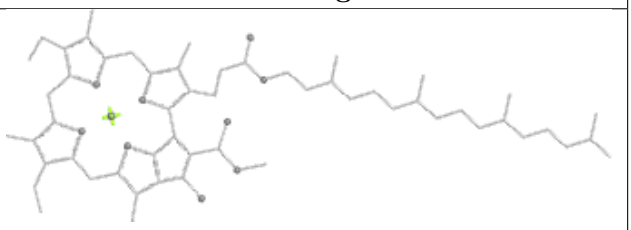
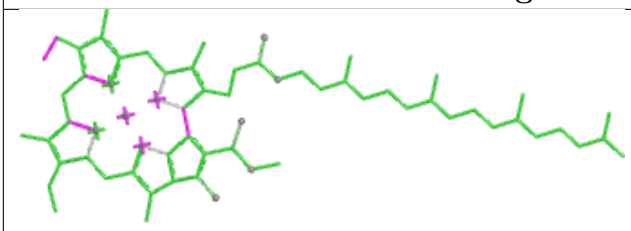


Rings

Ligand CLA B1 605



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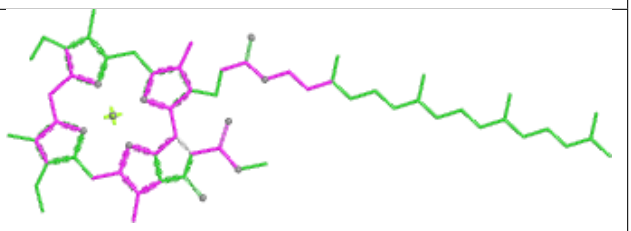
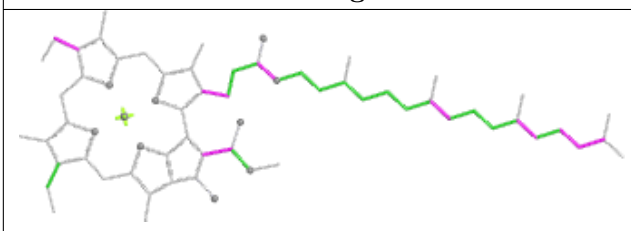
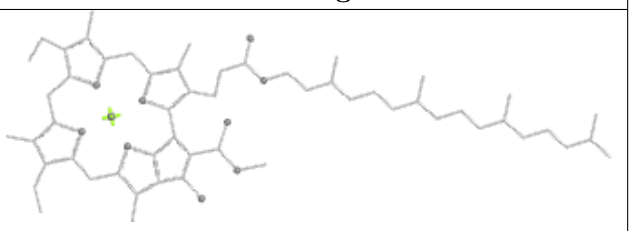


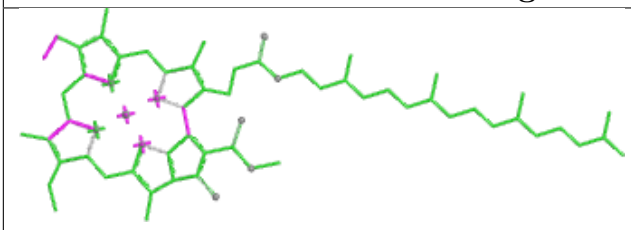
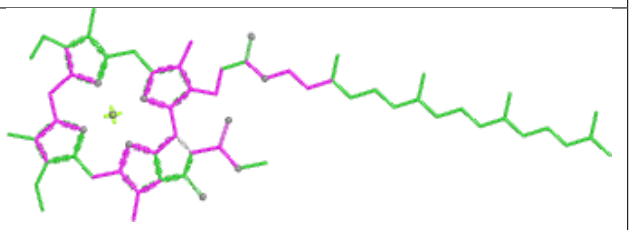
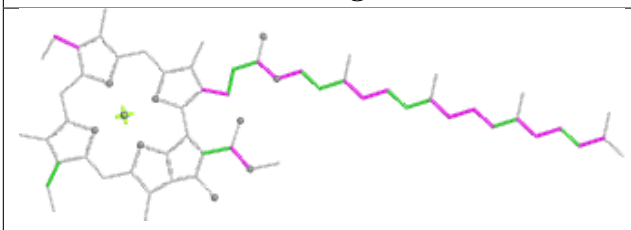
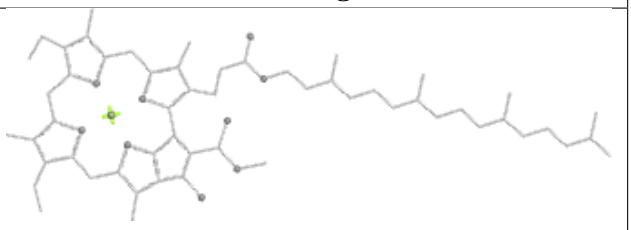
Bond angles

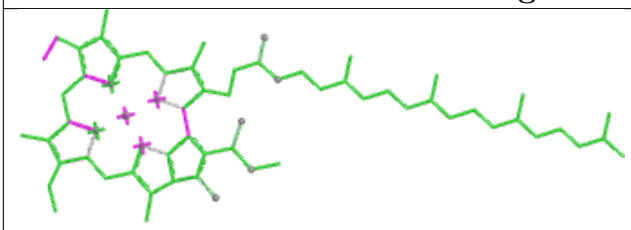
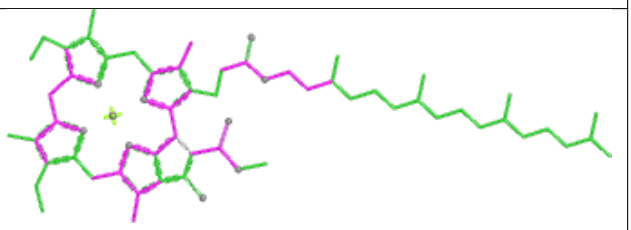
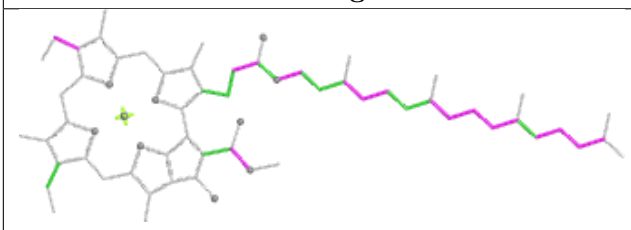
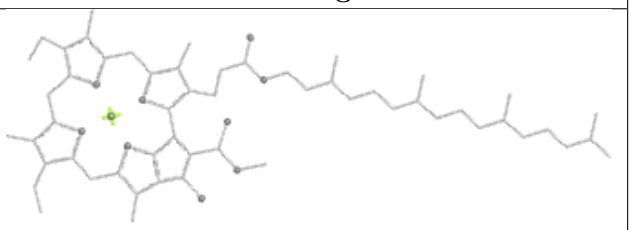


Torsions

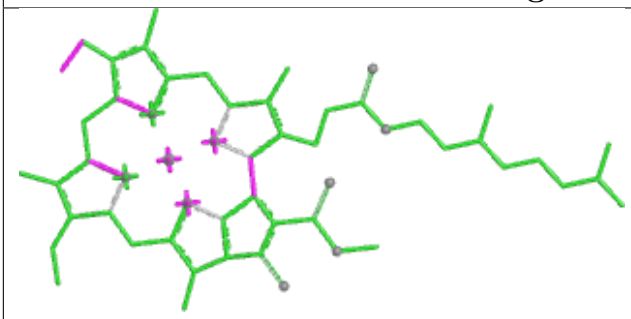


Rings

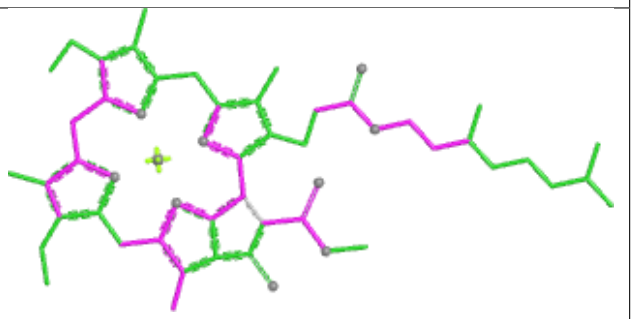
Ligand CLA n1 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b1 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA S 614



Bond lengths



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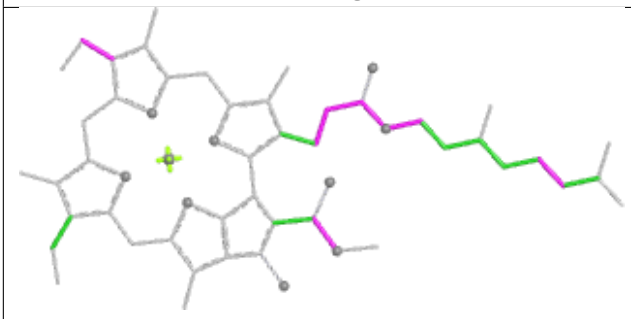

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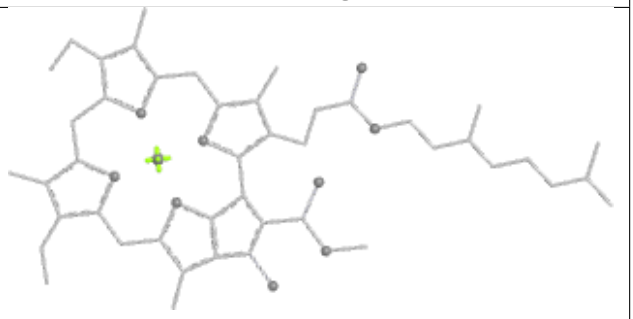
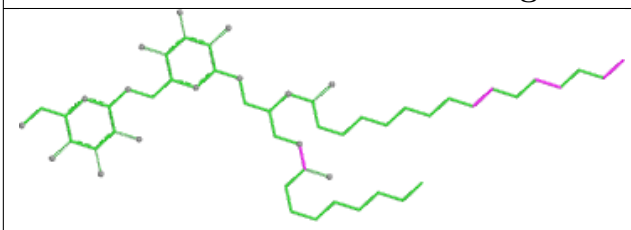


Rings

Ligand DGD C 518



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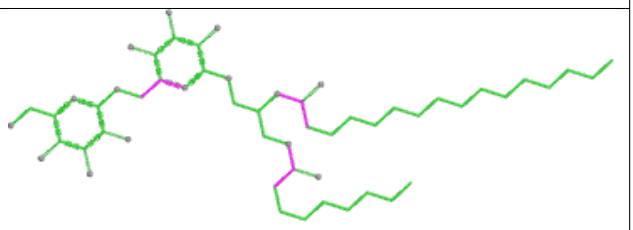

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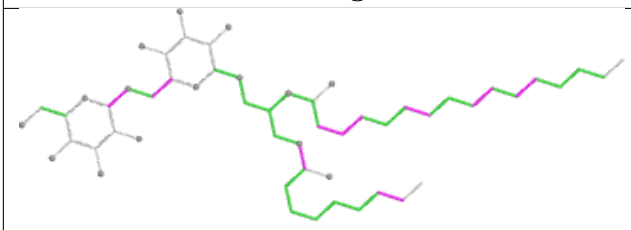

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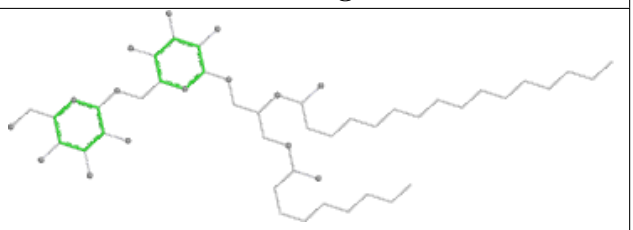
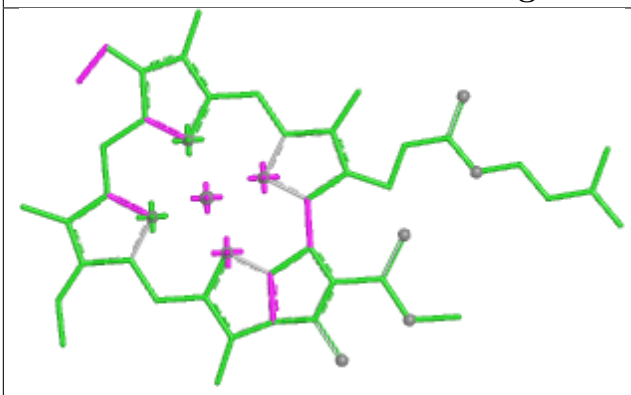


Rings

Ligand CLA S1 605



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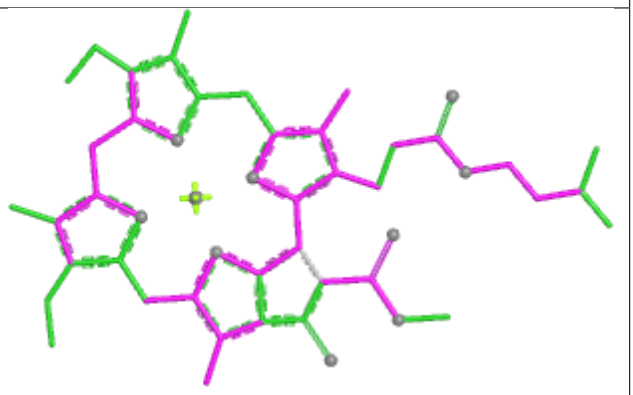

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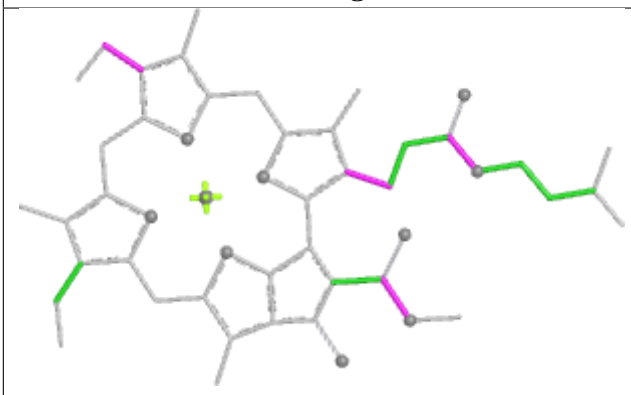

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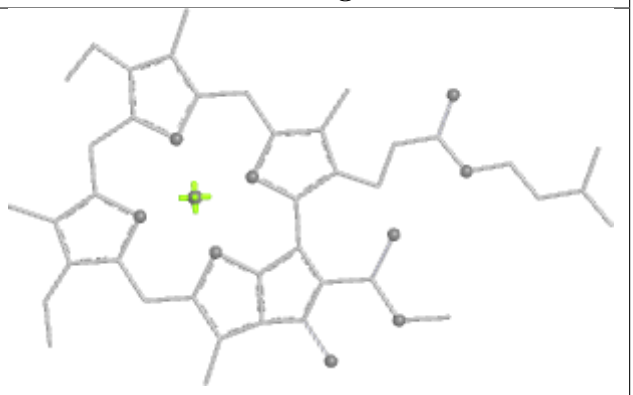
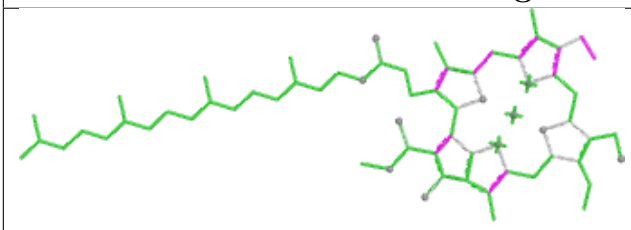


Rings

Ligand CHL Y1 606



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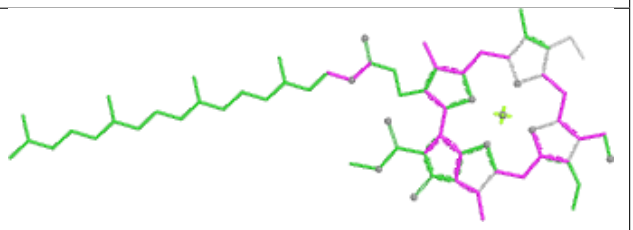

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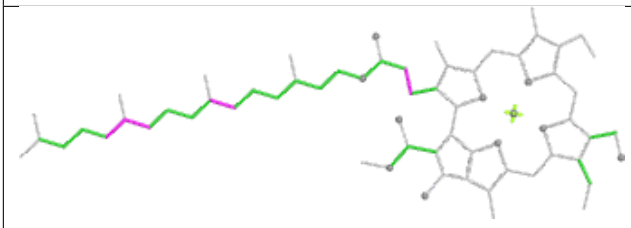

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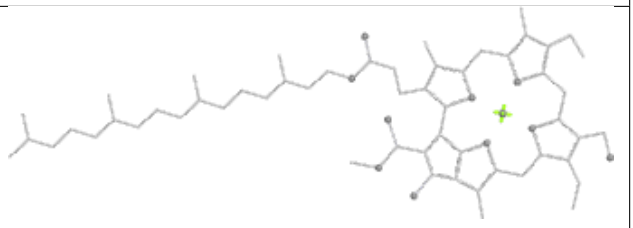
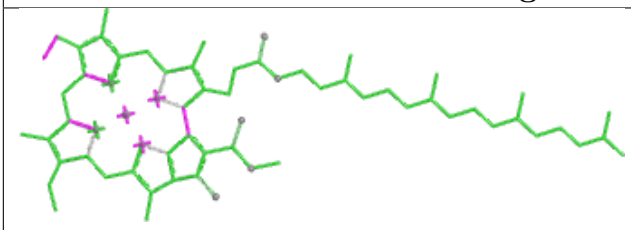


Rings

Ligand CLA g1 611



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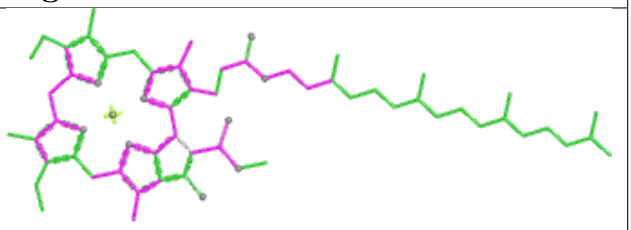

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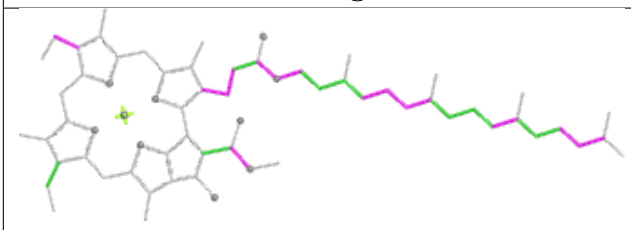

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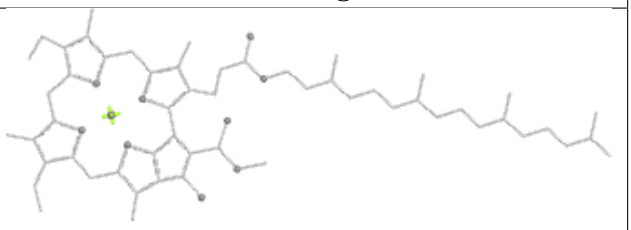
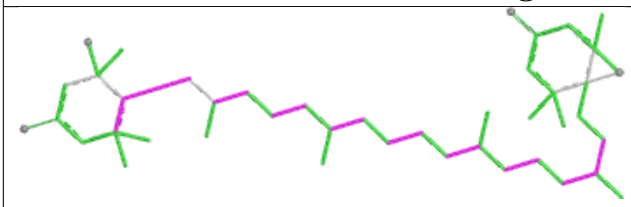


Rings

Ligand NEX g1 623



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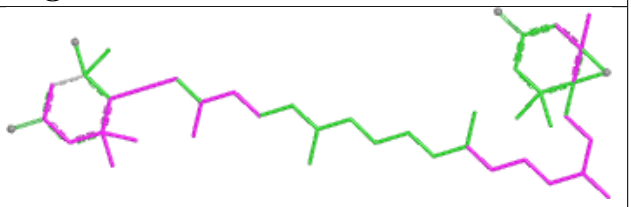
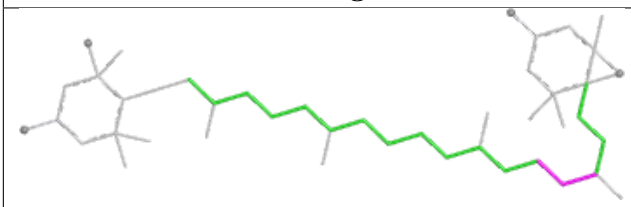


Bond angles



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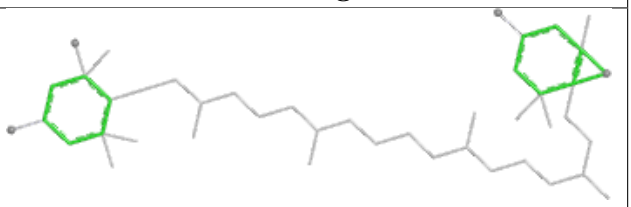
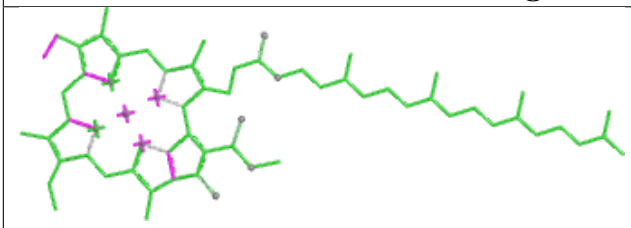


Rings

Ligand CLA B 617



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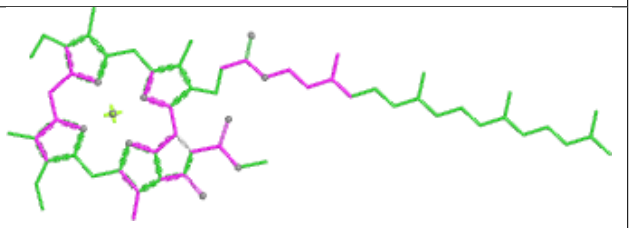
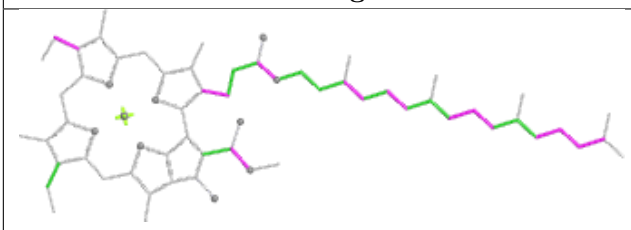


Bond angles



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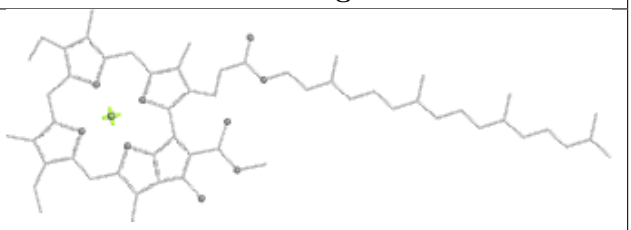
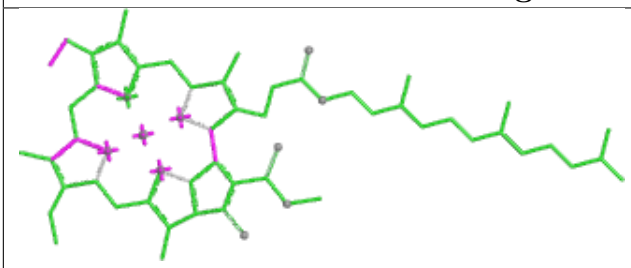
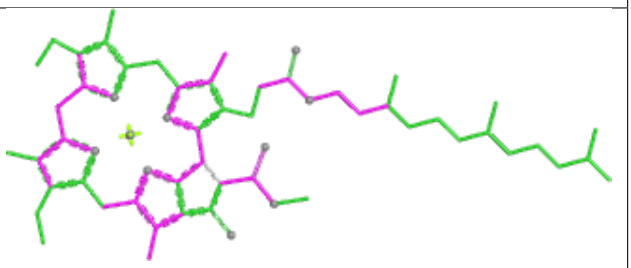


Rings

Ligand CLA R1 608	
	
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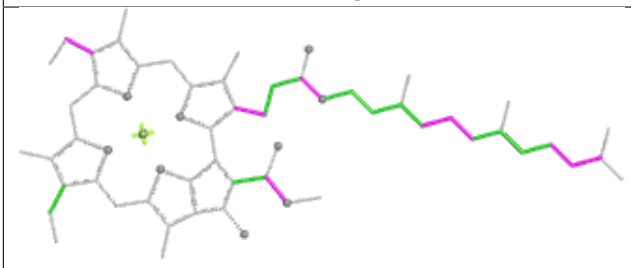
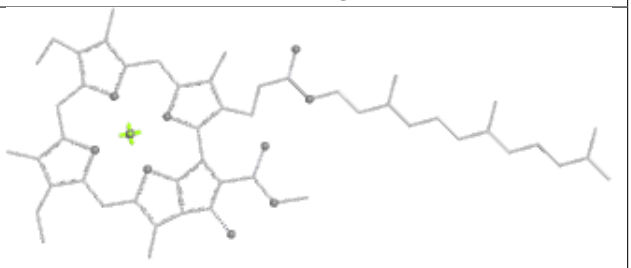
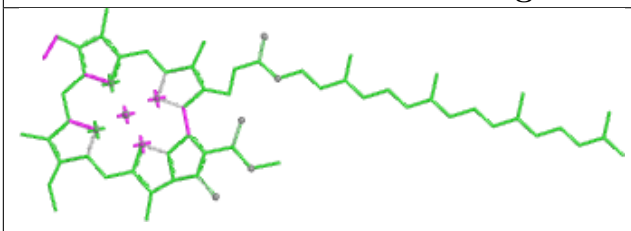
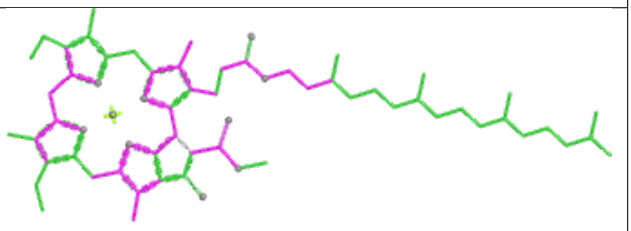
	
Torsions	**Rings**

Ligand CLA B1 603	
	
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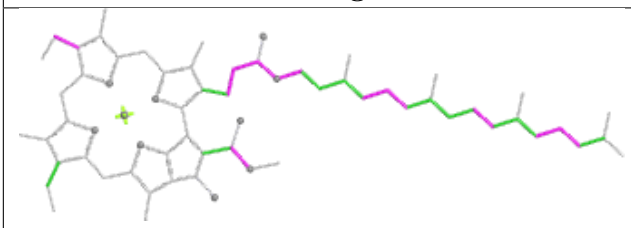
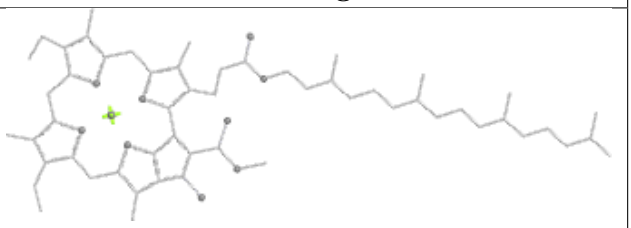
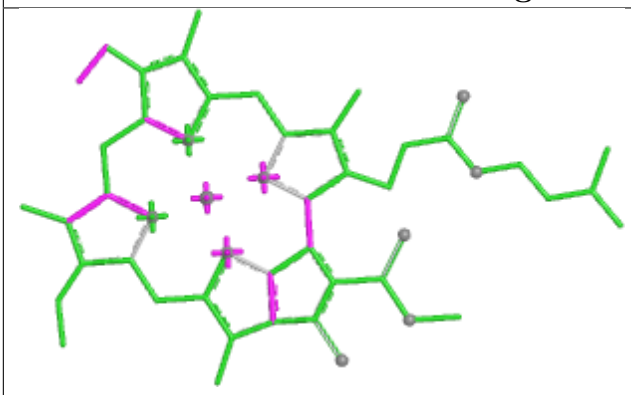
	
Torsions	**Rings**

Ligand CLA Y1 608



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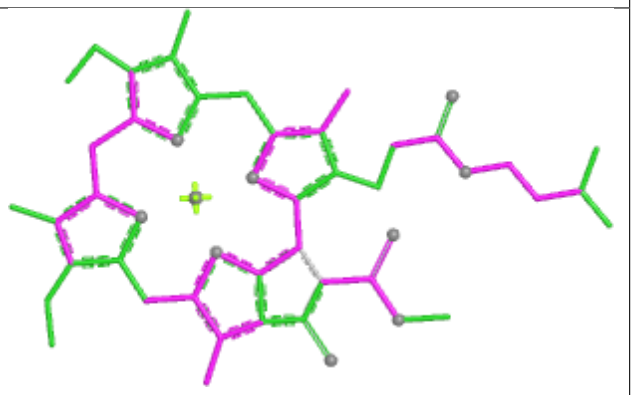
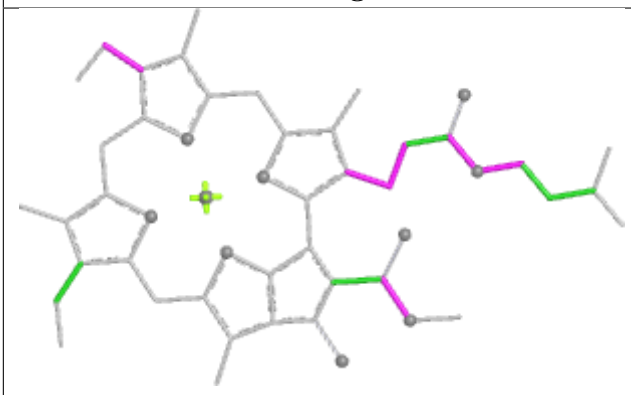
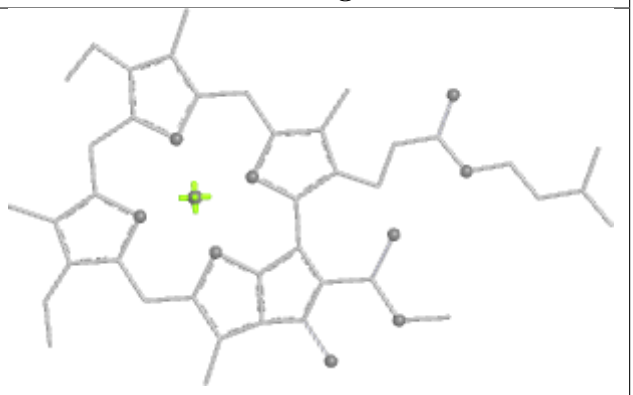


Bond angles

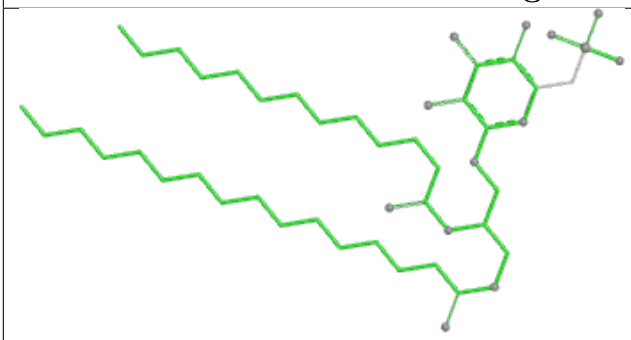


Torsions



Rings

Ligand SQD A 412



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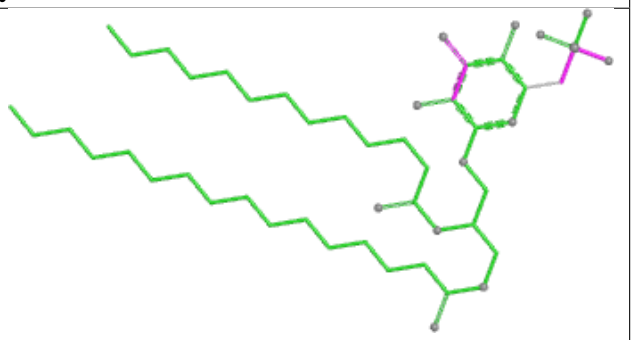
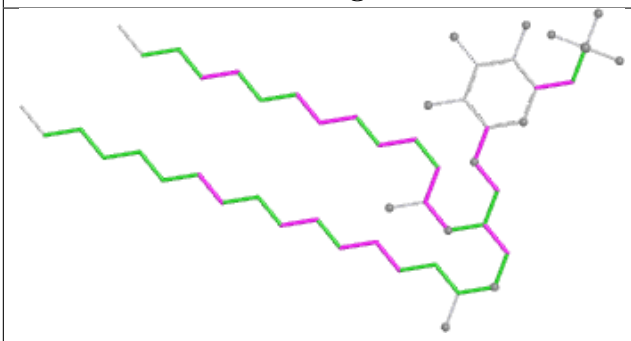


Bond angles



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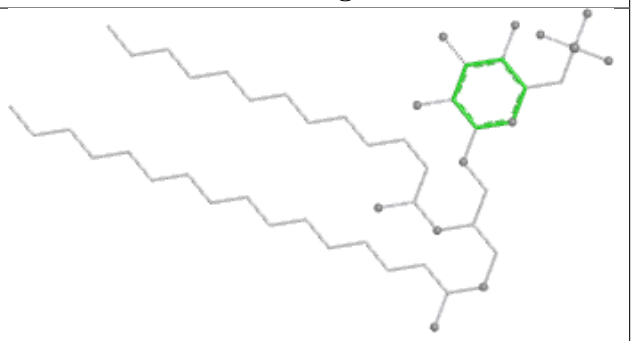
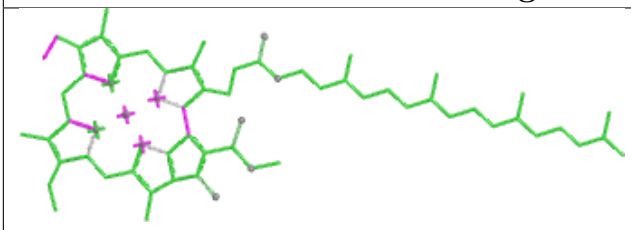


Rings

Ligand CLA S1 603



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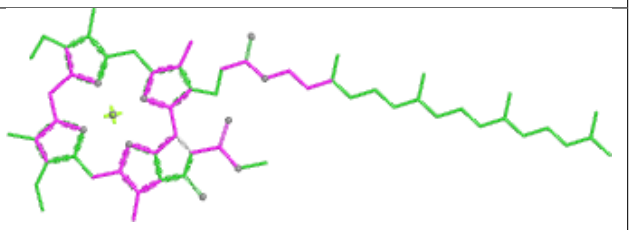
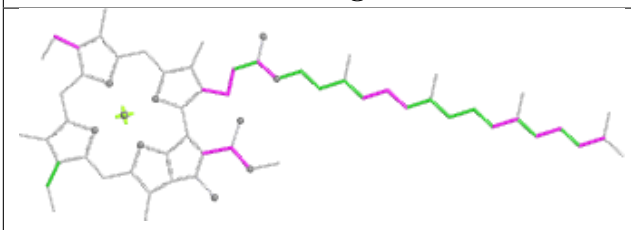


Bond angles



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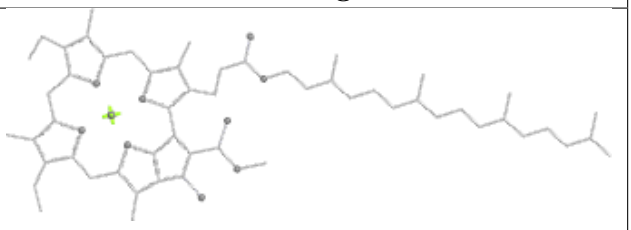
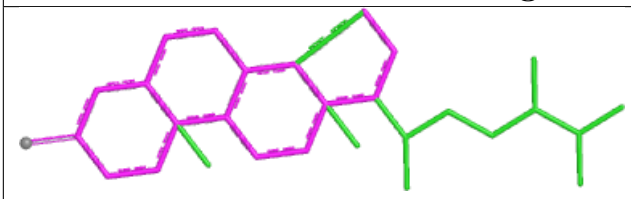
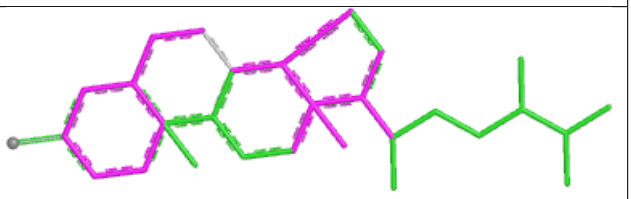


Rings

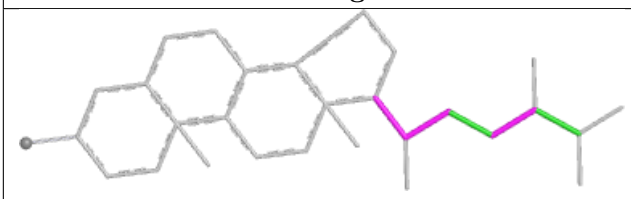
Ligand ERG r1 626



Bond lengths



Bond angles



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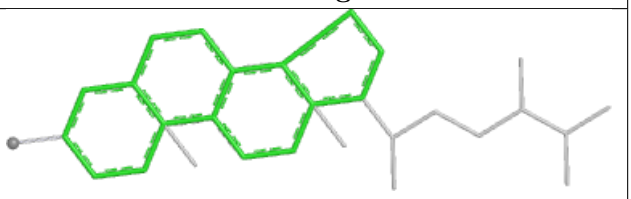
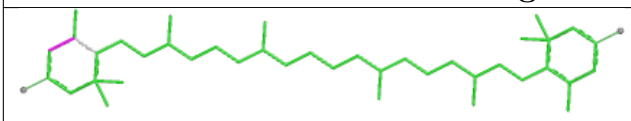


Rings

Ligand LUT n1 620



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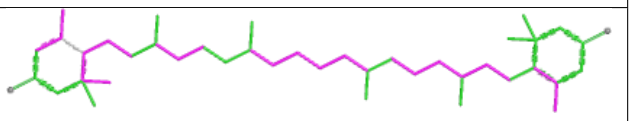
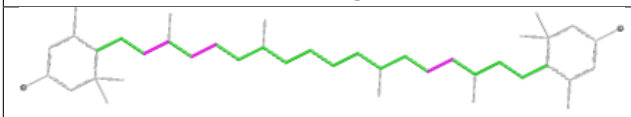
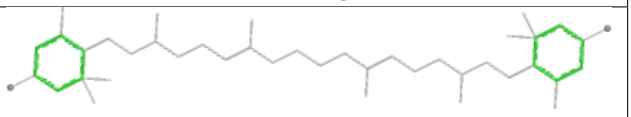


Bond angles

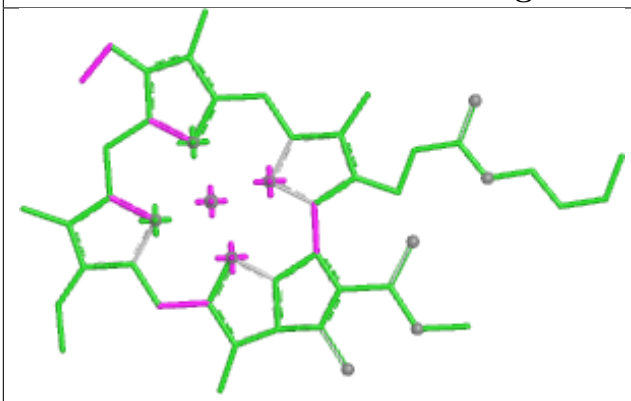


Torsions

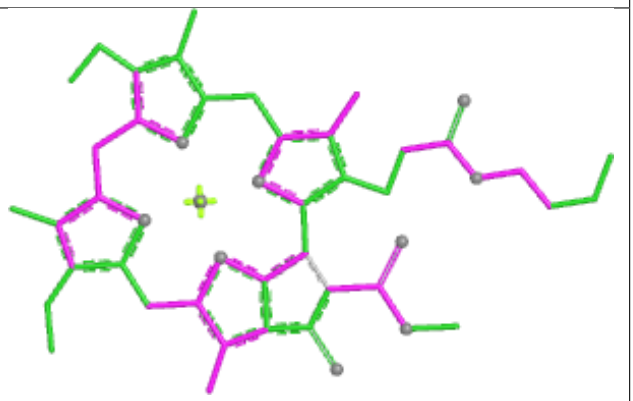


Rings

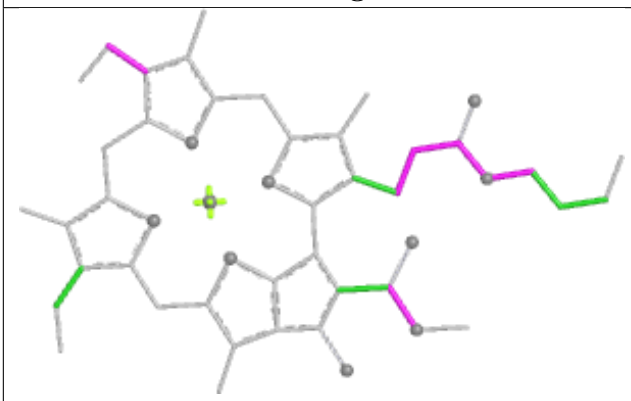
Ligand CLA R1 604



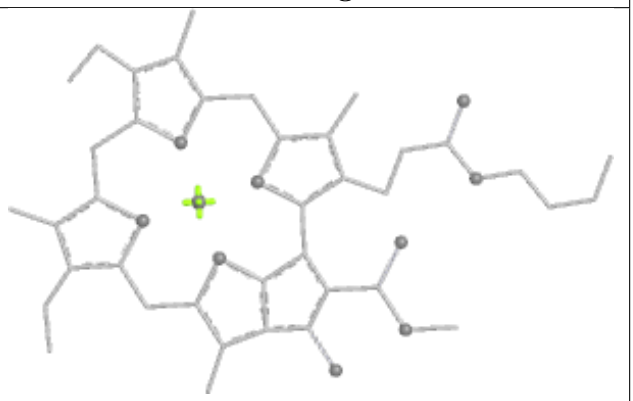
Bond lengths



Bond angles

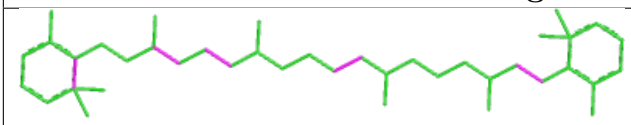


Torsions

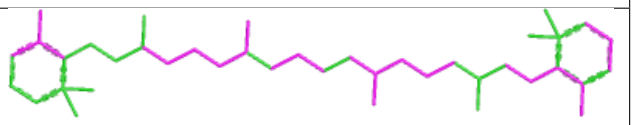


Rings

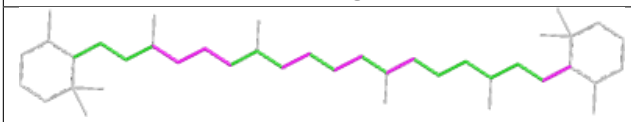
Ligand BCR a 411



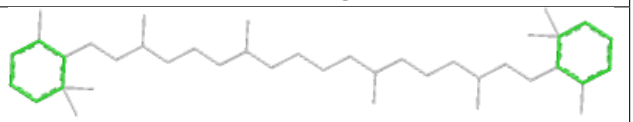
Bond lengths



Bond angles

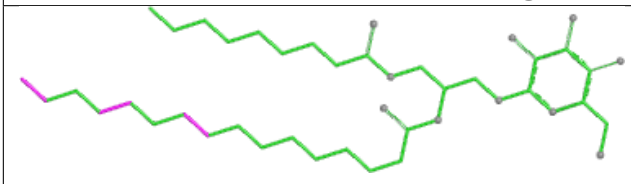


Torsions



Rings

Ligand LMG B 622



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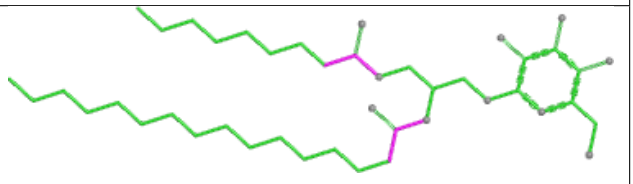
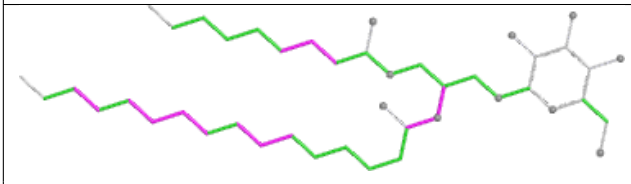


Bond angles



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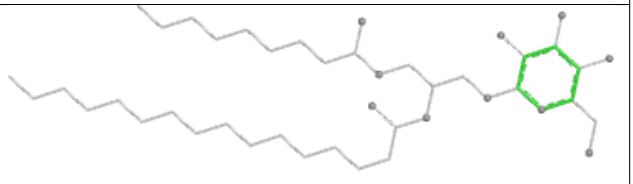
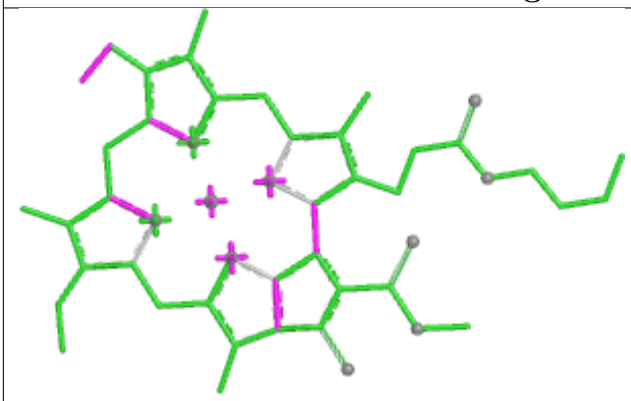
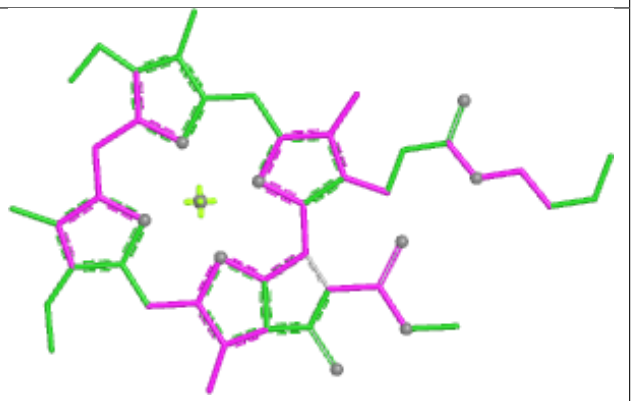


Rings

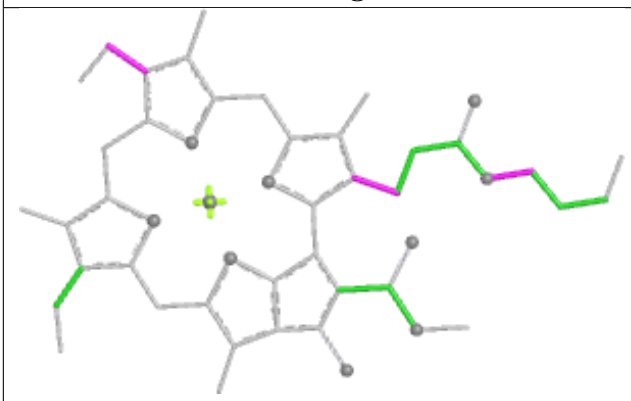
Ligand CLA A 407



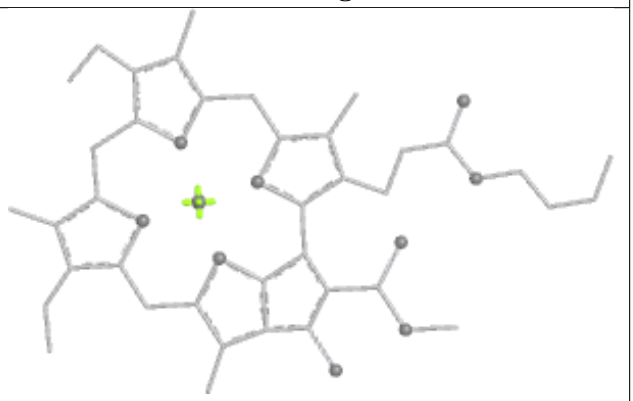
Bond lengths



Bond angles

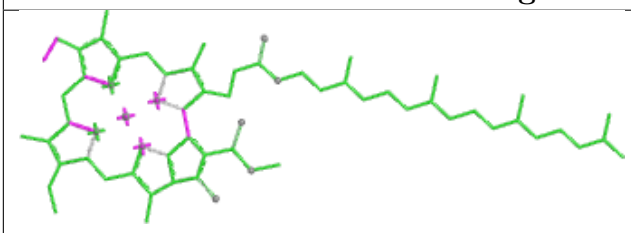


Torsions



Rings

Ligand CLA b1 615



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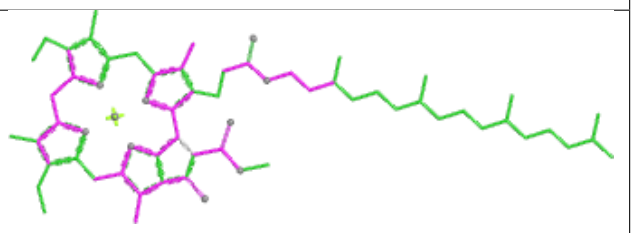
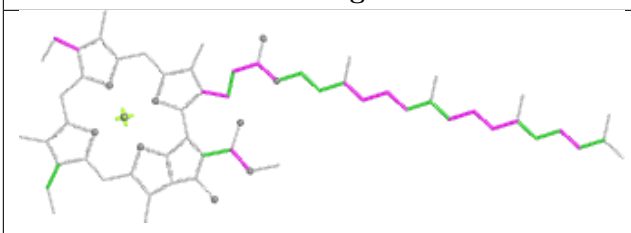


Bond angles



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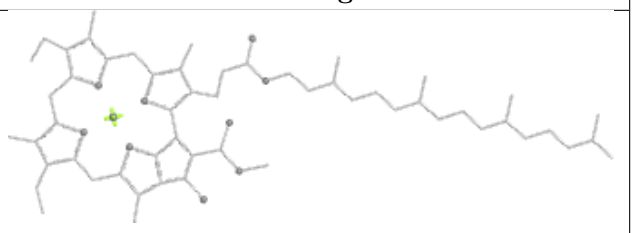
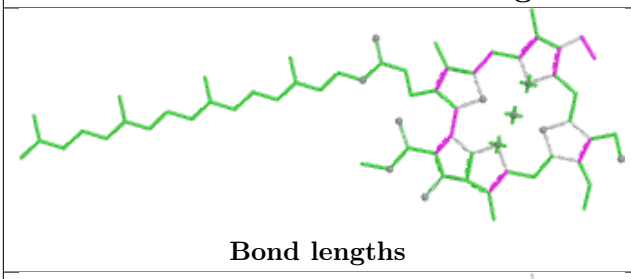
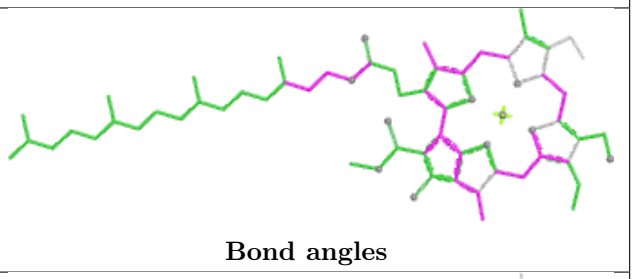


Rings

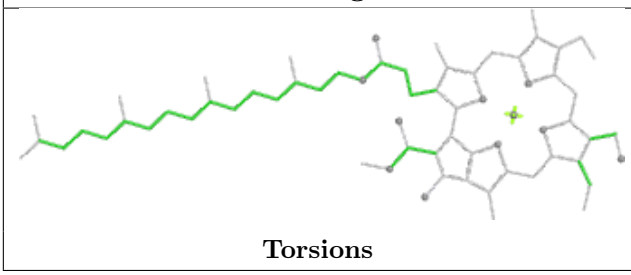
Ligand CHL Y1 601



Bond lengths



Bond angles



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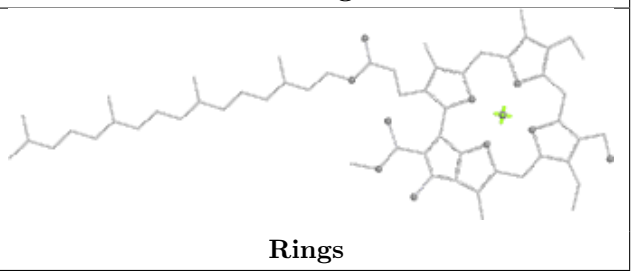
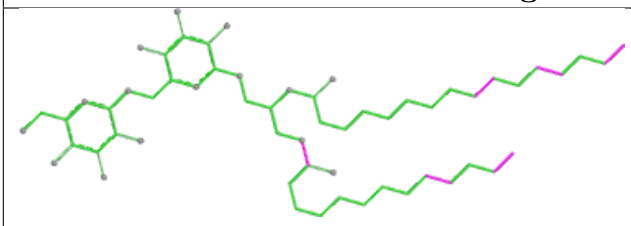


Rings

Ligand DGD C 520



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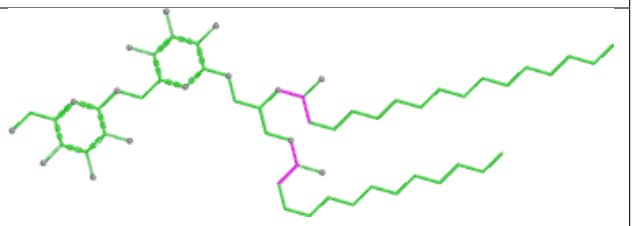
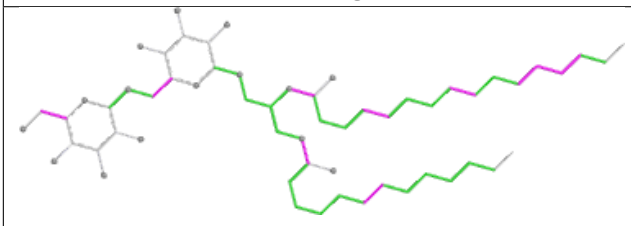


Bond angles



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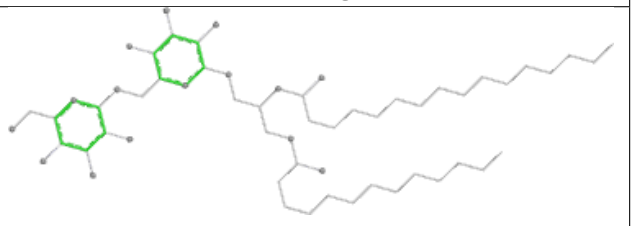
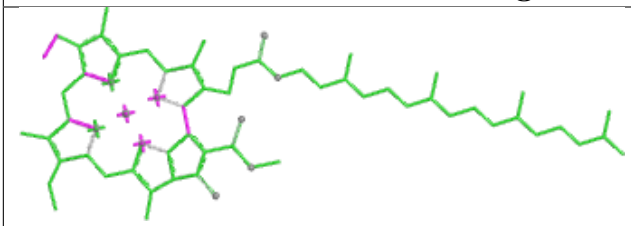
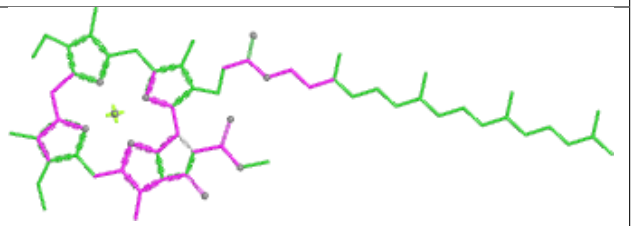


Rings

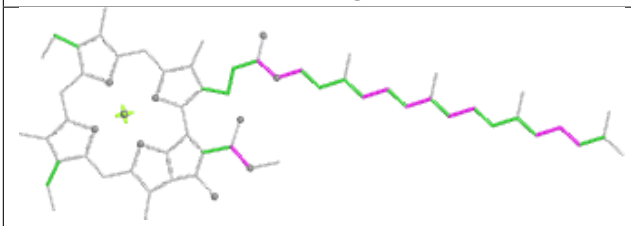
Ligand CLA B1 614



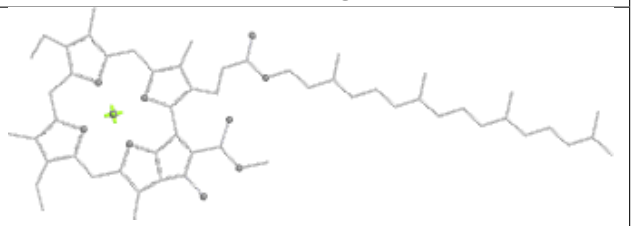
Bond lengths



Bond angles

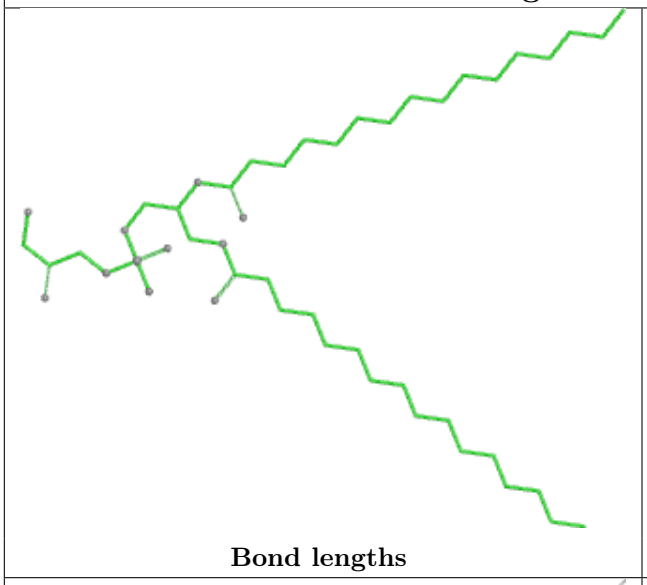


Torsions



Rings

Ligand LHG G 630



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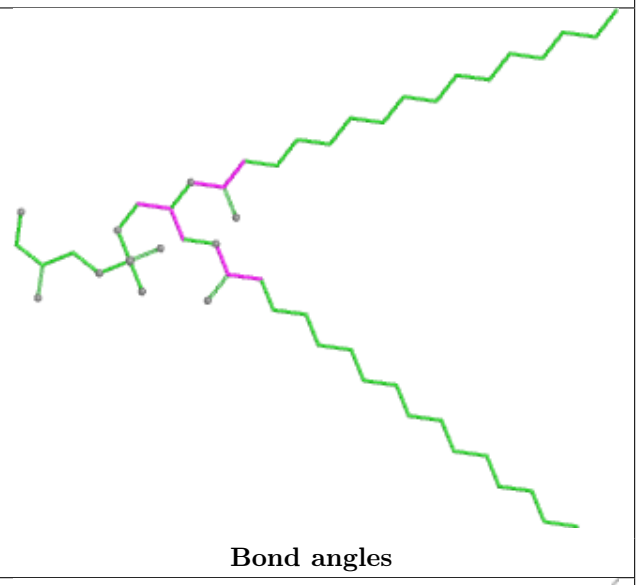
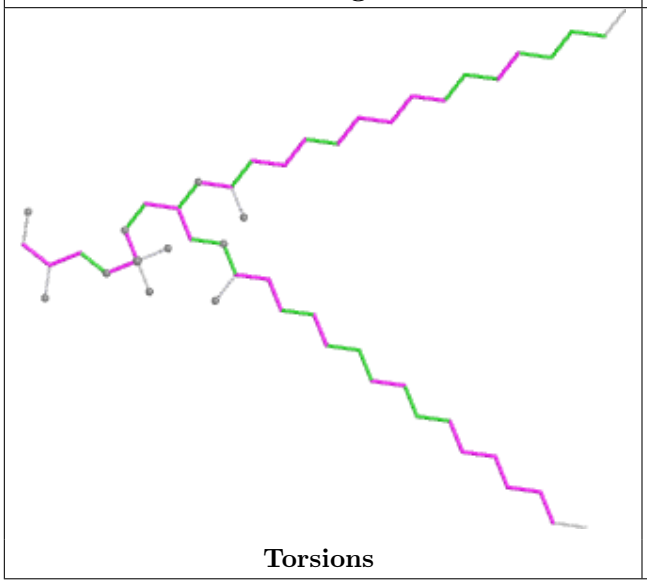
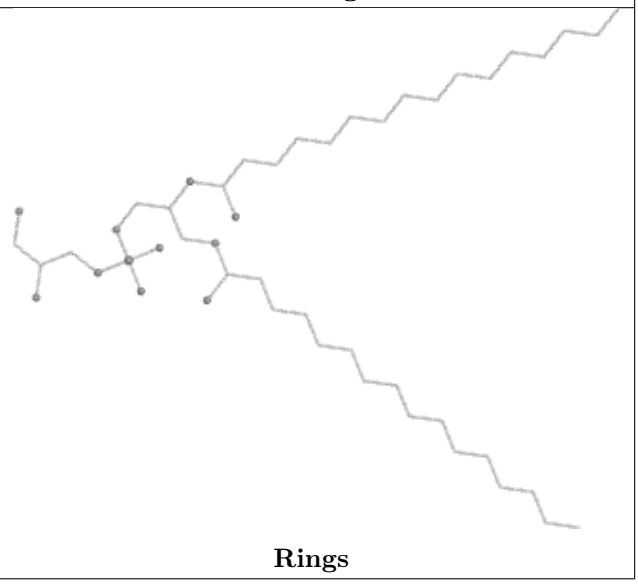


Bond angles

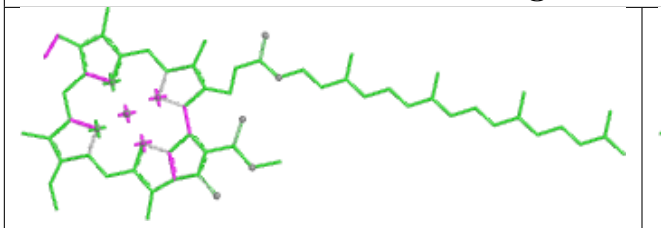


Torsions

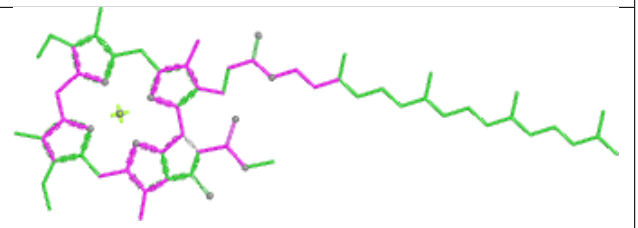


Rings

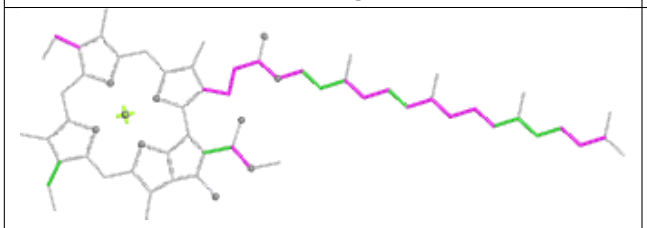
Ligand CLA b 602



Bond lengths



Bond angles



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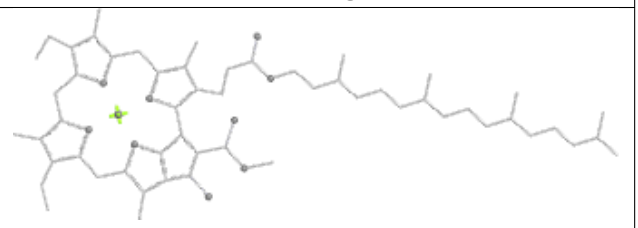
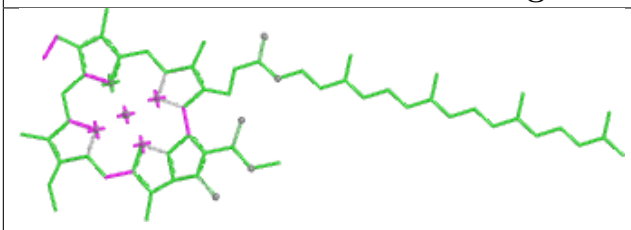


Rings

Ligand CLA b 615



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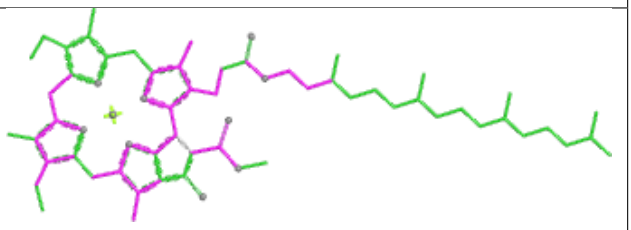
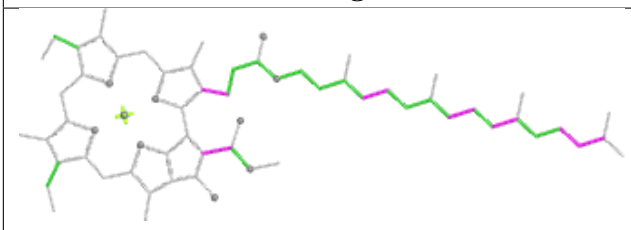
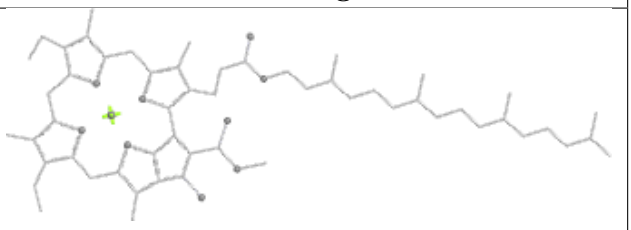


Bond angles

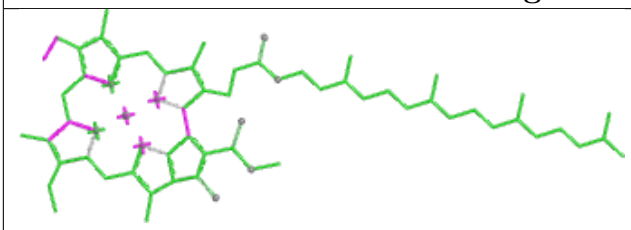


Torsions

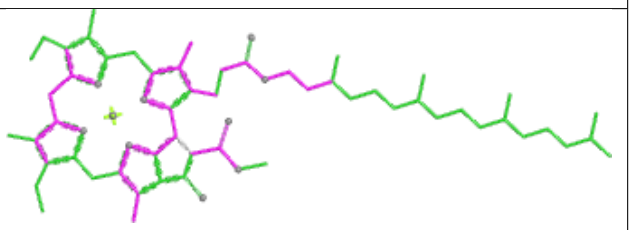


Rings

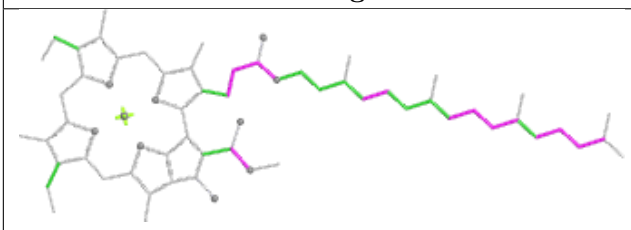
Ligand CLA Y 613



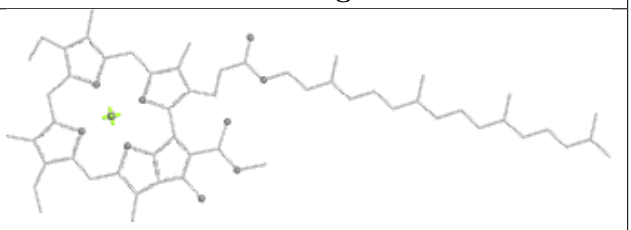
Bond lengths



Bond angles

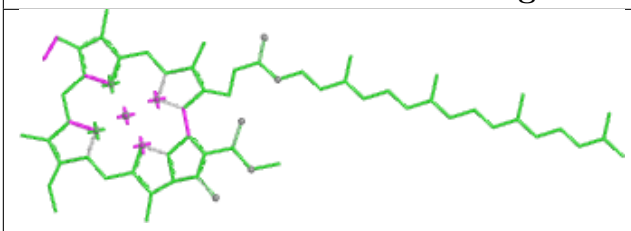


Torsions

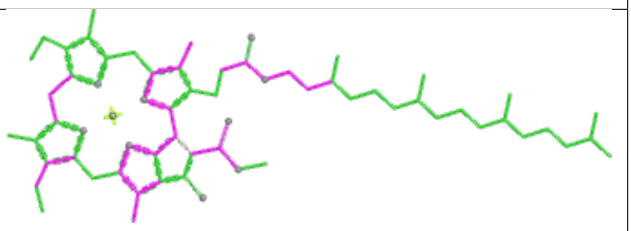


Rings

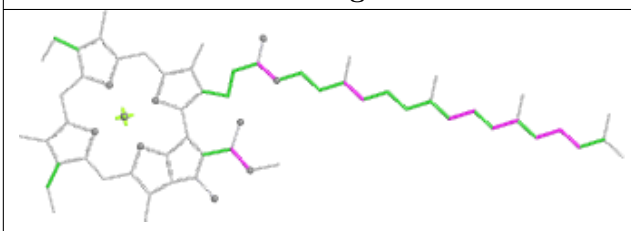
Ligand CLA b1 612



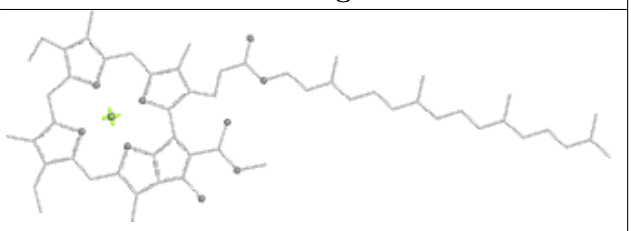
Bond lengths



Bond angles



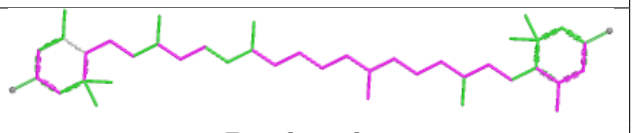
Torsions



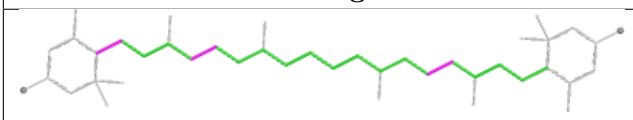
Rings

Ligand LUT n1 621

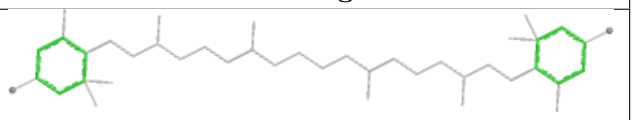
Bond lengths



Bond angles

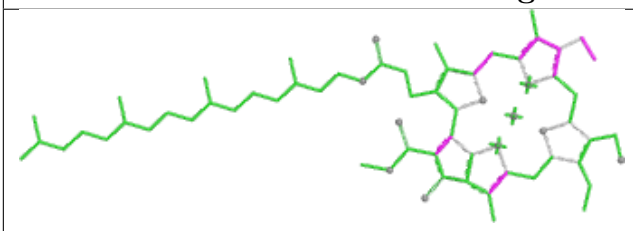


Torsions



Rings

Ligand CHL n1 606



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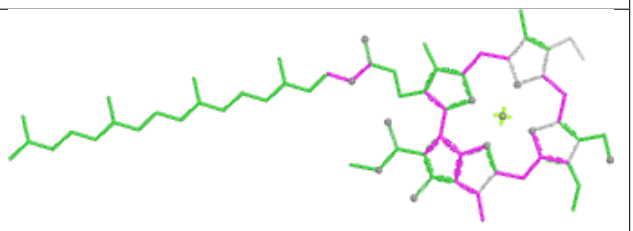

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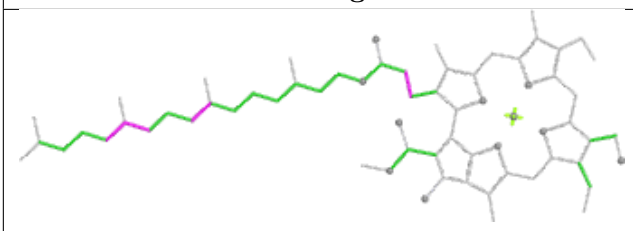

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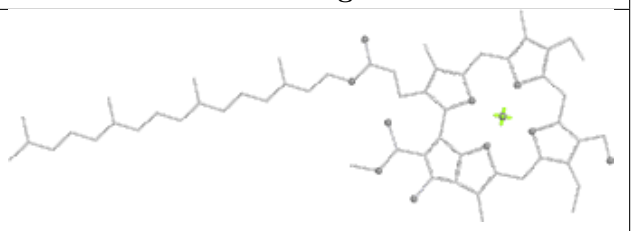
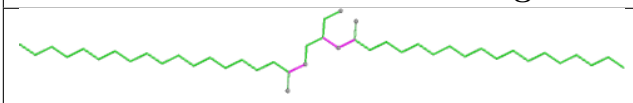


Rings

Ligand DGA b1 625



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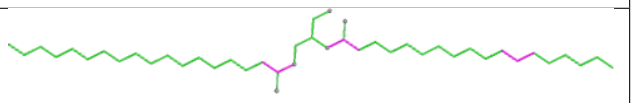

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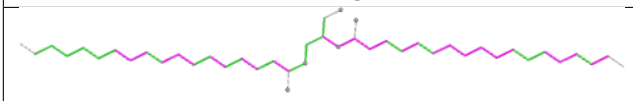
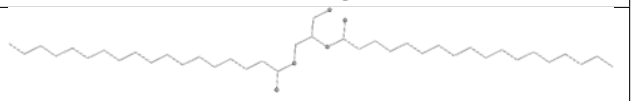
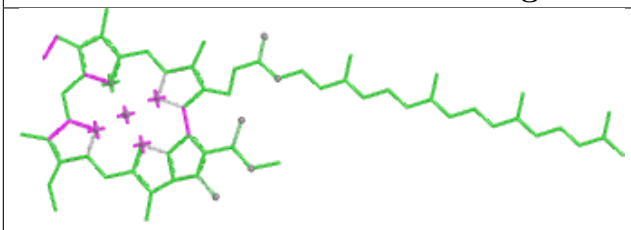


Torsions



Rings

Ligand CLA s1 603



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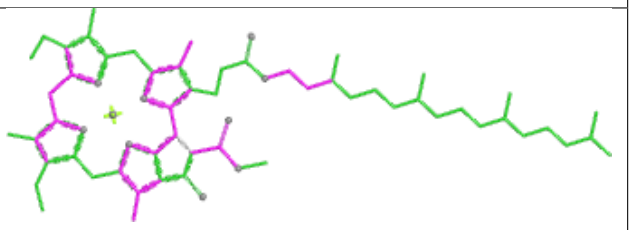
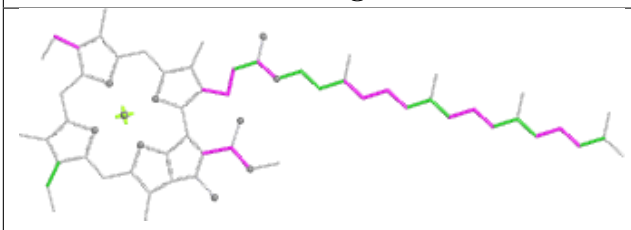


Bond angles



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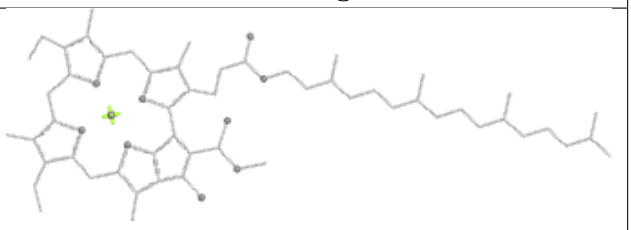
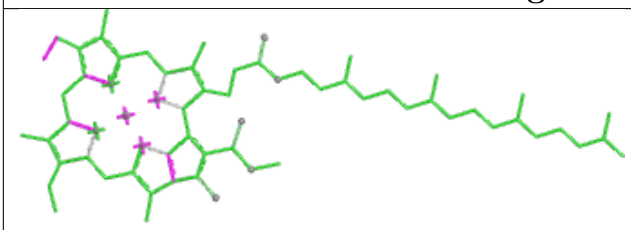


Rings

Ligand CLA b 613



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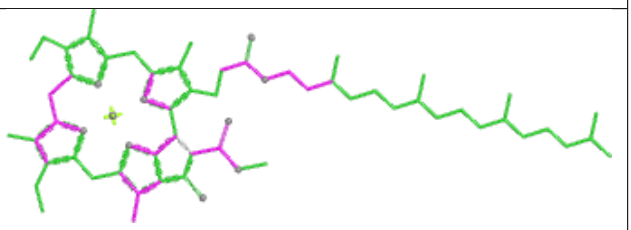
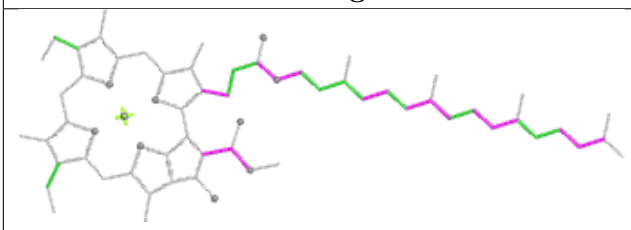


Bond angles



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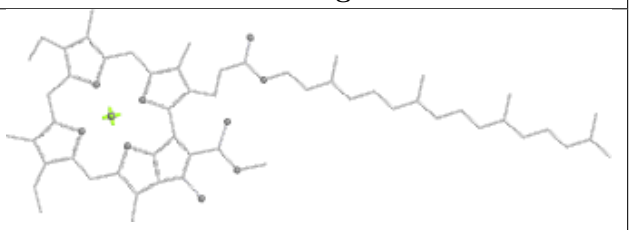
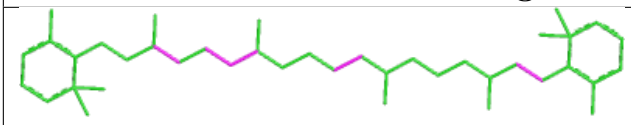


Rings

Ligand BCR d1 404



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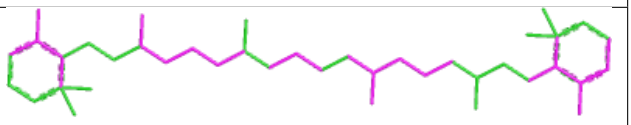
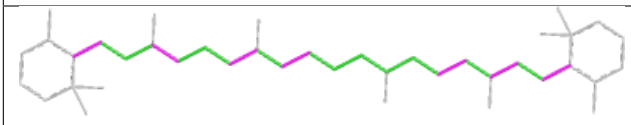


Bond angles



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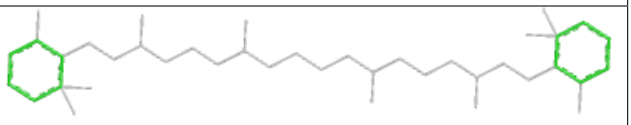
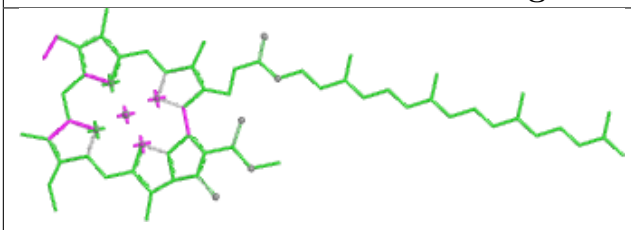


Rings

Ligand CLA g 603



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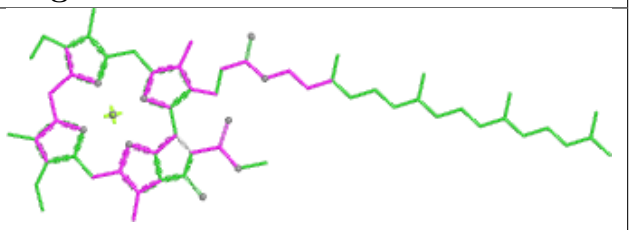
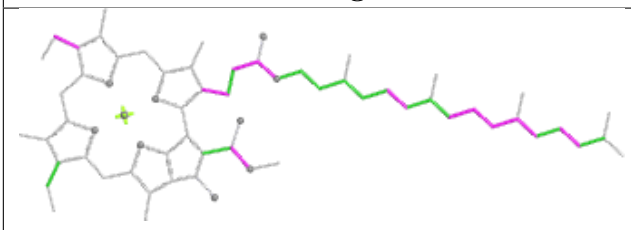
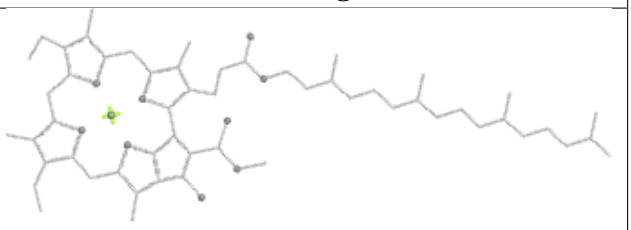


Bond angles

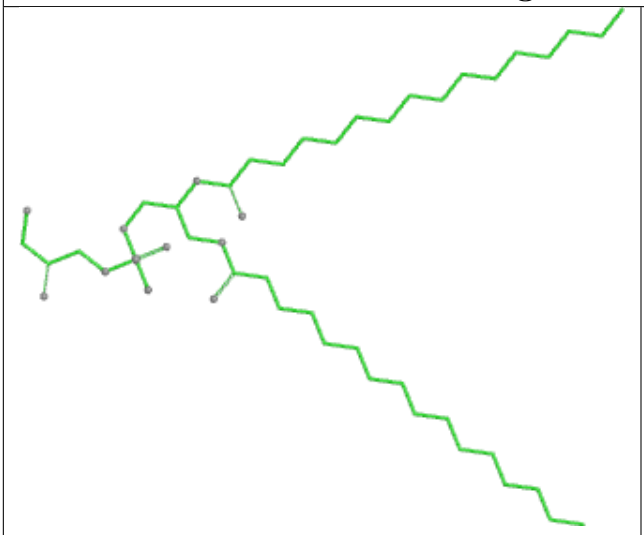


Torsions



Rings

Ligand LHG n1 624



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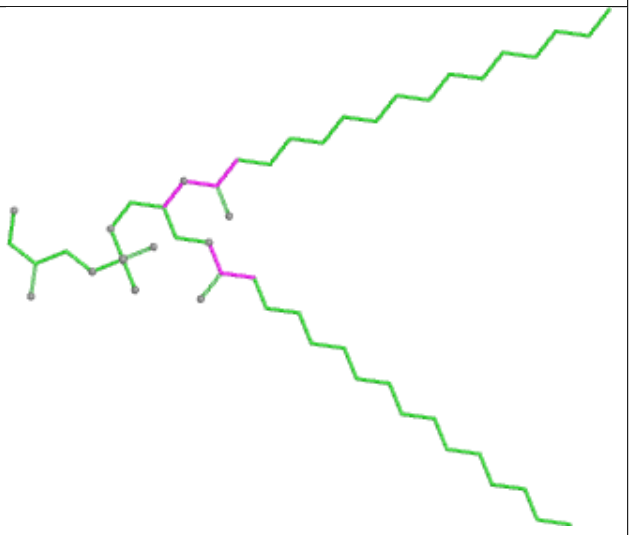

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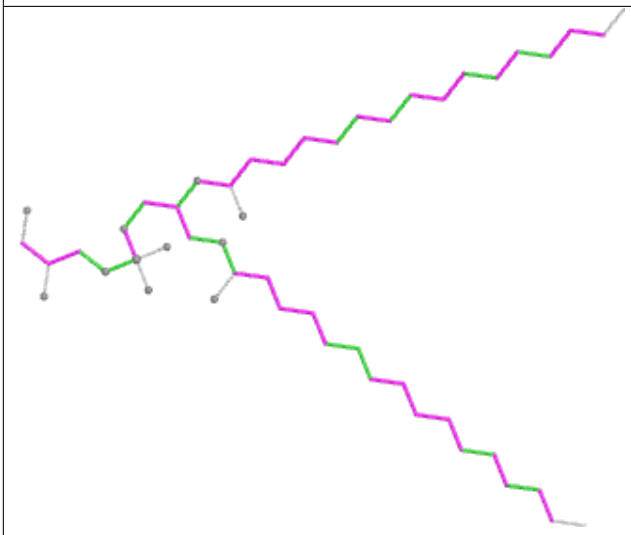

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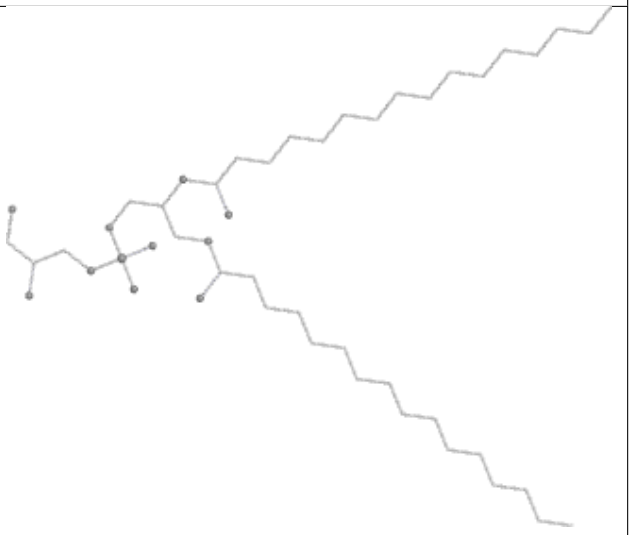
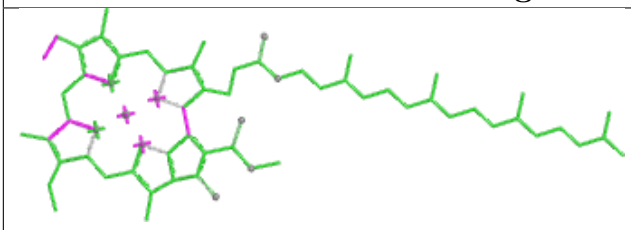


Rings

Ligand CLA A1 406



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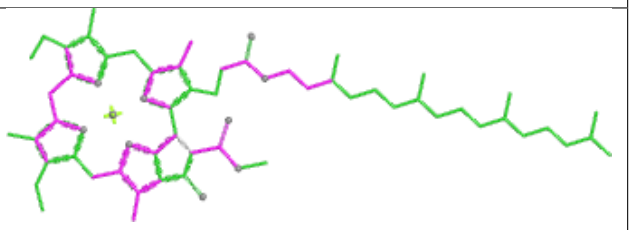
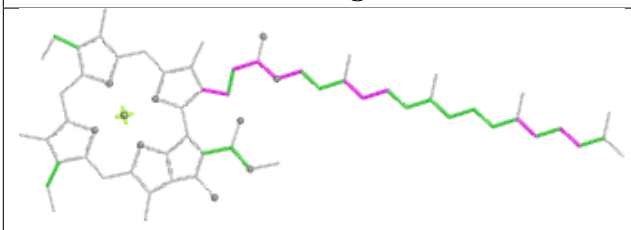
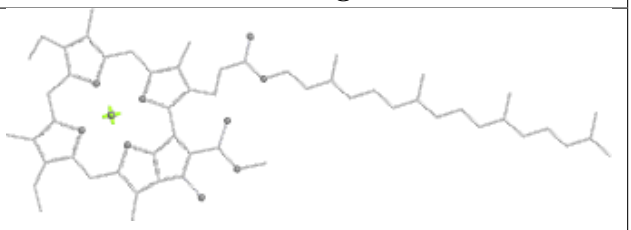


Bond angles

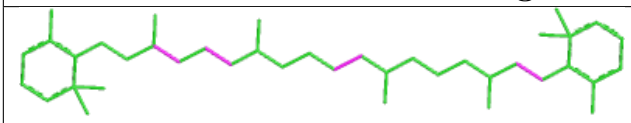


Torsions



Rings

Ligand BCR b1 619



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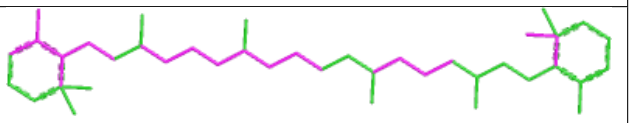
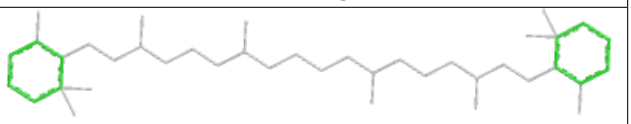


Bond angles

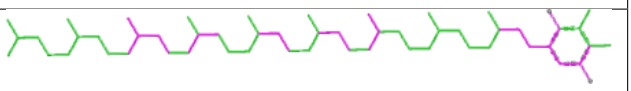
Torsions



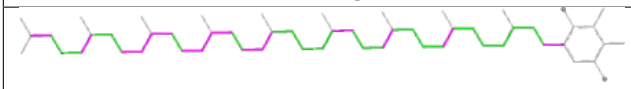
Rings

Ligand PL9 d1 405

Bond lengths



Bond angles



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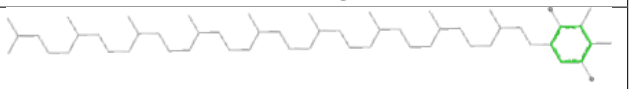
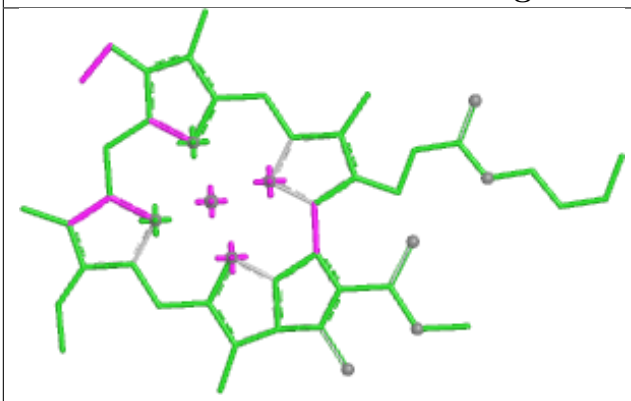


Rings

Ligand CLA G1 614



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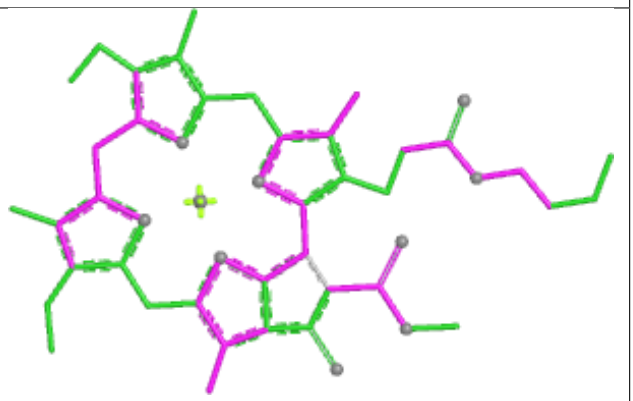
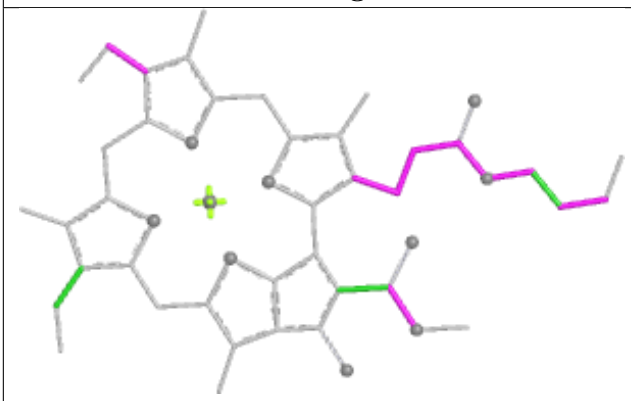


Bond angles



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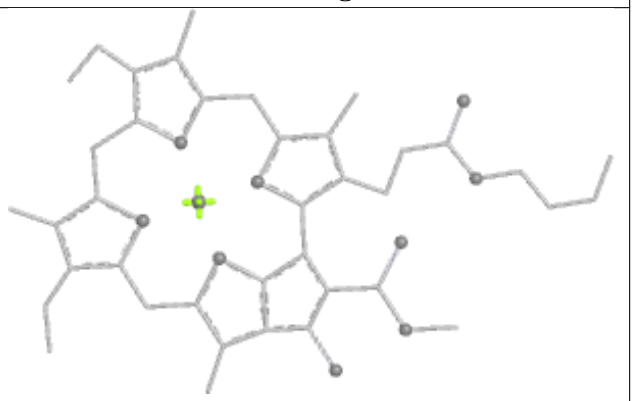
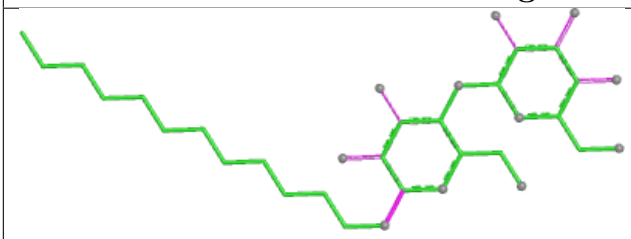


Rings

Ligand LMT r1 625



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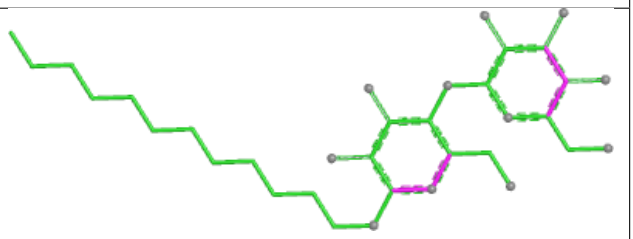
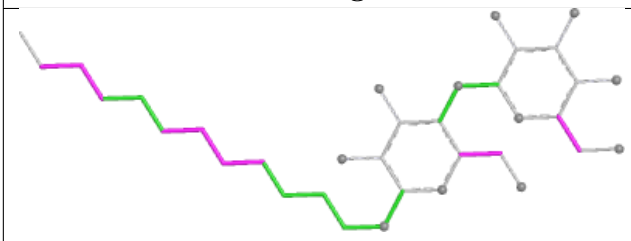
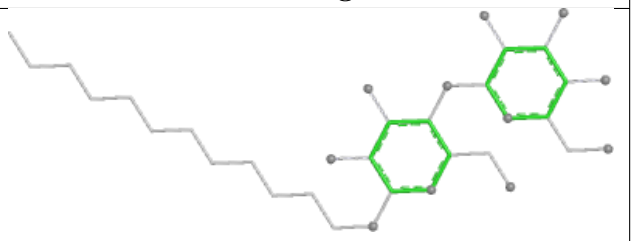


Bond angles

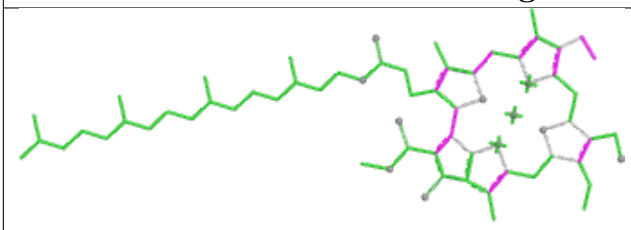


Torsions



Rings

Ligand CHL y1 601



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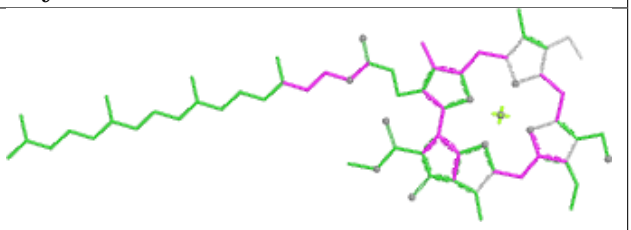
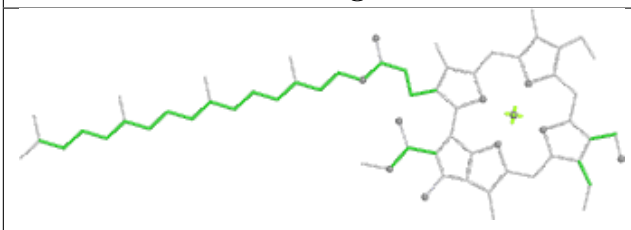
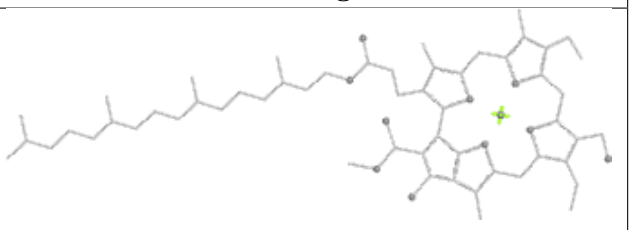


Bond angles

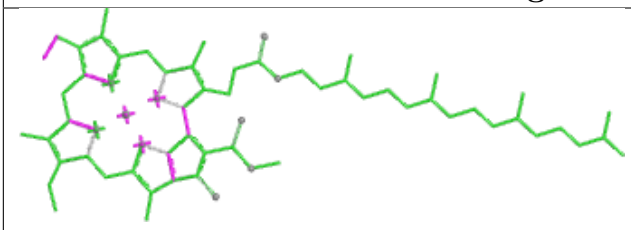


Torsions



Rings

Ligand CLA b 606



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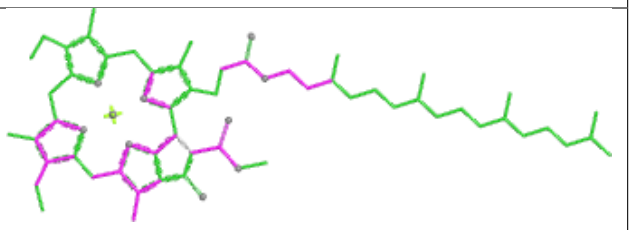
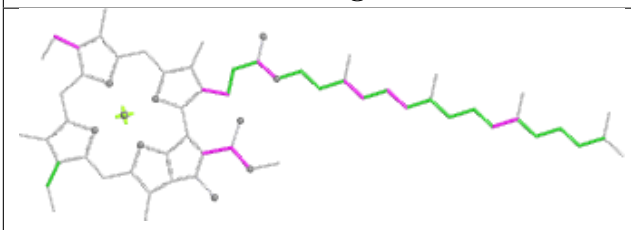
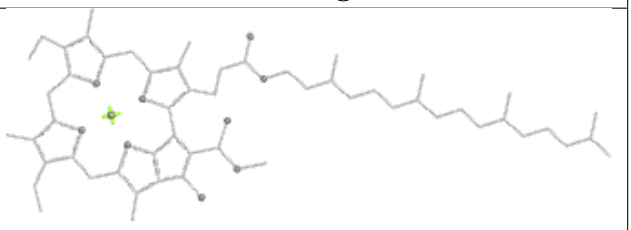


Bond angles

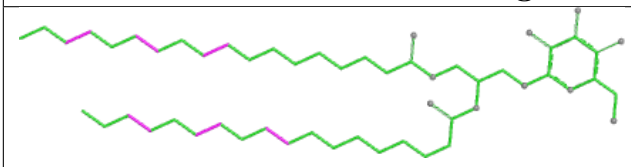


Torsions



Rings

Ligand LMG c1 523



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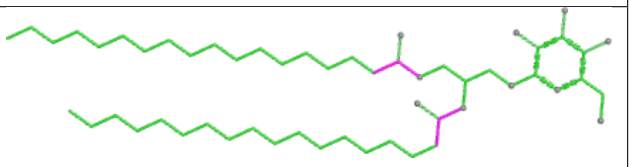
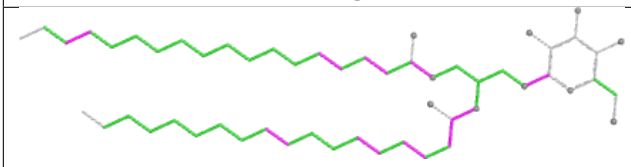


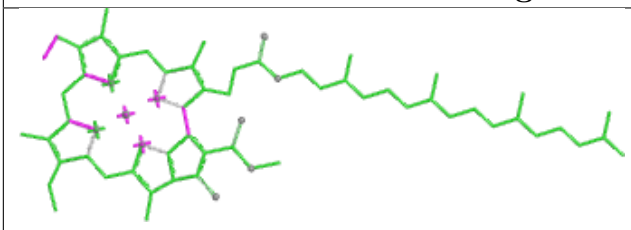
Bond angles



Torsions

Rings

Ligand CLA C1 504



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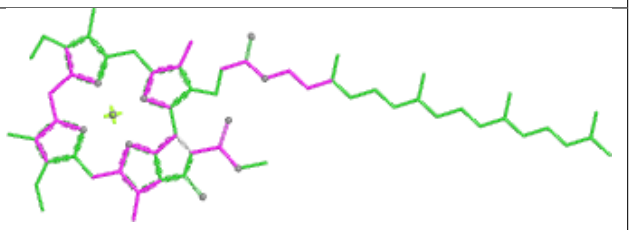

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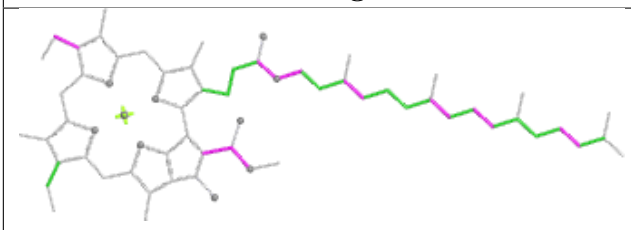

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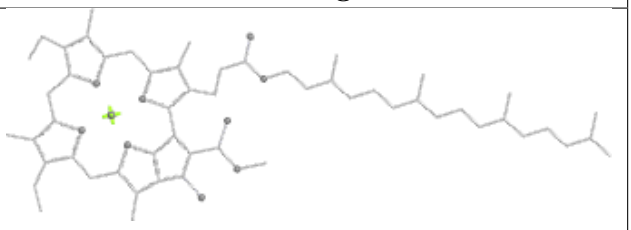
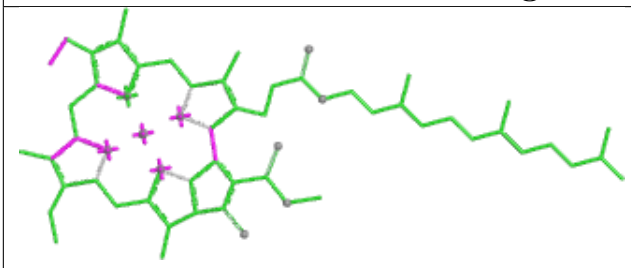


Rings

Ligand CLA r1 612



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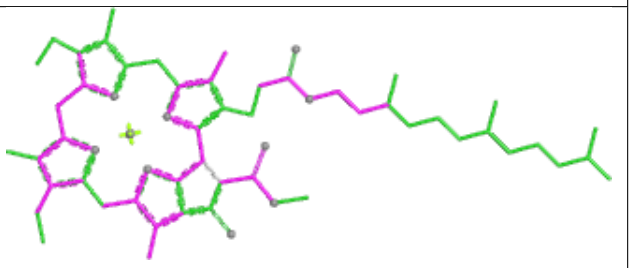

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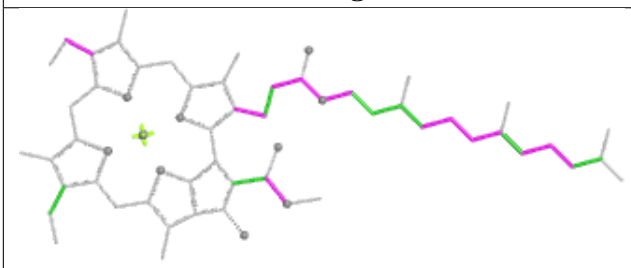

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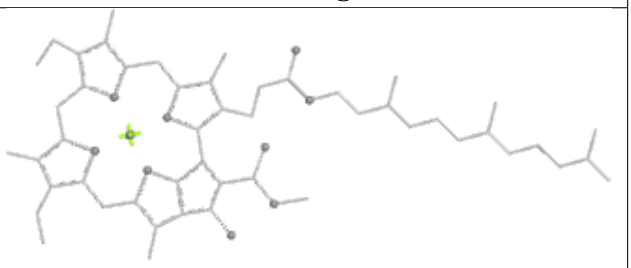

Rings

Ligand XAT G 622

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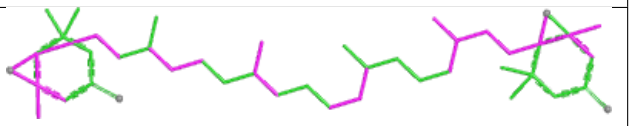

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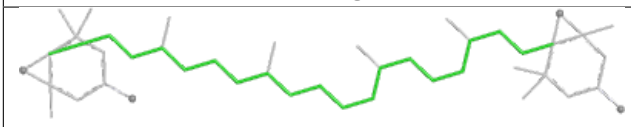

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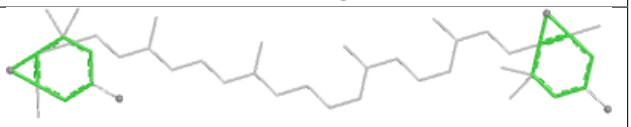
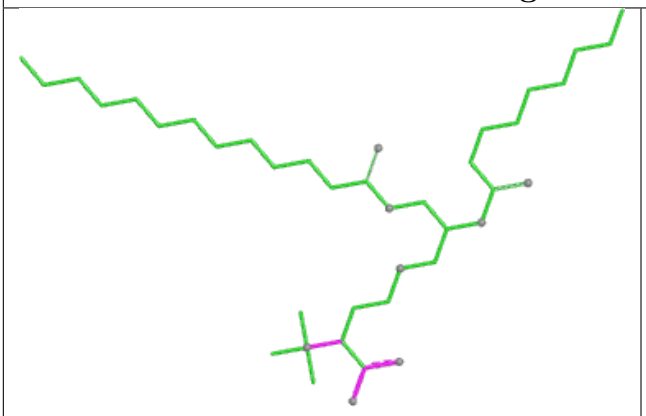


Rings

Ligand LMK C 527



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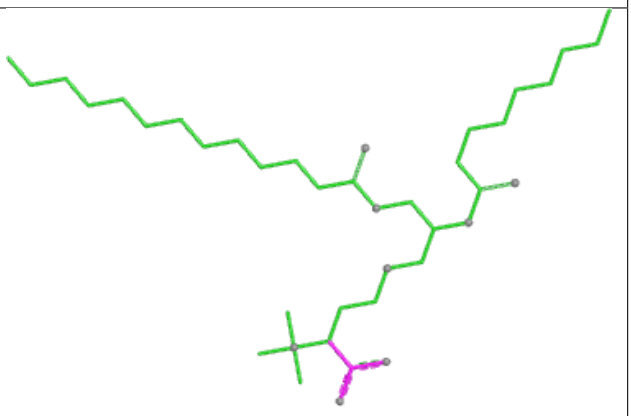

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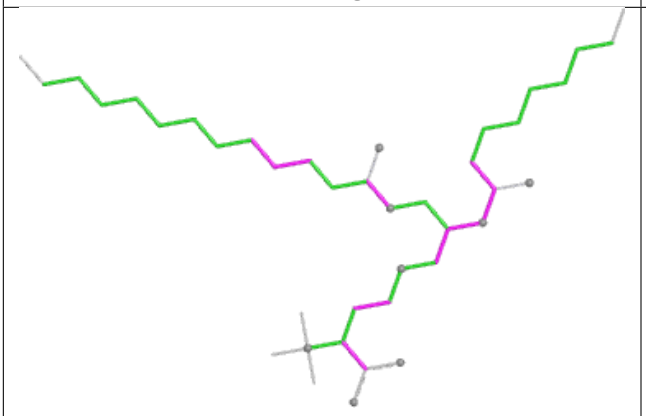

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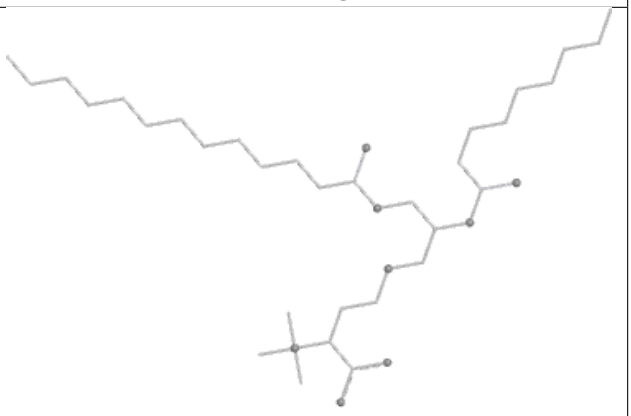
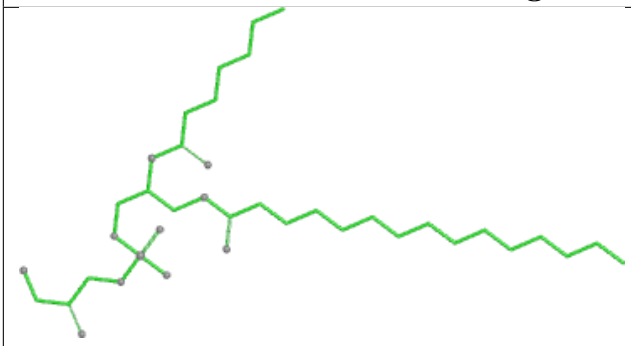


Rings

Ligand LHG d 410



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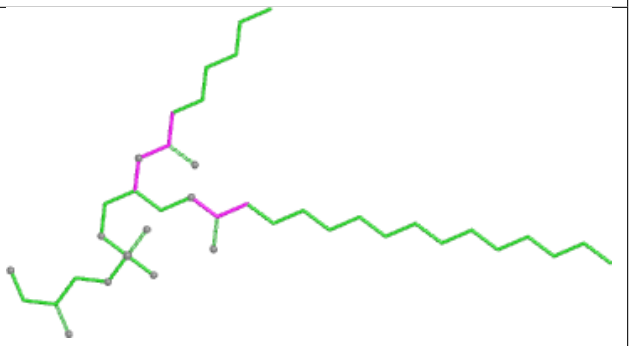

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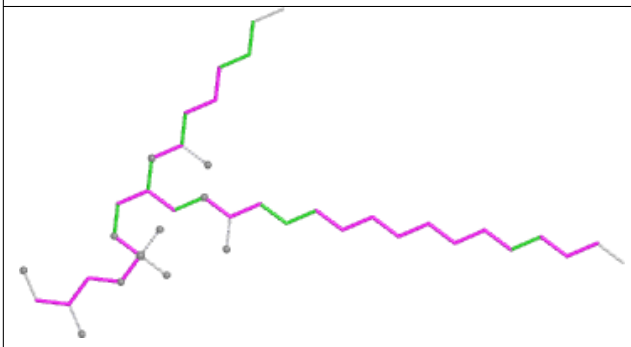

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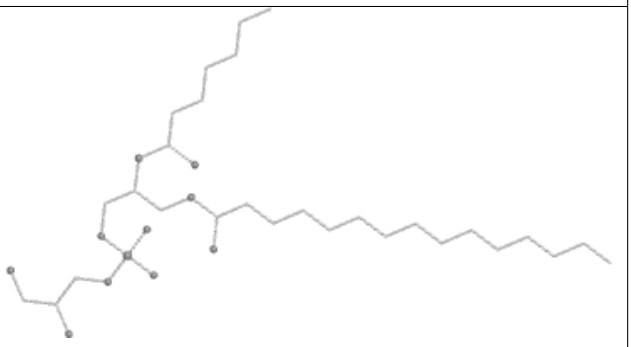
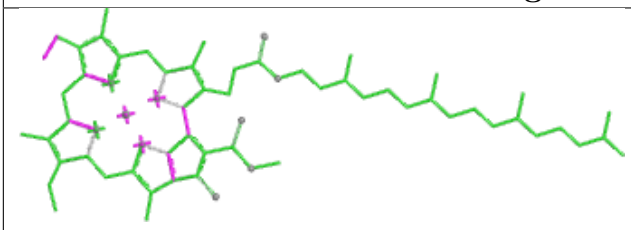


Rings

Ligand CLA B 609



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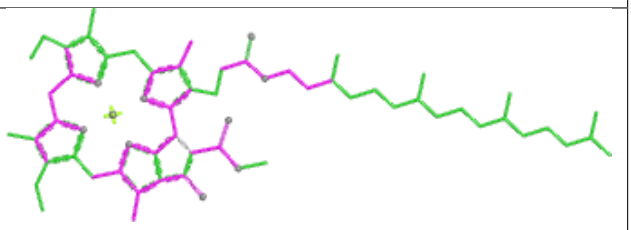

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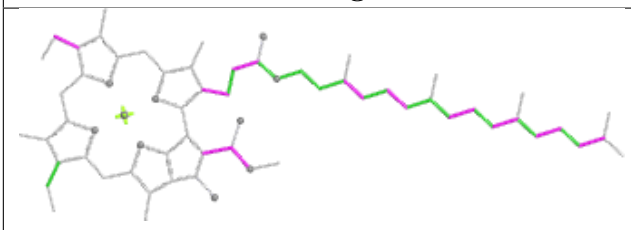

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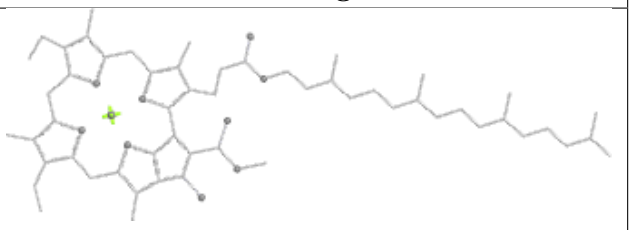
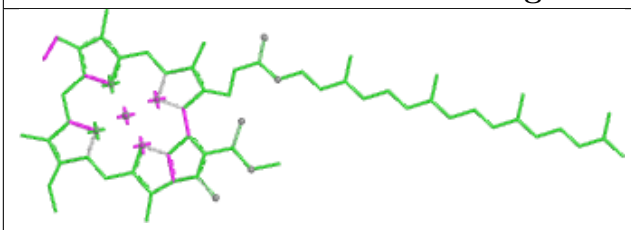


Rings

Ligand CLA C 506



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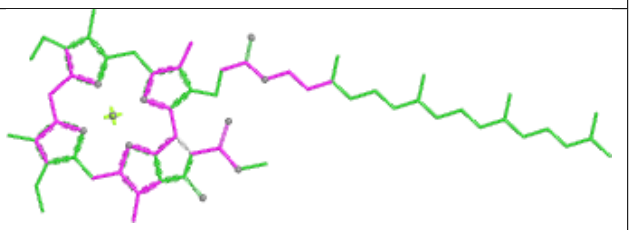

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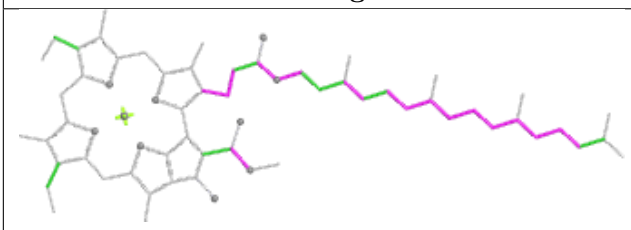

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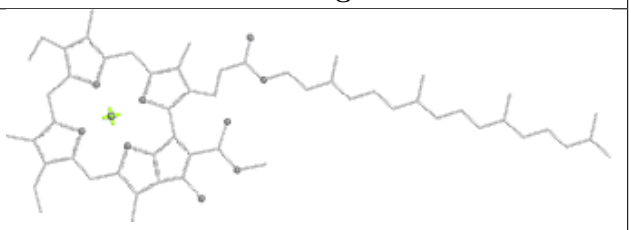
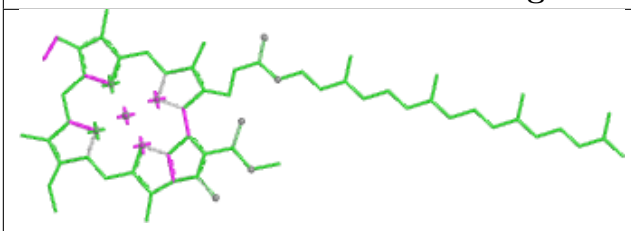


Rings

Ligand CLA b 610



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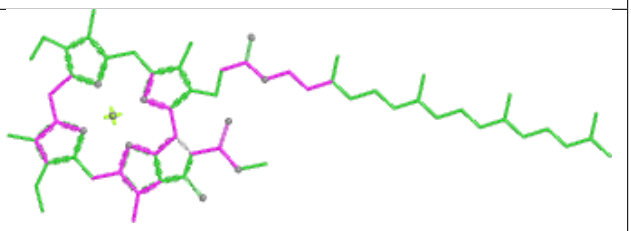

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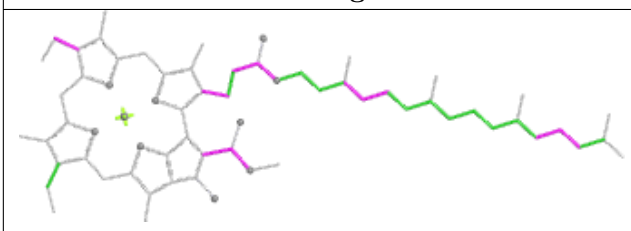

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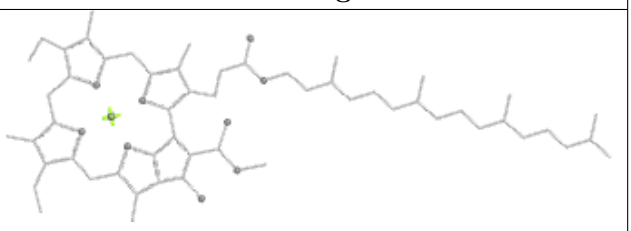
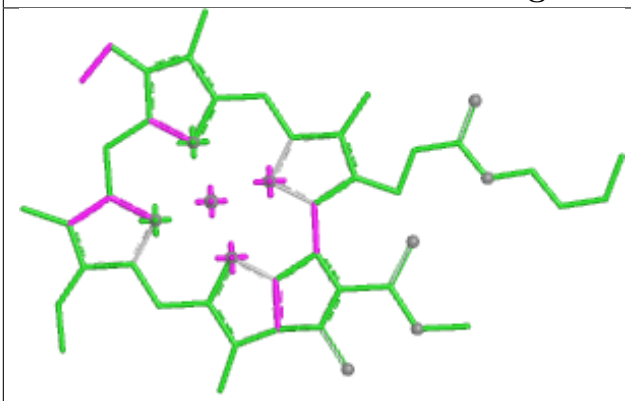


Rings

Ligand CLA g 604



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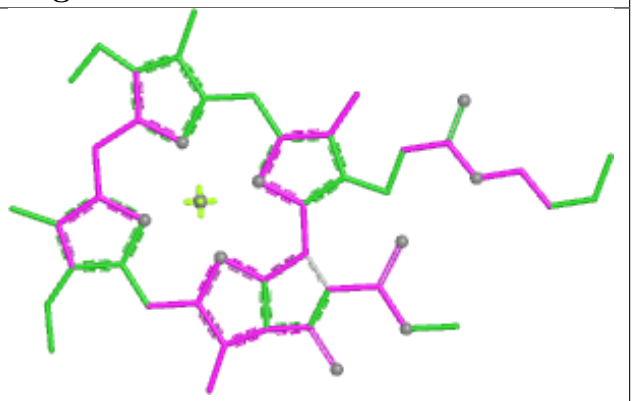

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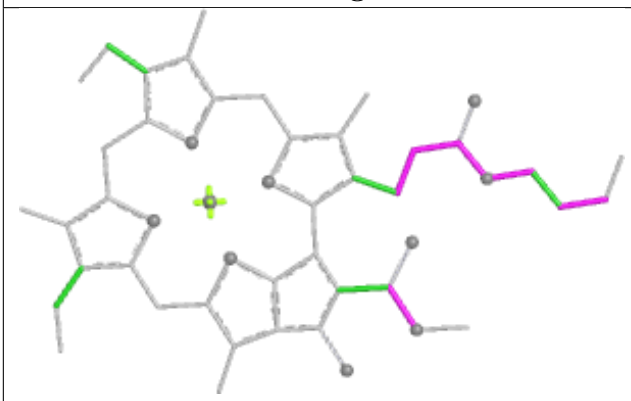

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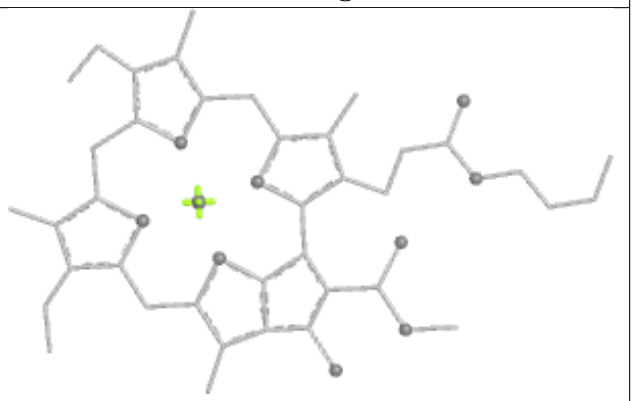
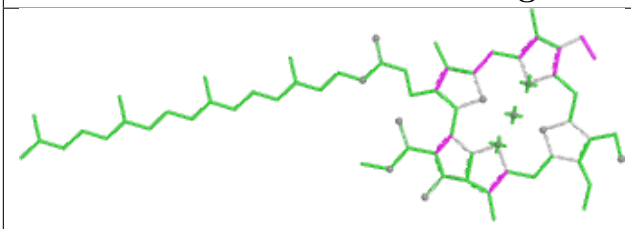


Rings

Ligand CHL y1 607



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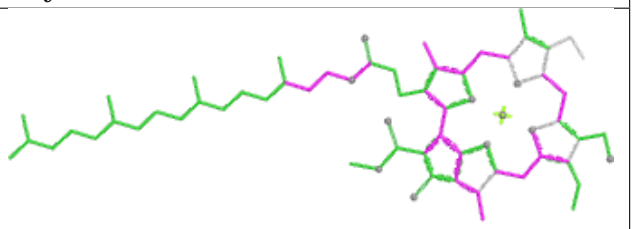

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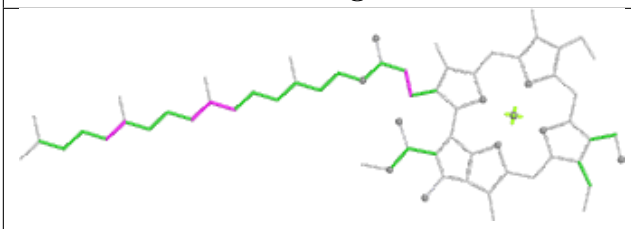

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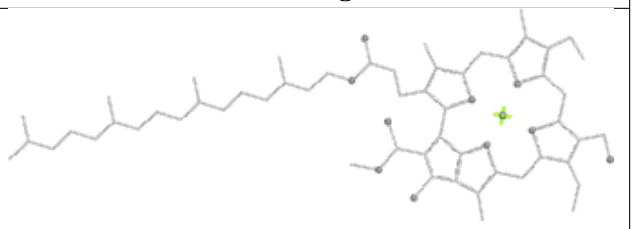
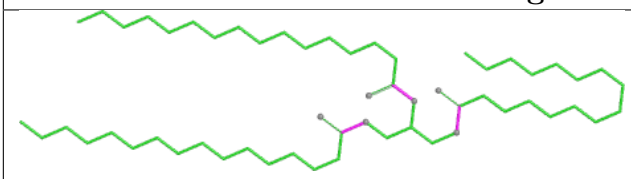


Rings

Ligand 4RF i1 101



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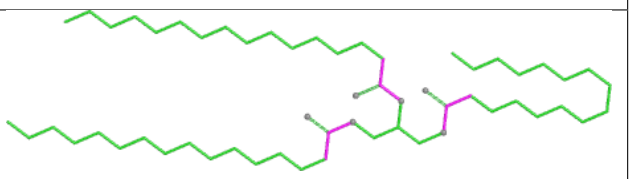

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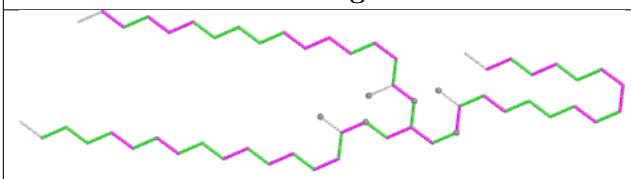

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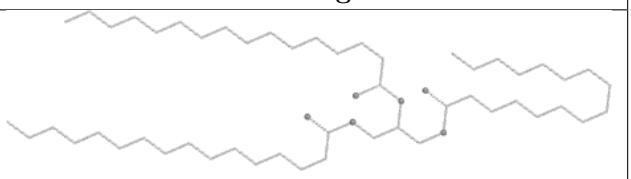
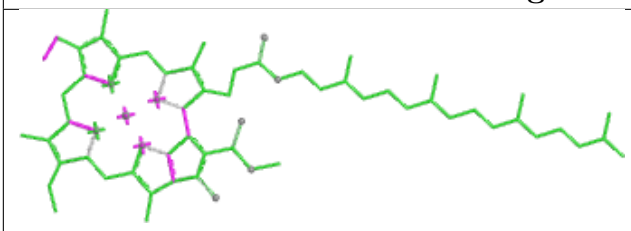


Rings

Ligand CLA b 612



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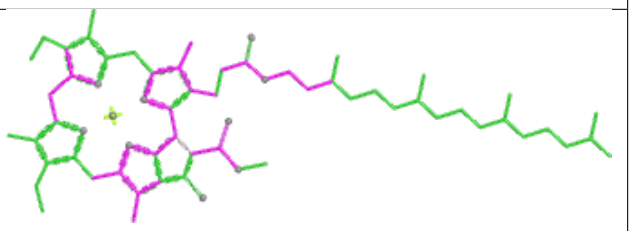
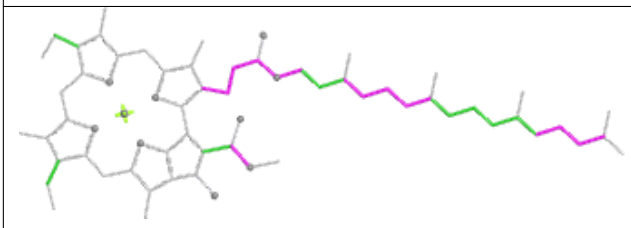


Bond angles



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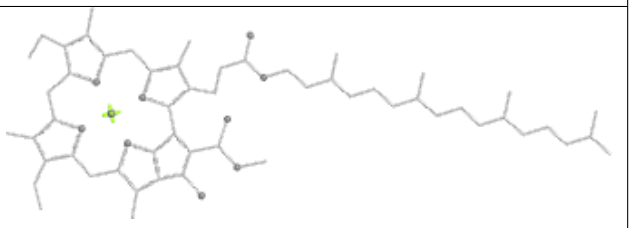
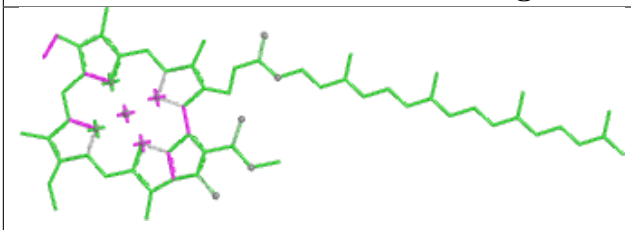


Rings

Ligand CLA B1 606



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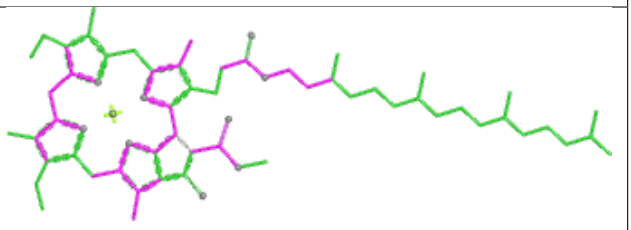
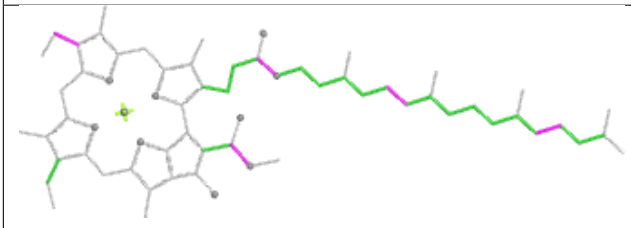


Bond angles



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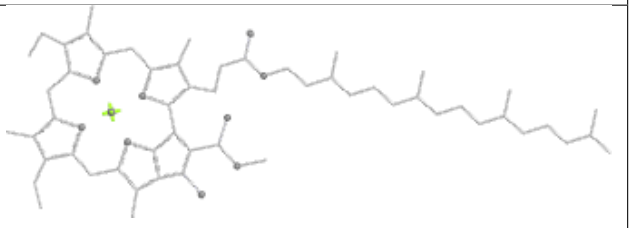
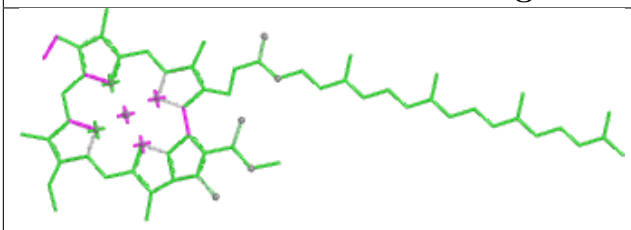
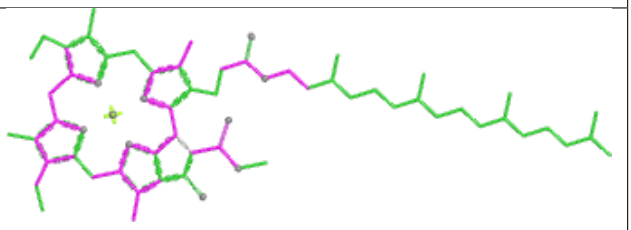
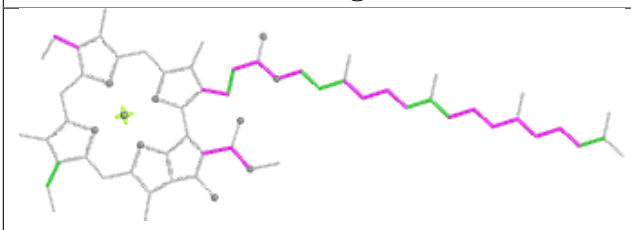
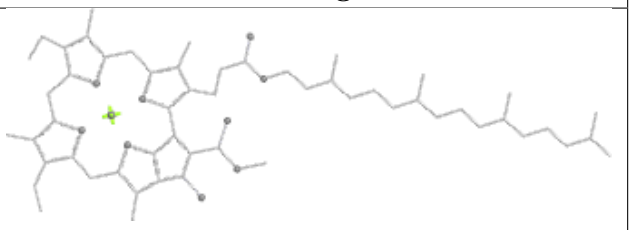
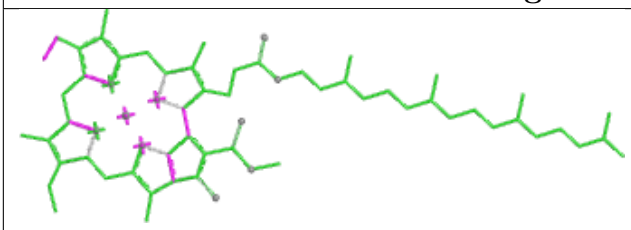
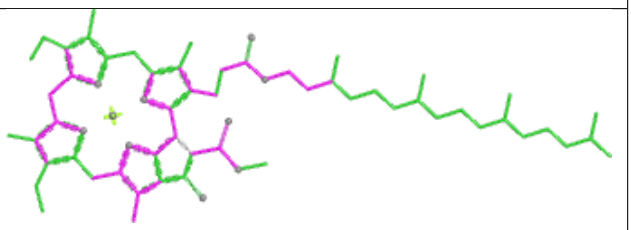
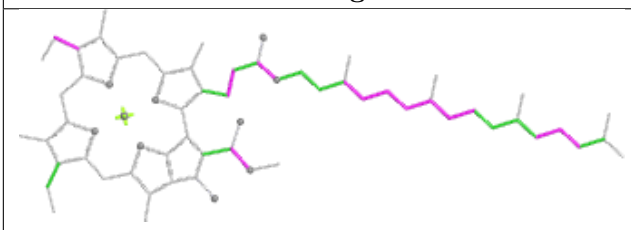
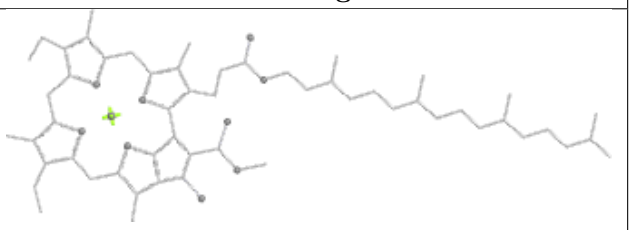
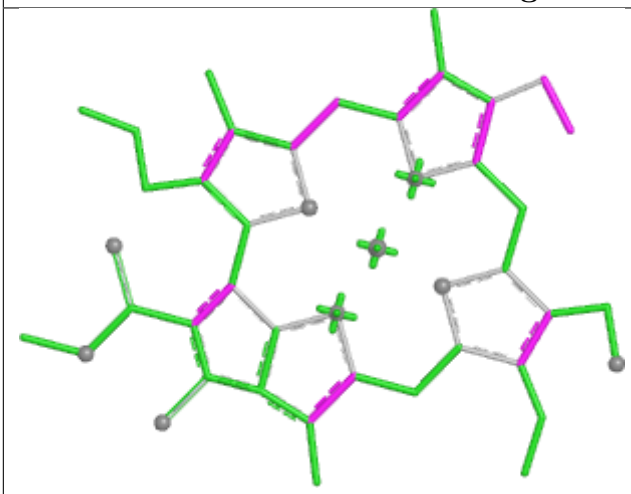


Rings

Ligand CLA B1 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C 510	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CHL r1 606



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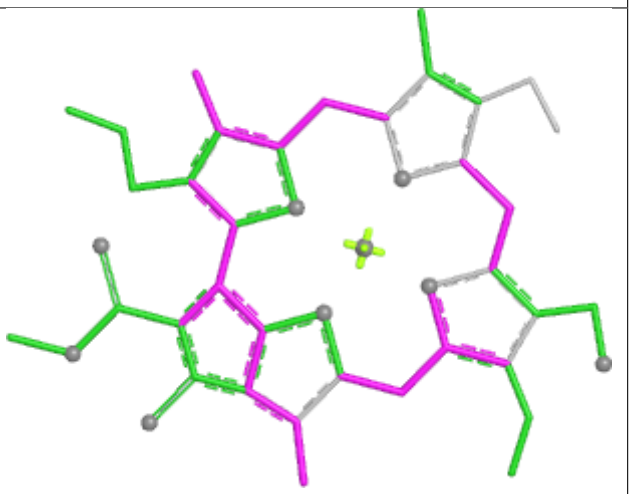

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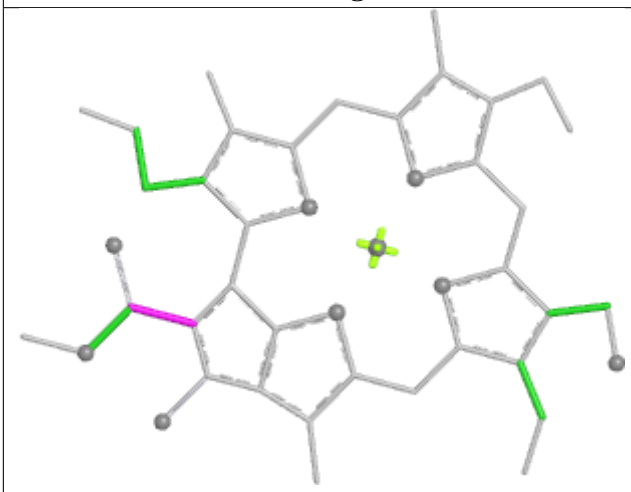
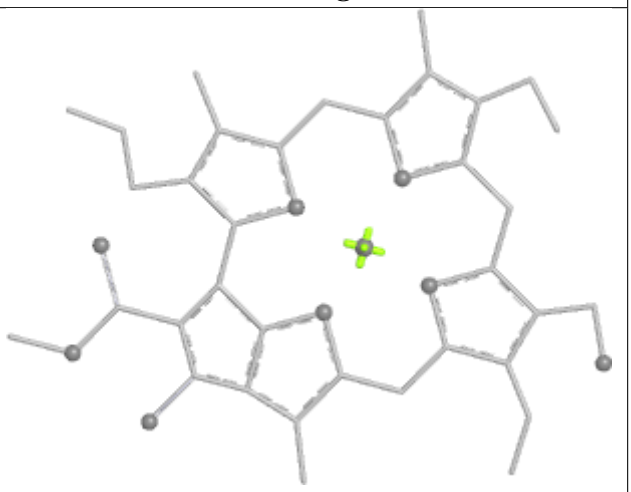
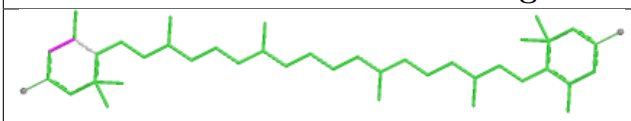


Torsions



Rings

Ligand LUT g1 621



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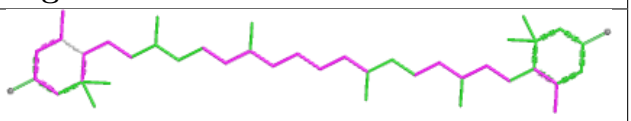

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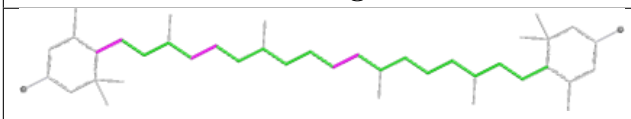

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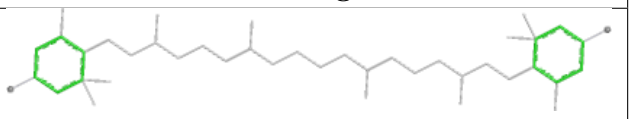
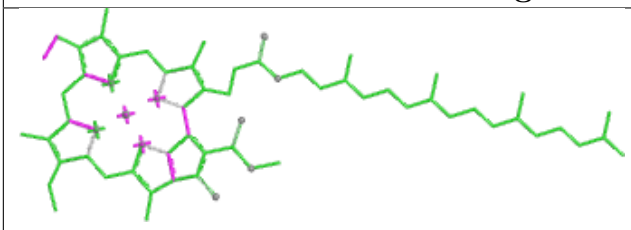
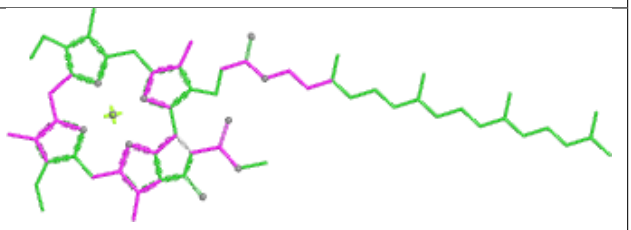
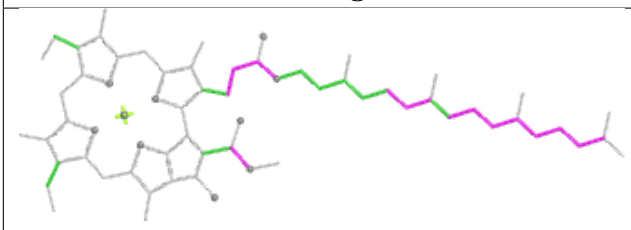
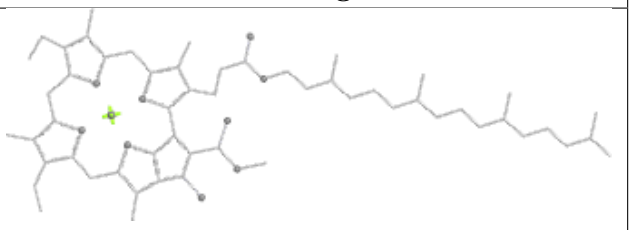


Rings

Ligand CLA Y1 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

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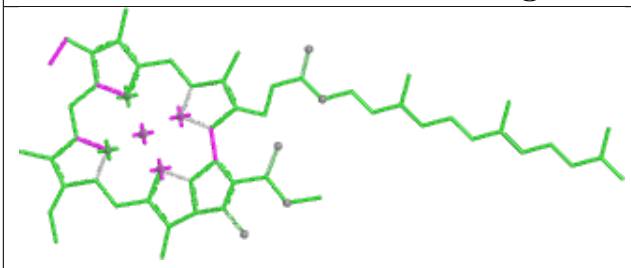
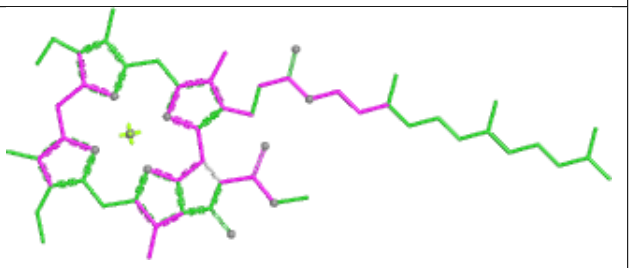
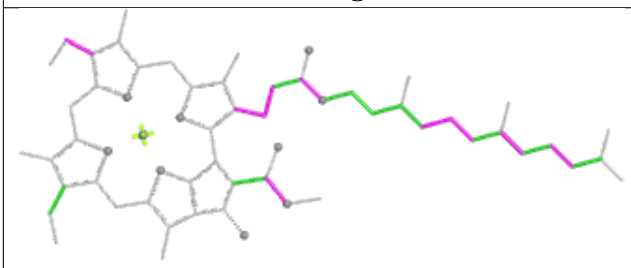
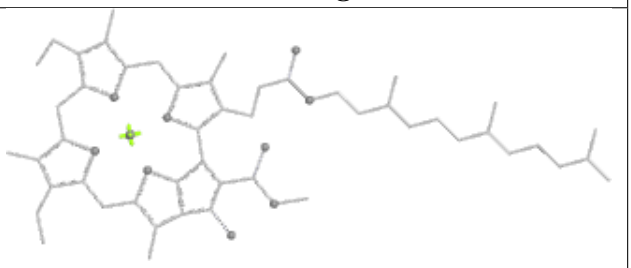
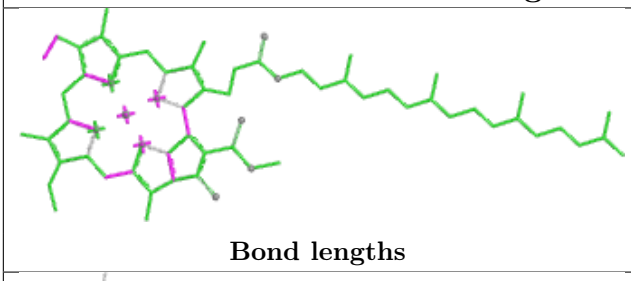
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA B 607



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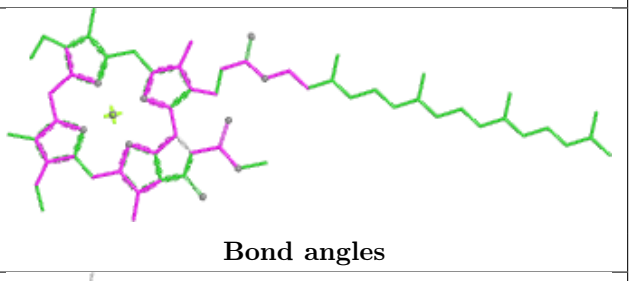
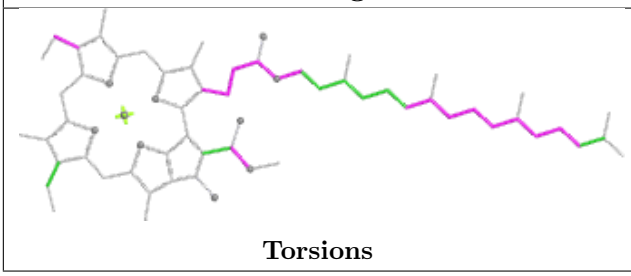
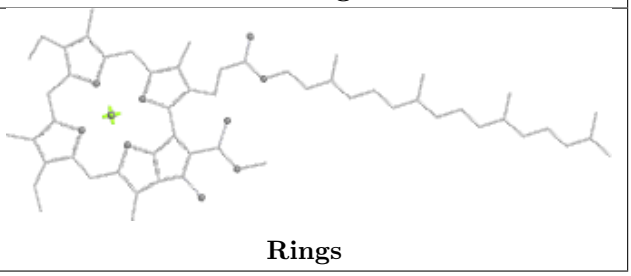


Bond angles

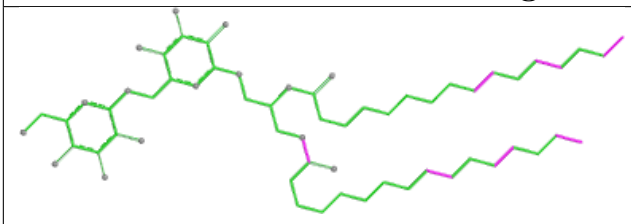


Torsions



Rings

Ligand DGD C 519



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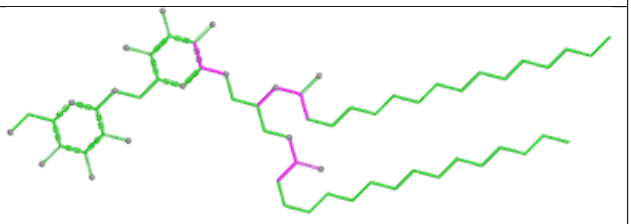

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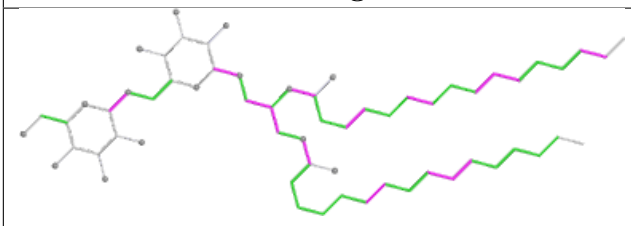

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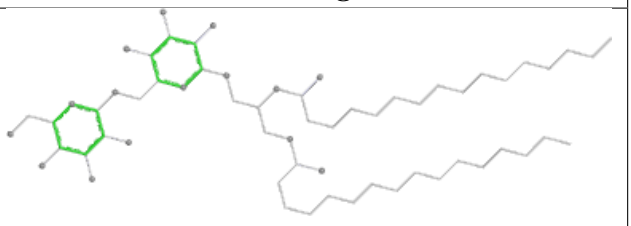
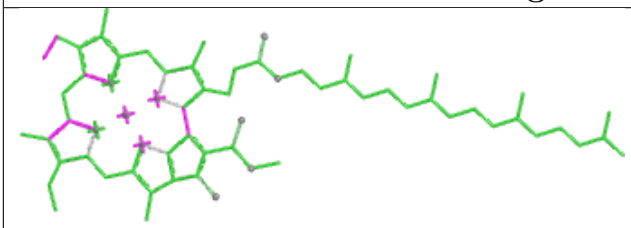


Rings

Ligand CLA n 602



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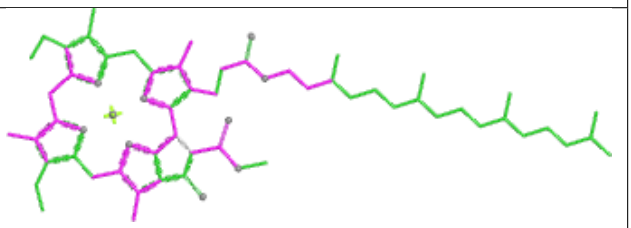
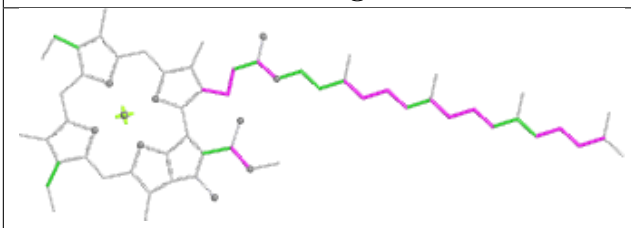
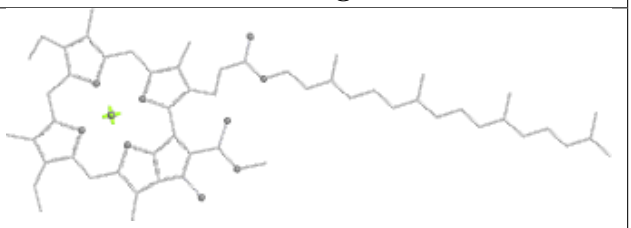


Bond angles

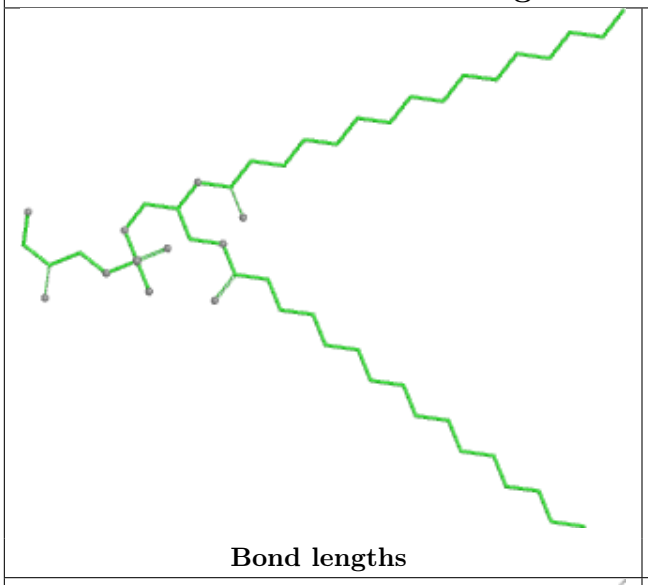


Torsions



Rings

Ligand LHG D1 409



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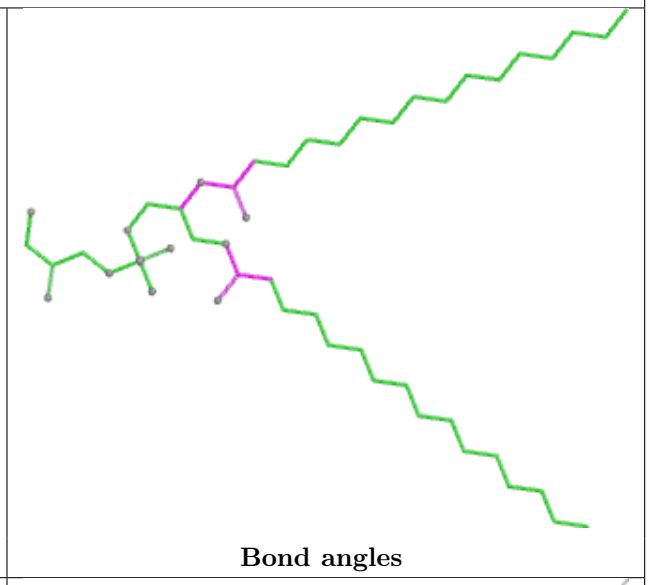
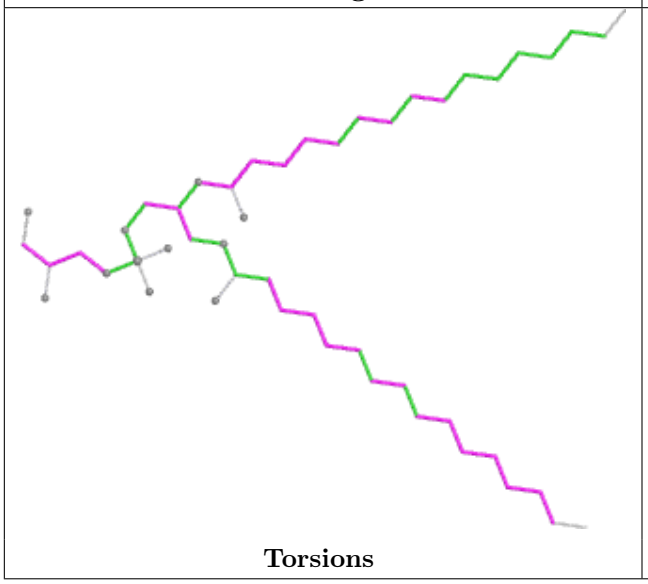
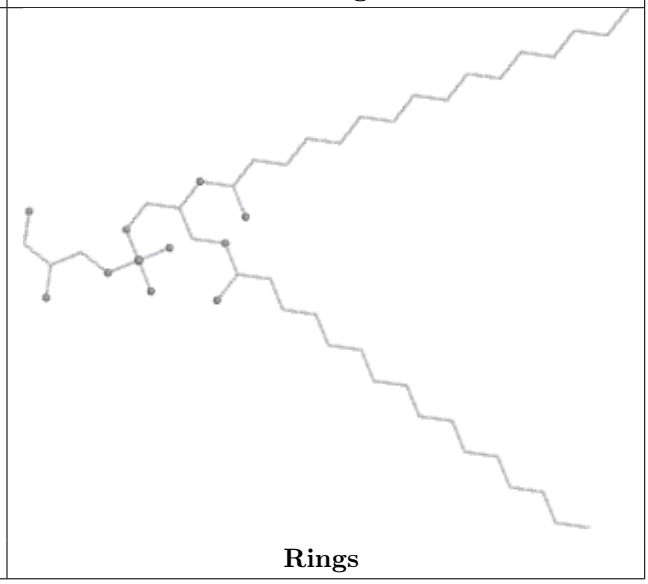


Bond angles

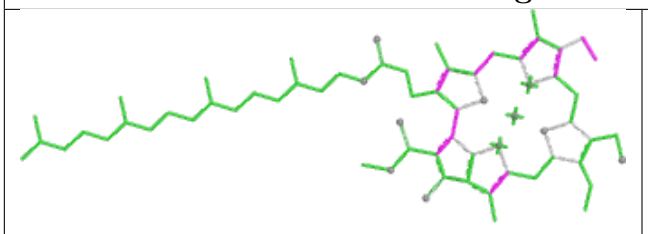


Torsions



Rings

Ligand CHL N1 605



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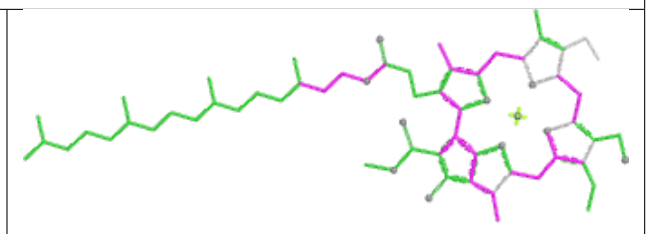
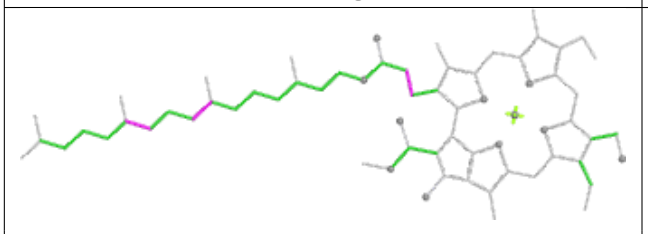


Bond angles



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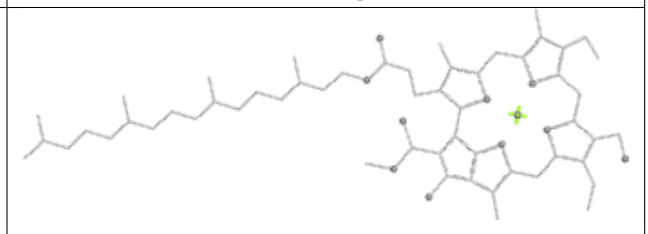
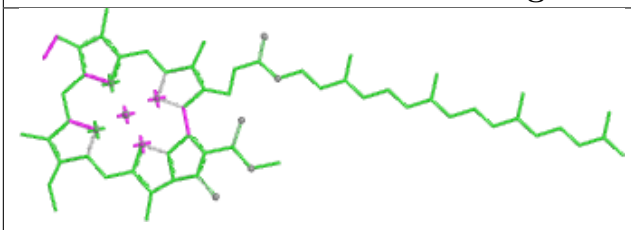


Rings

Ligand CLA b 614



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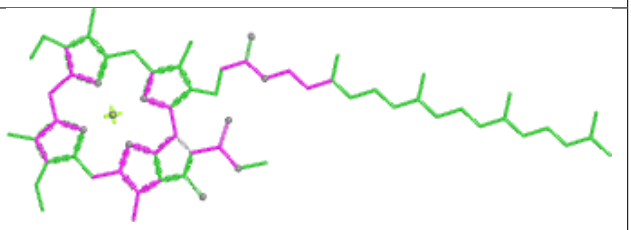
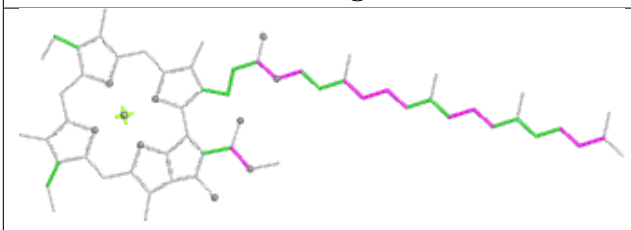
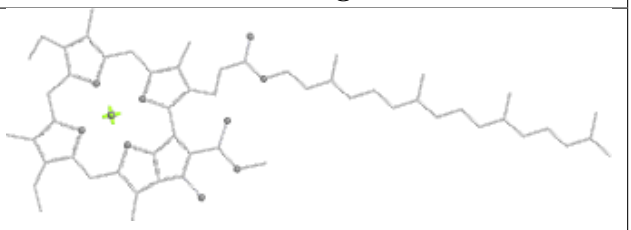


Bond angles

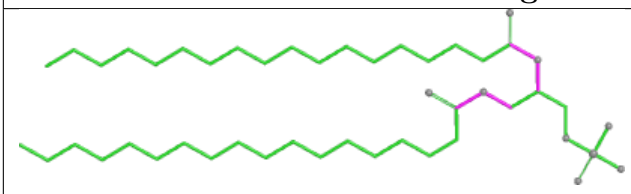


Torsions



Rings

Ligand 3PH S1 626



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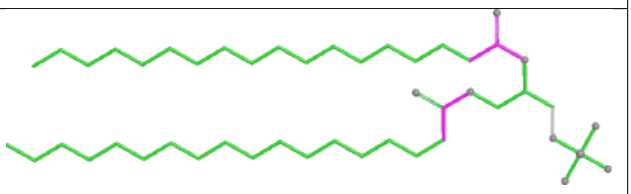
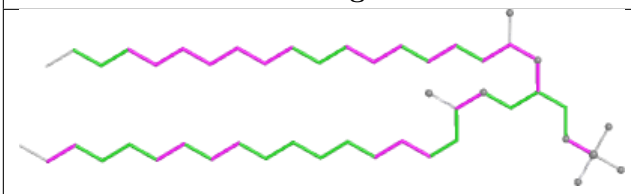
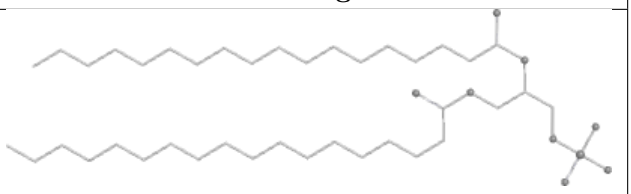


Bond angles

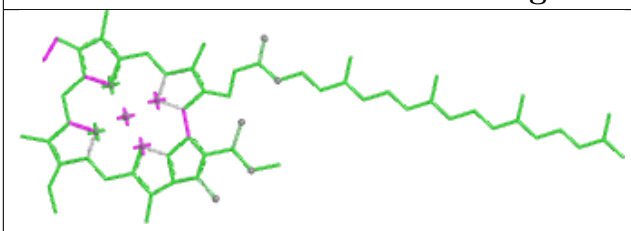


Torsions

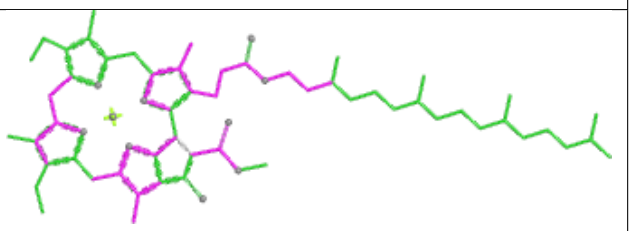


Rings

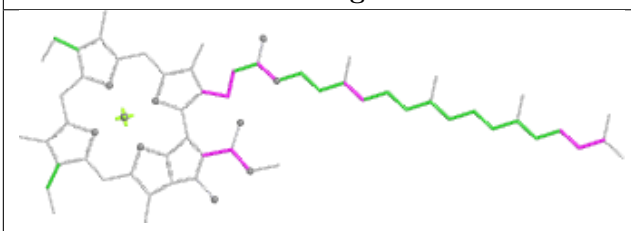
Ligand CLA c 504



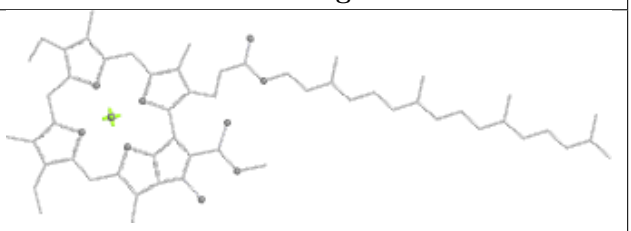
Bond lengths



Bond angles

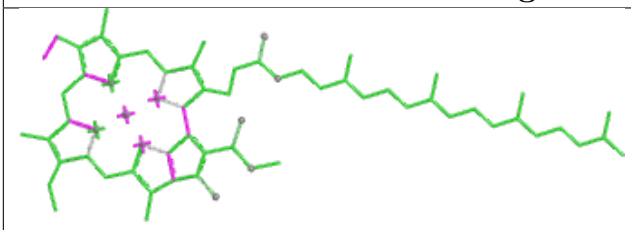


Torsions

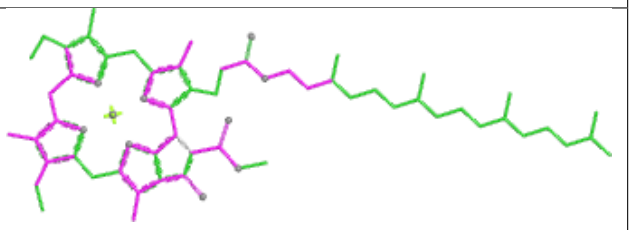


Rings

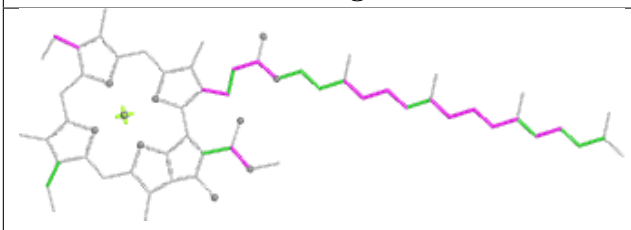
Ligand CLA S1 610



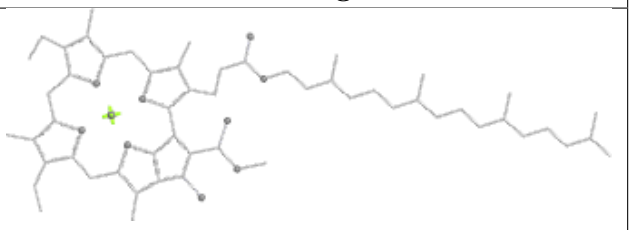
Bond lengths



Bond angles

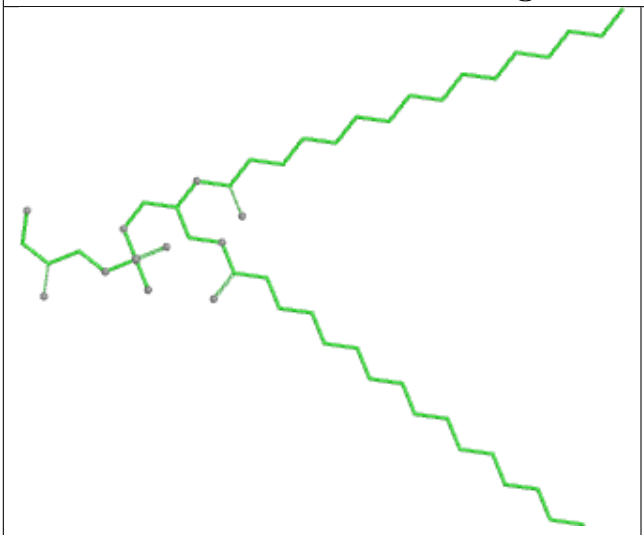


Torsions



Rings

Ligand LHG d1 409



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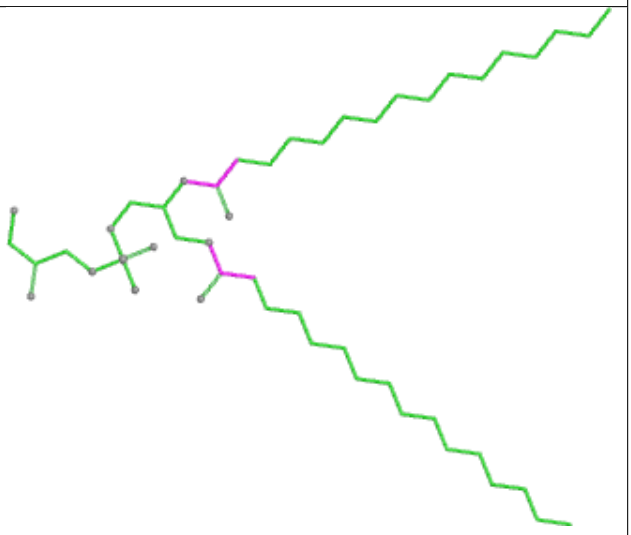

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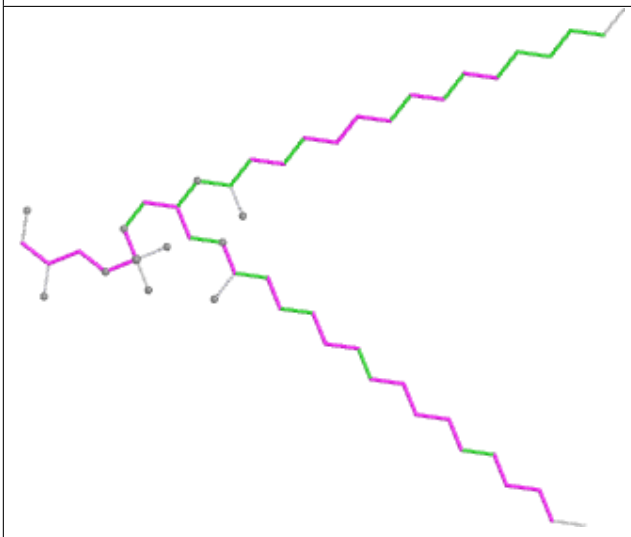

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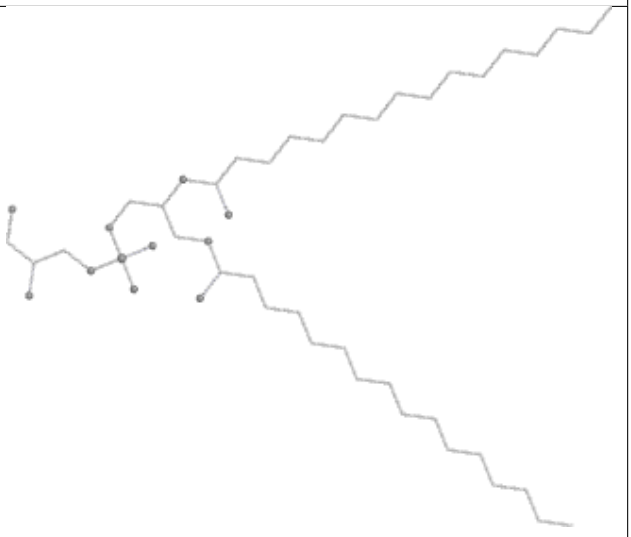
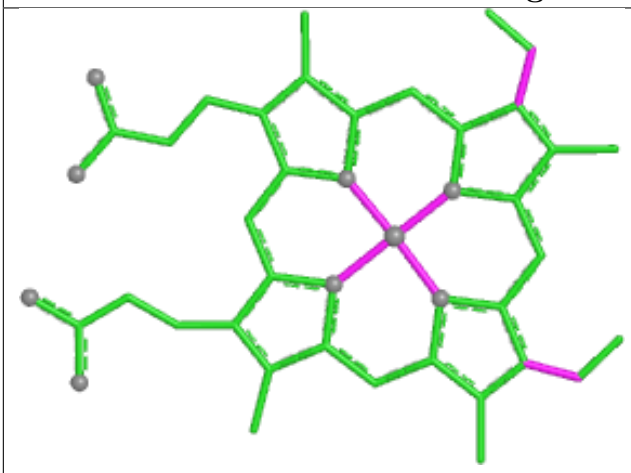


Rings

Ligand HEM f 101



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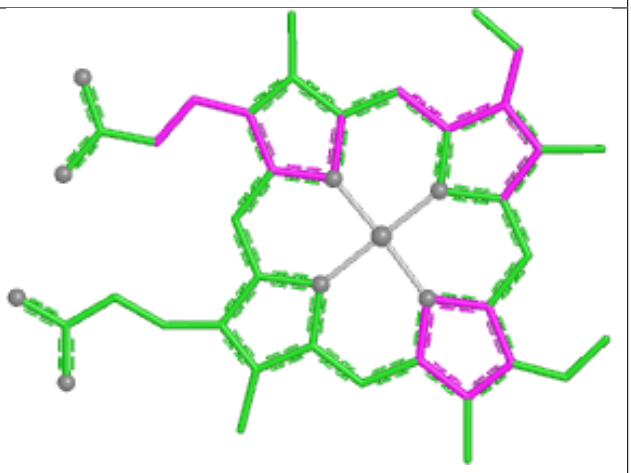

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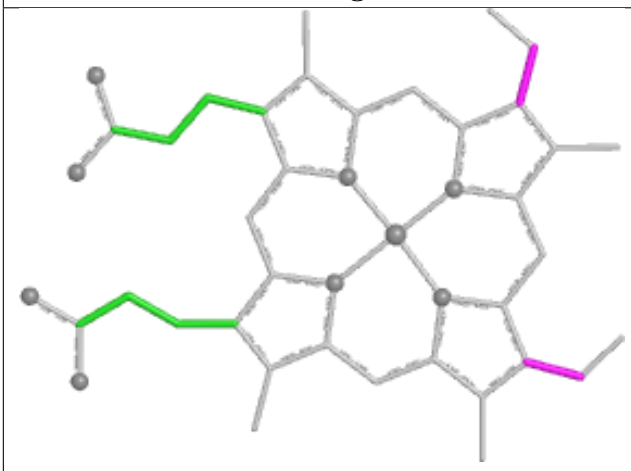

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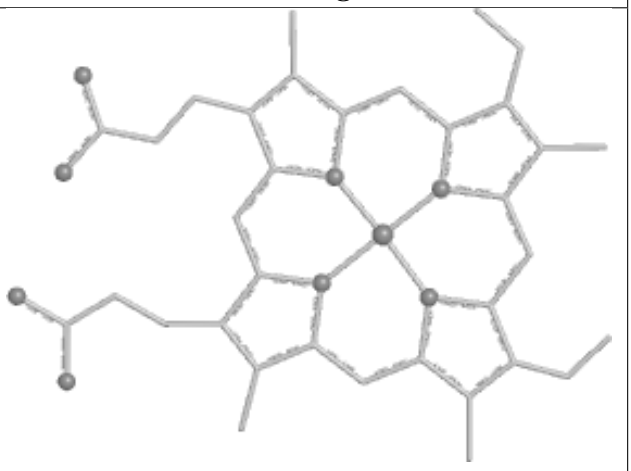
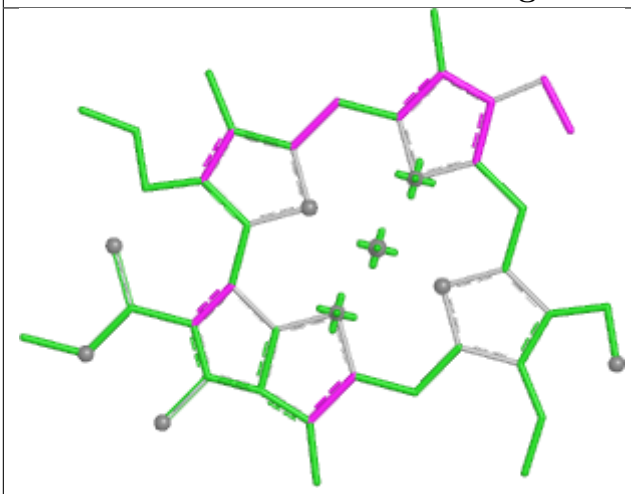


Rings

Ligand CHL g1 608



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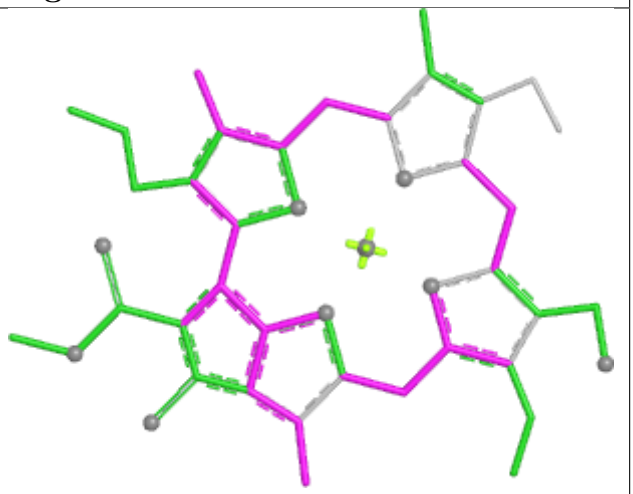

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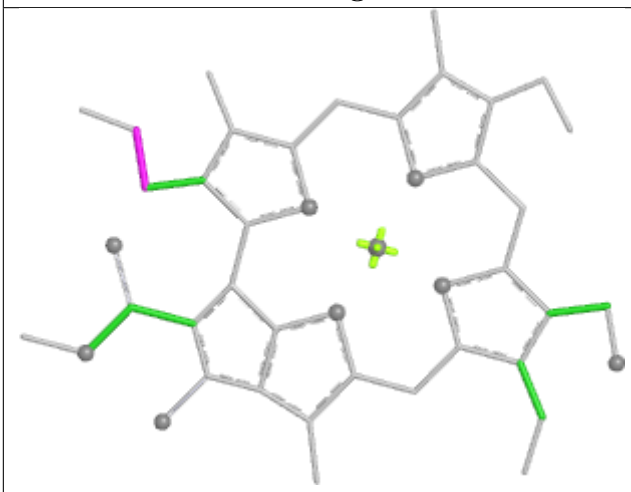

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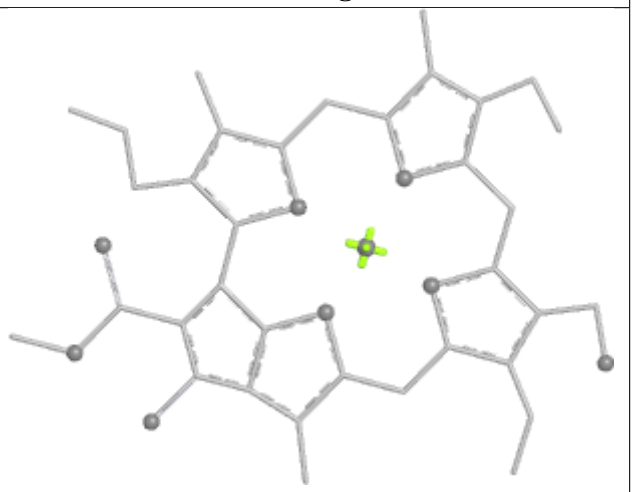
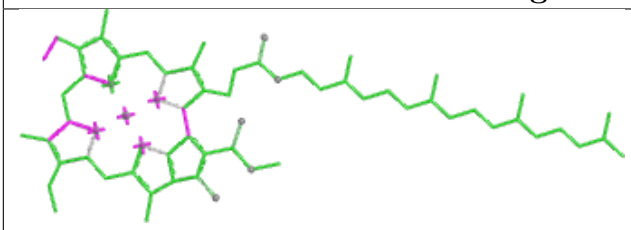


Rings

Ligand CLA s 603



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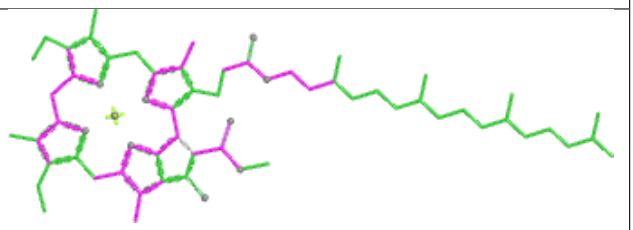

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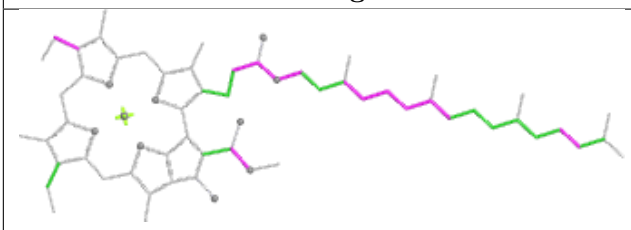

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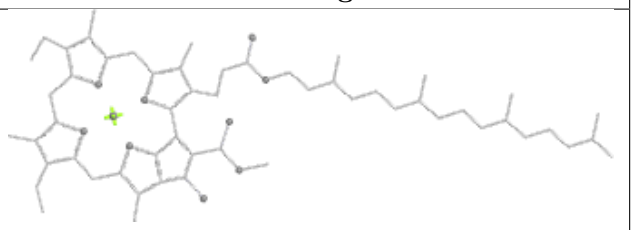
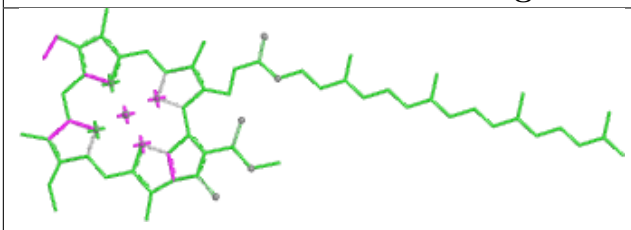


Rings

Ligand CLA Y1 602



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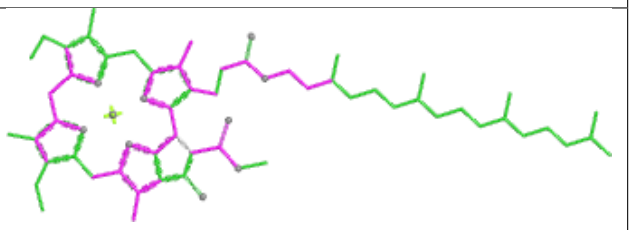

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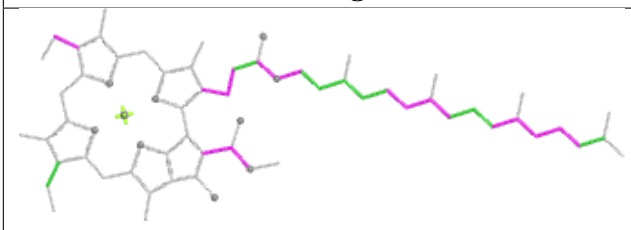

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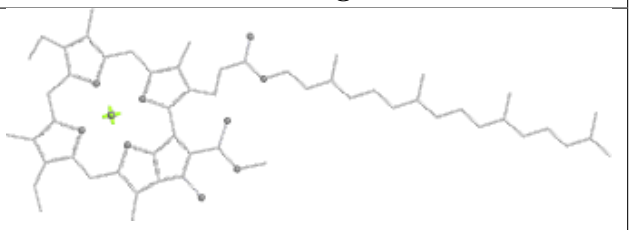
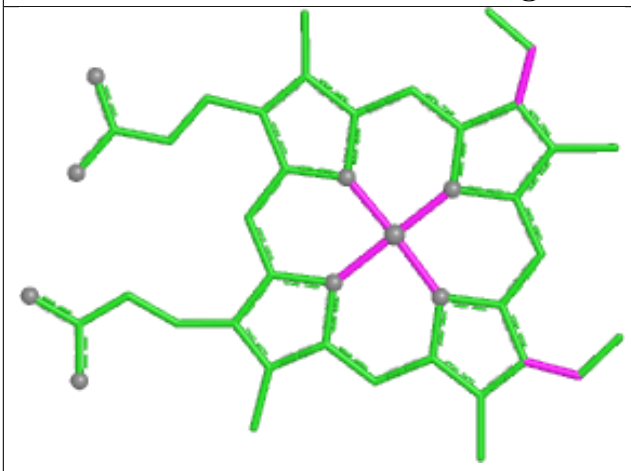


Rings

Ligand HEM F 101



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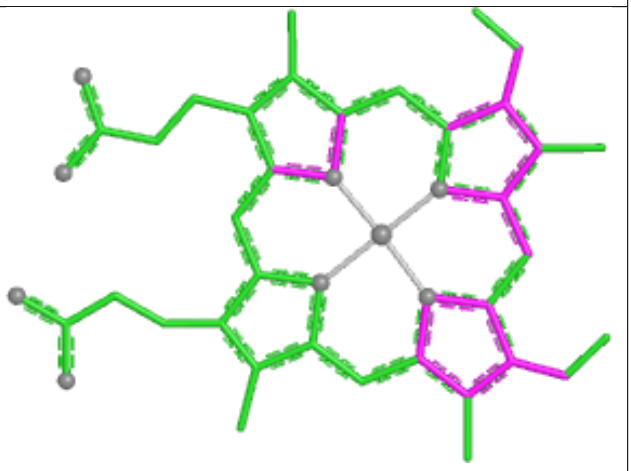

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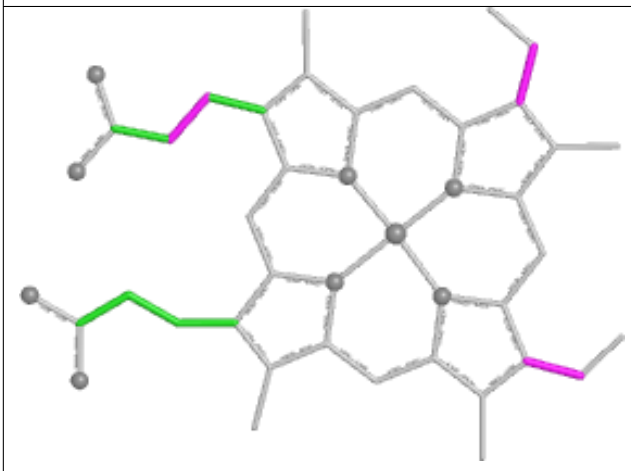

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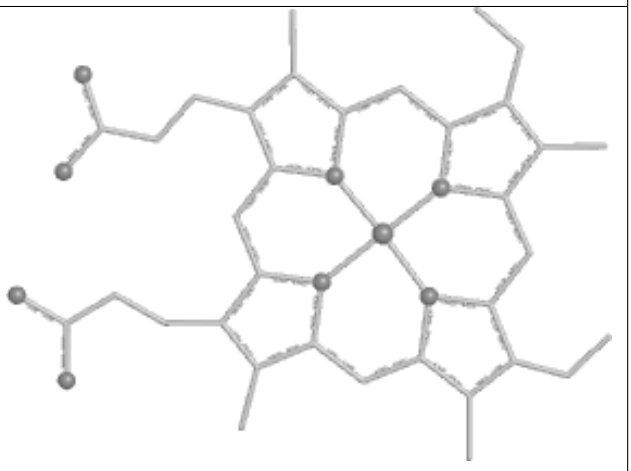
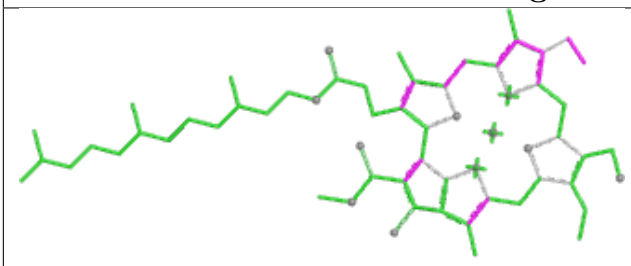


Rings

Ligand CHL s 608



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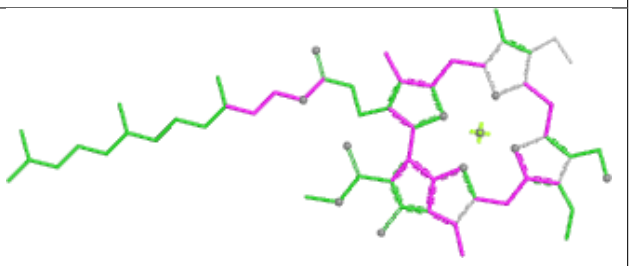

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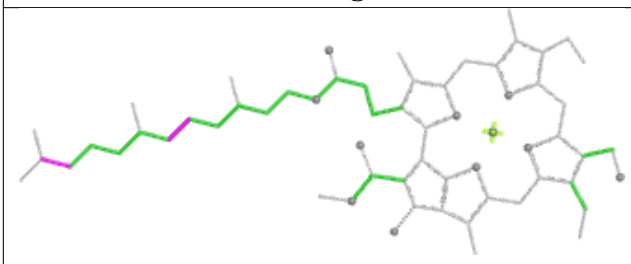

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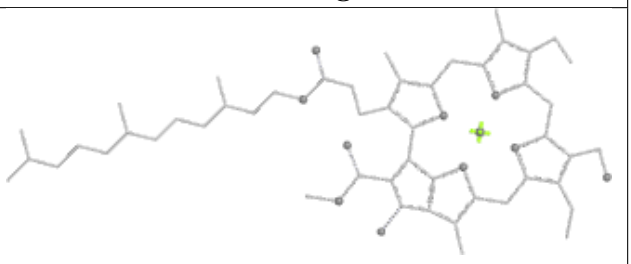
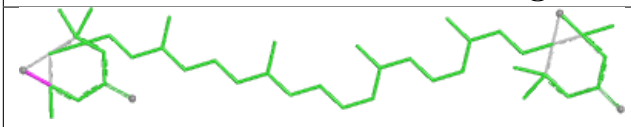


Rings

Ligand XAT r 622



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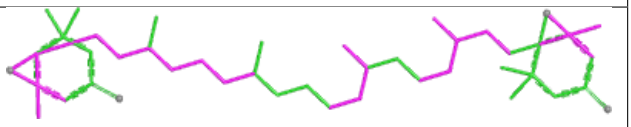
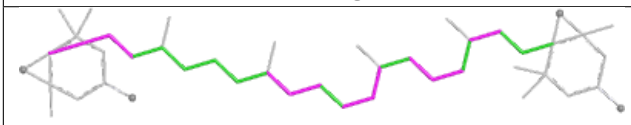


Bond angles



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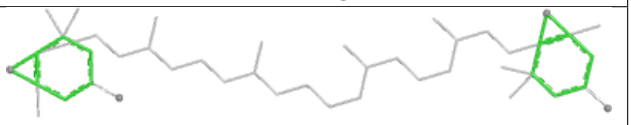
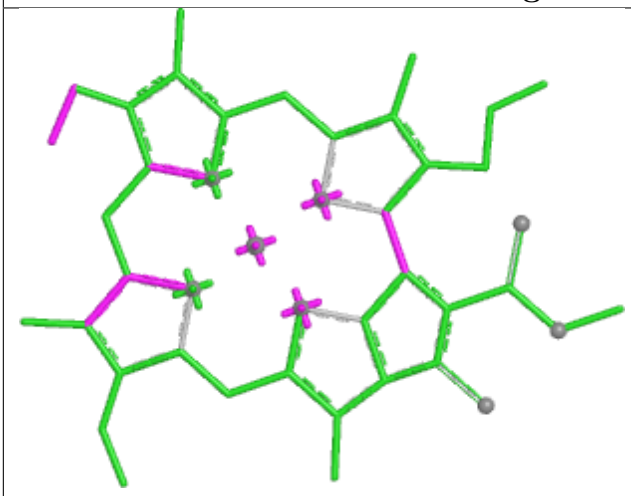


Rings

Ligand CLA G 612



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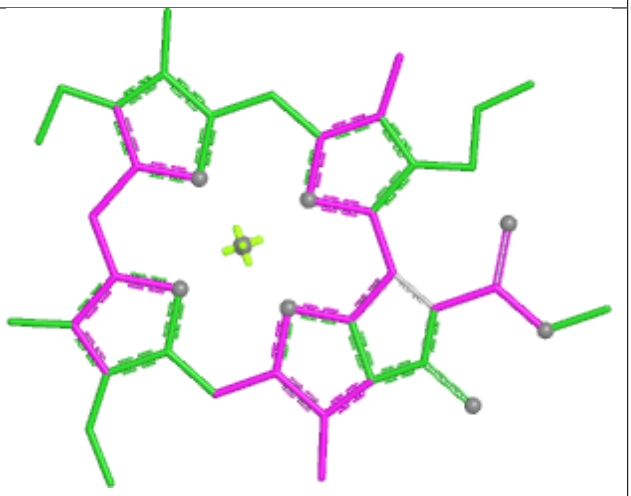
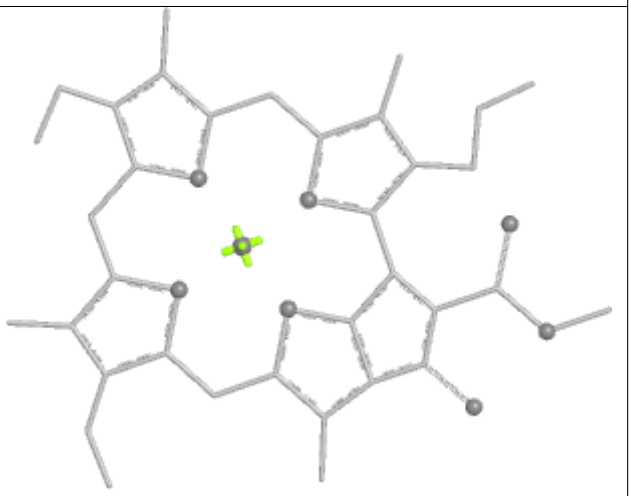


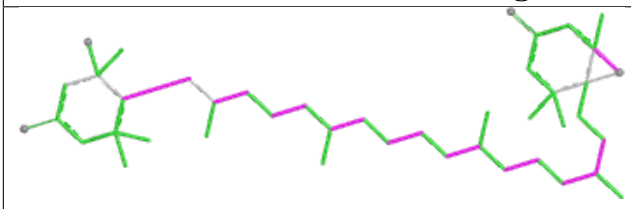
Bond angles

Torsions



Rings

Ligand NEX R1 622



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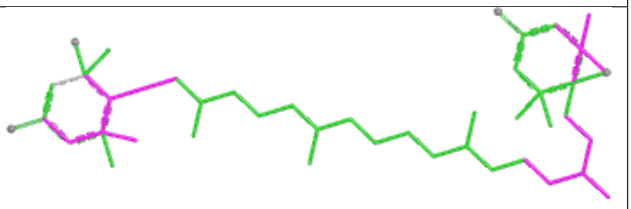

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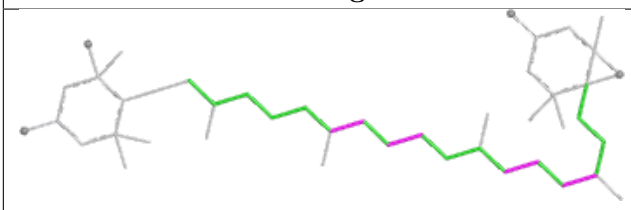

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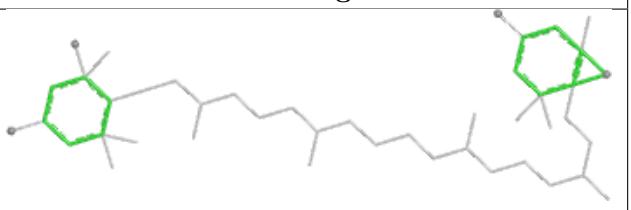
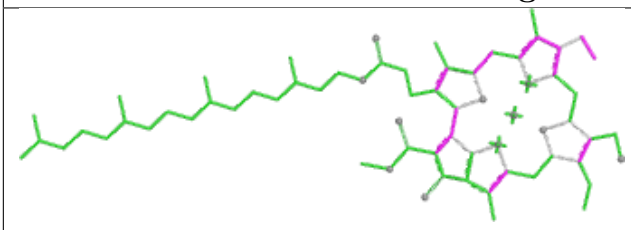


Rings

Ligand CHL g1 609



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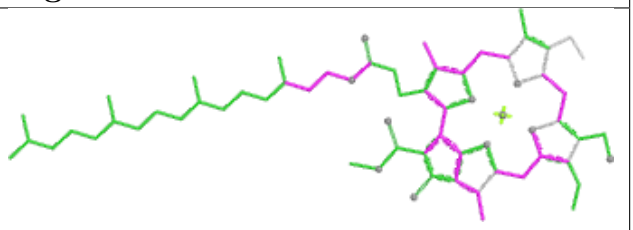

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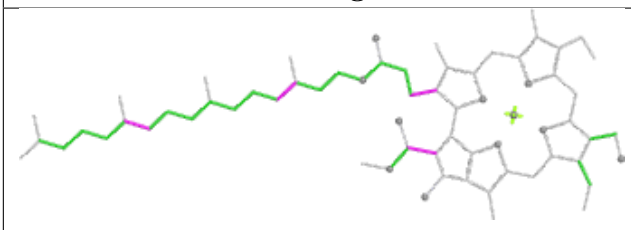

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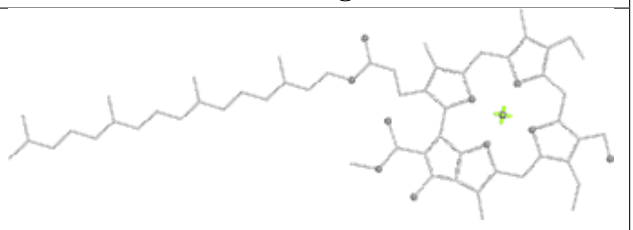
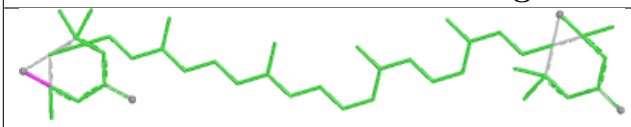


Rings

Ligand XAT G1 622



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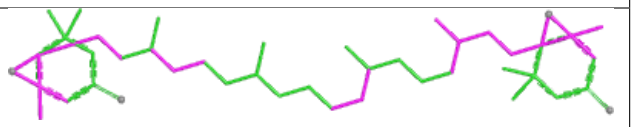
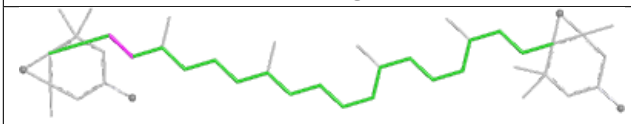


Bond angles



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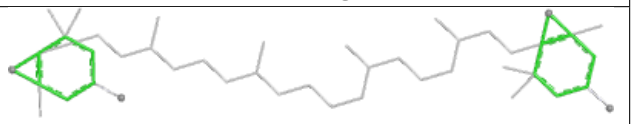
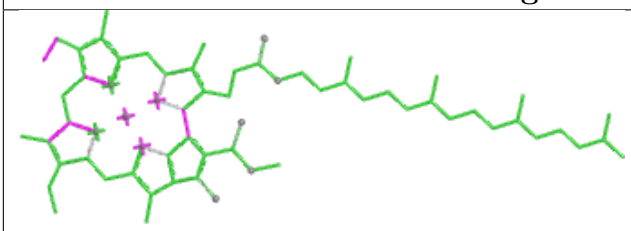


Rings

Ligand CLA s1 611



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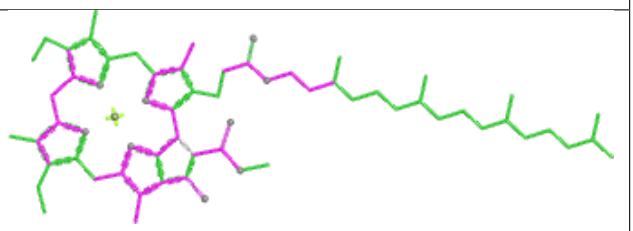
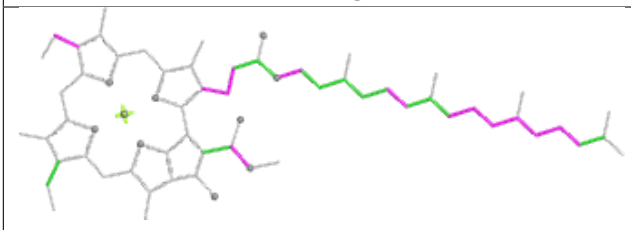


Bond angles



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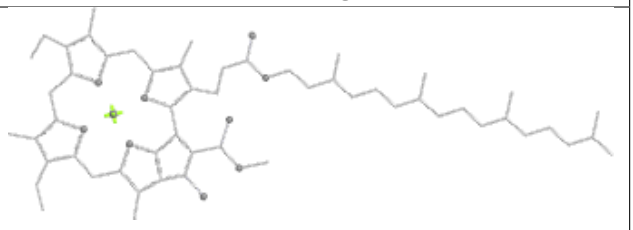
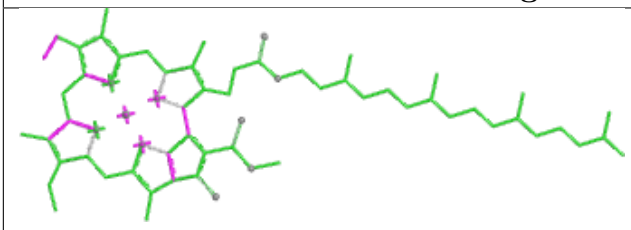
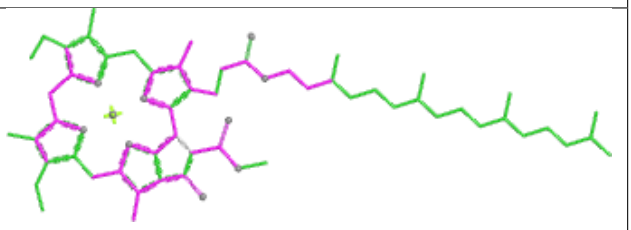


Rings

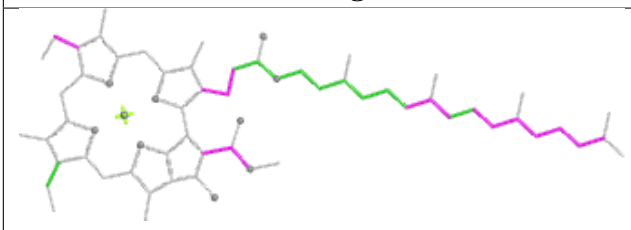
Ligand CLA c1 507



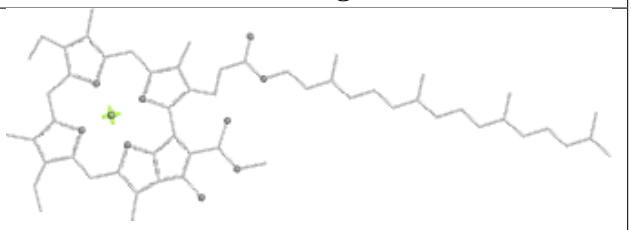
Bond lengths



Bond angles

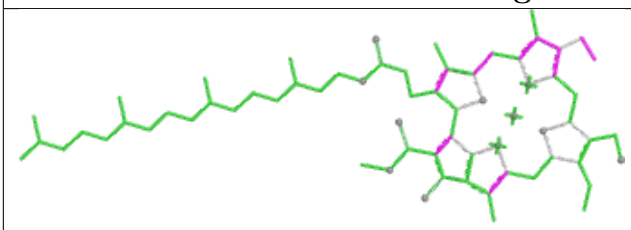


Torsions



Rings

Ligand CHL G1 601



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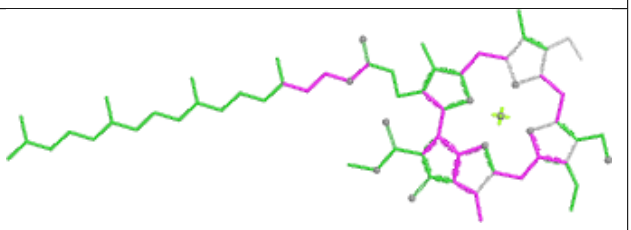
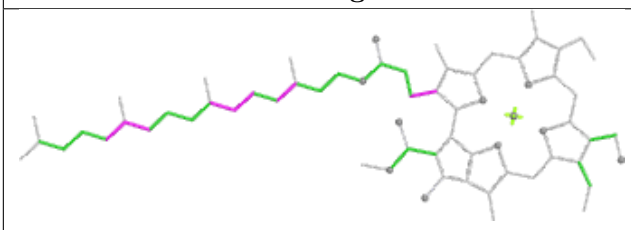


Bond angles



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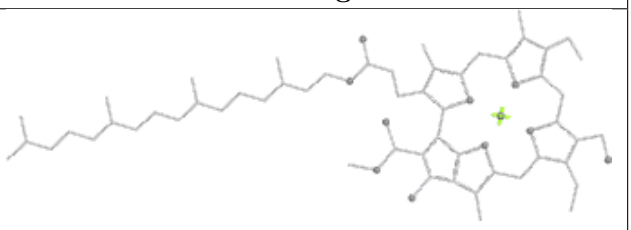
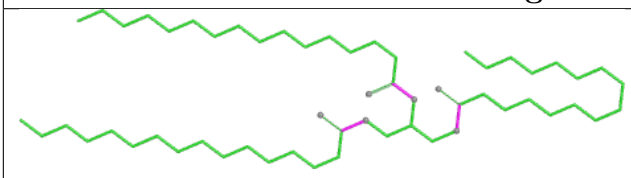


Rings

Ligand 4RF I1 102



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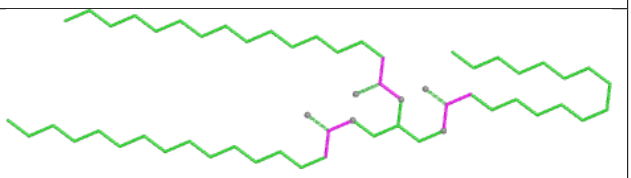
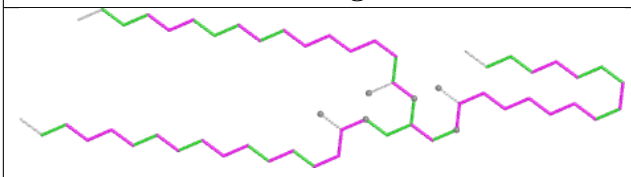
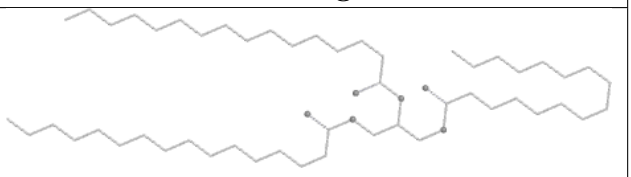


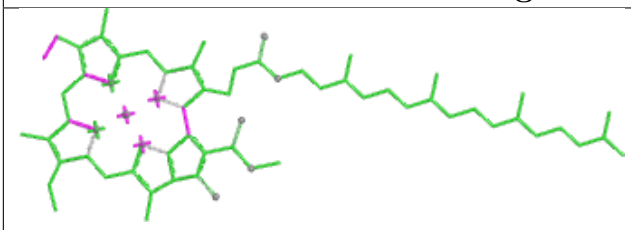
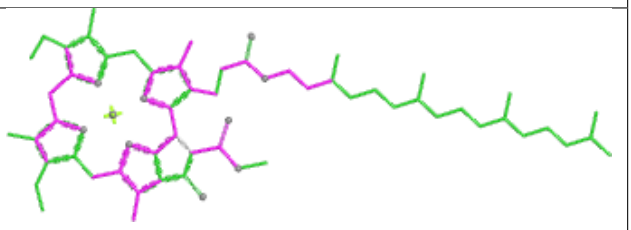
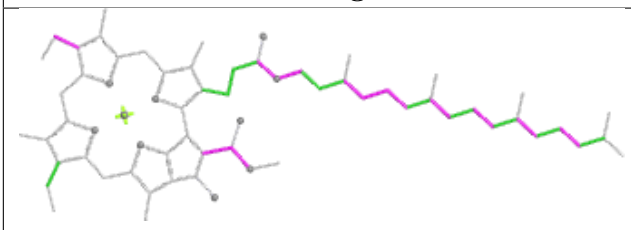
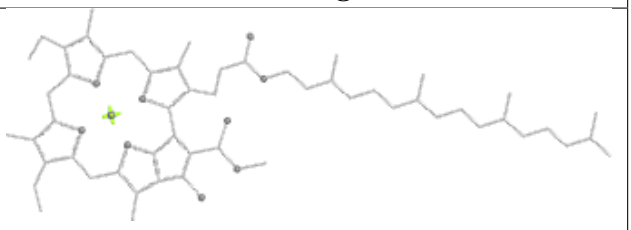
Bond angles

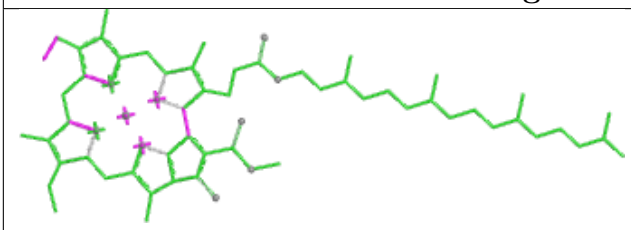
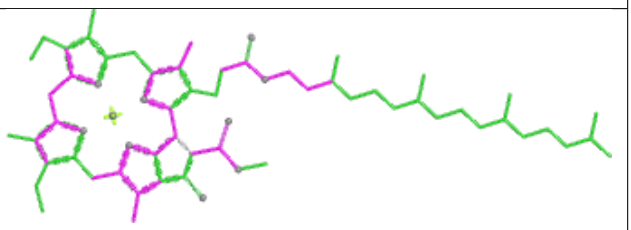
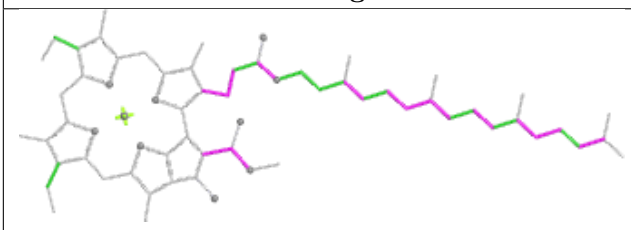
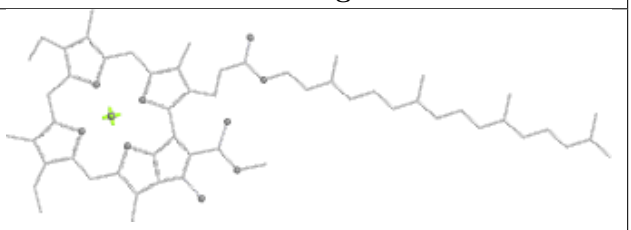


Torsions

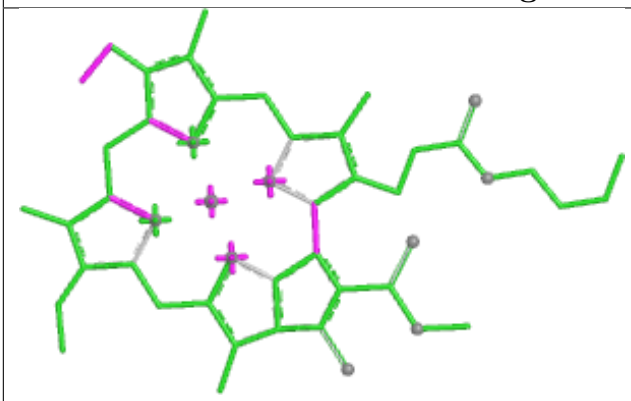


Rings

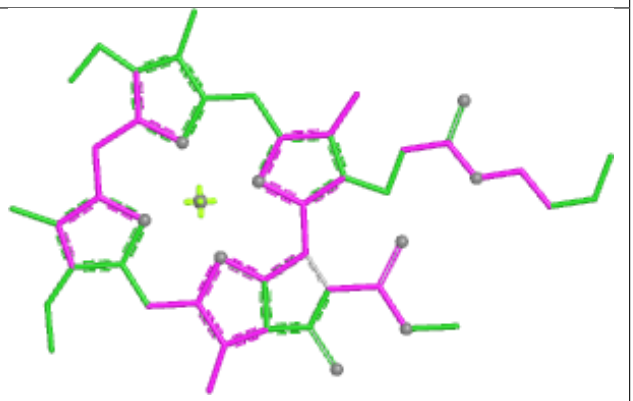
Ligand CLA C1 506	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA G 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

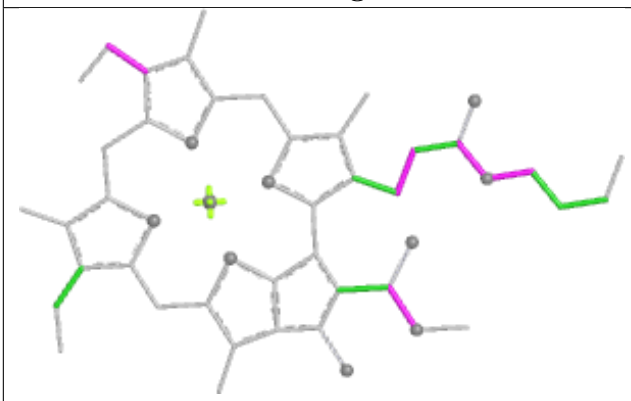
Ligand CLA a1 407



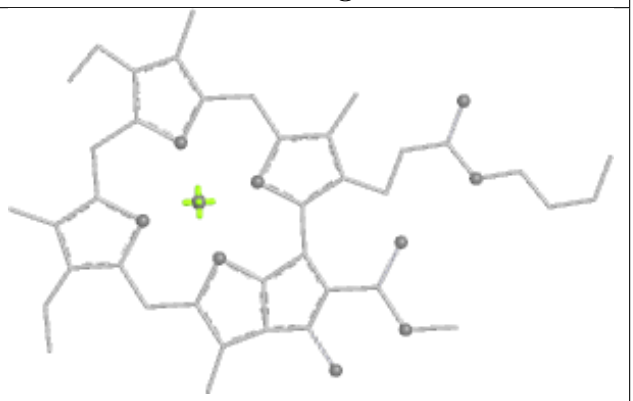
Bond lengths



Bond angles

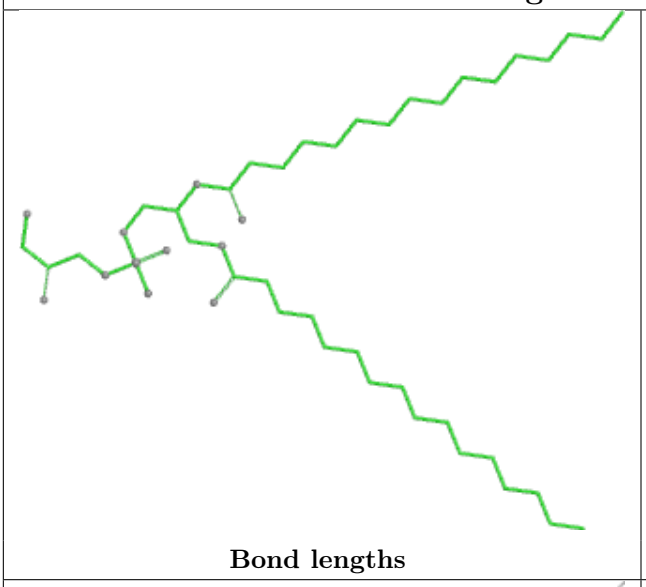


Torsions



Rings

Ligand LHG n 624



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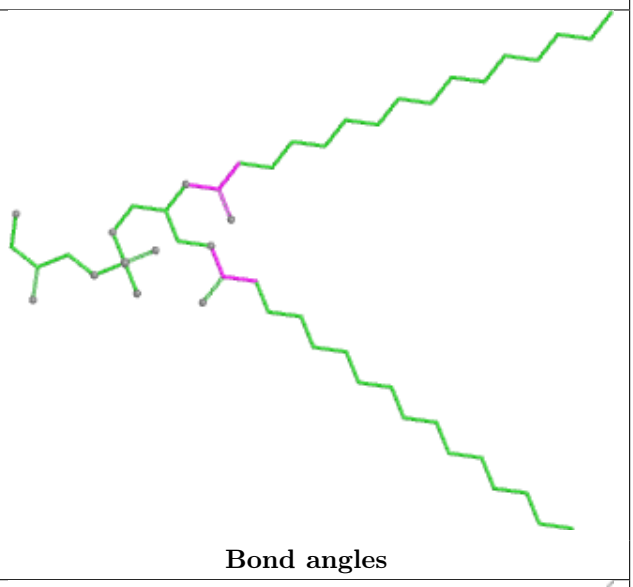
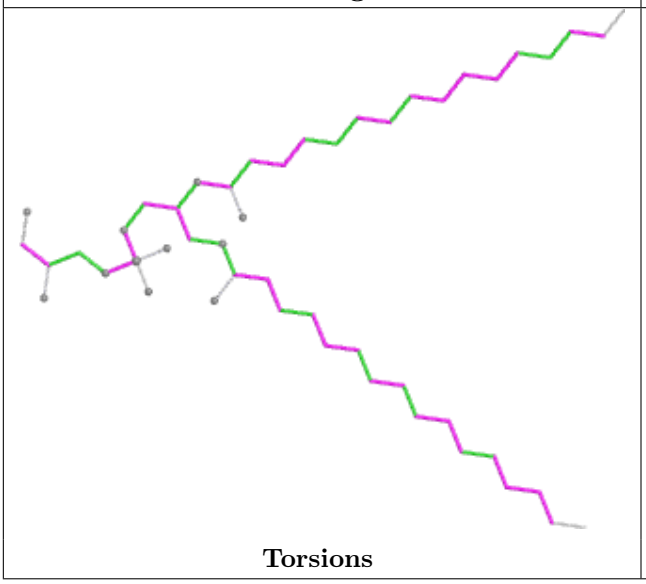
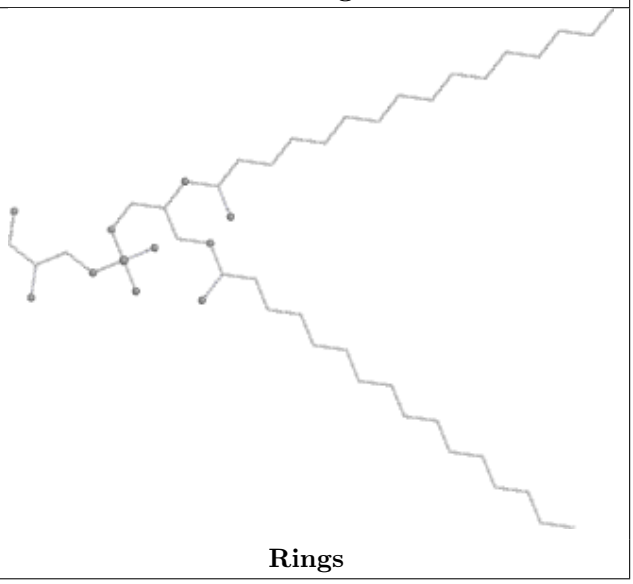


Bond angles



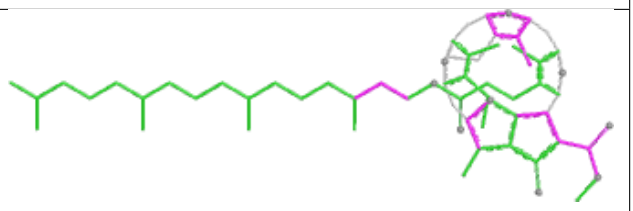
Torsions



Rings

Ligand PHO a1 408

Bond lengths



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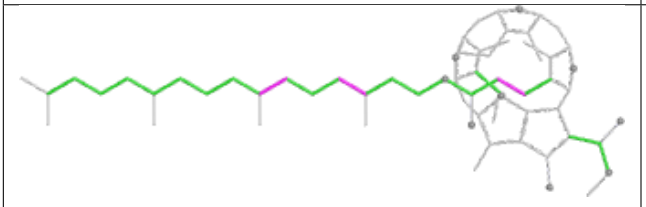
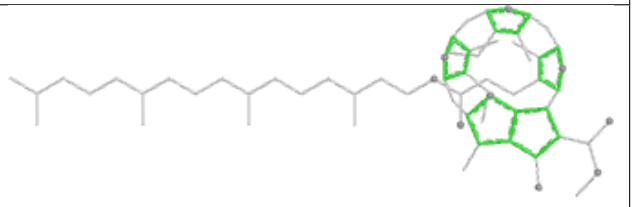
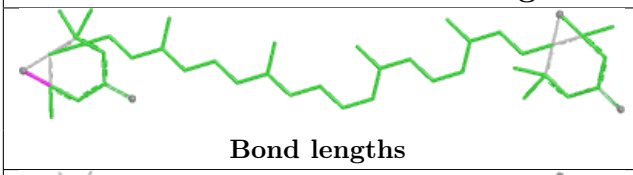


Torsions



Rings

Ligand XAT g1 622



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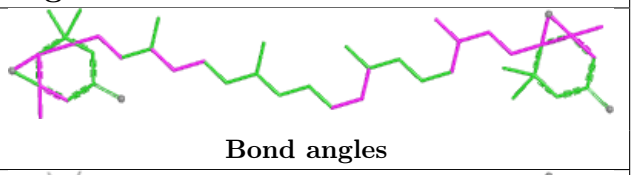
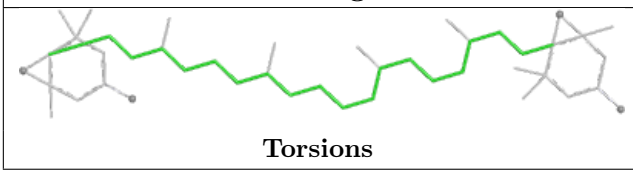
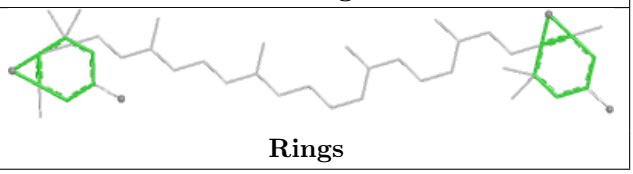


Bond angles

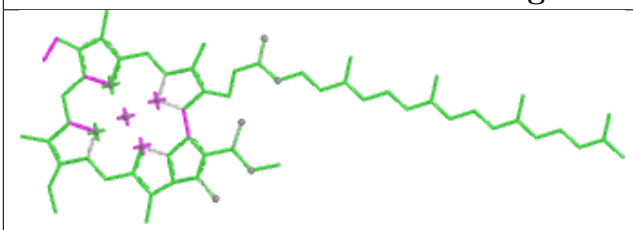


Torsions



Rings

Ligand CLA y 612



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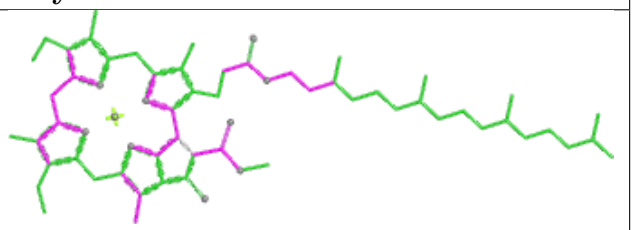

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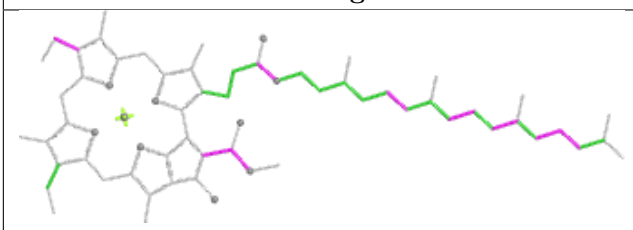
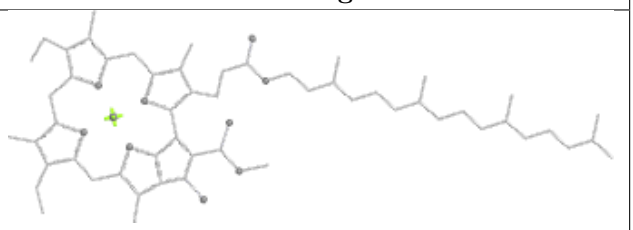
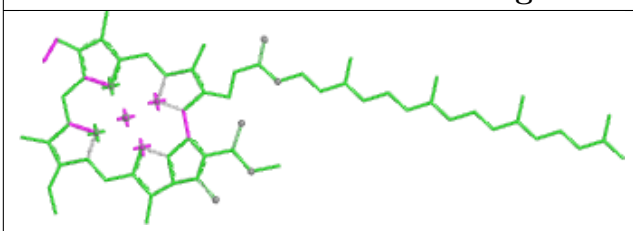


Torsions



Rings

Ligand CLA B1 616



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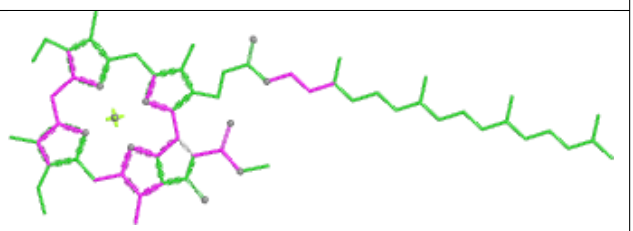
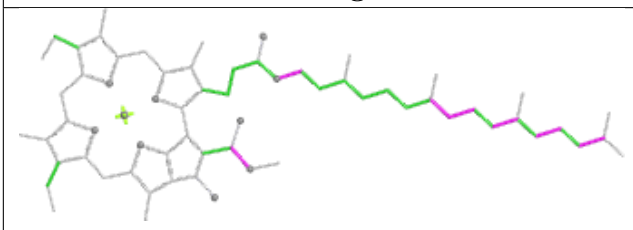


Bond angles



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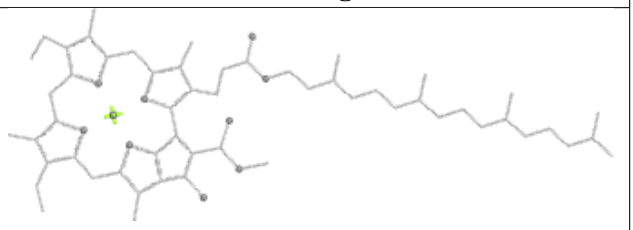
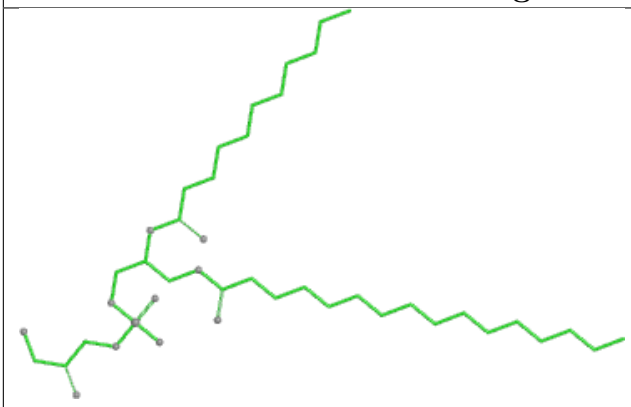


Rings

Ligand LHG D1 408



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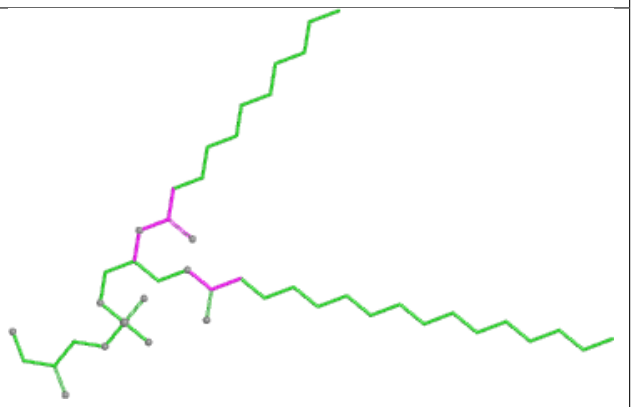
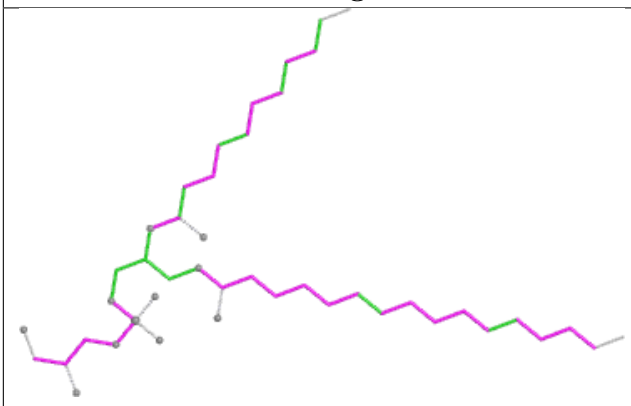


Bond angles



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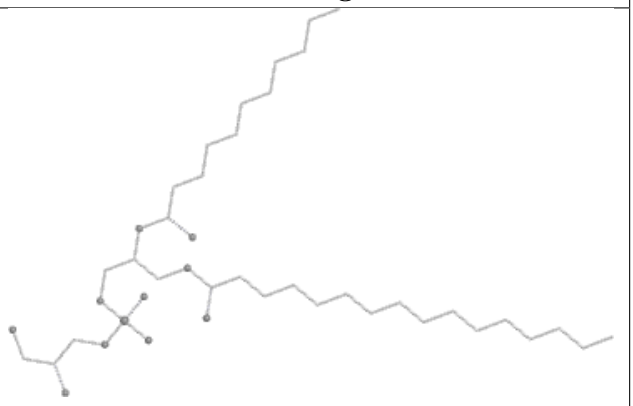
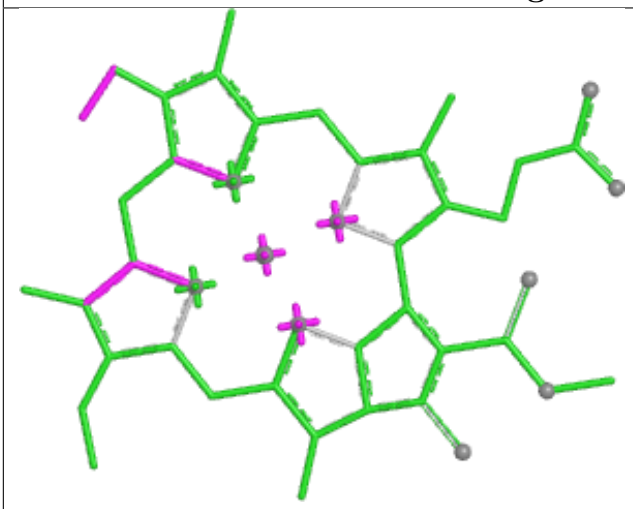


Rings

Ligand CLA n 612



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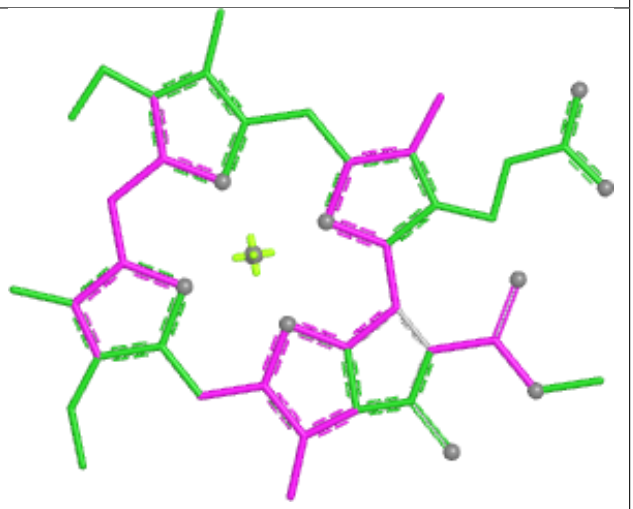
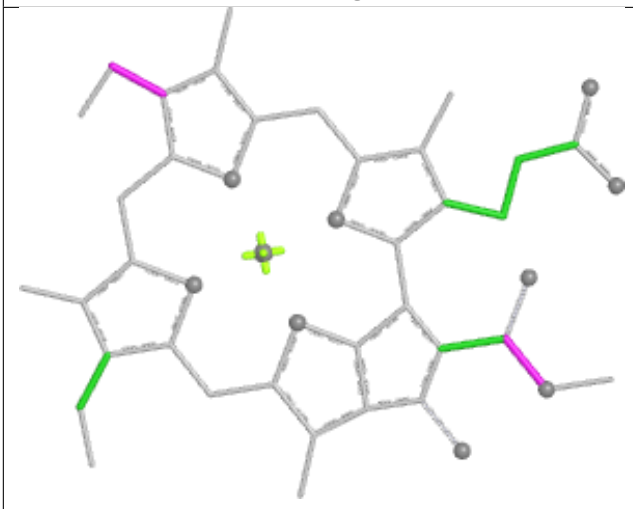


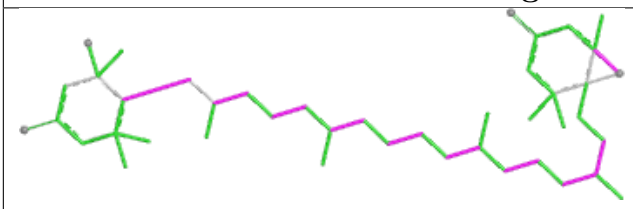
Bond angles



Torsions

Rings

Ligand NEX Y 623



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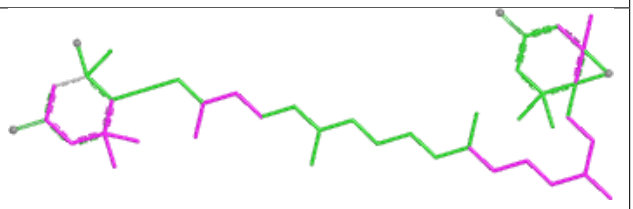
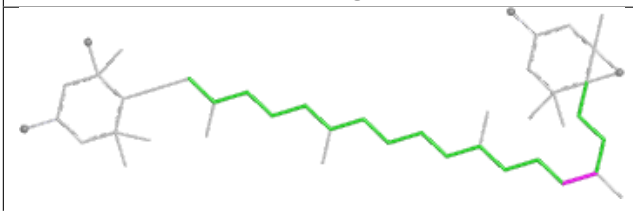


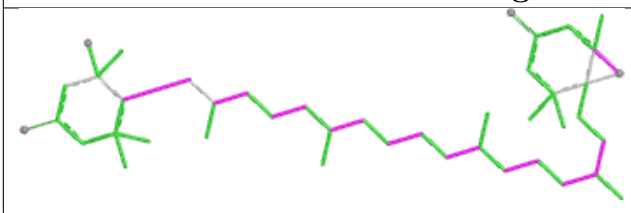
Bond angles



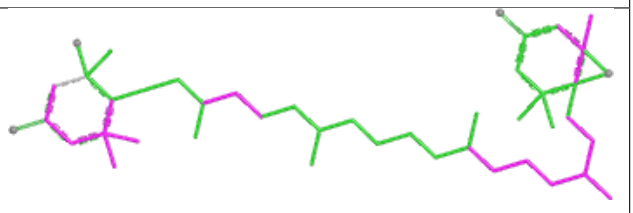
Torsions

Rings

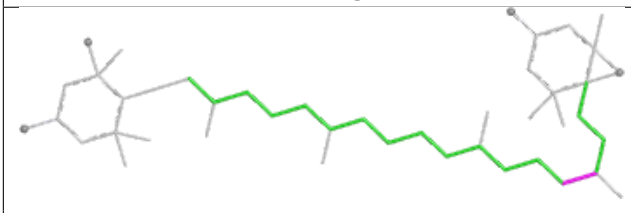
Ligand NEX G1 623



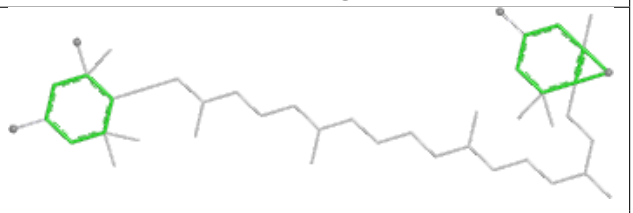
Bond lengths



Bond angles

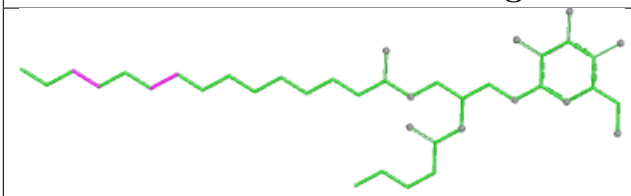


Torsions

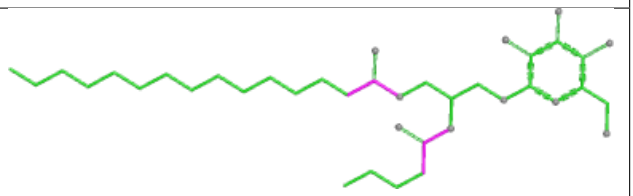


Rings

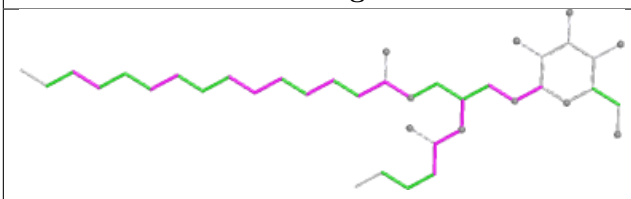
Ligand LMG W1 201



Bond lengths



Bond angles



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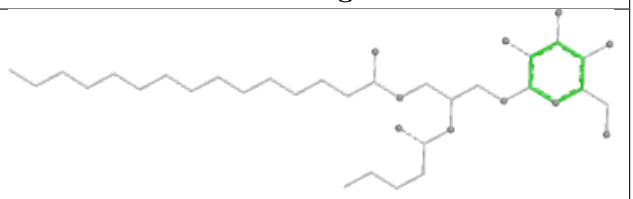
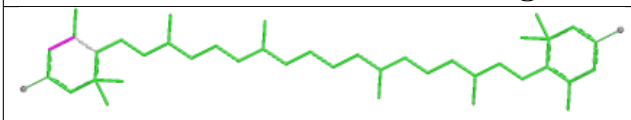


Rings

Ligand LUT S1 621



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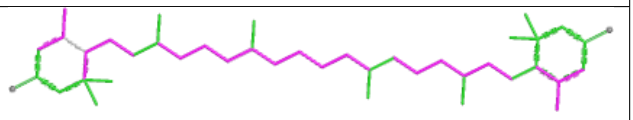
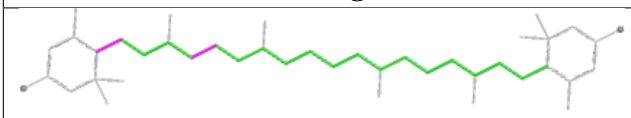


Bond angles



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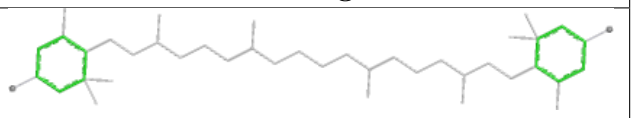
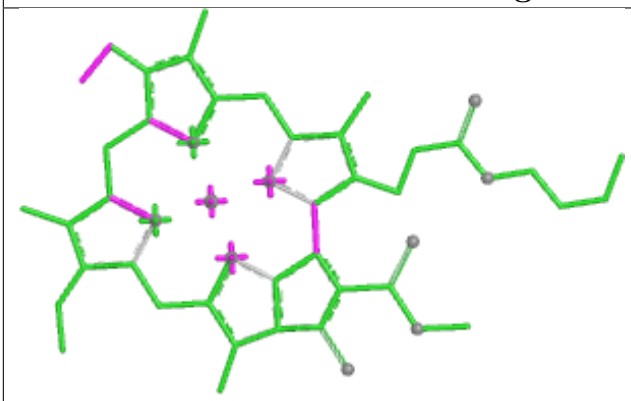


Rings

Ligand CLA N1 611



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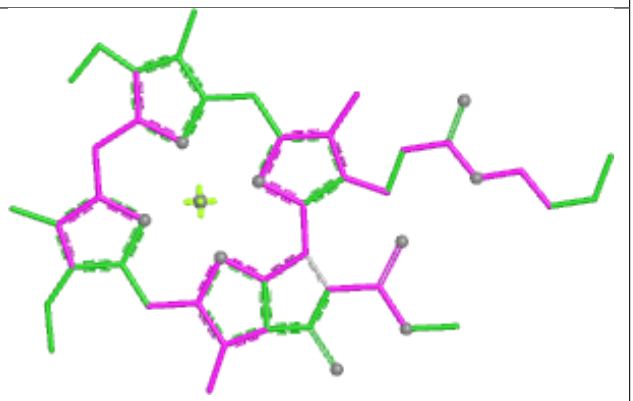
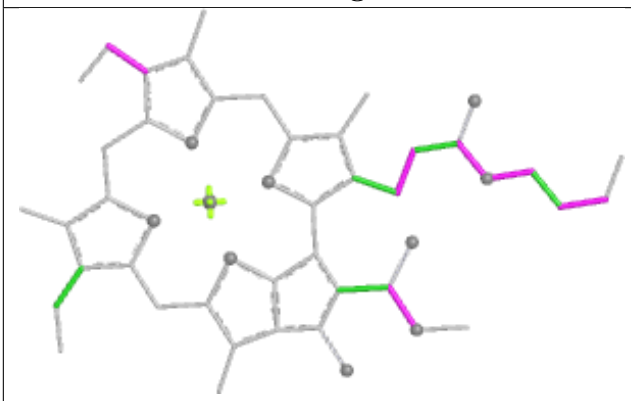


Bond angles



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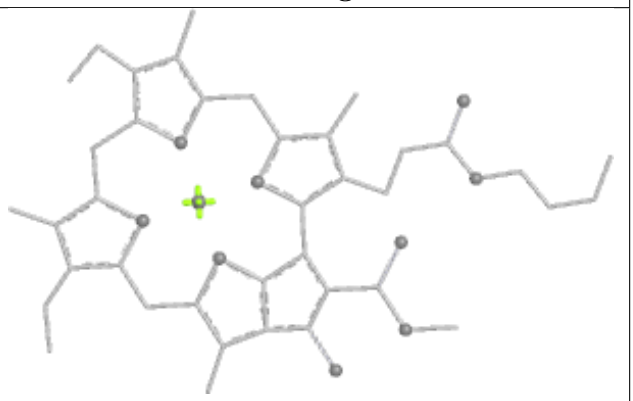
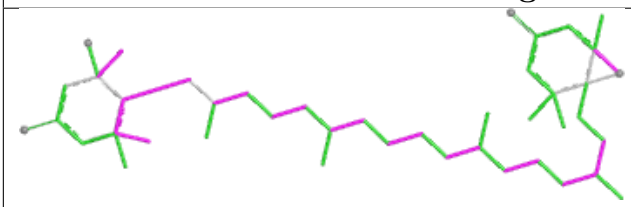


Rings

Ligand NEX s1 623



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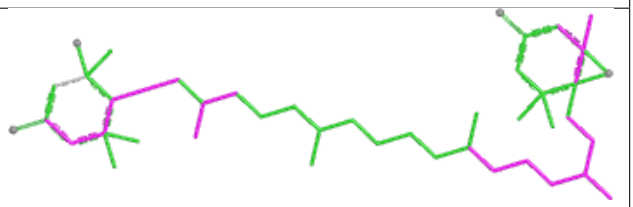

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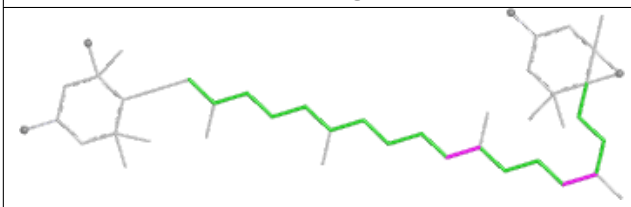

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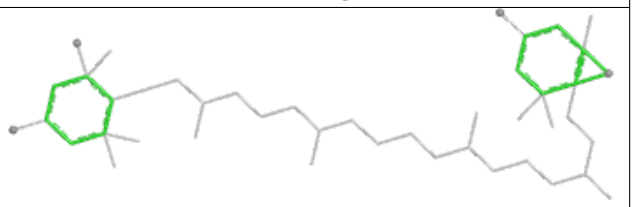
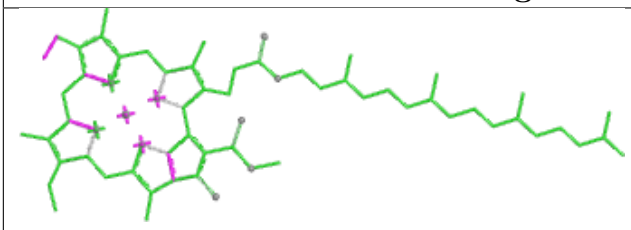


Rings

Ligand CLA D1 402



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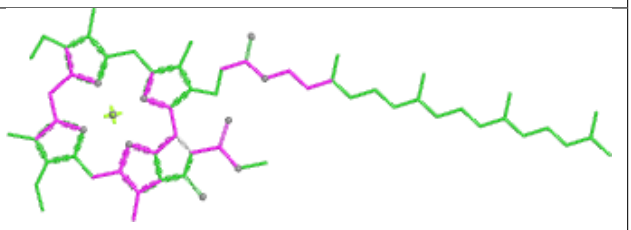
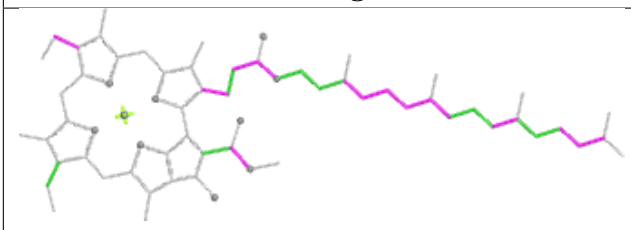


Bond angles



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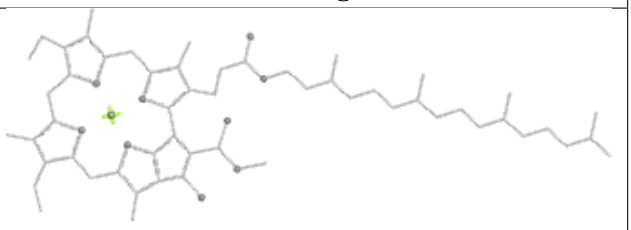
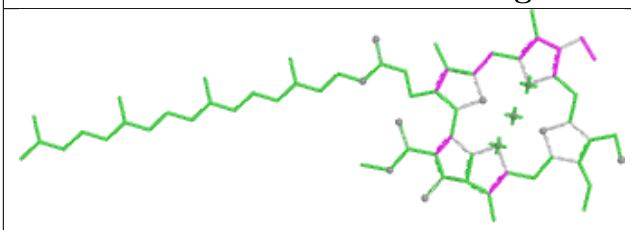


Rings

Ligand CHL Y1 609



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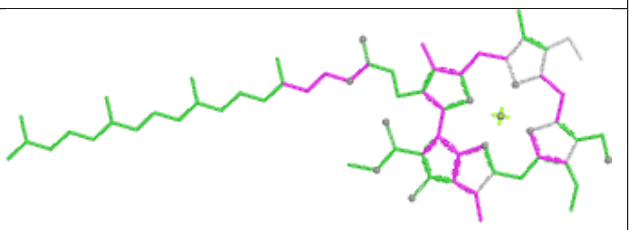
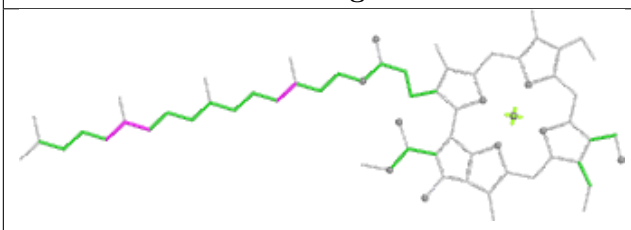


Bond angles



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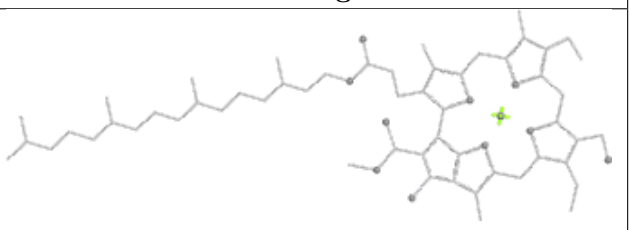
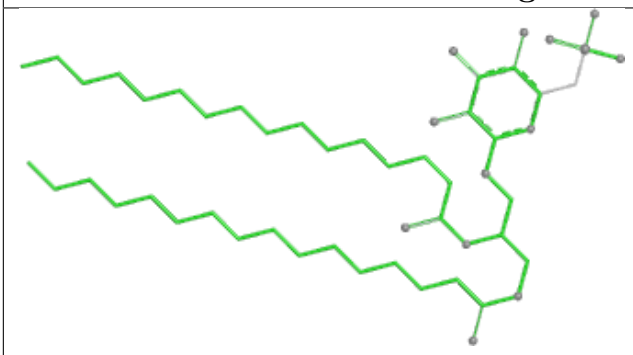


Rings

Ligand SQD b1 626



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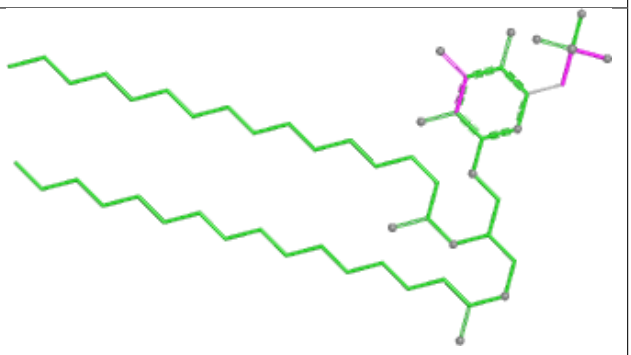

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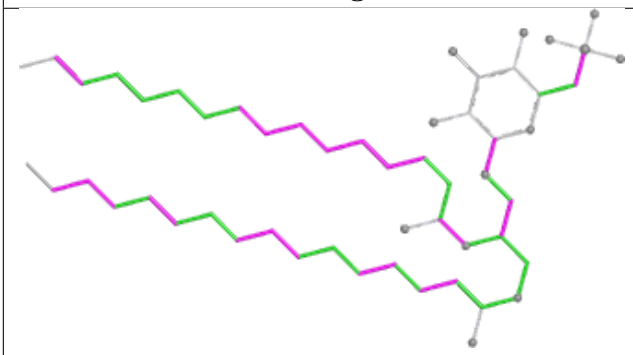

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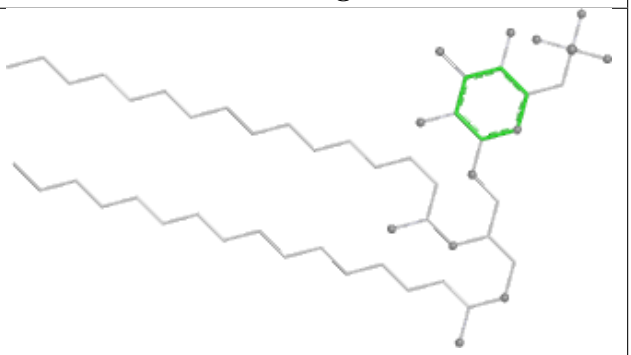
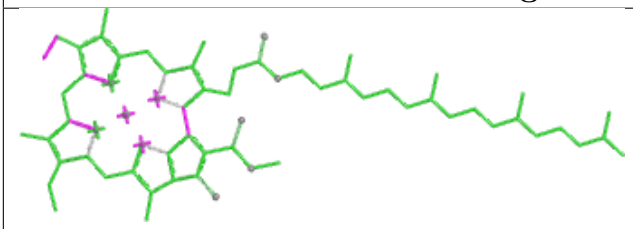


Rings

Ligand CLA c1 512



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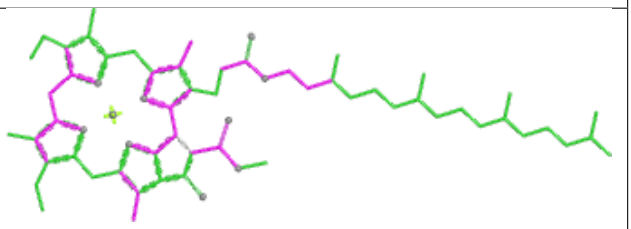
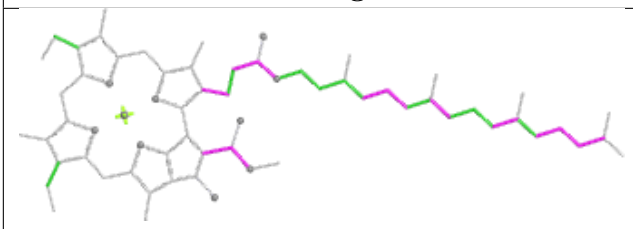


Bond angles



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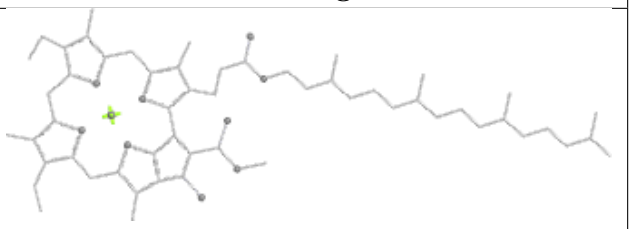
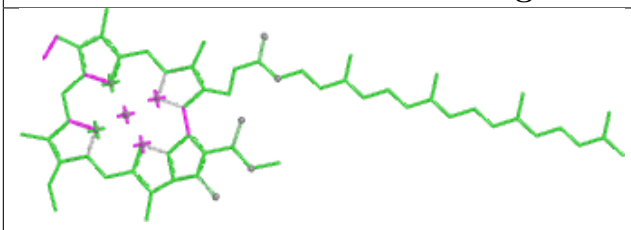


Rings

Ligand CLA C1 509



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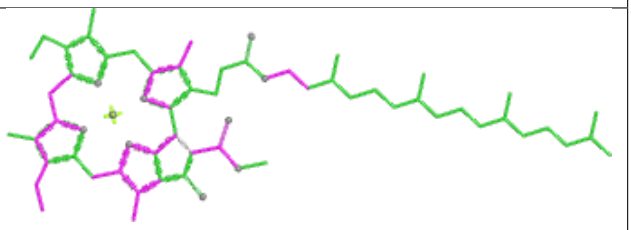
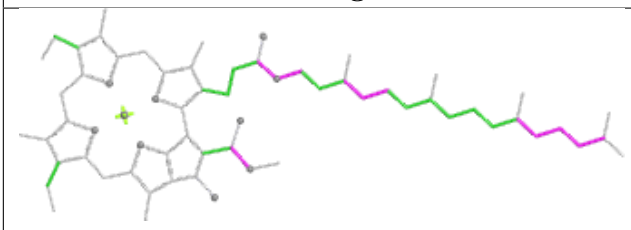


Bond angles



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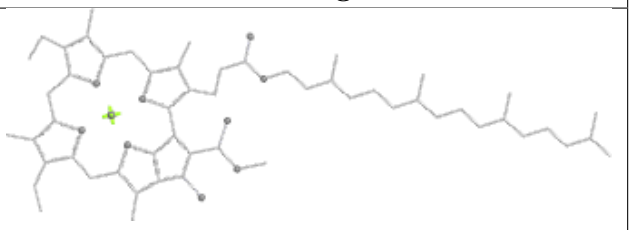
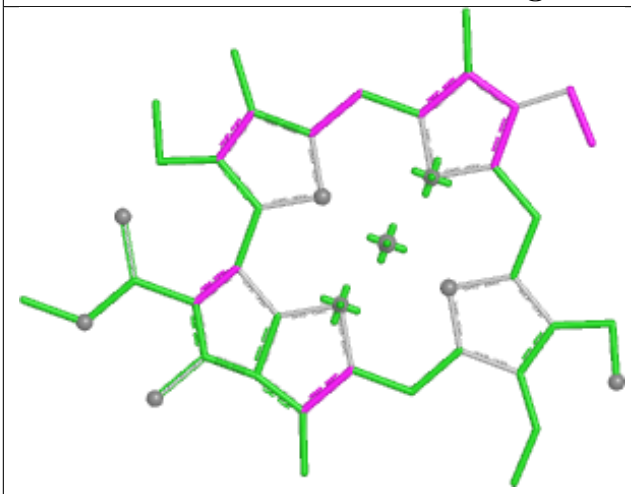


Rings

Ligand CHL S 607



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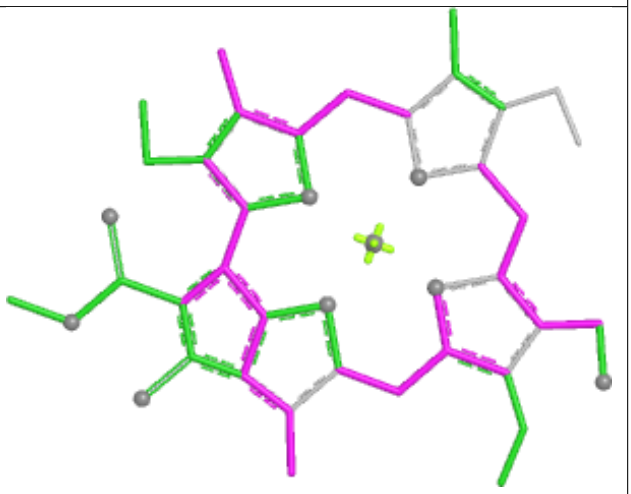
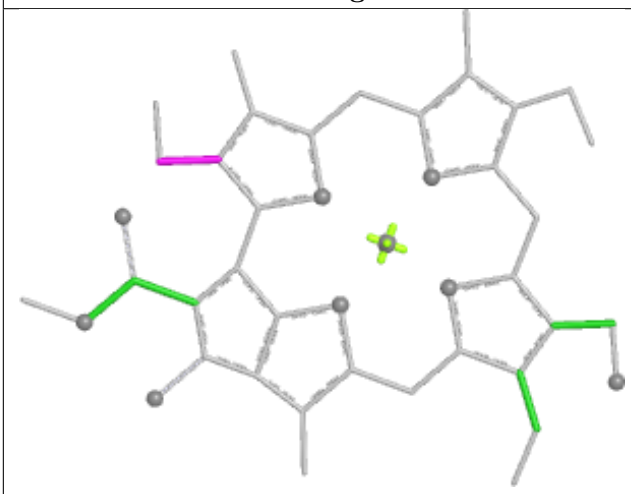


Bond angles



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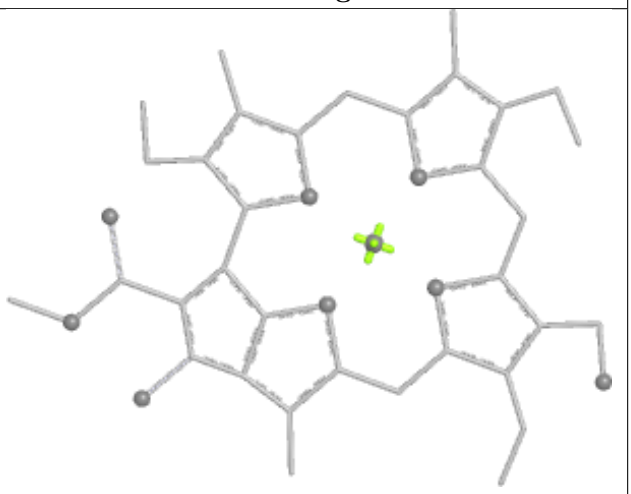
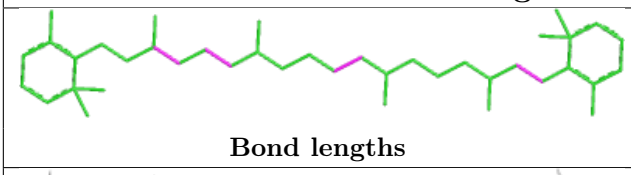


Rings

Ligand BCR B1 619



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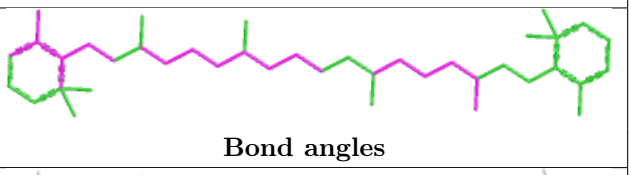
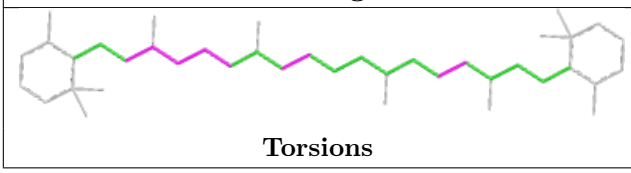


Bond angles



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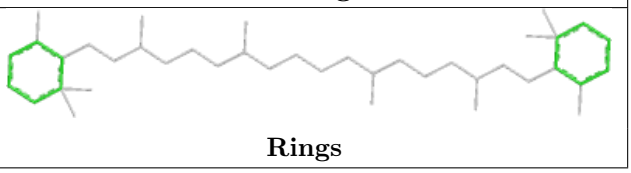
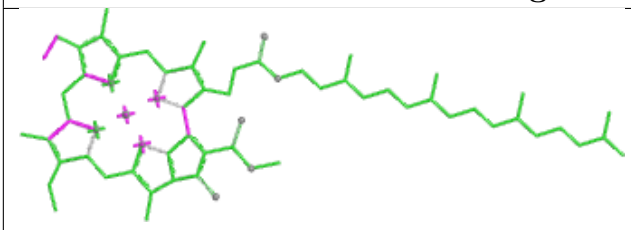
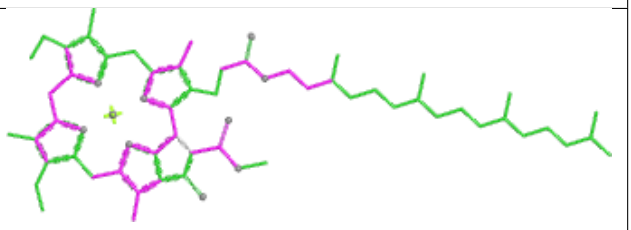


Rings

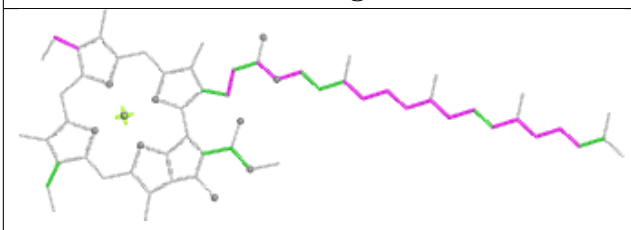
Ligand CLA c 512



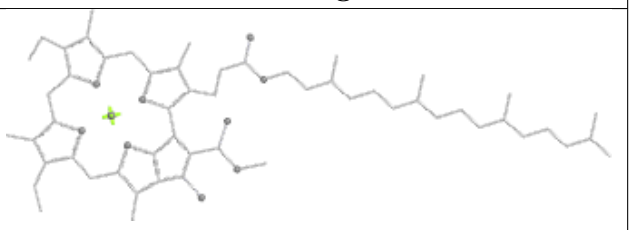
Bond lengths



Bond angles

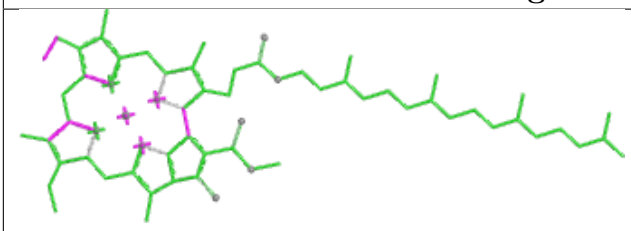


Torsions

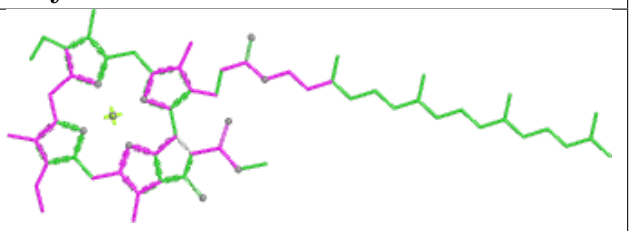


Rings

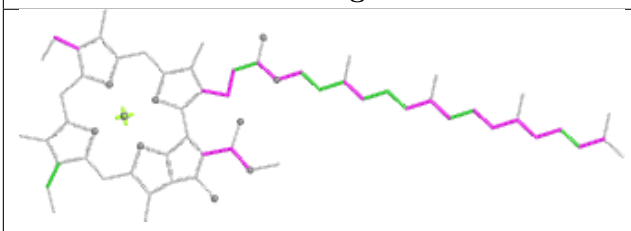
Ligand CLA y 602



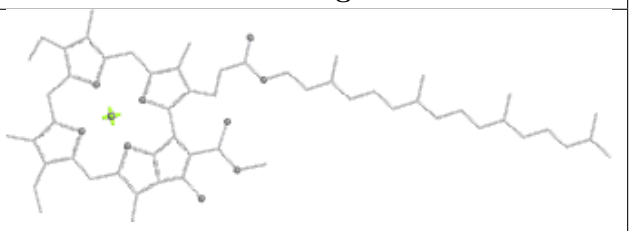
Bond lengths



Bond angles

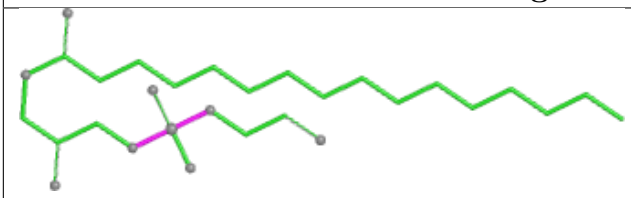


Torsions



Rings

Ligand LPX s 625



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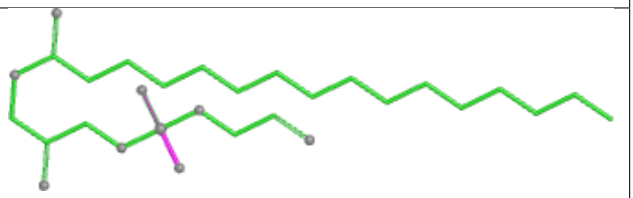
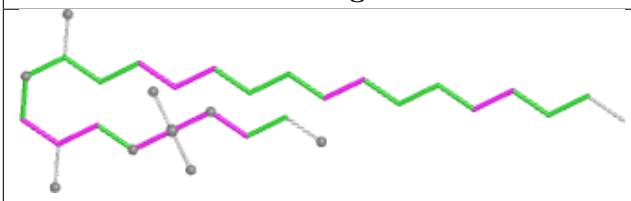
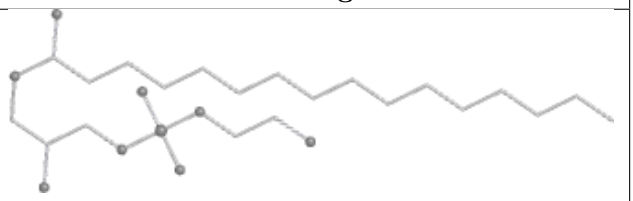


Bond angles

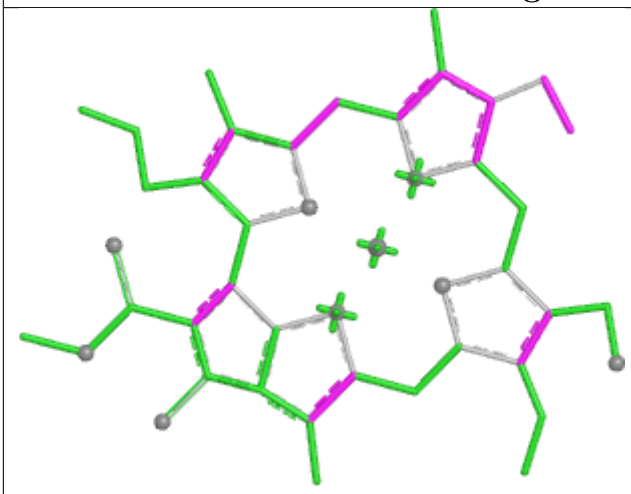


Torsions



Rings

Ligand CHL R 606



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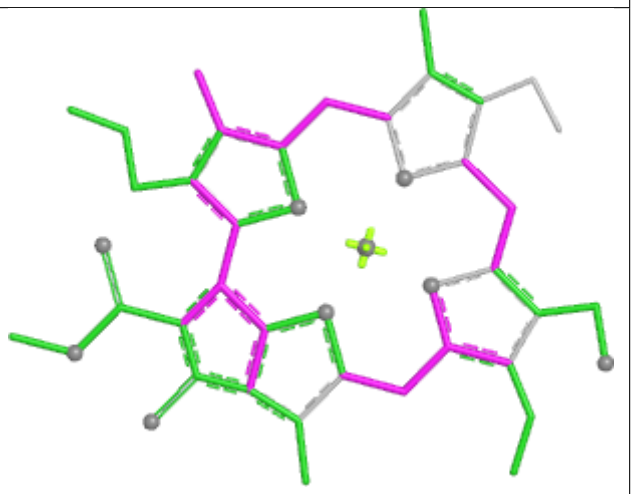
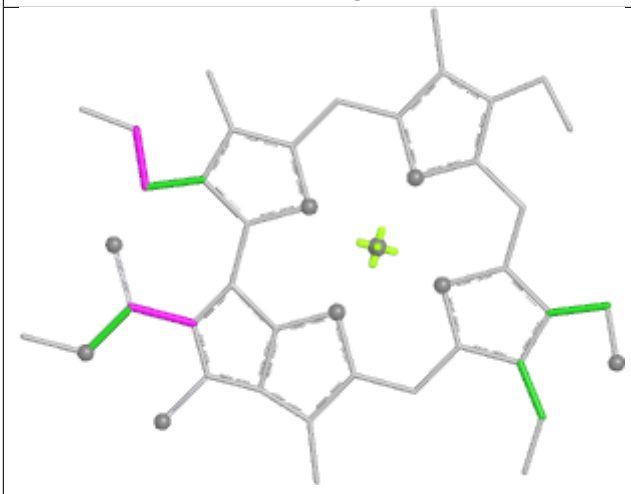


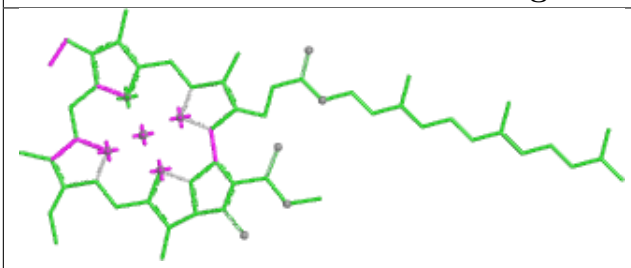
Bond angles



Torsions

Rings

Ligand CLA r 612



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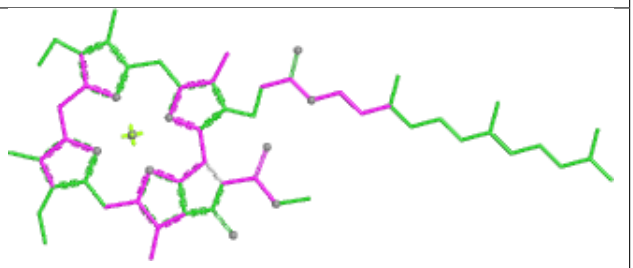
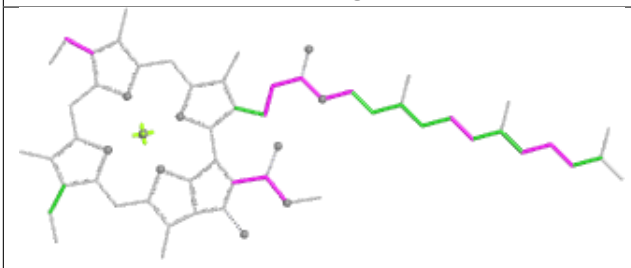


Bond angles



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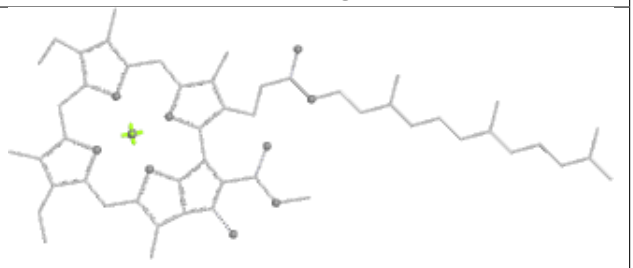
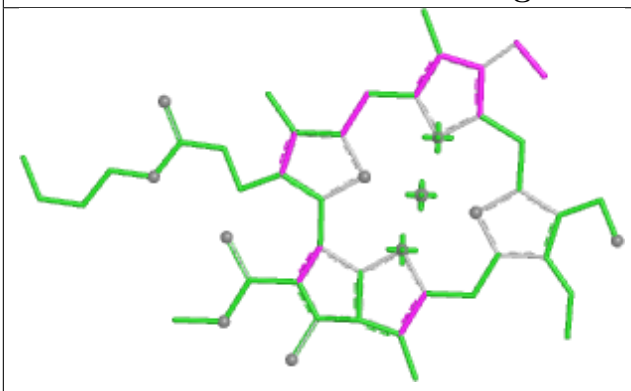


Rings

Ligand CHL G1 606



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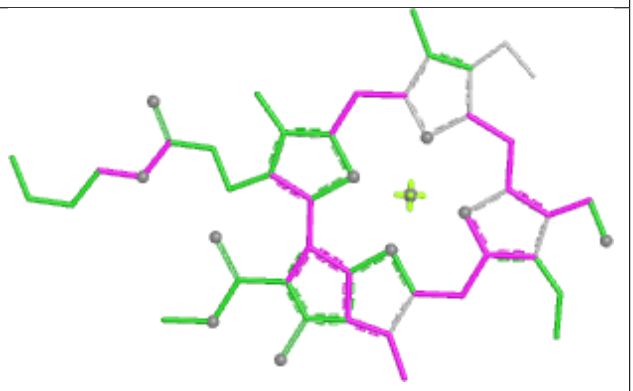

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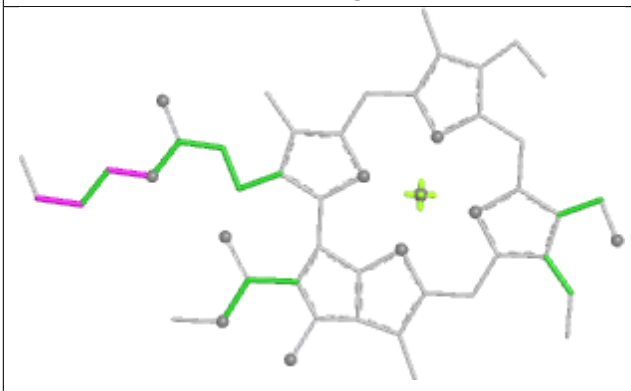

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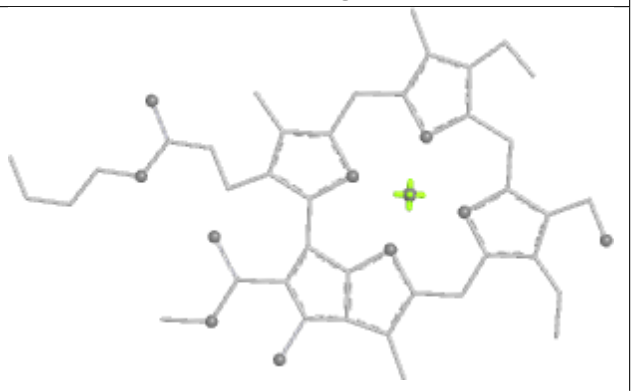
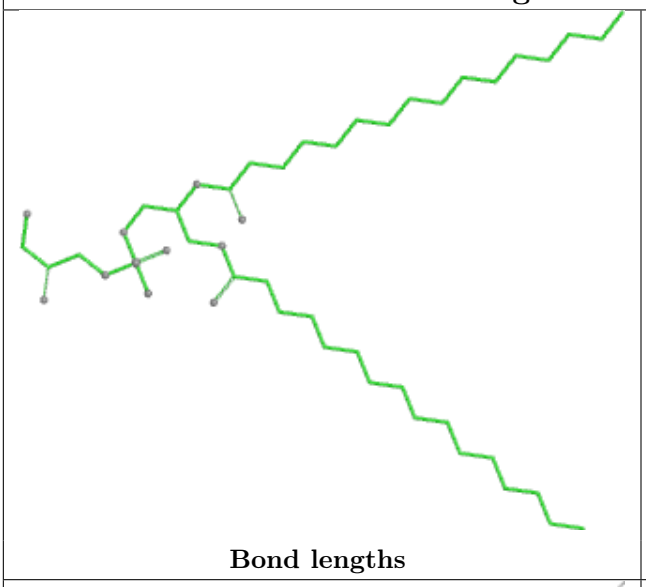


Rings

Ligand LHG G1 624



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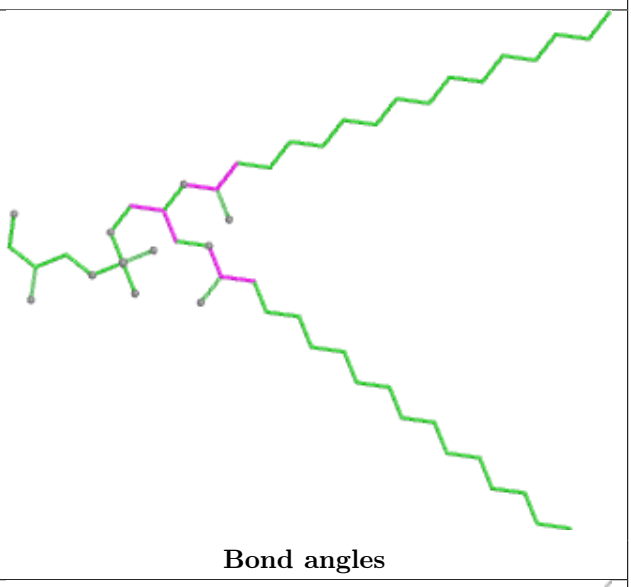

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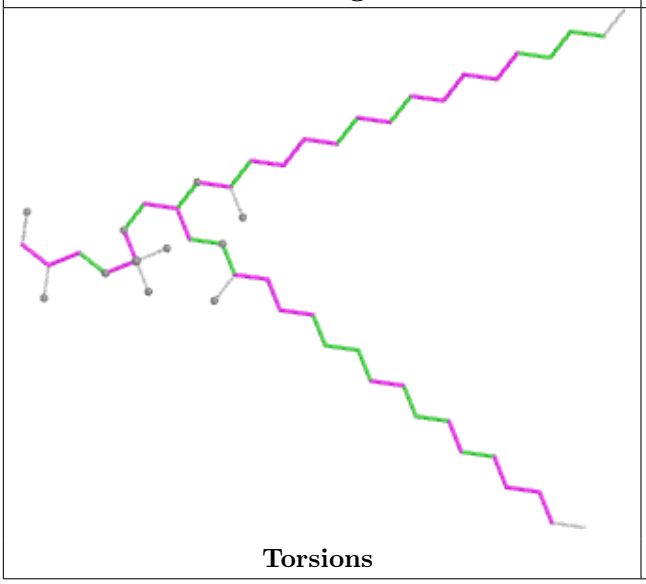

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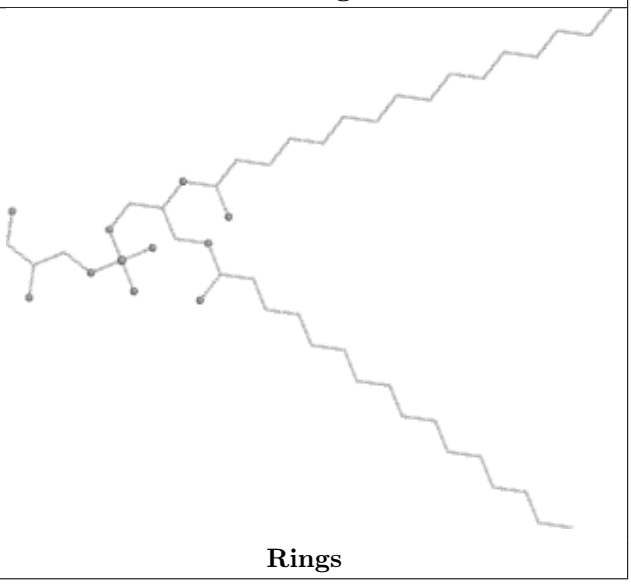
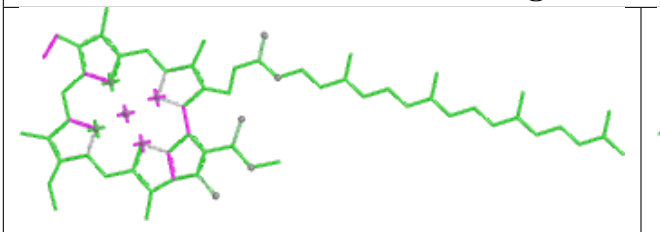


Rings

Ligand CLA b 607



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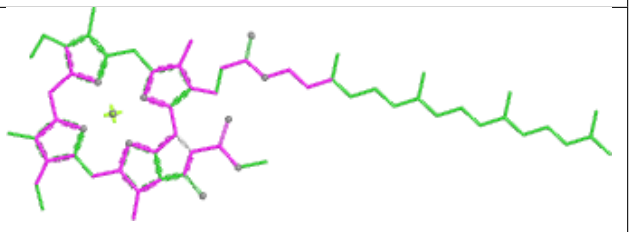

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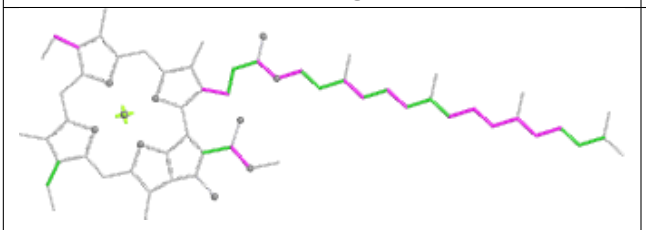

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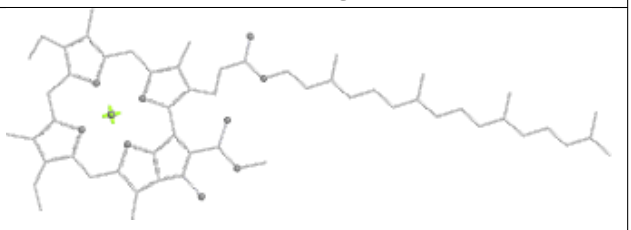
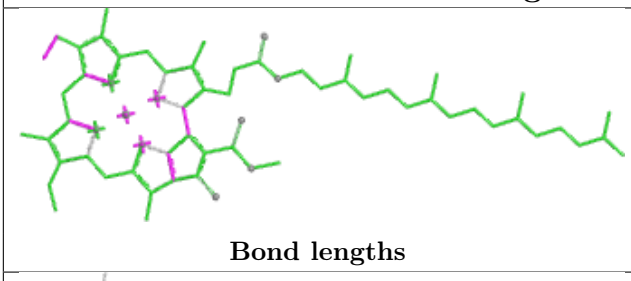


Rings

Ligand CLA Y 603



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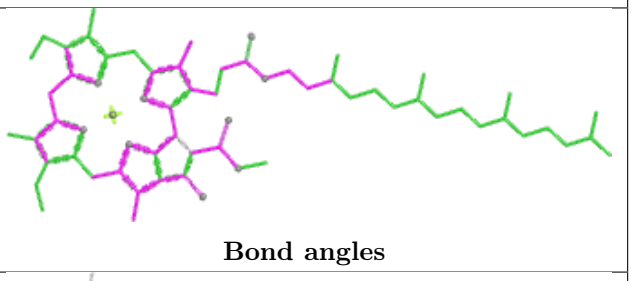

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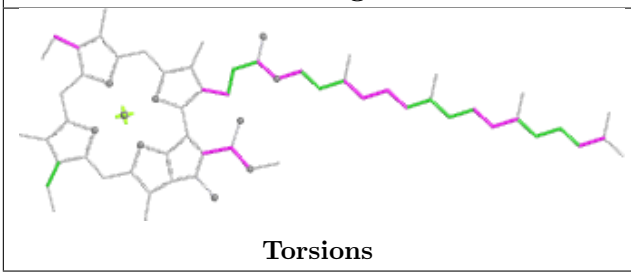

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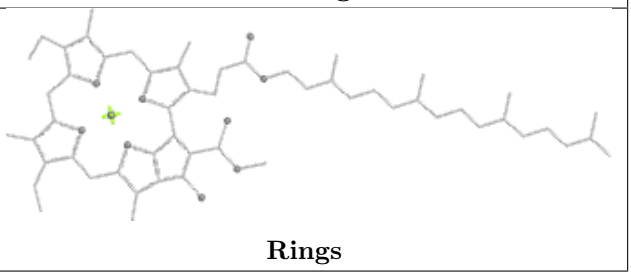
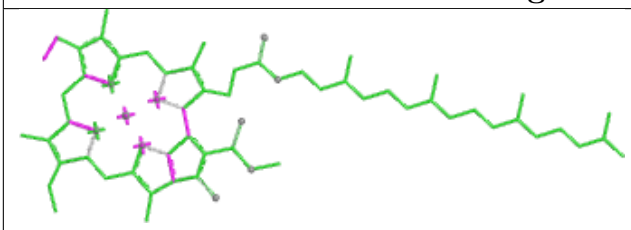


Rings

Ligand CLA y 613



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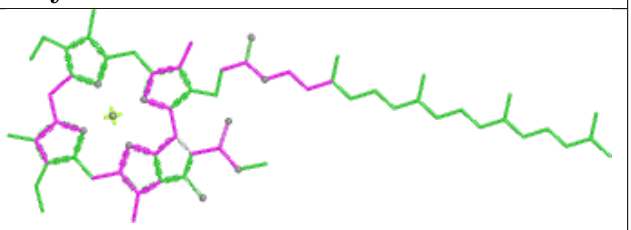
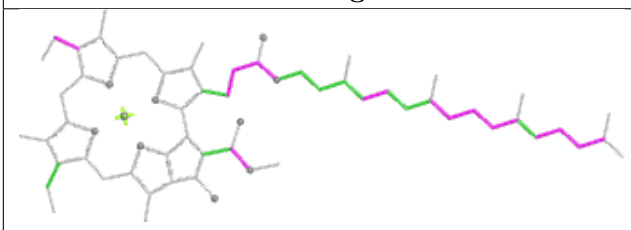


Bond angles



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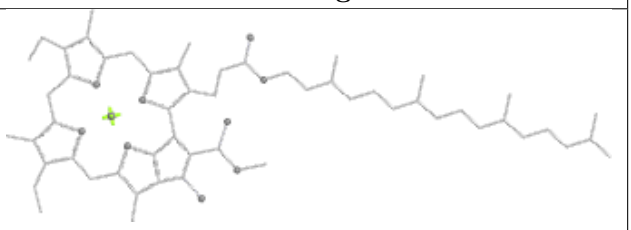
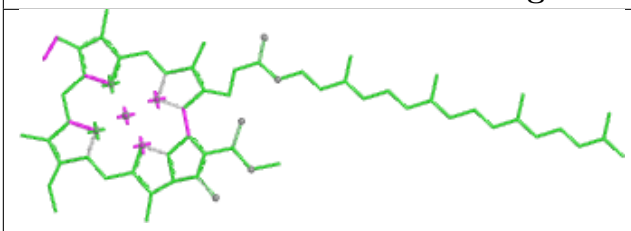


Rings

Ligand CLA n 604



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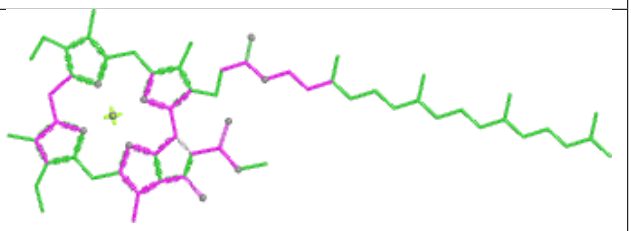
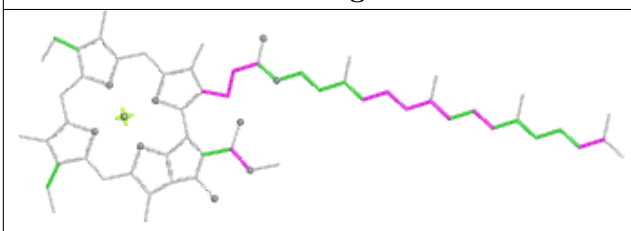


Bond angles



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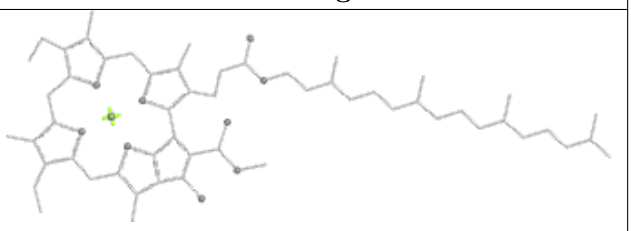
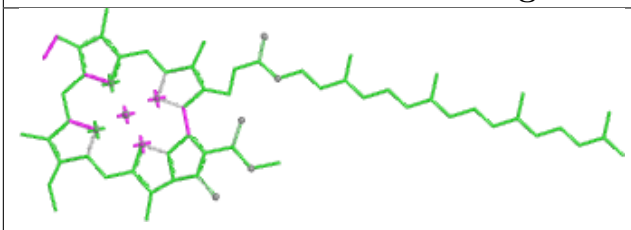


Rings

Ligand CLA y1 603



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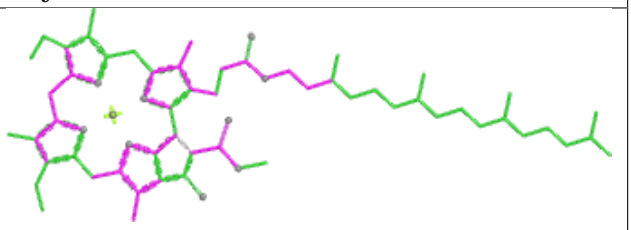

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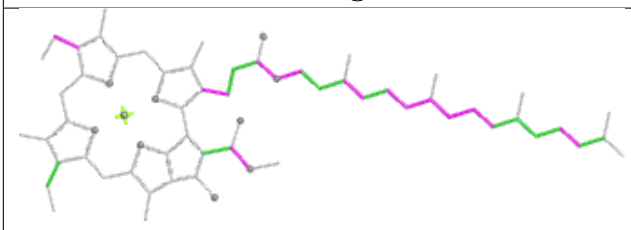

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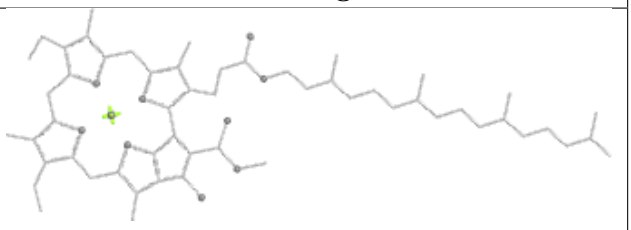
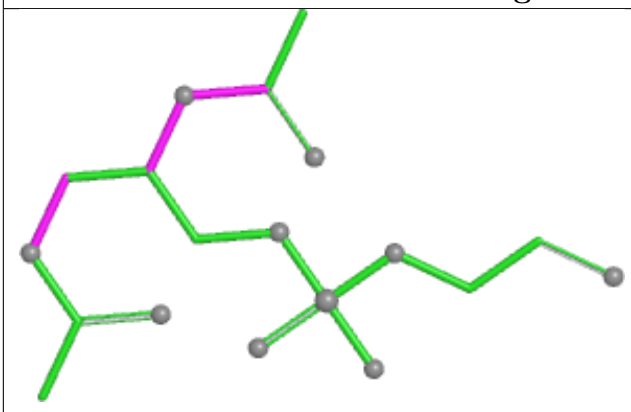


Rings

Ligand PTY Y1 627



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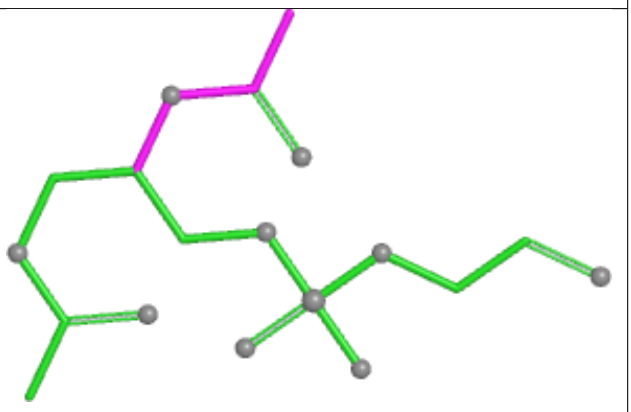
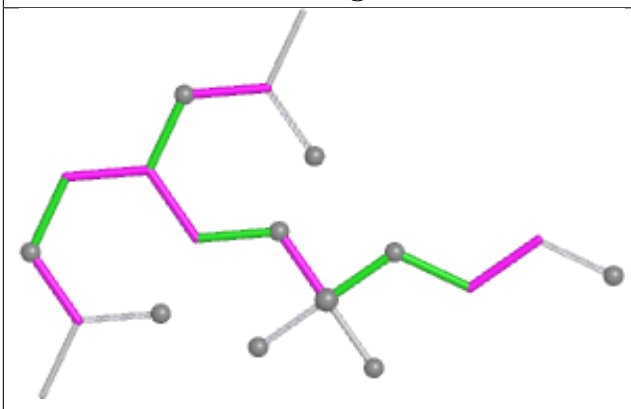


Bond angles



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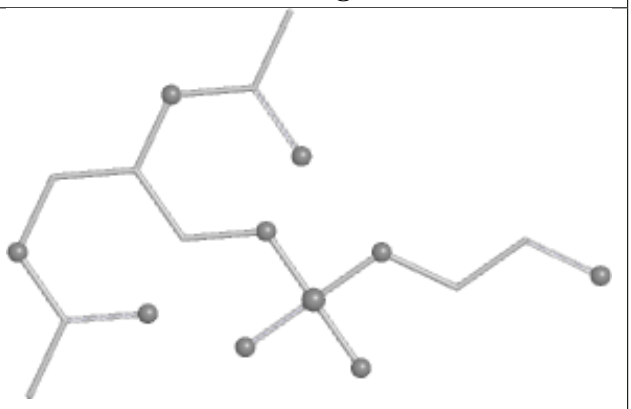
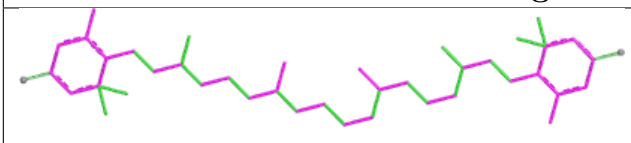


Rings

Ligand C7Z b 620



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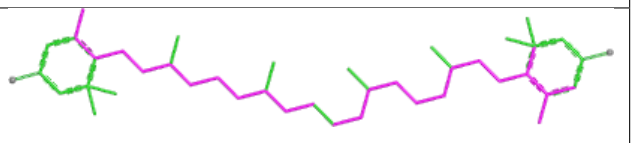
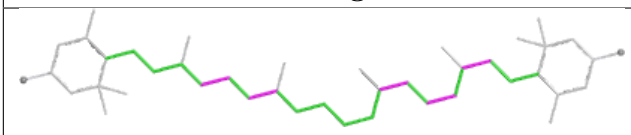


Bond angles



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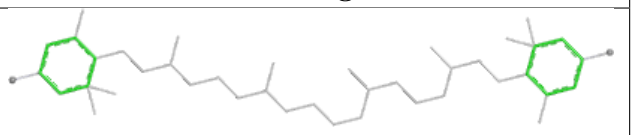
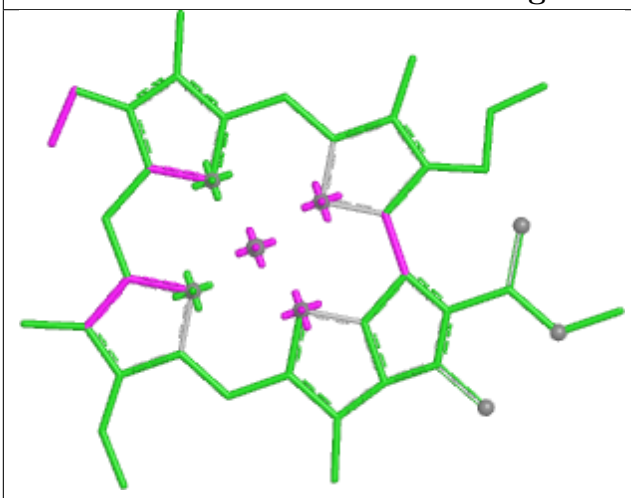


Rings

Ligand CLA g 612



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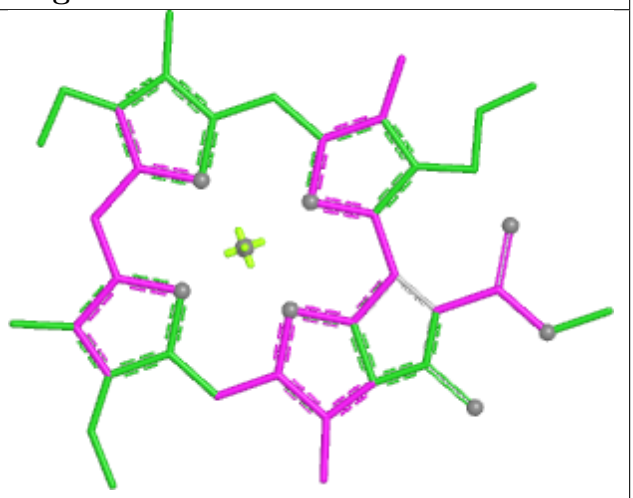
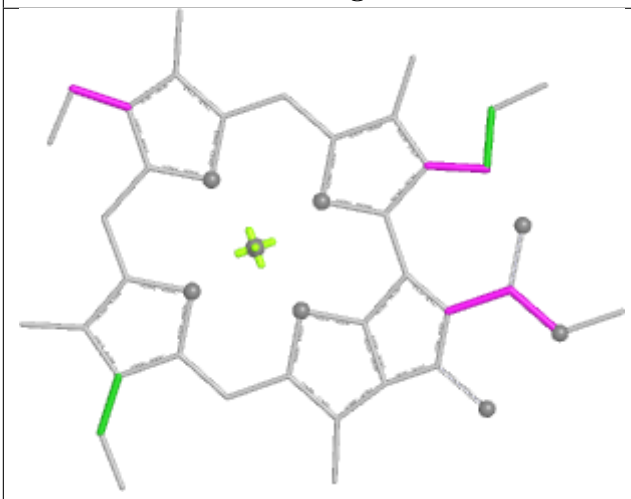


Bond angles



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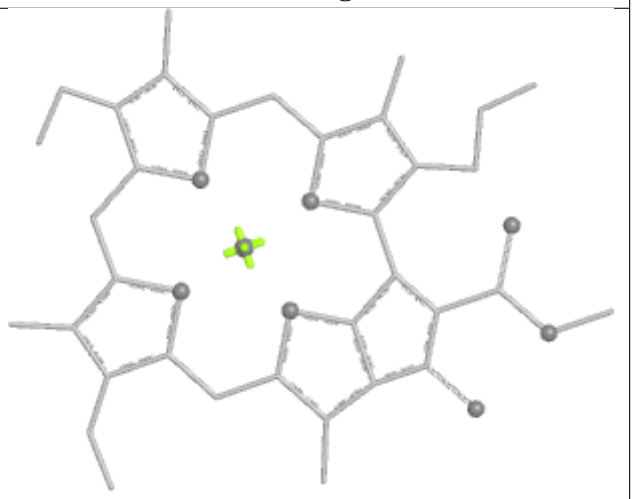
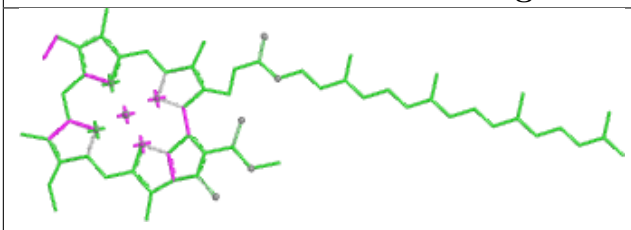
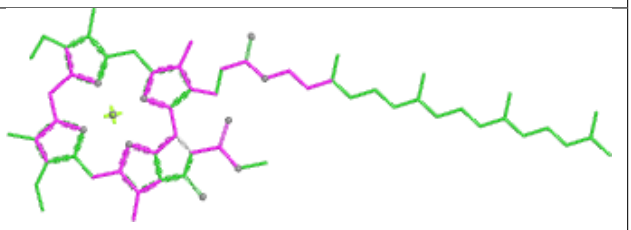


Rings

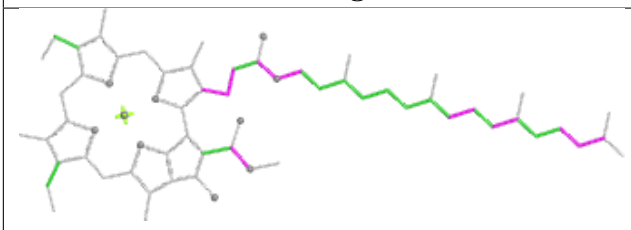
Ligand CLA C1 501



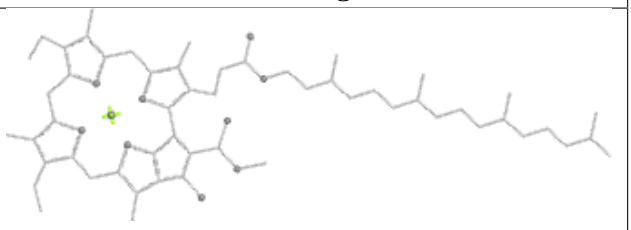
Bond lengths



Bond angles

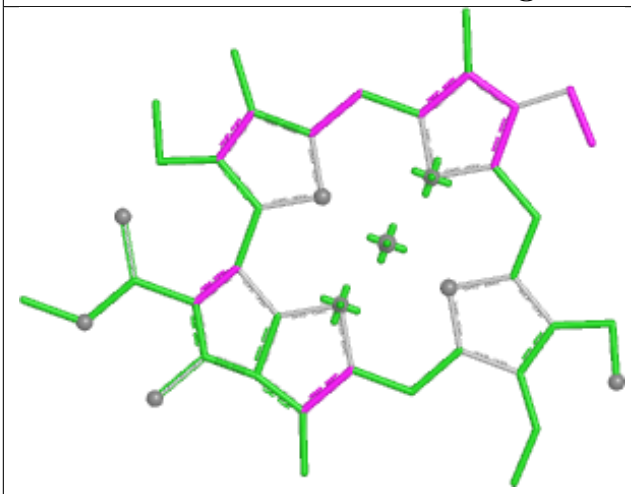


Torsions



Rings

Ligand CHL S1 607



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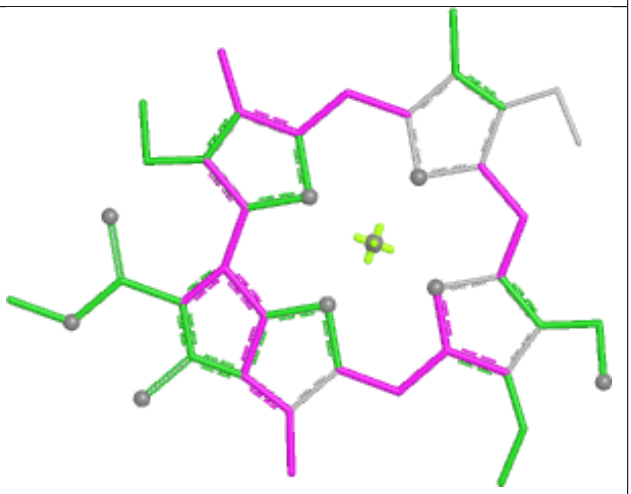
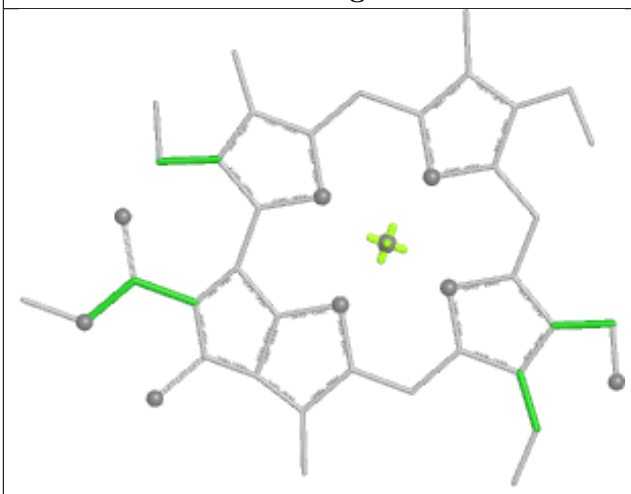
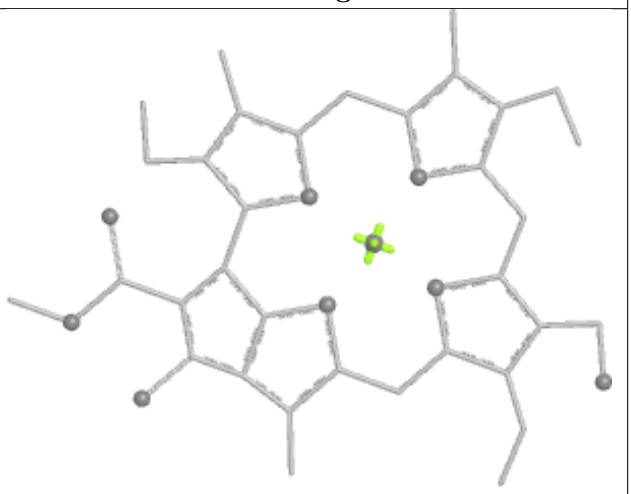


Bond angles

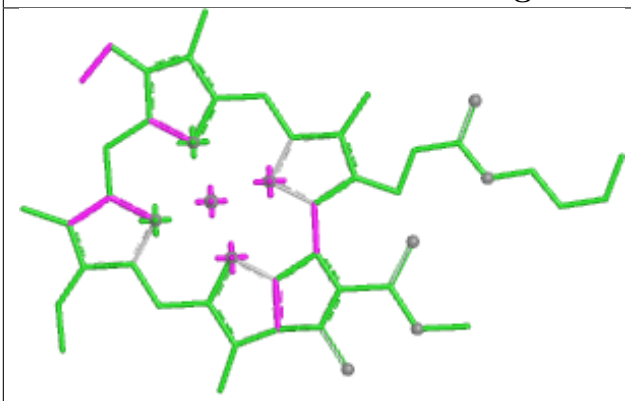


Torsions

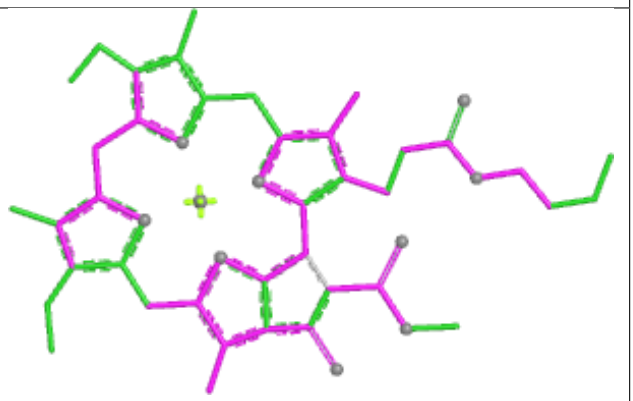


Rings

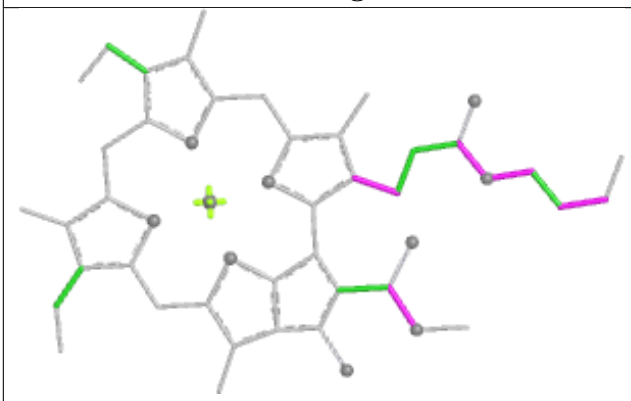
Ligand CLA G1 604



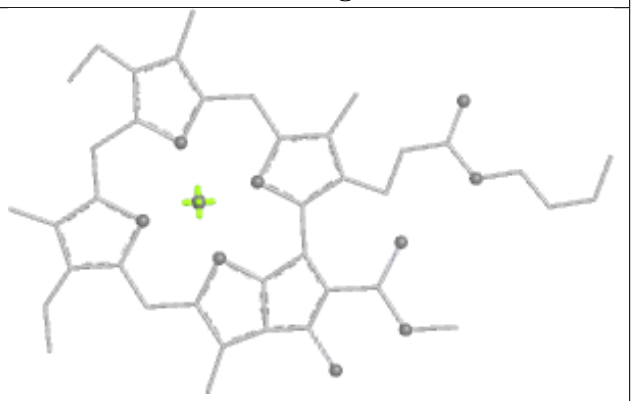
Bond lengths



Bond angles

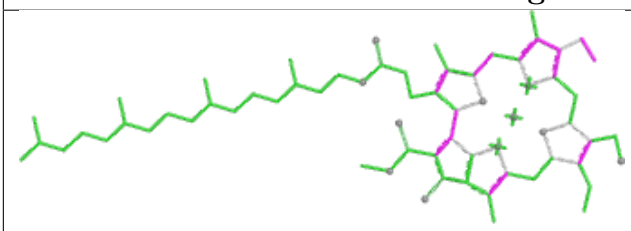


Torsions

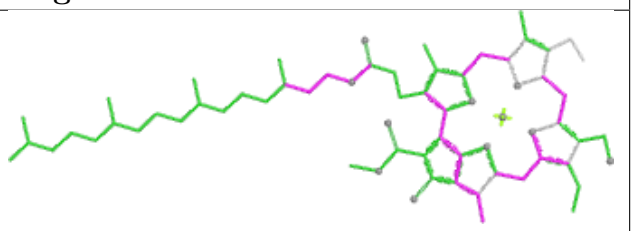


Rings

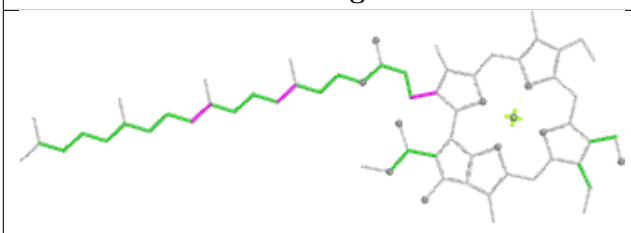
Ligand CHL g 609



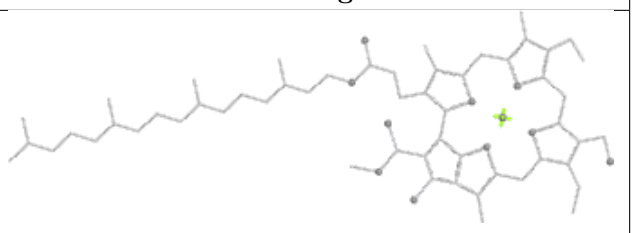
Bond lengths



Bond angles

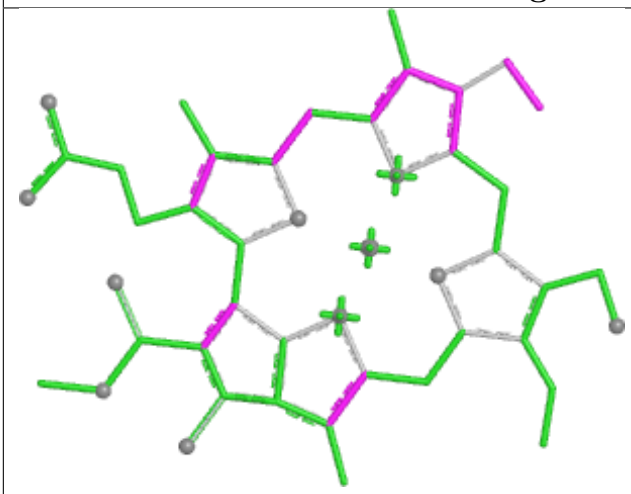


Torsions



Rings

Ligand CHL s 601



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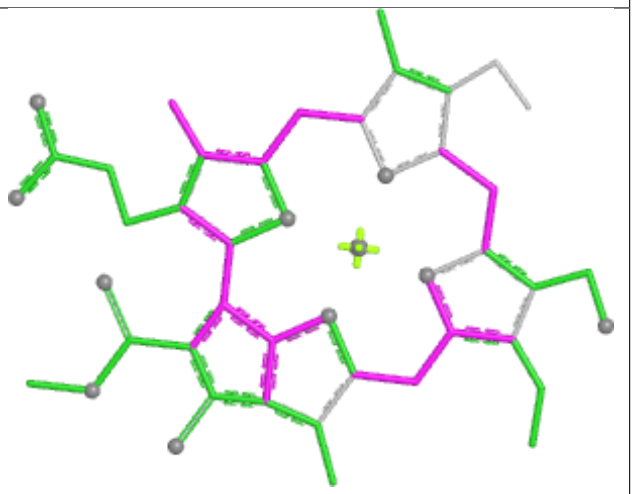
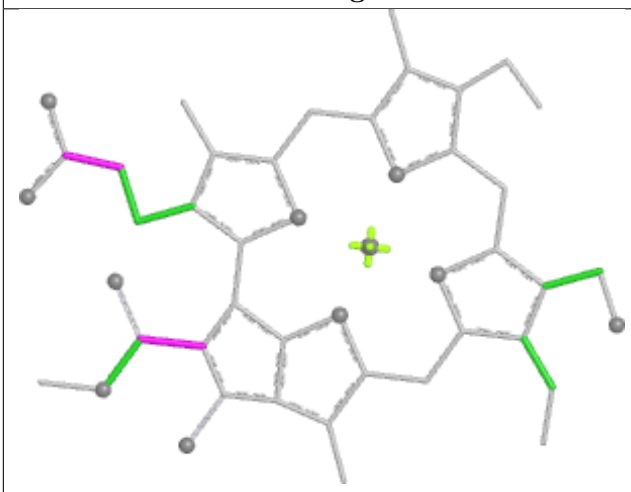
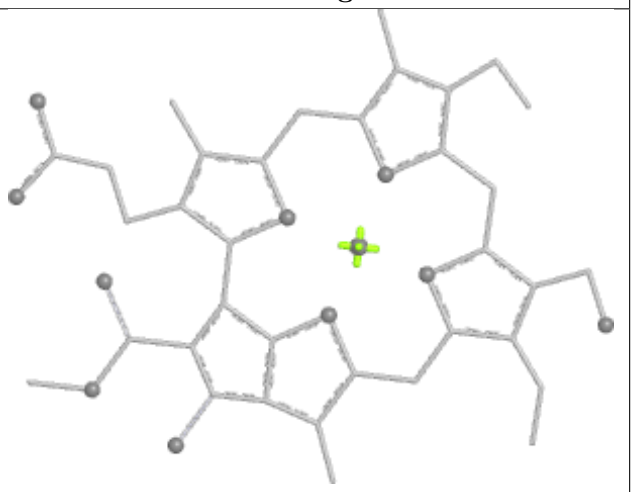


Bond angles

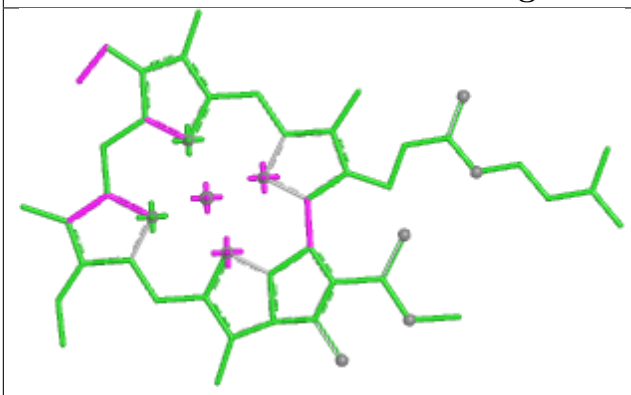


Torsions

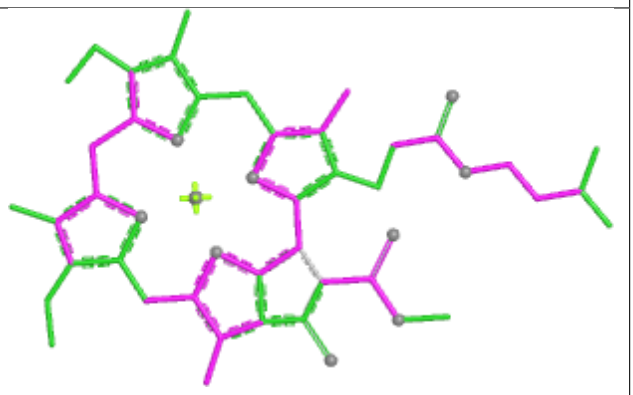


Rings

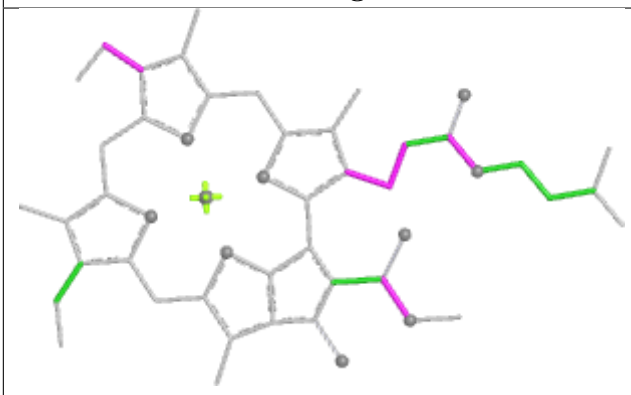
Ligand CLA S1 617



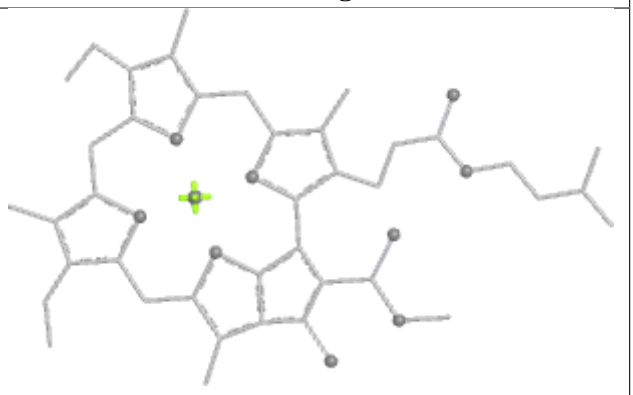
Bond lengths



Bond angles

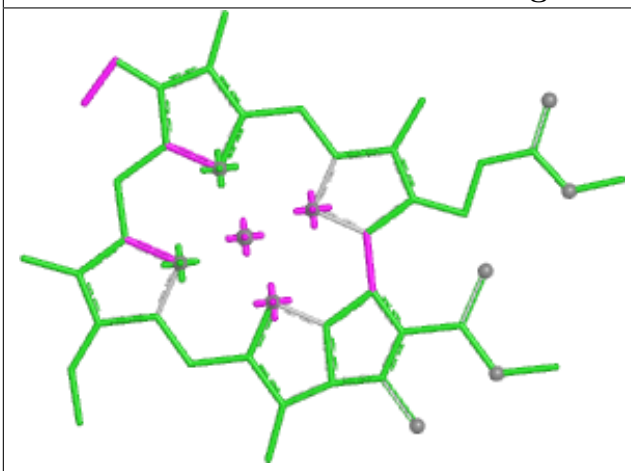


Torsions



Rings

Ligand CLA r 613



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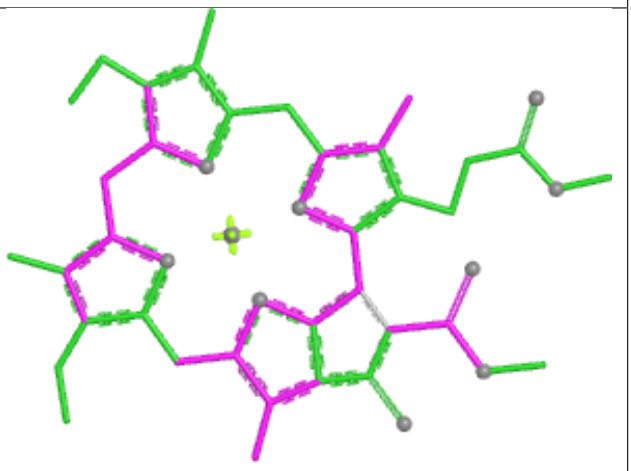
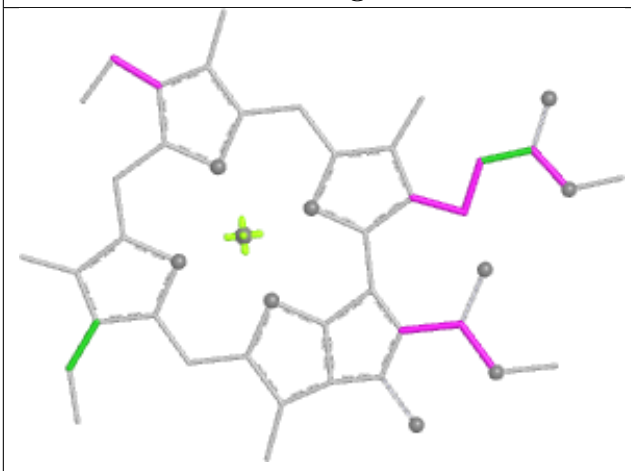
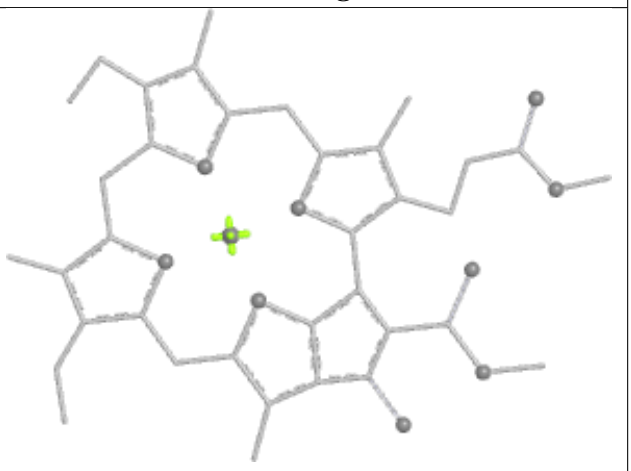


Bond angles

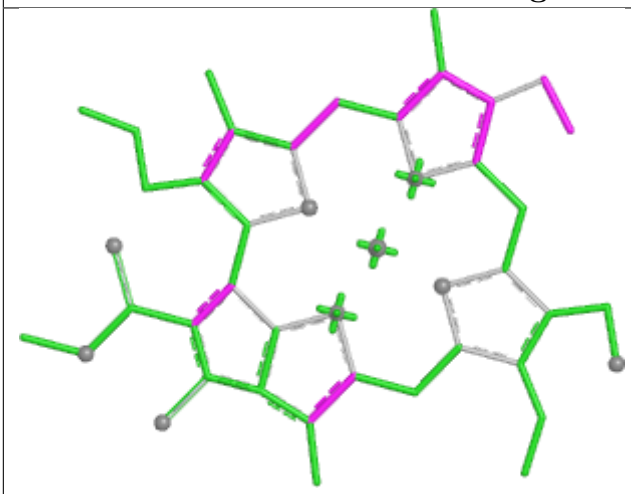


Torsions

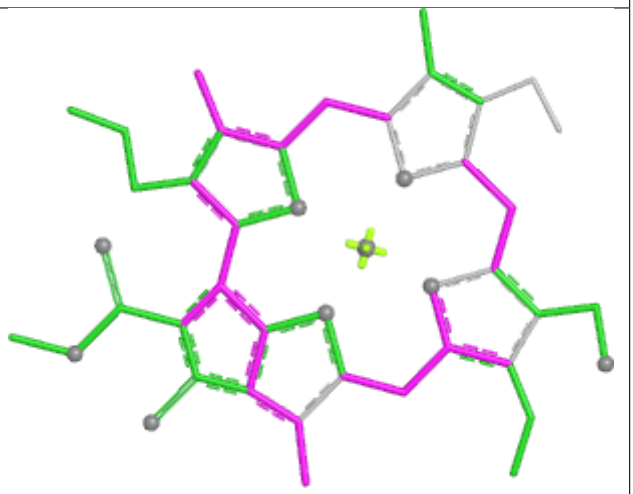


Rings

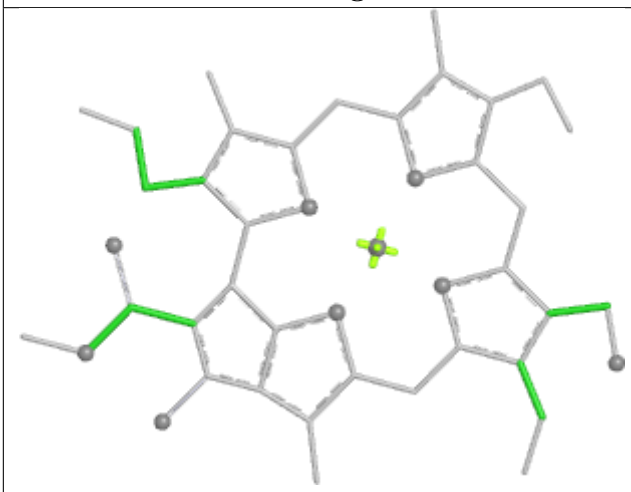
Ligand CHL s 606



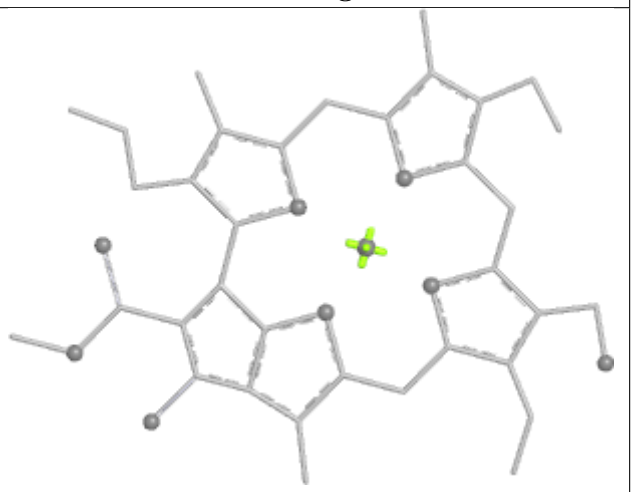
Bond lengths



Bond angles

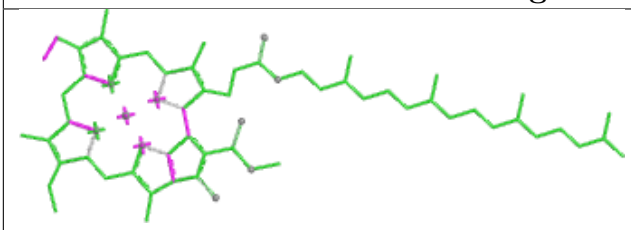


Torsions

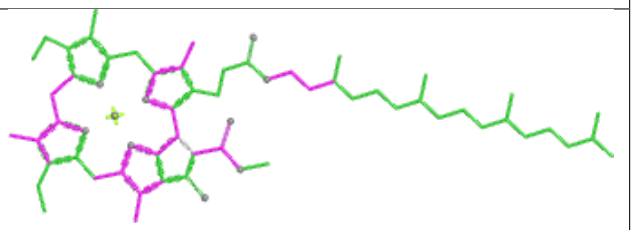


Rings

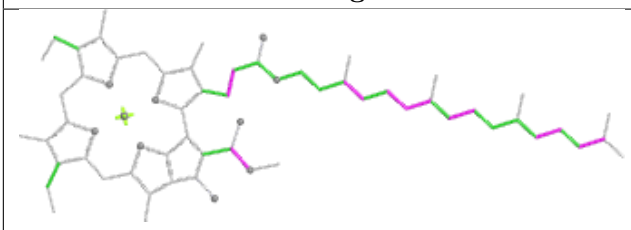
Ligand CLA c 502



Bond lengths



Bond angles



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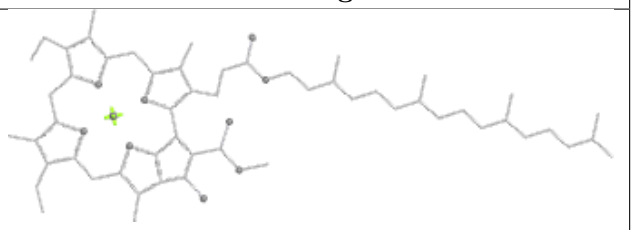
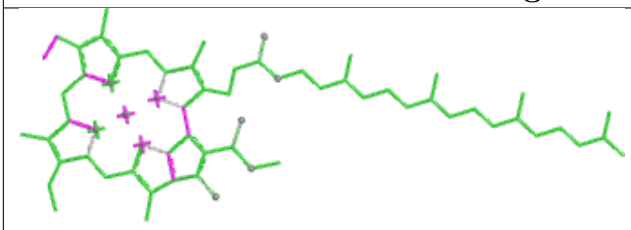
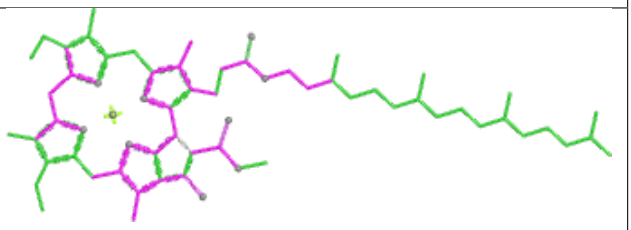


Rings

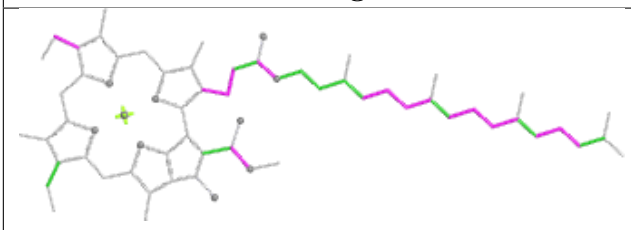
Ligand CLA Y 610



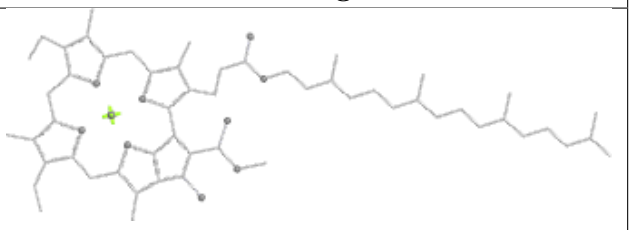
Bond lengths



Bond angles

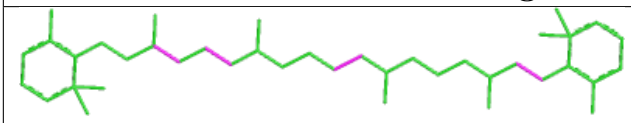


Torsions



Rings

Ligand BCR c1 517



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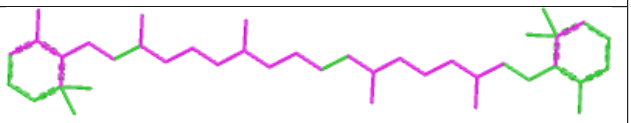
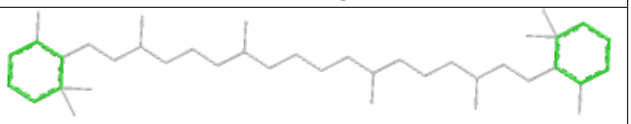


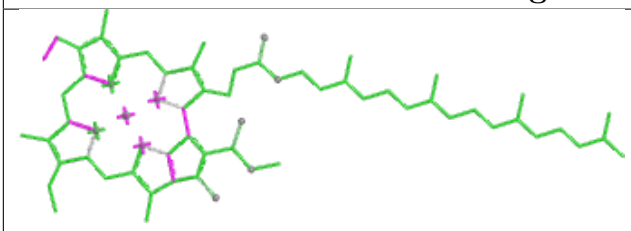
Bond angles

Torsions

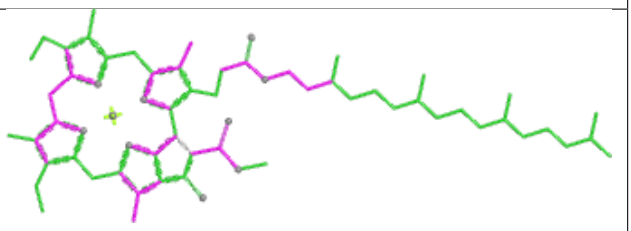


Rings

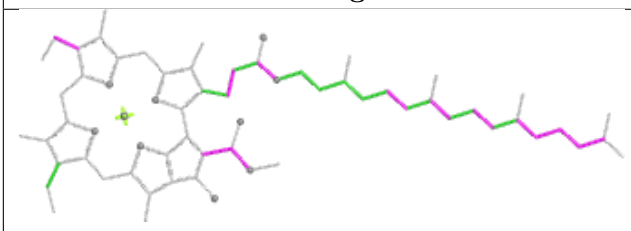
Ligand CLA c 505



Bond lengths



Bond angles



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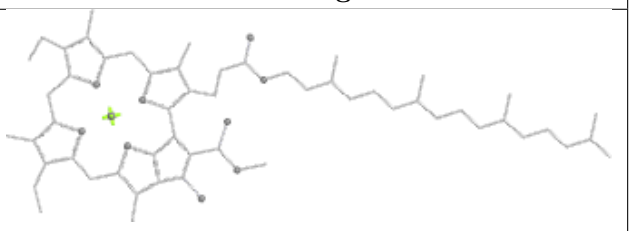
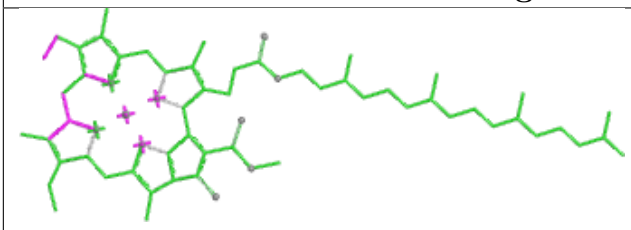
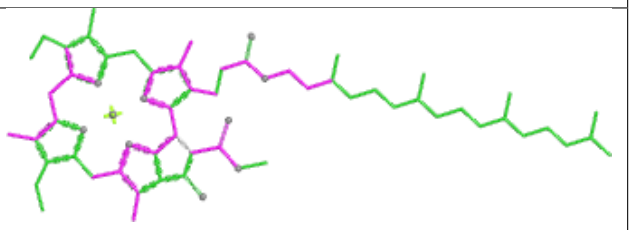
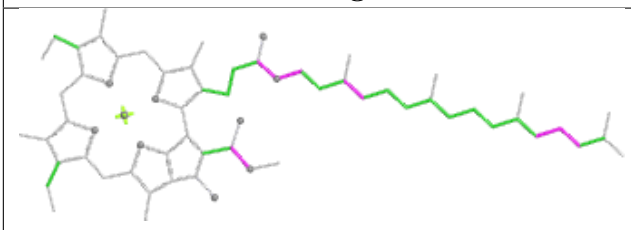
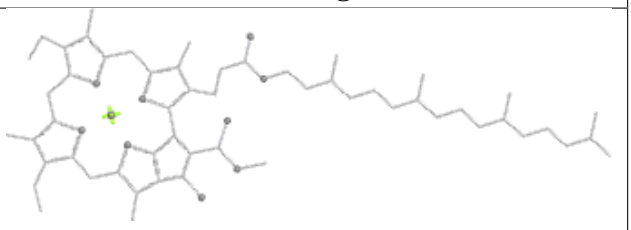
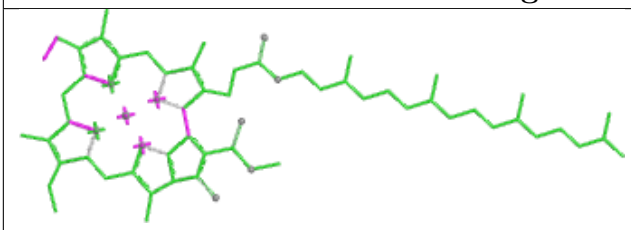
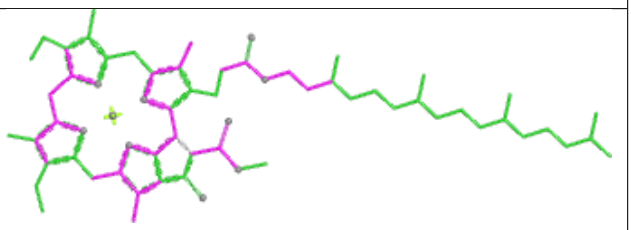
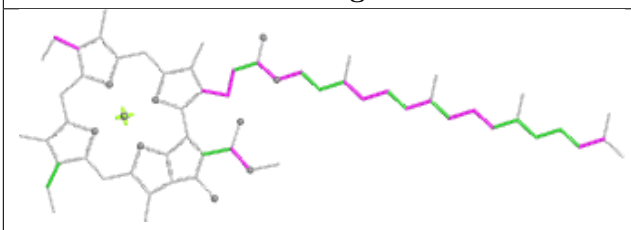
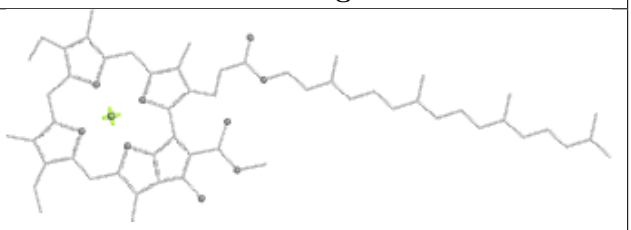
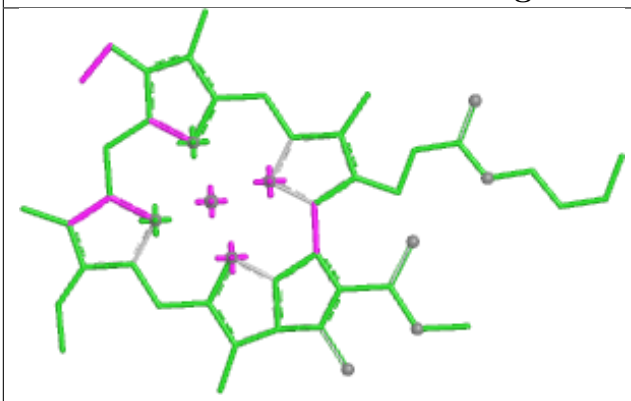


Rings

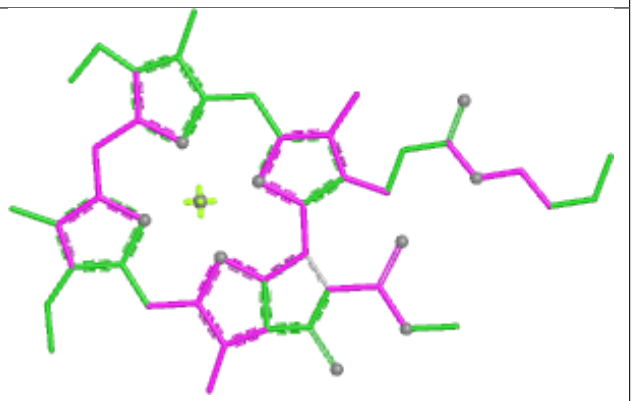
Ligand CLA B1 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA s1 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

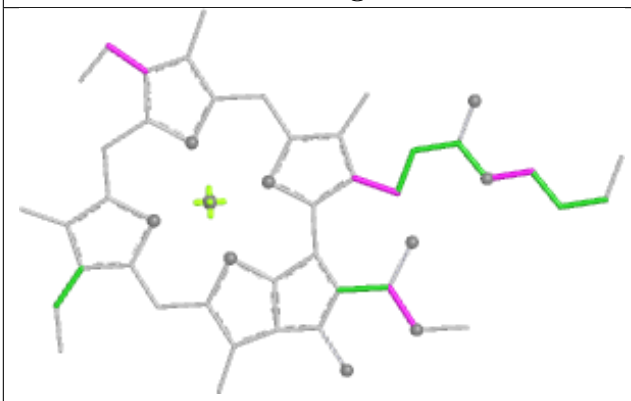
Ligand CLA N1 614



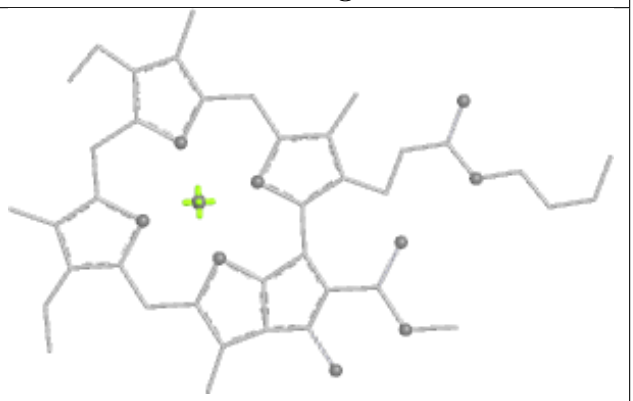
Bond lengths



Bond angles

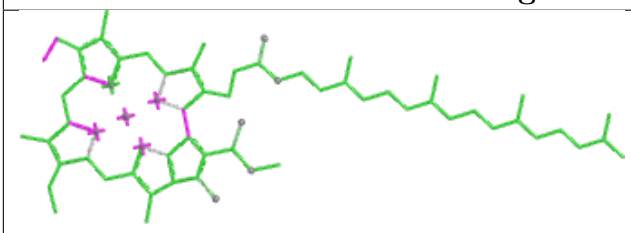


Torsions

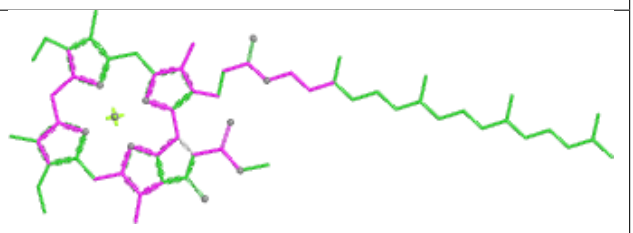


Rings

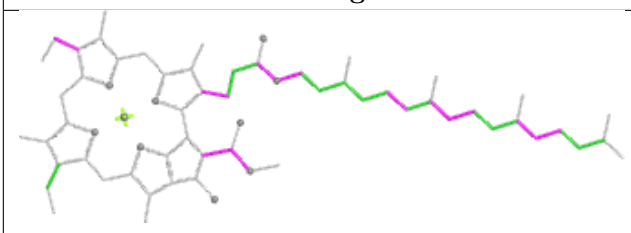
Ligand CLA n1 603



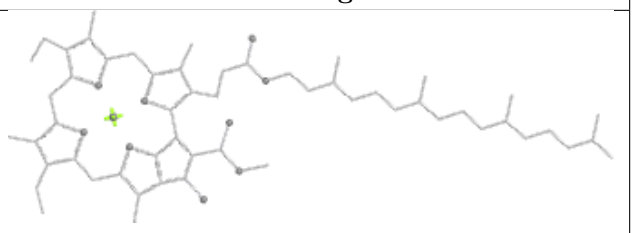
Bond lengths



Bond angles

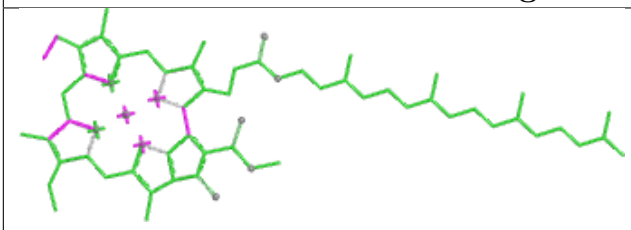


Torsions

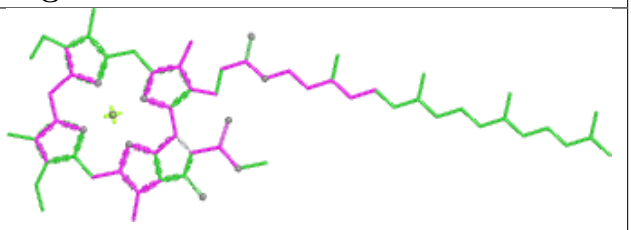


Rings

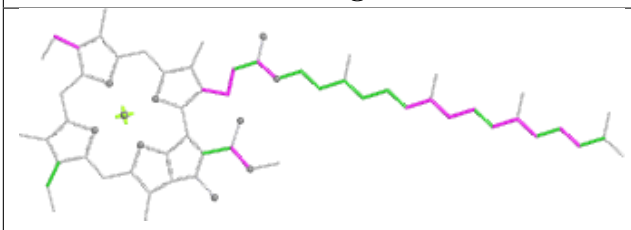
Ligand CLA g1 610



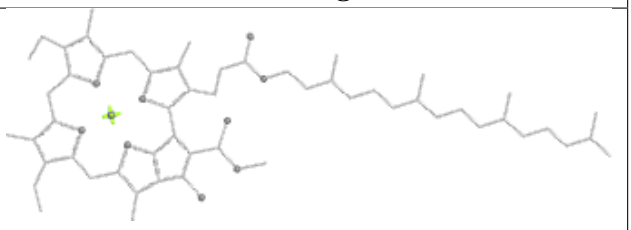
Bond lengths



Bond angles

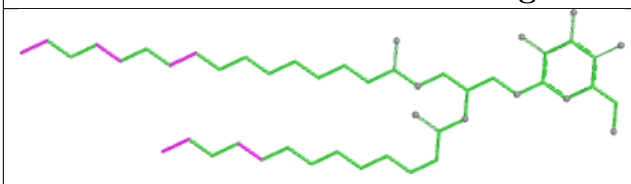


Torsions



Rings

Ligand LMG H 102



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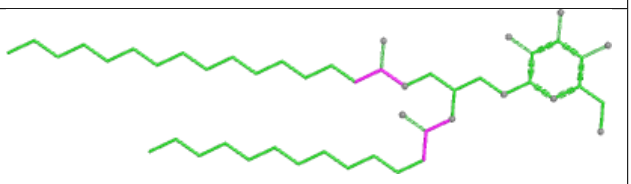

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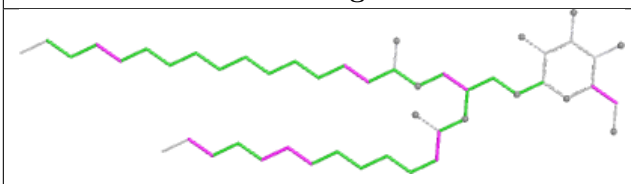

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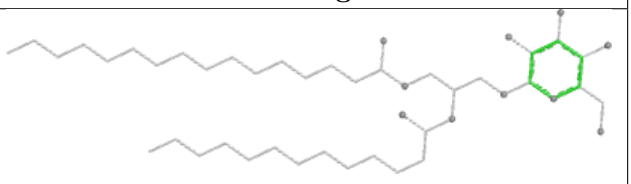
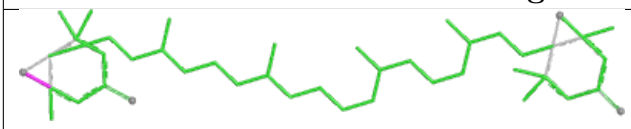


Rings

Ligand XAT g 622



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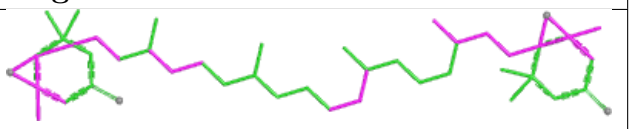
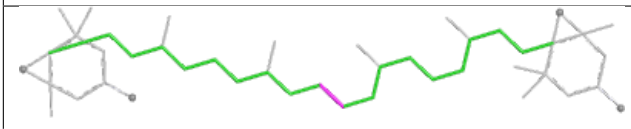
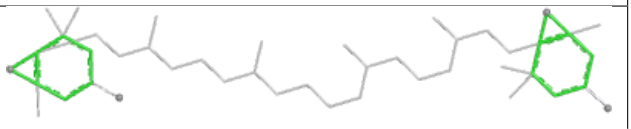


Bond angles

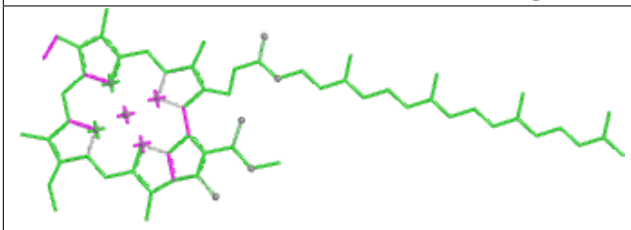


Torsions

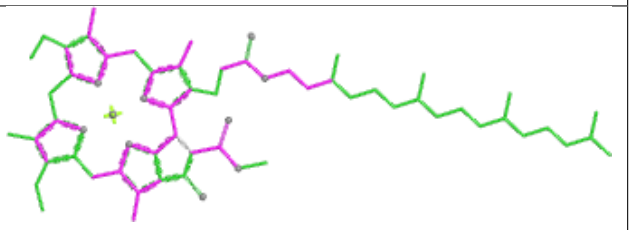


Rings

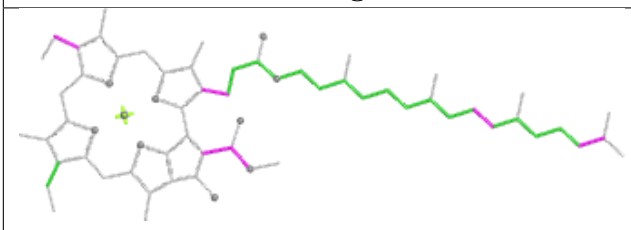
Ligand CLA b 609



Bond lengths



Bond angles



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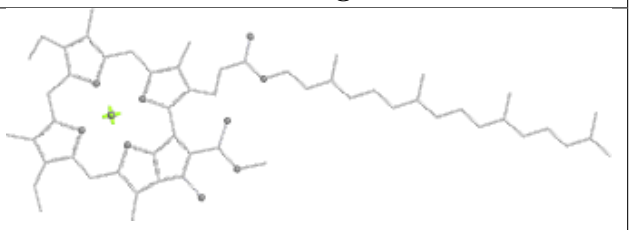
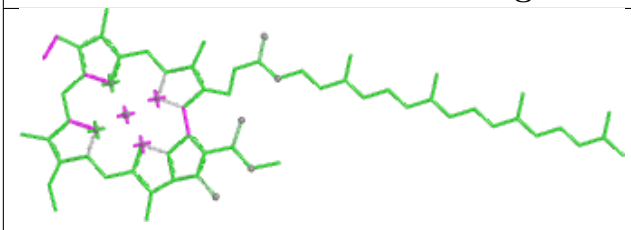


Rings

Ligand CLA Y1 612



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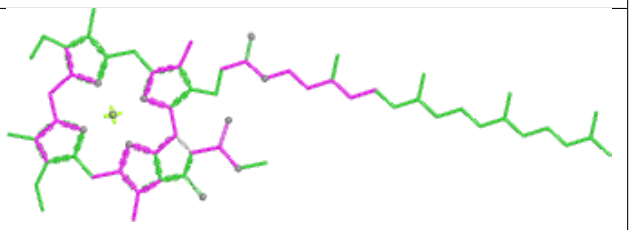
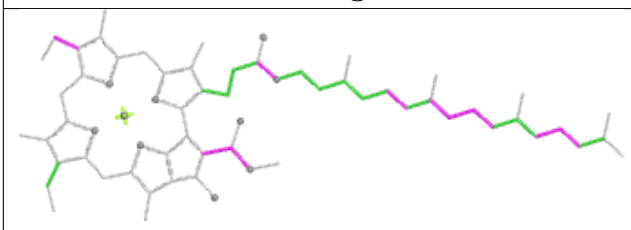
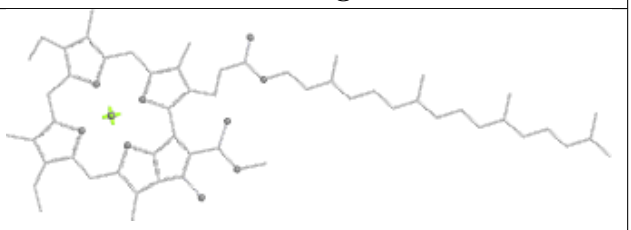


Bond angles

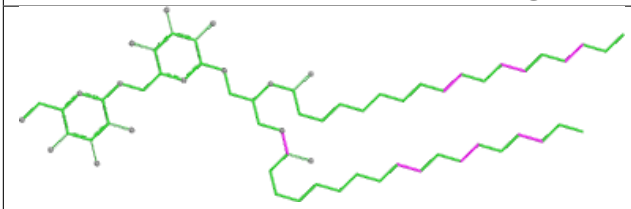


Torsions



Rings

Ligand DGD c 523



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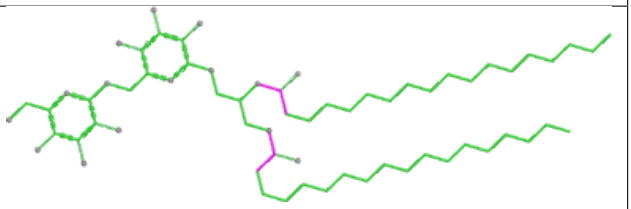
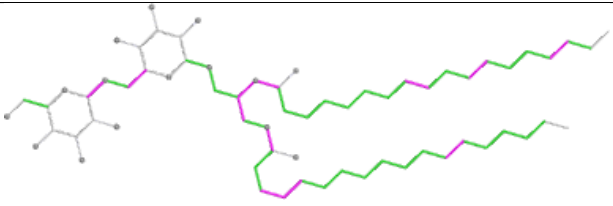


Bond angles



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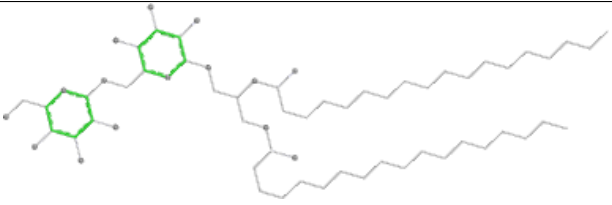
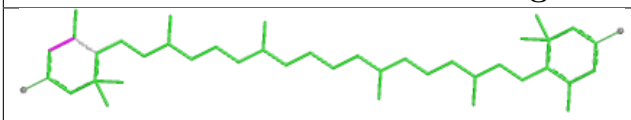


Rings

Ligand LUT r 620



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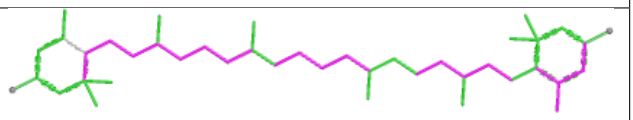
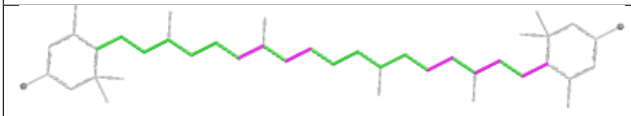


Bond angles



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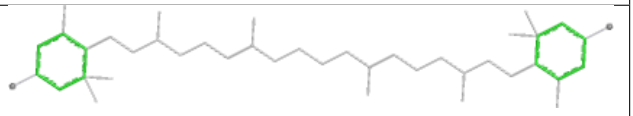
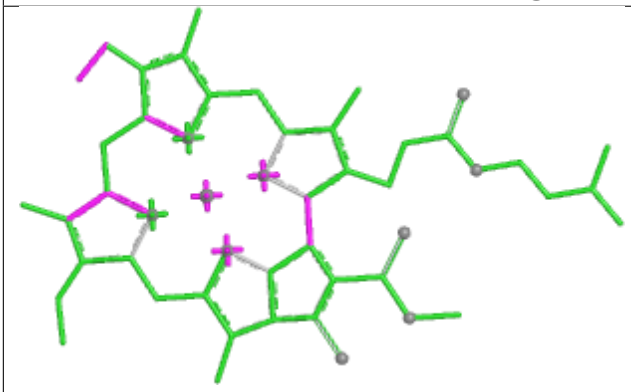


Rings

Ligand CLA y 608



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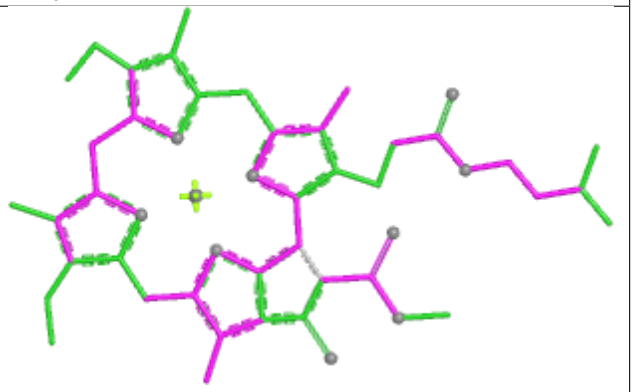
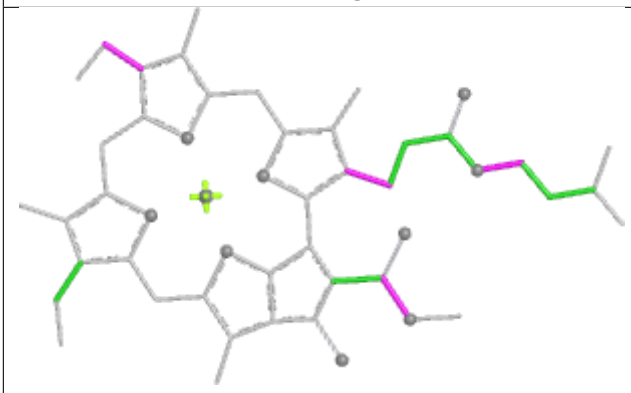
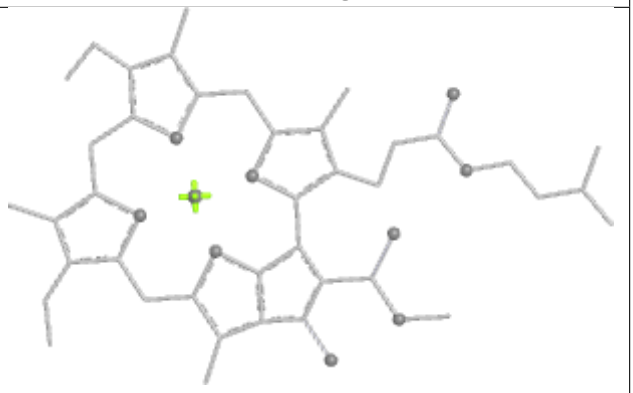


Bond angles

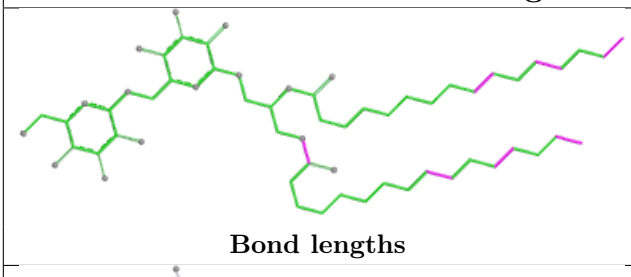


Torsions



Rings

Ligand DGD c 519



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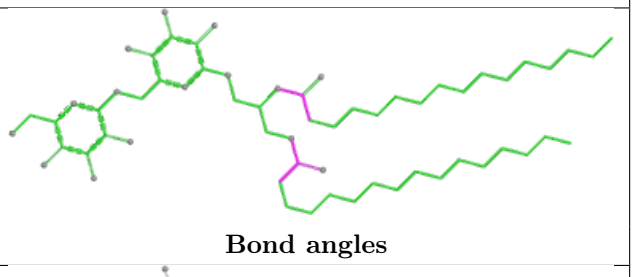
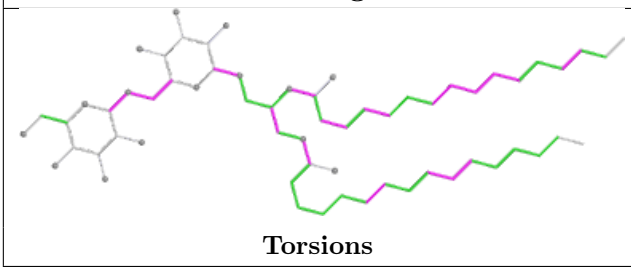


Bond angles



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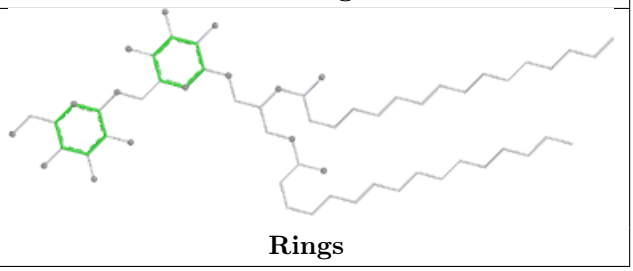
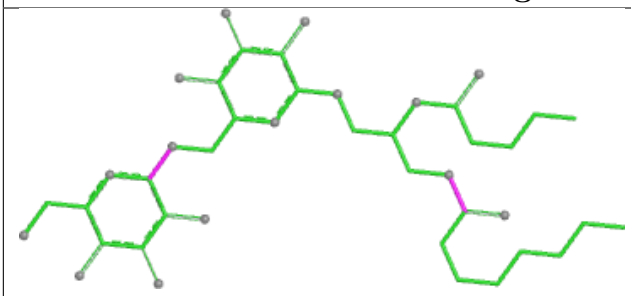


Rings

Ligand DGD b1 623



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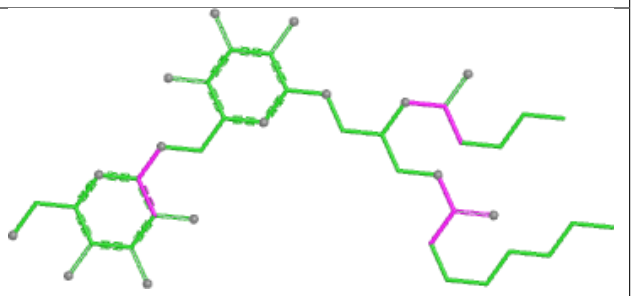
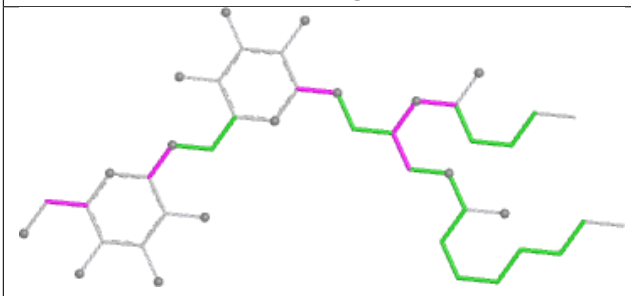
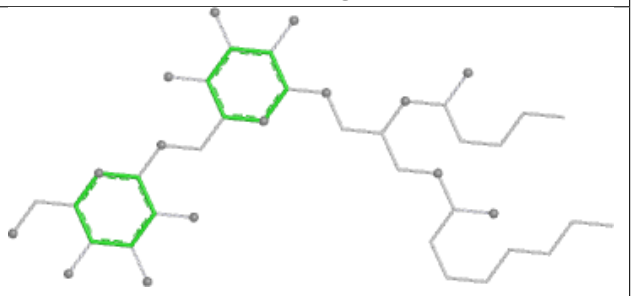


Bond angles

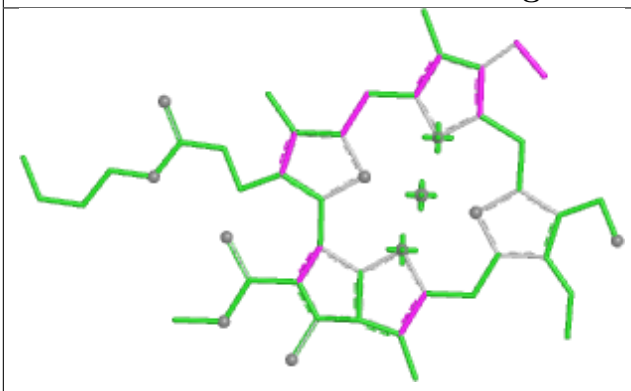


Torsions



Rings

Ligand CHL G 607



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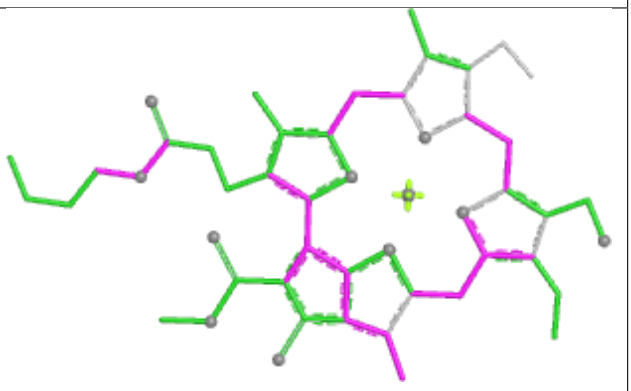
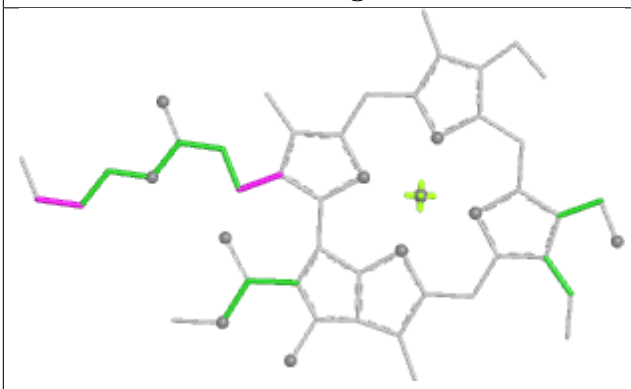
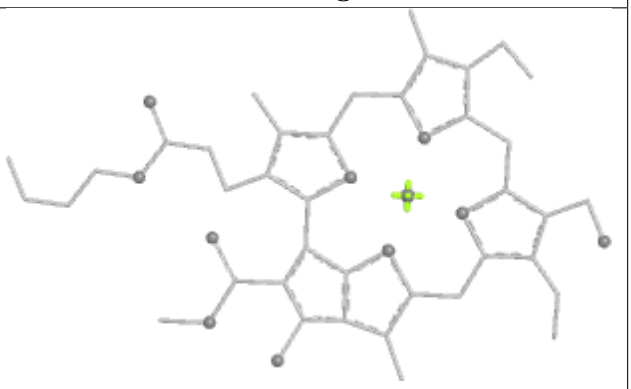


Bond angles

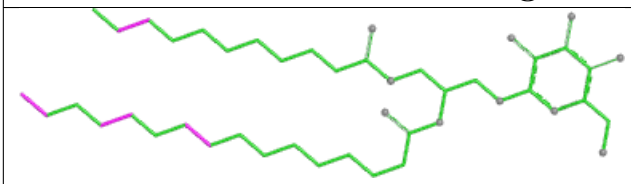


Torsions

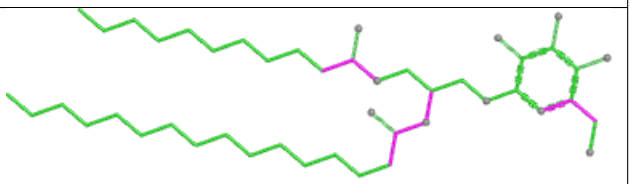


Rings

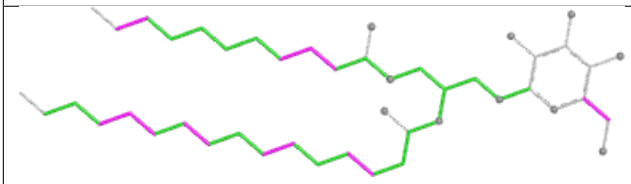
Ligand LMG D 411



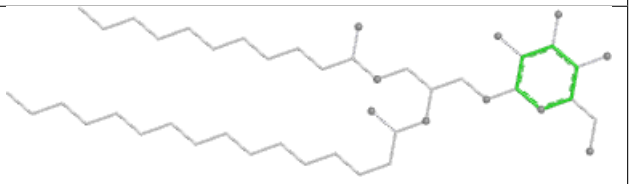
Bond lengths



Bond angles

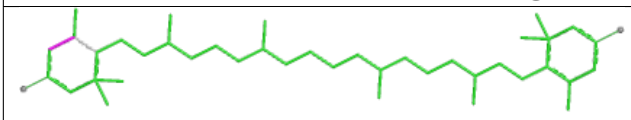


Torsions

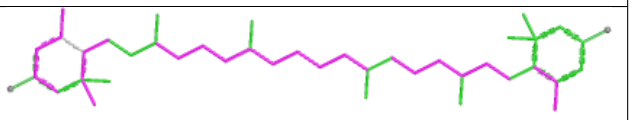


Rings

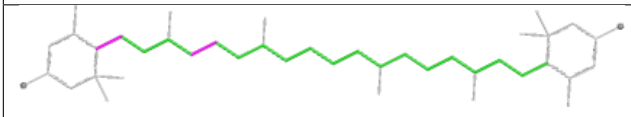
Ligand LUT S 620



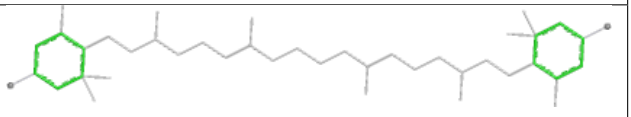
Bond lengths



Bond angles

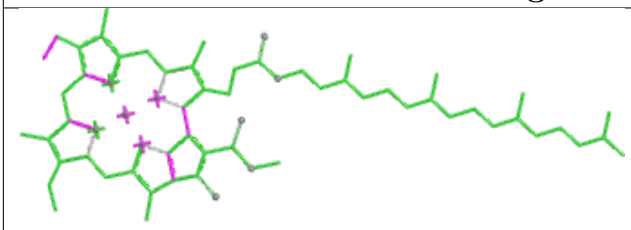


Torsions

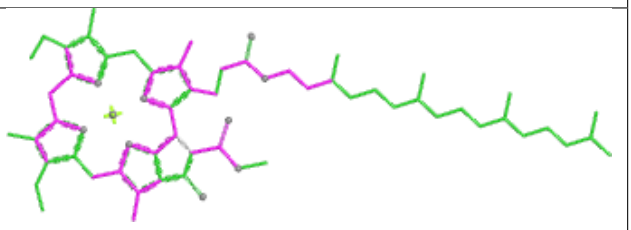


Rings

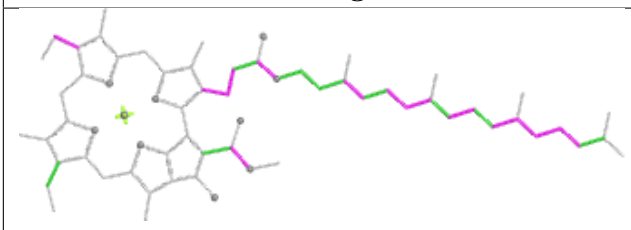
Ligand CLA b 604



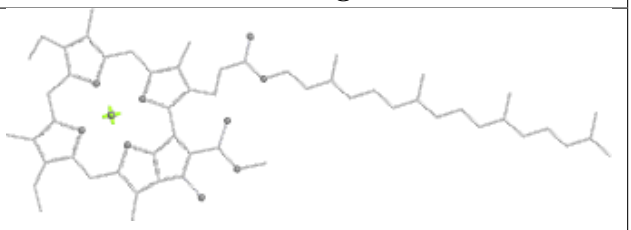
Bond lengths



Bond angles

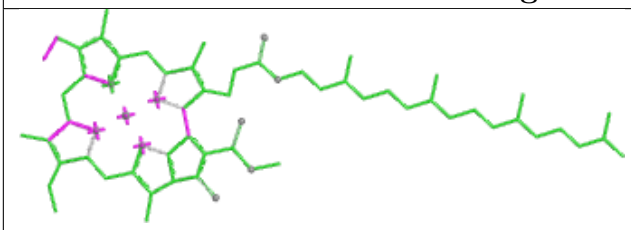


Torsions



Rings

Ligand CLA c1 505



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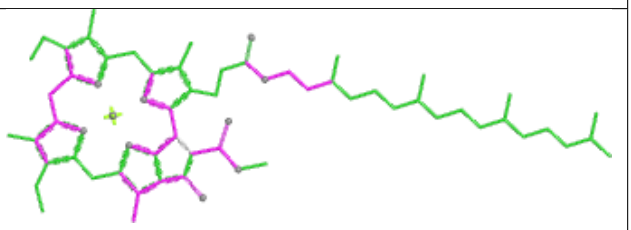
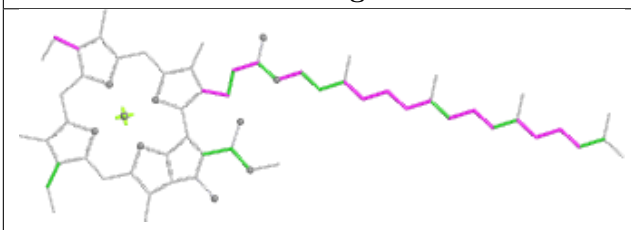
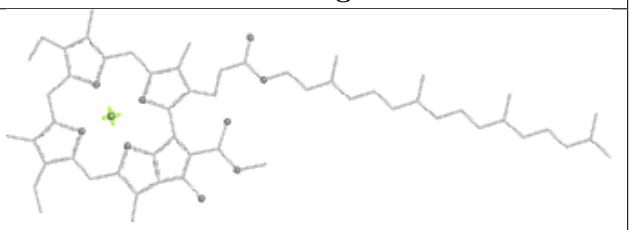


Bond angles

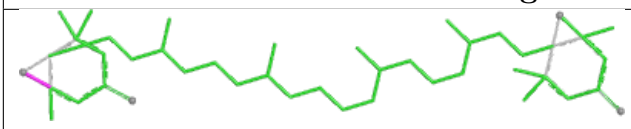


Torsions

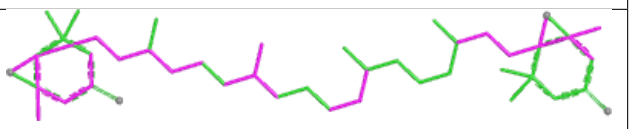


Rings

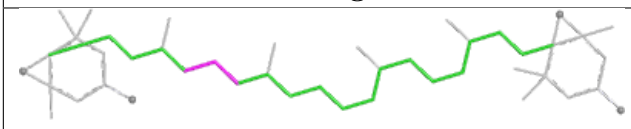
Ligand XAT r1 621



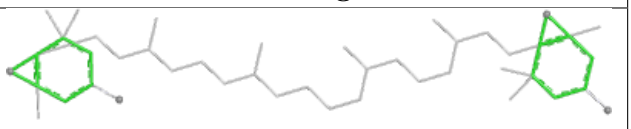
Bond lengths



Bond angles

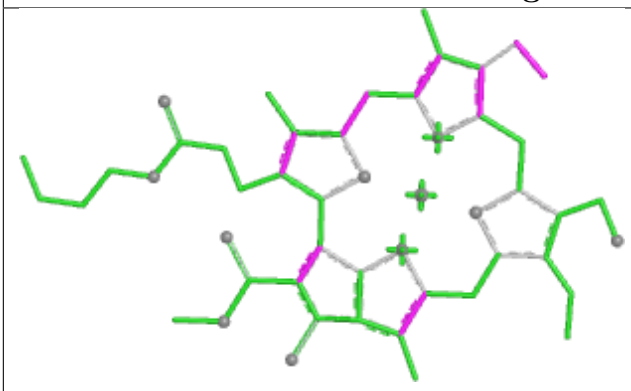


Torsions



Rings

Ligand CHL N 608



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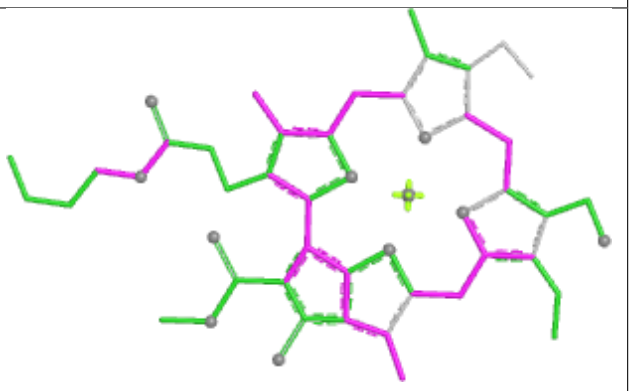
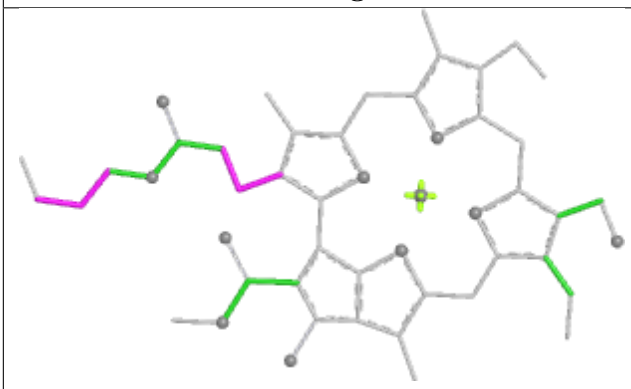


Bond angles



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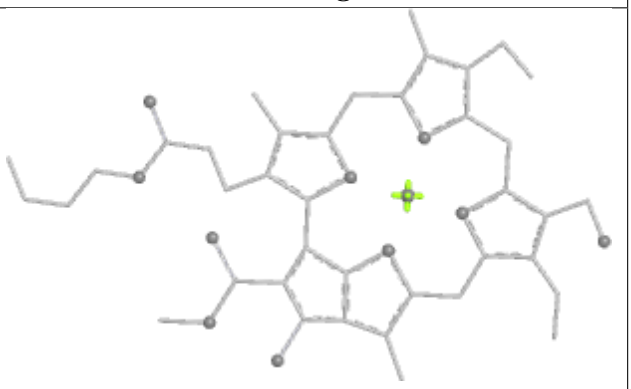
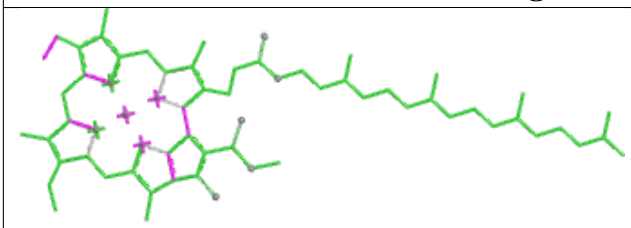
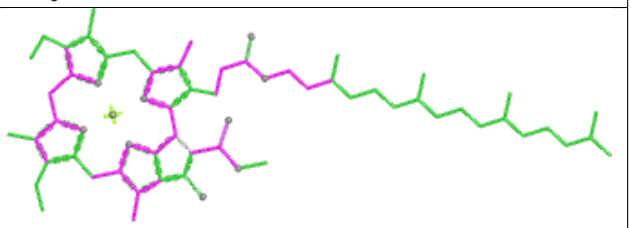


Rings

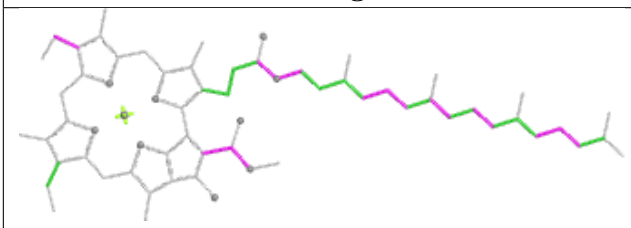
Ligand CLA y 614



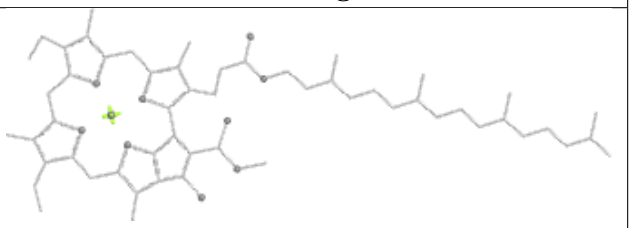
Bond lengths



Bond angles

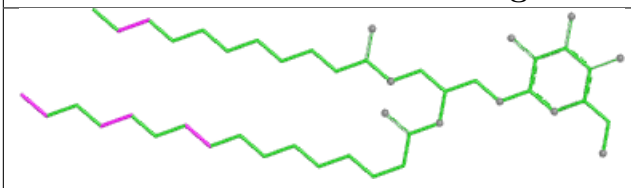


Torsions



Rings

Ligand LMG D1 411



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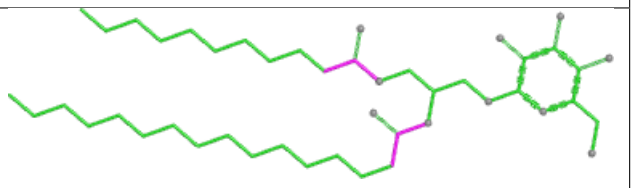
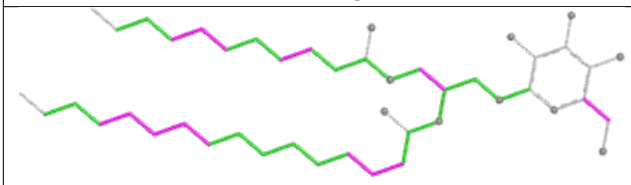
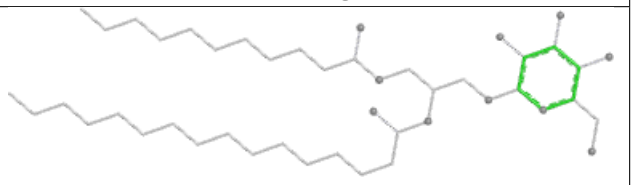


Bond angles

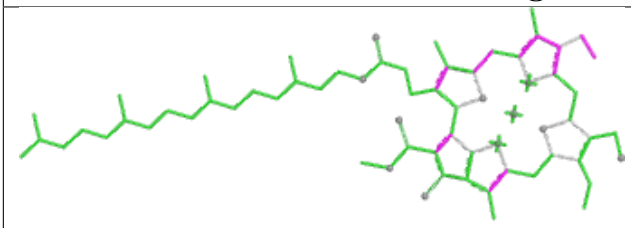


Torsions

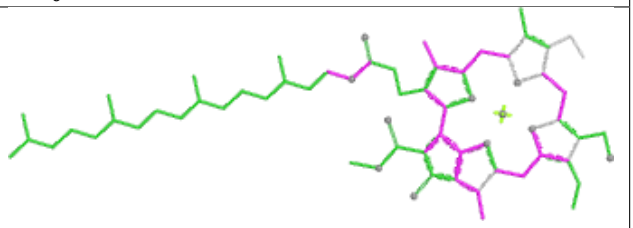


Rings

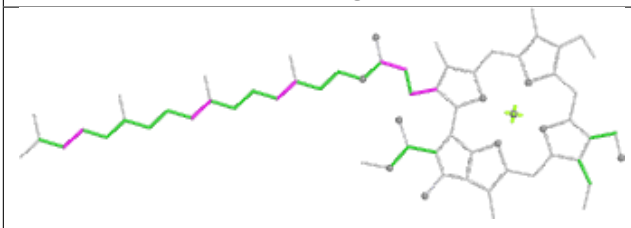
Ligand CHL y 606



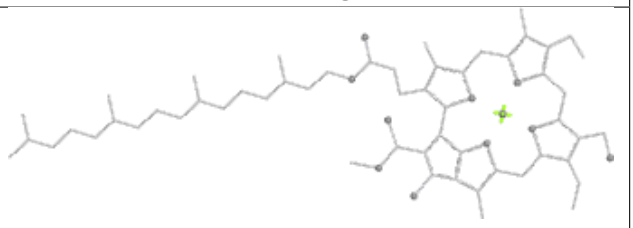
Bond lengths



Bond angles

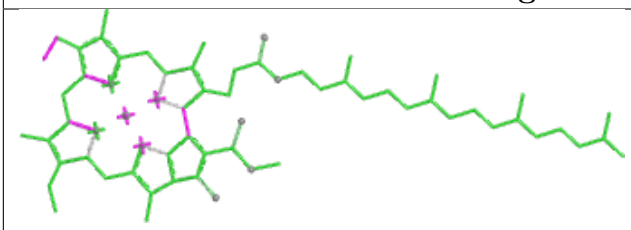


Torsions



Rings

Ligand CLA b1 607



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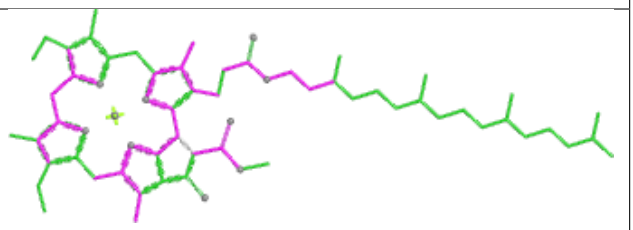
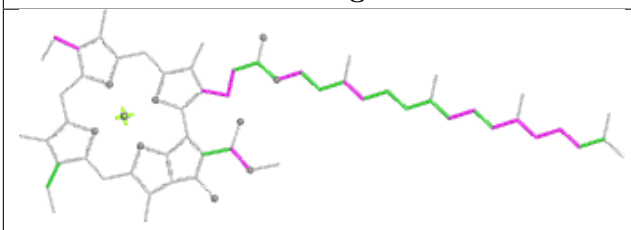
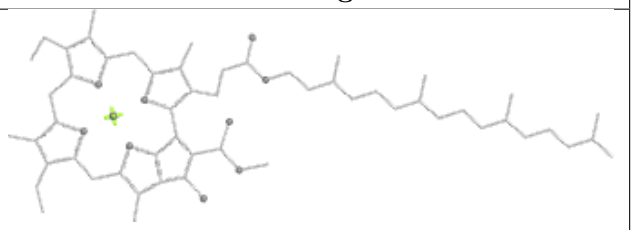


Bond angles

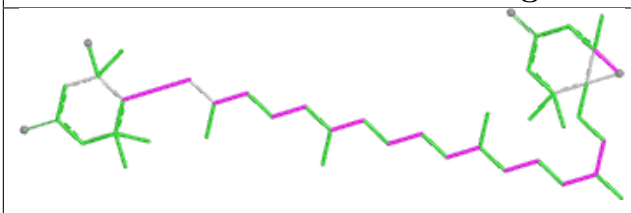


Torsions

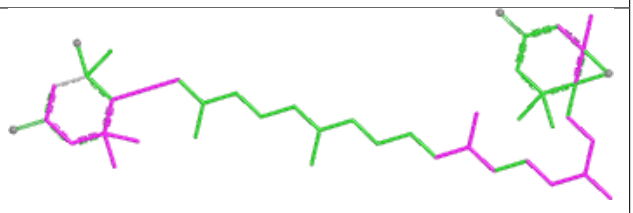


Rings

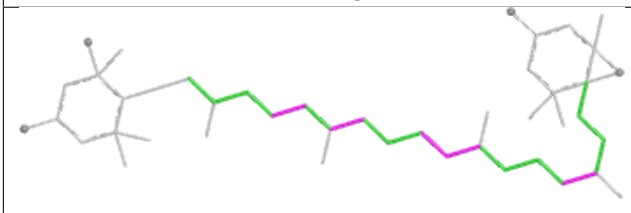
Ligand NEX N 623



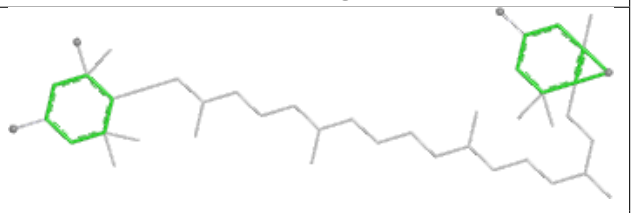
Bond lengths



Bond angles

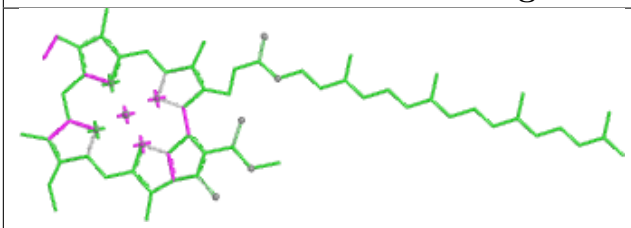


Torsions

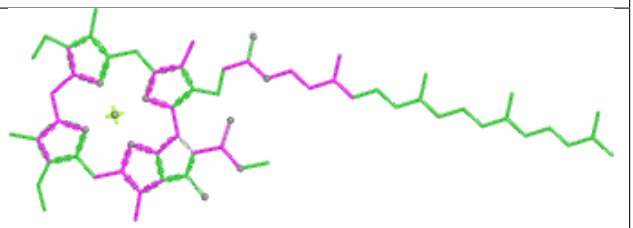


Rings

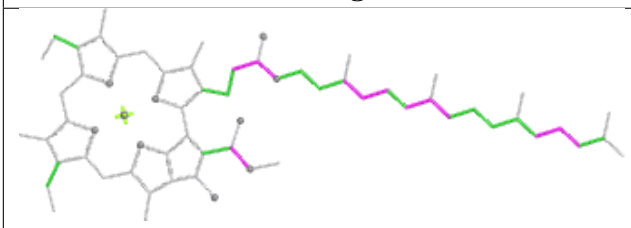
Ligand CLA d1 402



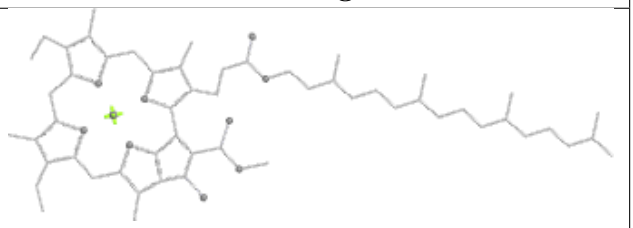
Bond lengths



Bond angles

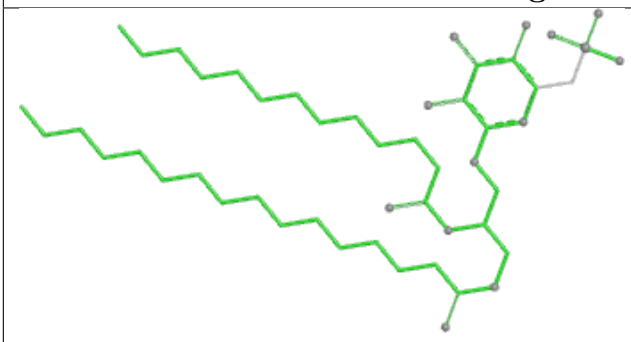


Torsions



Rings

Ligand SQD a 412



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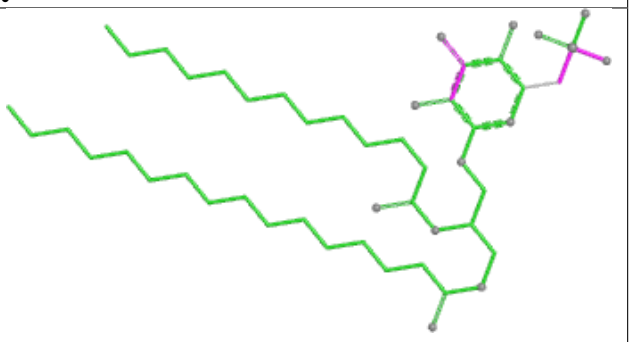
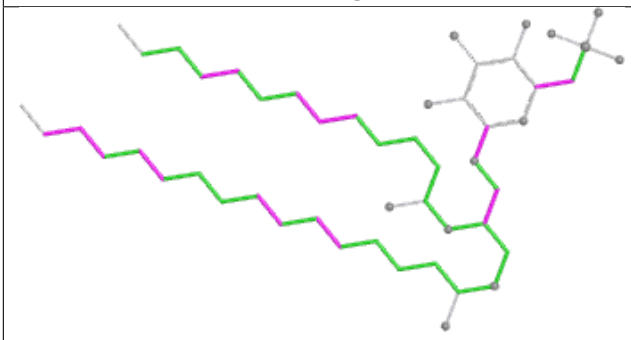
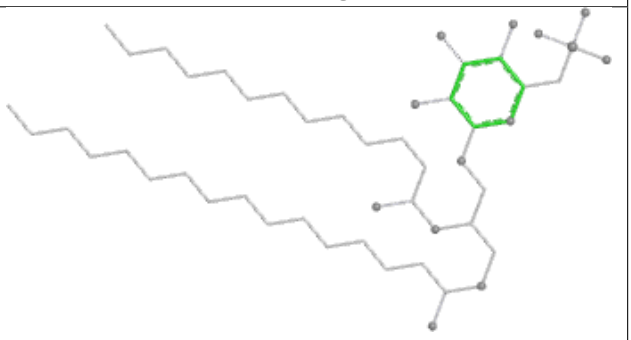


Bond angles

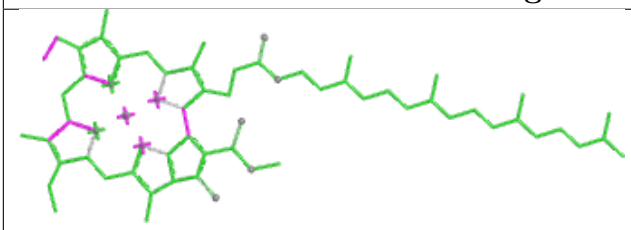


Torsions



Rings

Ligand CLA C 505



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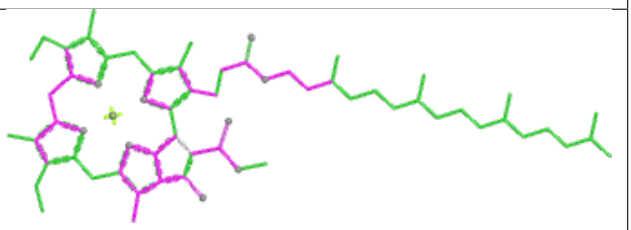
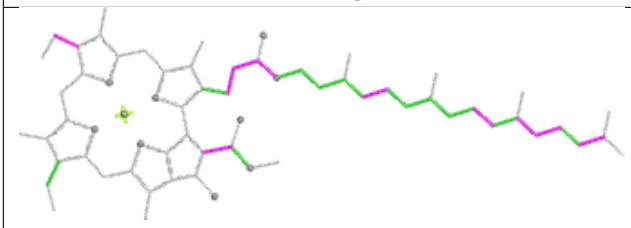


Bond angles



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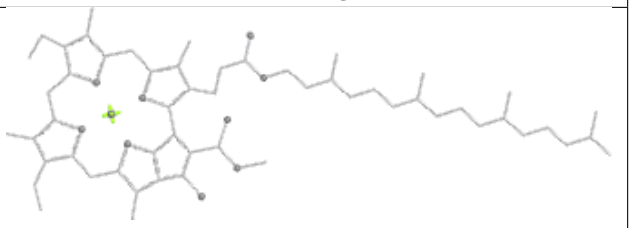
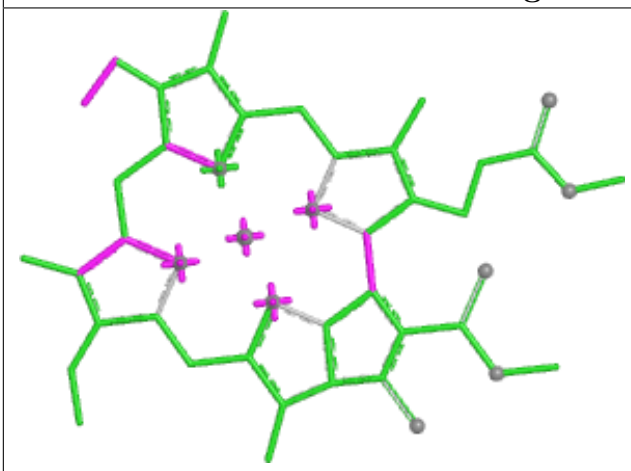
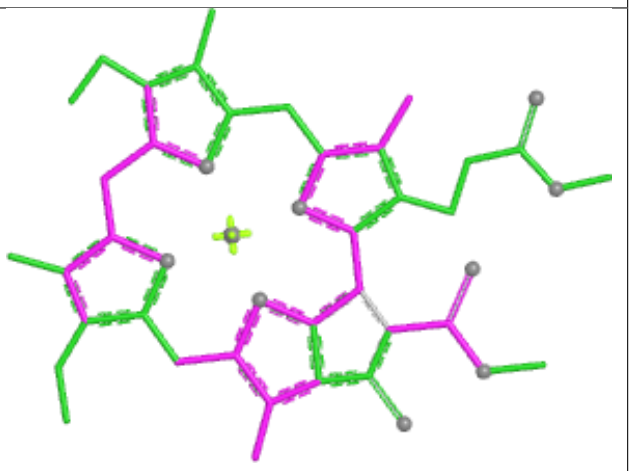


Rings

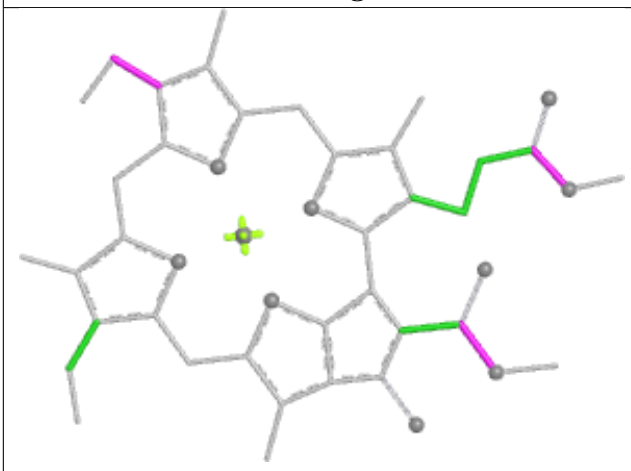
Ligand CLA R 611



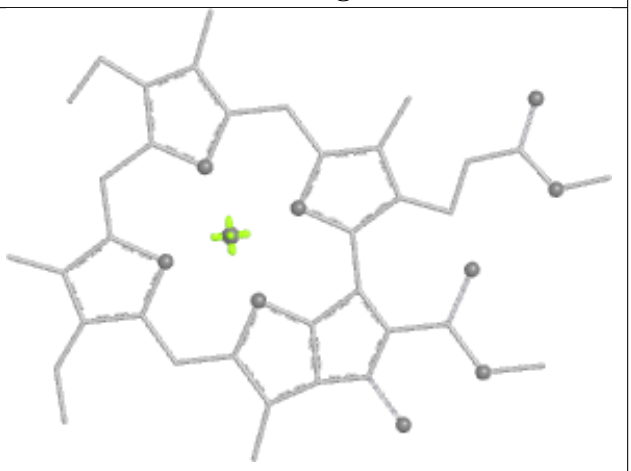
Bond lengths



Bond angles

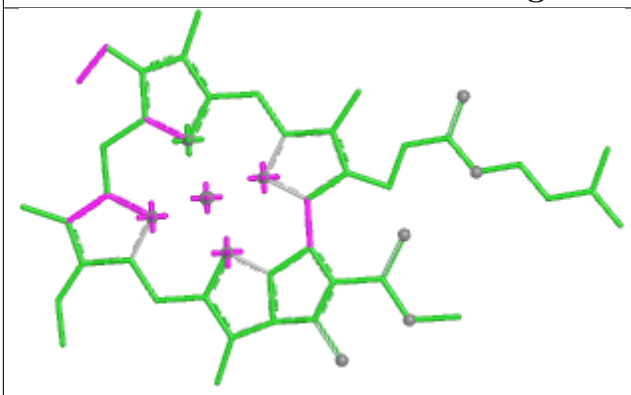


Torsions

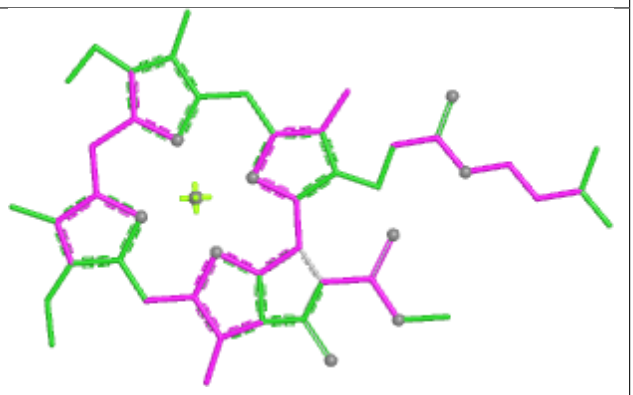


Rings

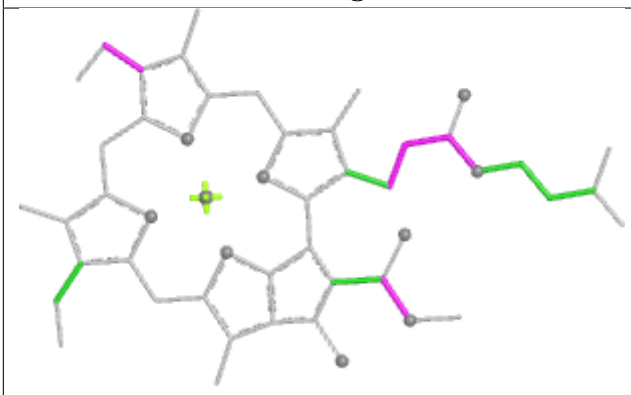
Ligand CLA S 617



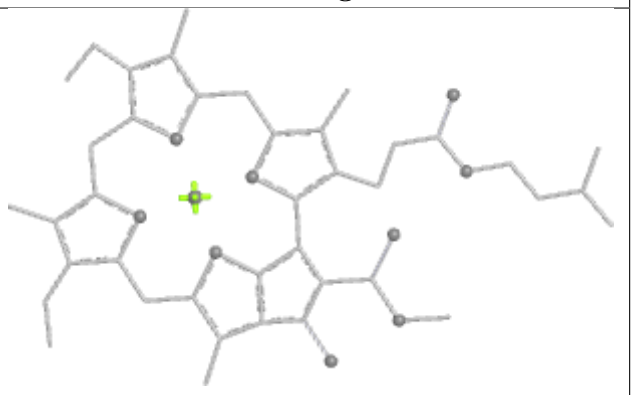
Bond lengths



Bond angles



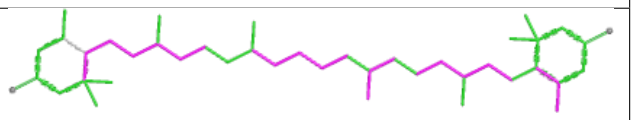
Torsions



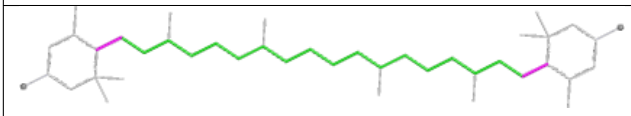
Rings

Ligand LUT S1 620

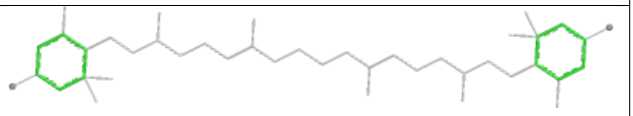
Bond lengths



Bond angles

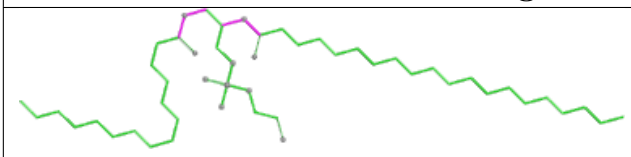


Torsions



Rings

Ligand PTY y1 626



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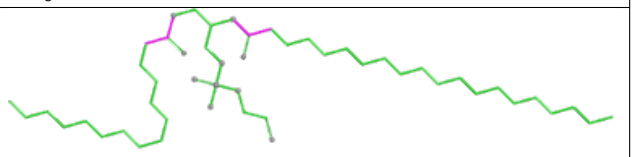

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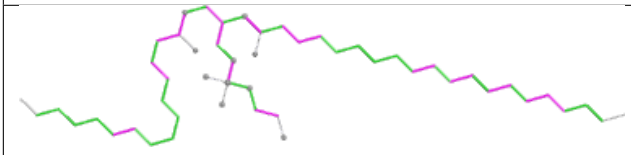
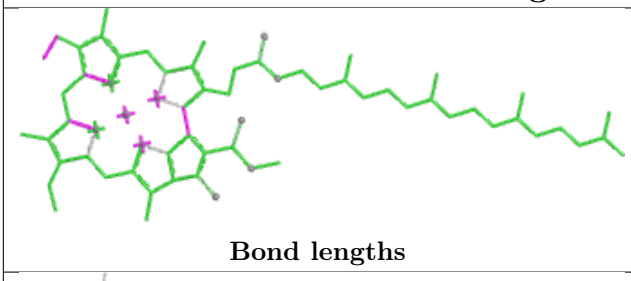


Torsions

Rings

Ligand CLA c 509



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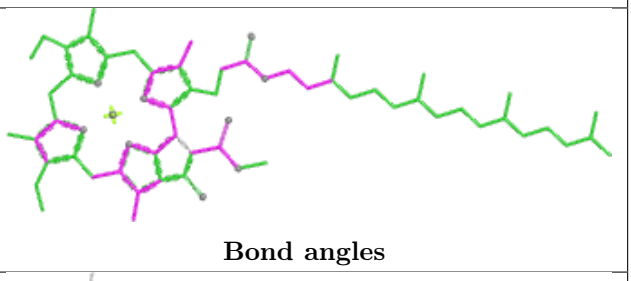

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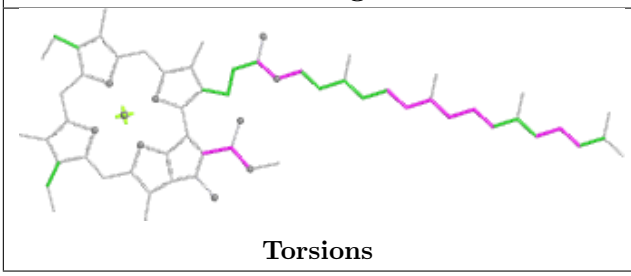

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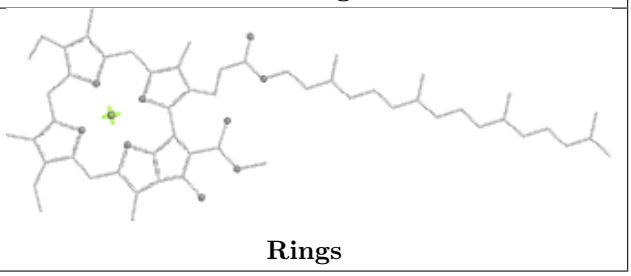
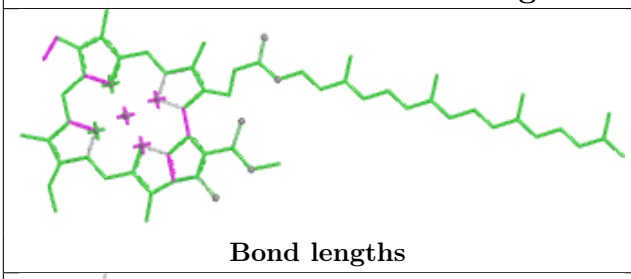


Rings

Ligand CLA y1 614



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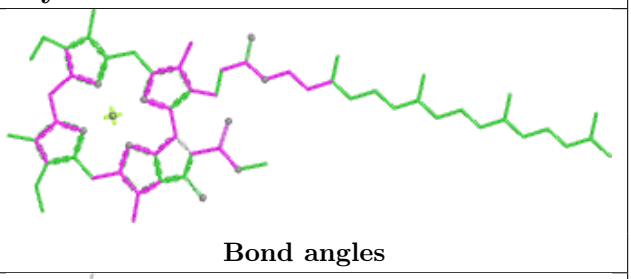
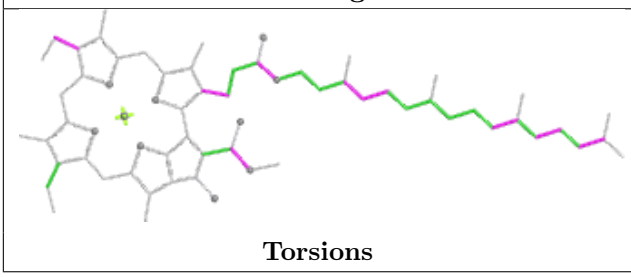


Bond angles



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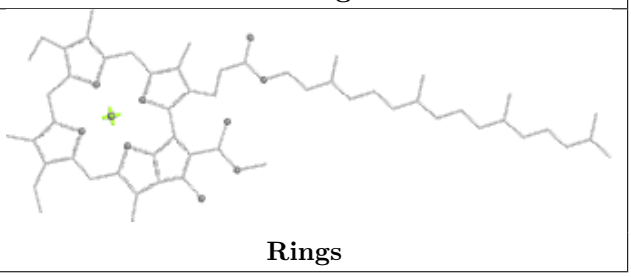
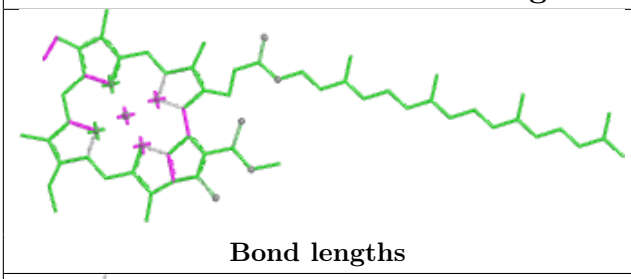


Rings

Ligand CLA c 503



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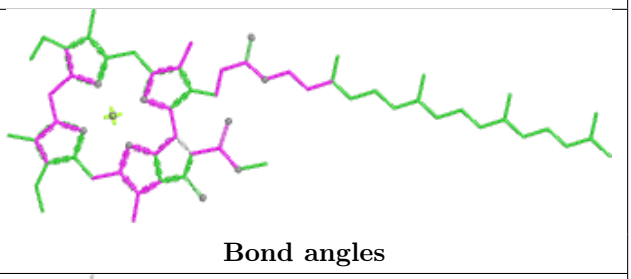
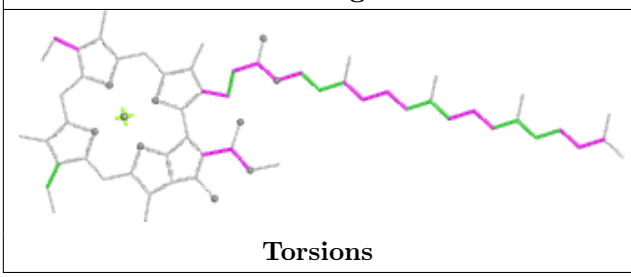


Bond angles



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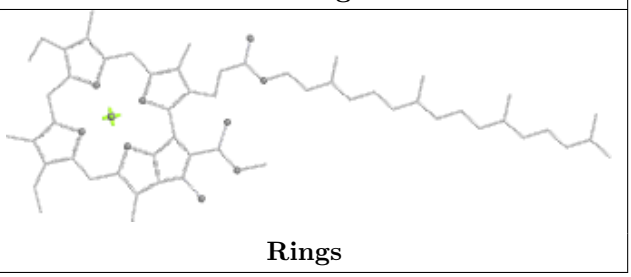
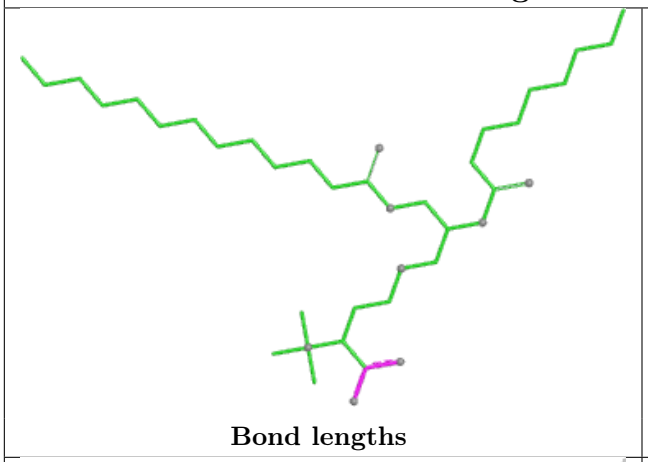


Rings

Ligand LMK C1 527



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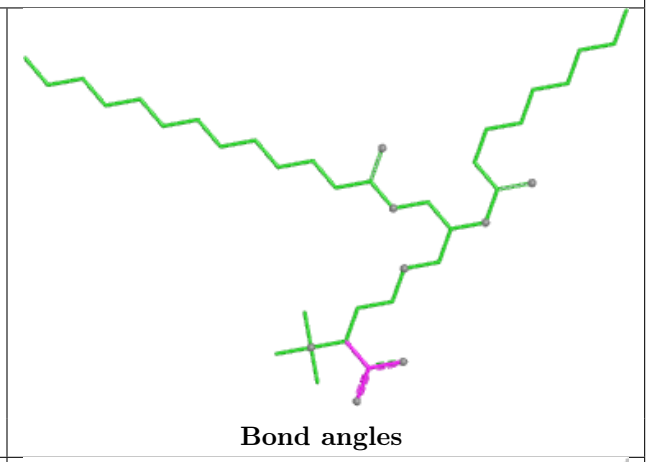

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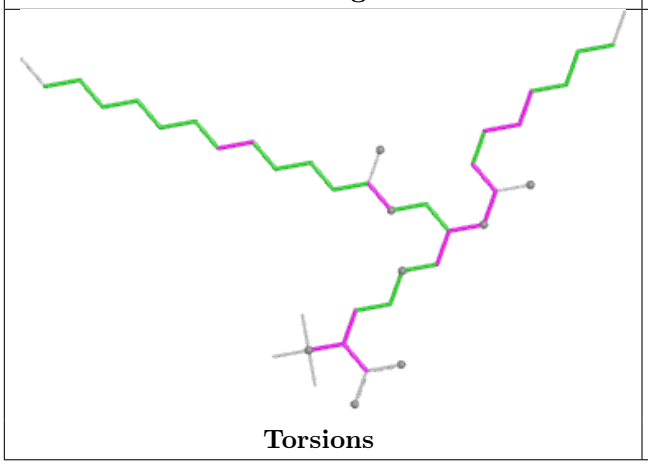

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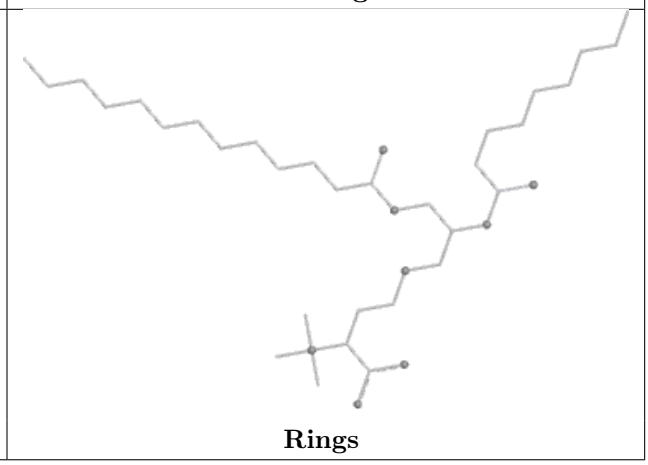
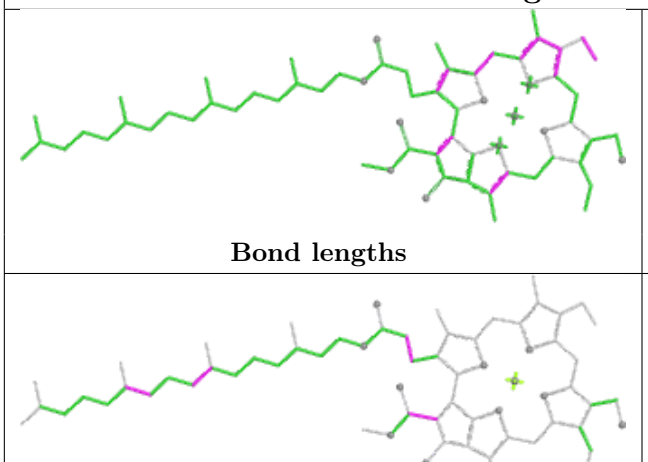


Rings

Ligand CHL N 606



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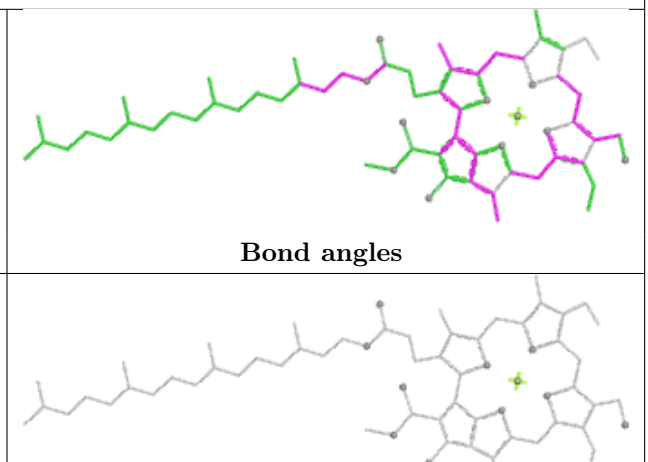
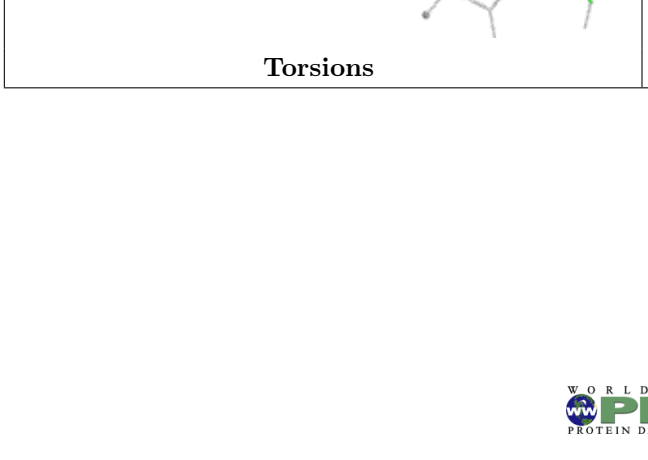


Bond angles



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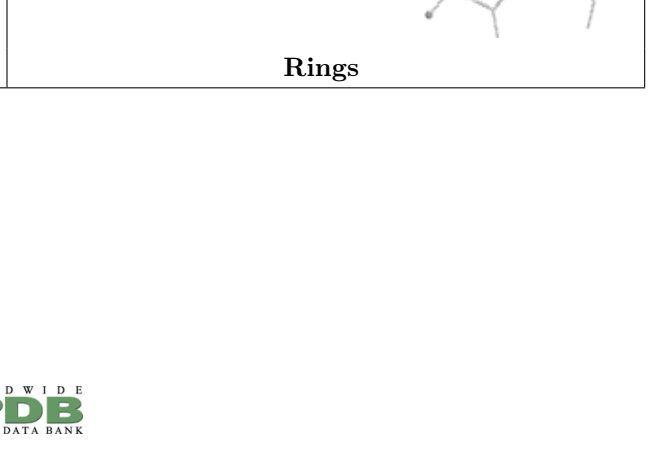
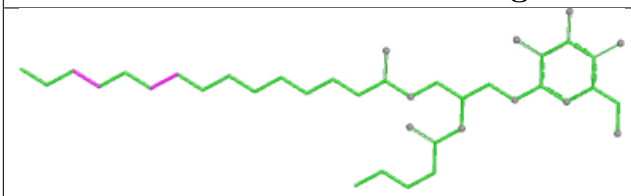


Rings

Ligand LMG w1 201



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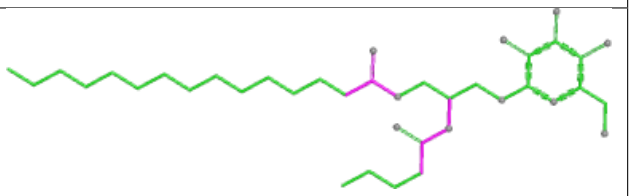

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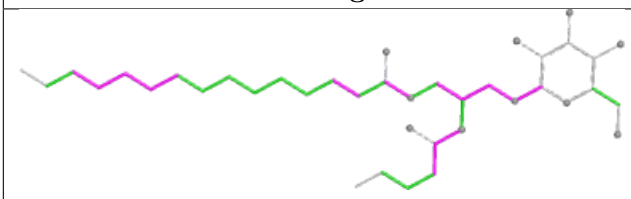

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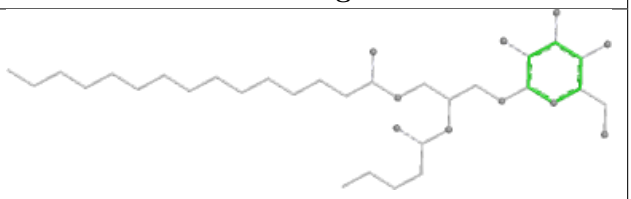
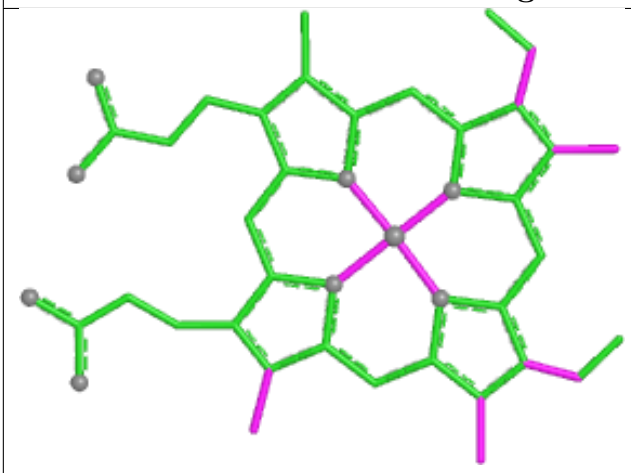


Rings

Ligand HEM f1 101



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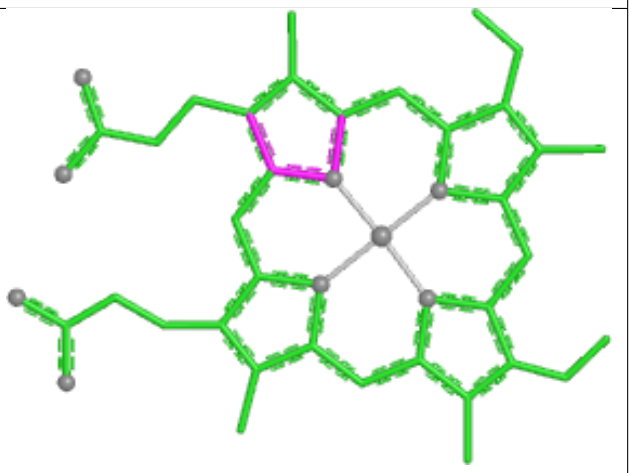
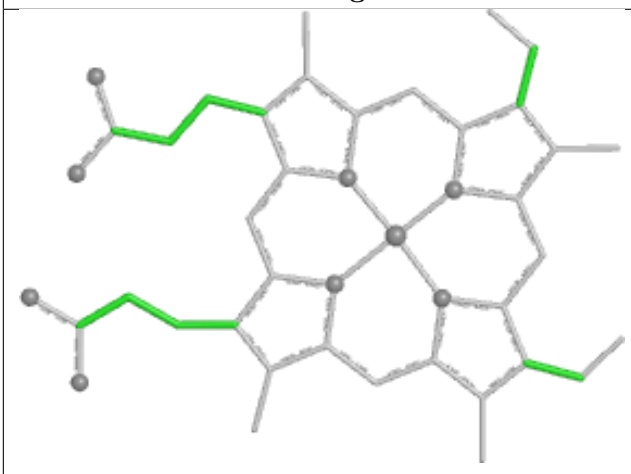


Bond angles



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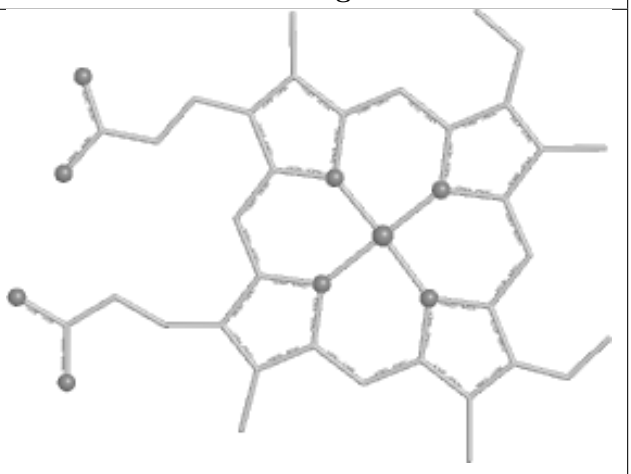
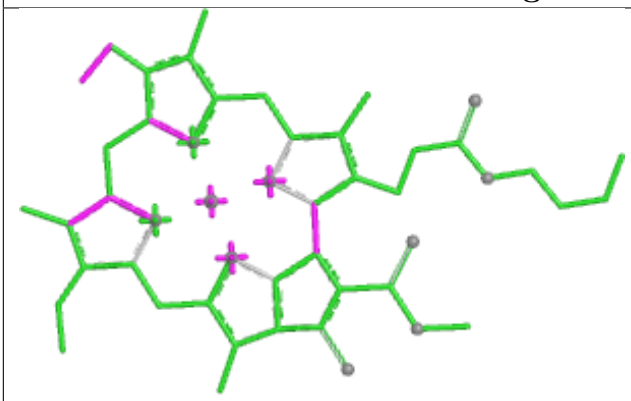


Rings

Ligand CLA G 614



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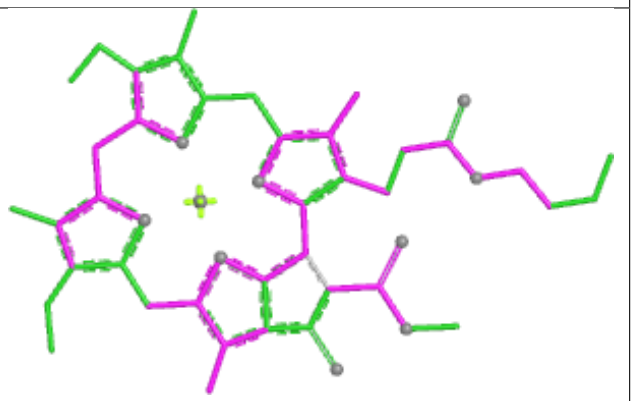

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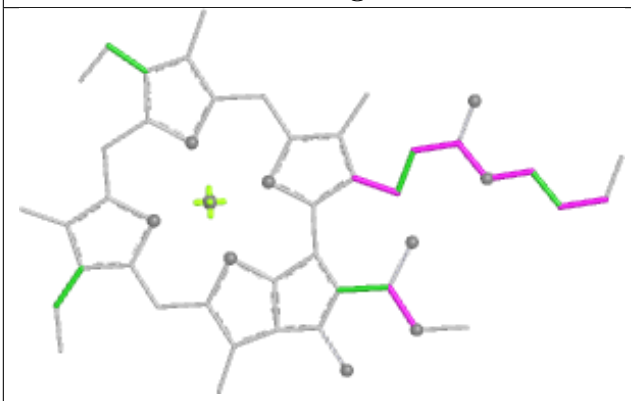

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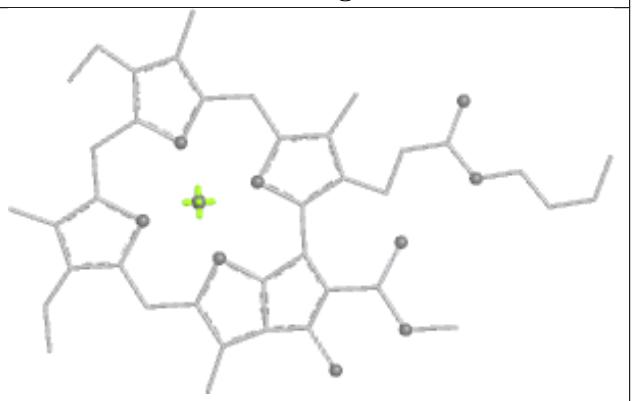
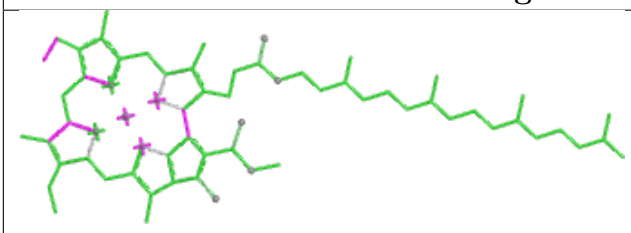


Rings

Ligand CLA N1 602



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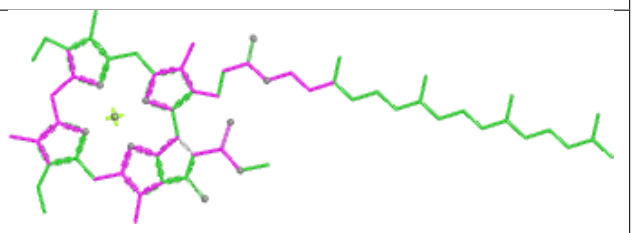
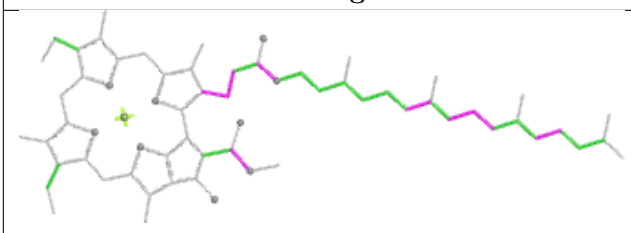


Bond angles



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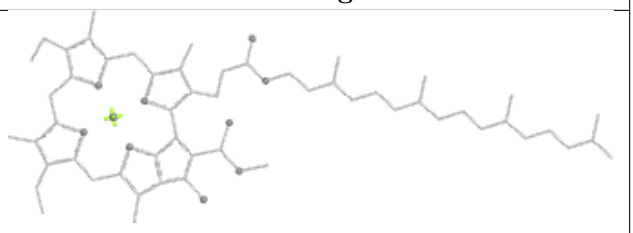

Rings

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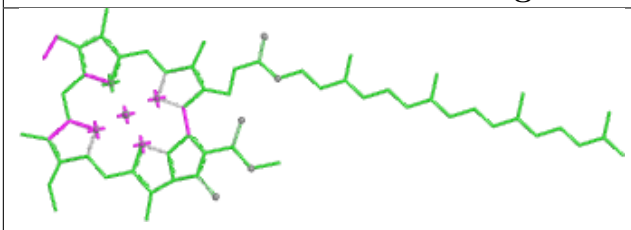

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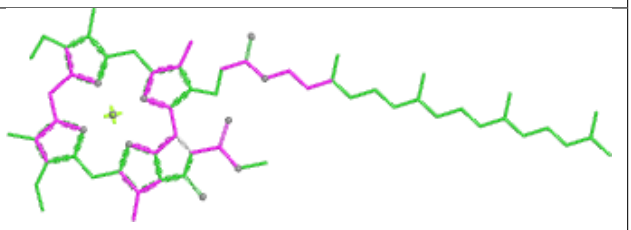

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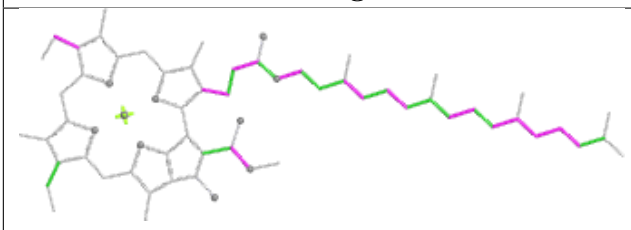

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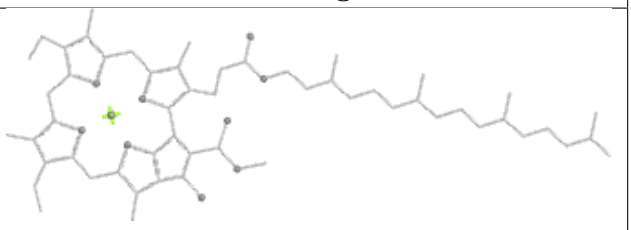
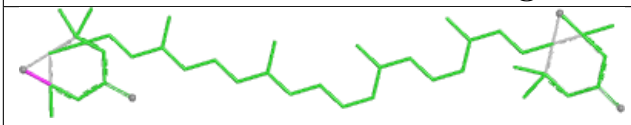


Rings

Ligand XAT y1 622



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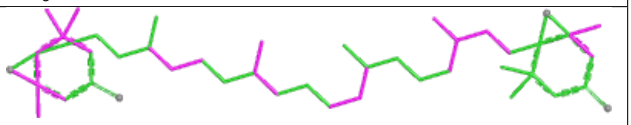
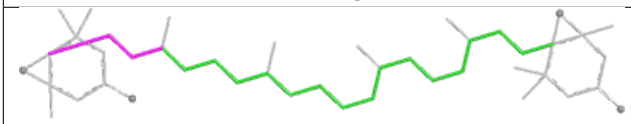


Bond angles



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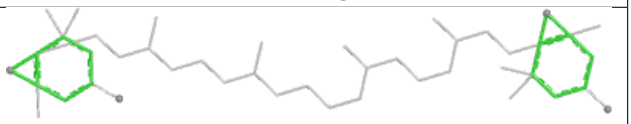
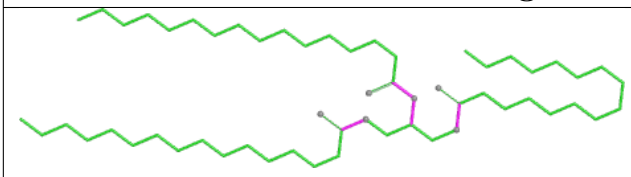


Rings

Ligand 4RF K1 101



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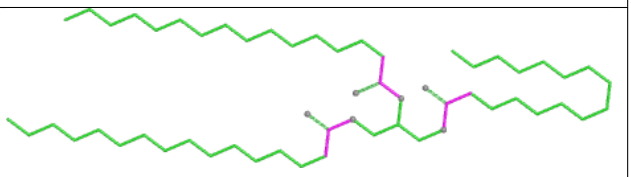
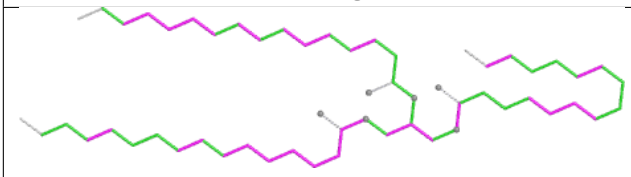
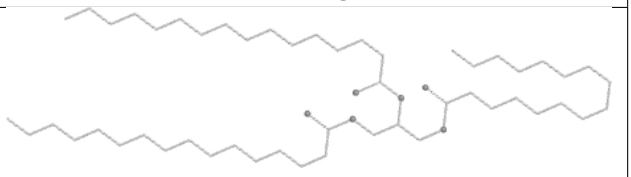


Bond angles

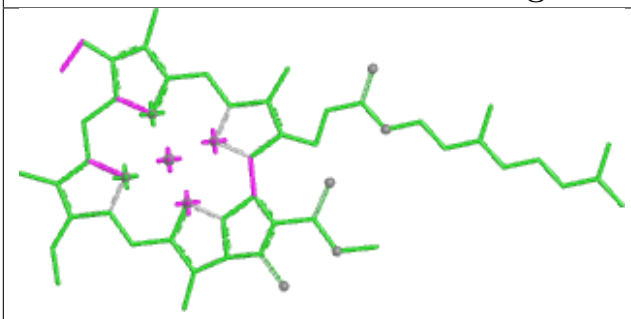


Torsions

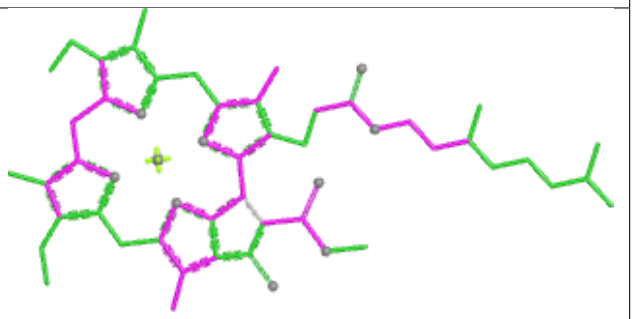


Rings

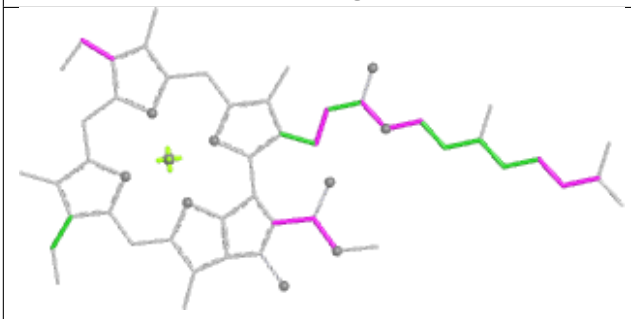
Ligand CLA S 613



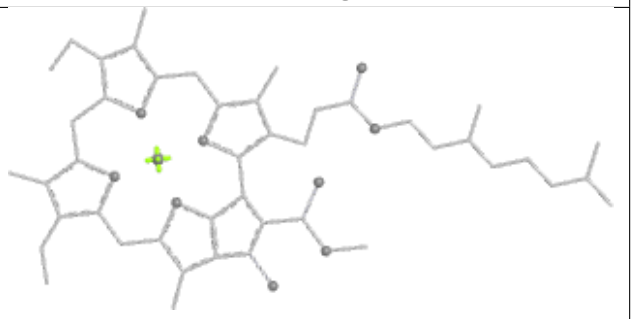
Bond lengths



Bond angles

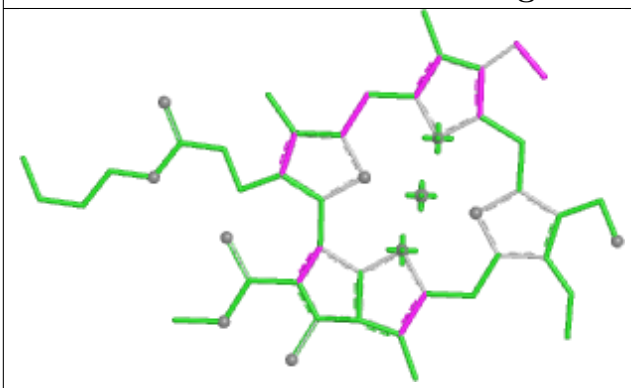


Torsions

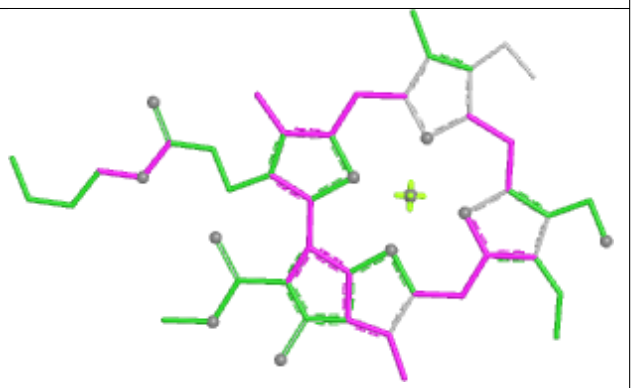


Rings

Ligand CHL n1 608



Bond lengths



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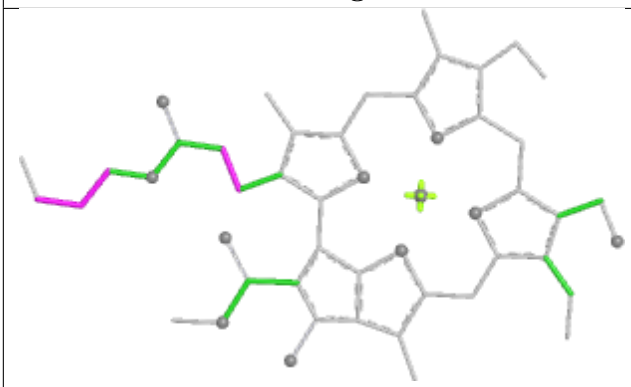

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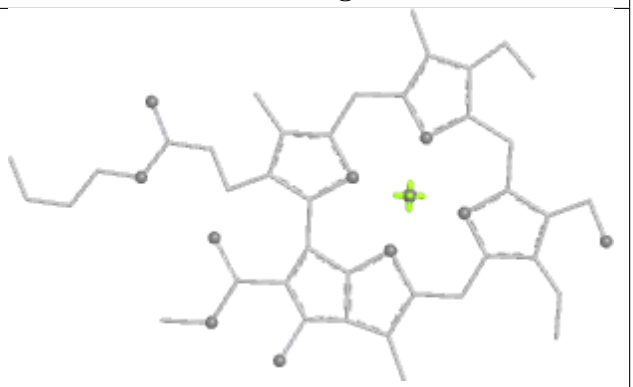
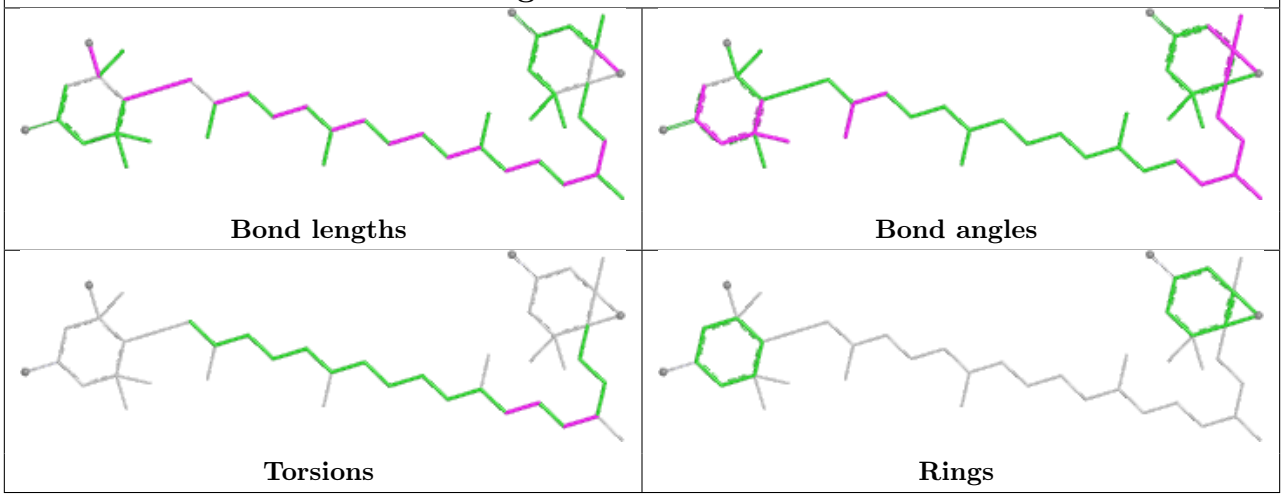
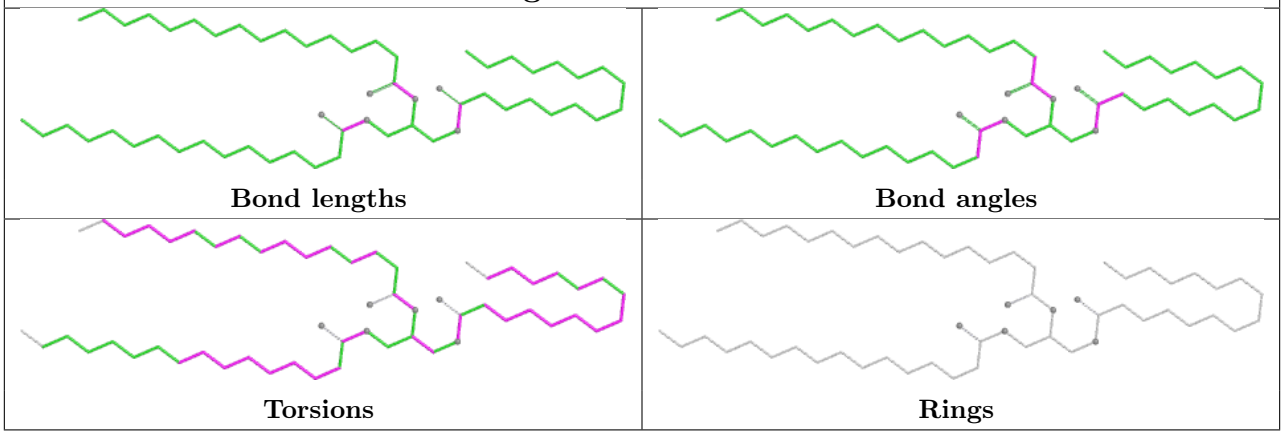


Rings

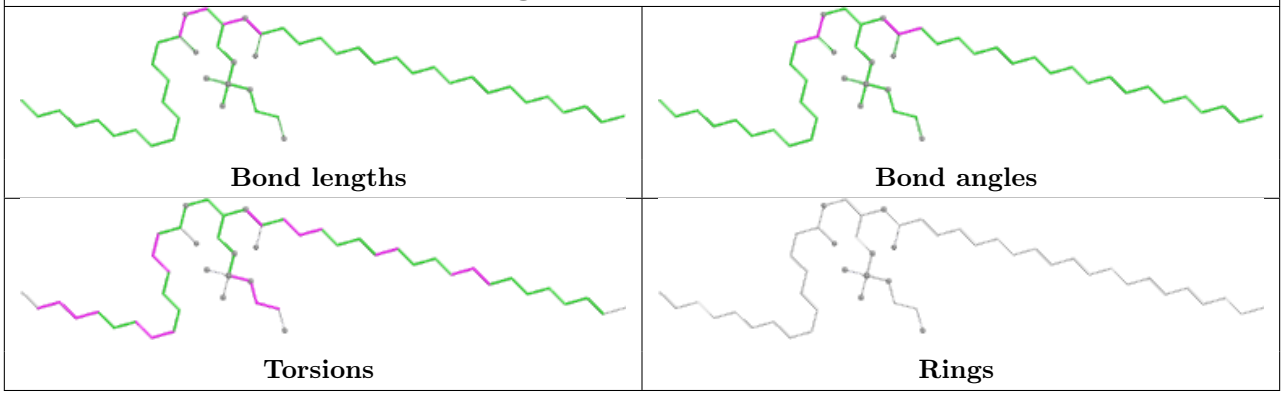
Ligand NEX S1 623



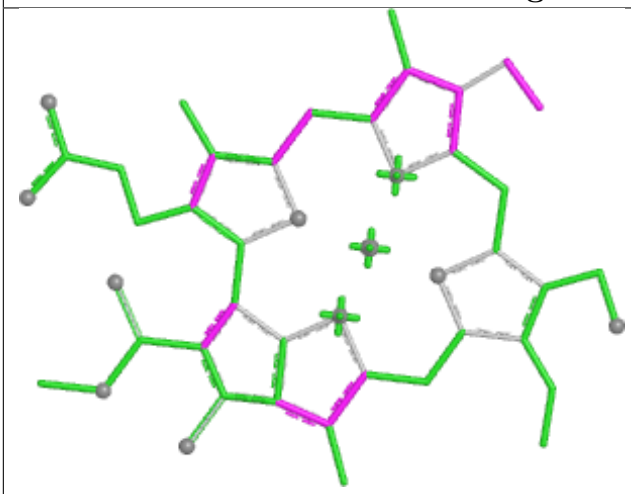
Ligand 4RF k1 101



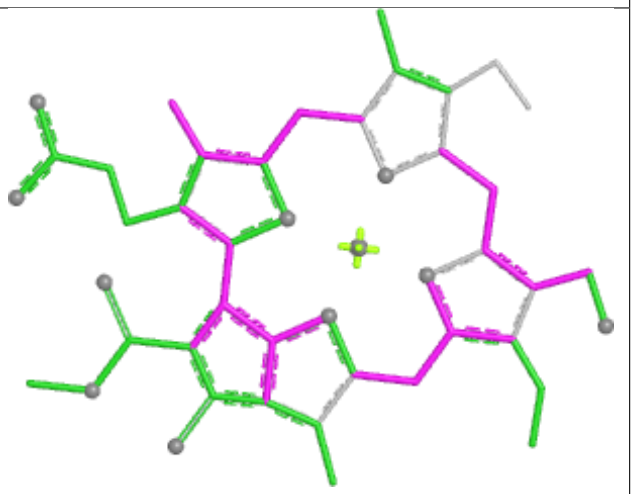
Ligand PTY Y1 626



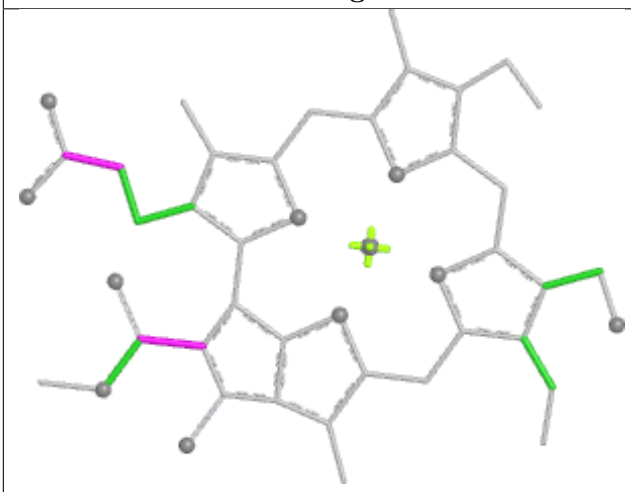
Ligand CHL S 601



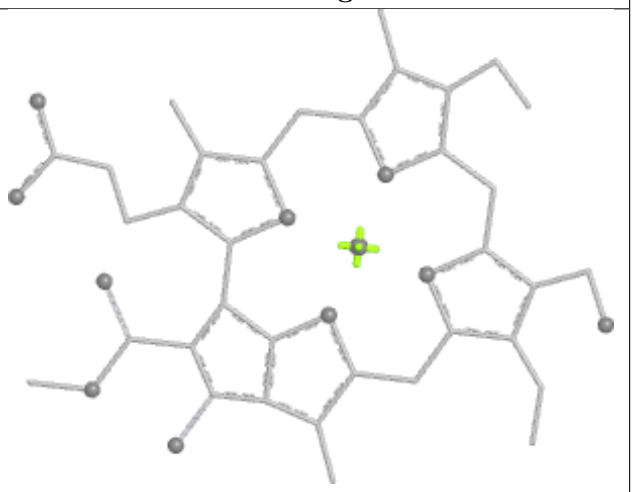
Bond lengths



Bond angles

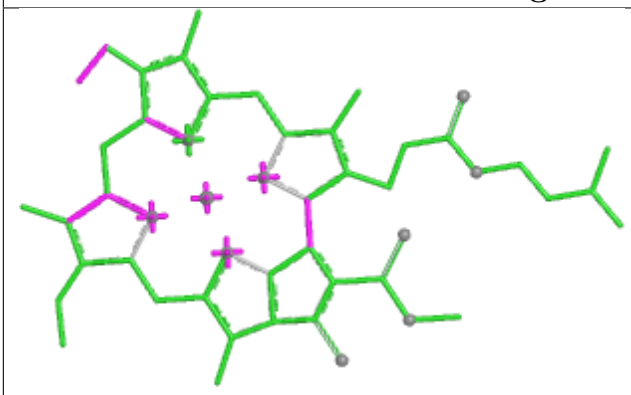


Torsions

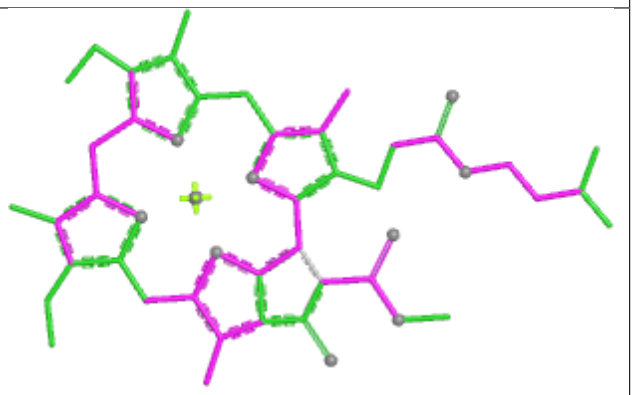


Rings

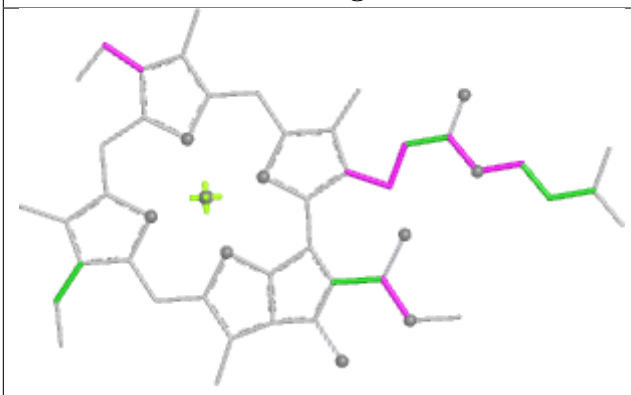
Ligand CLA s 617



Bond lengths



Bond angles



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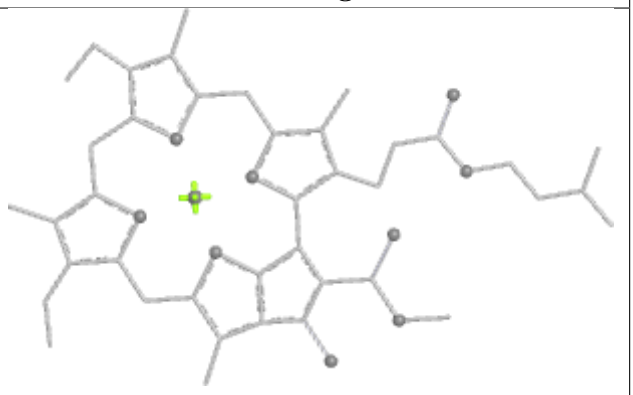
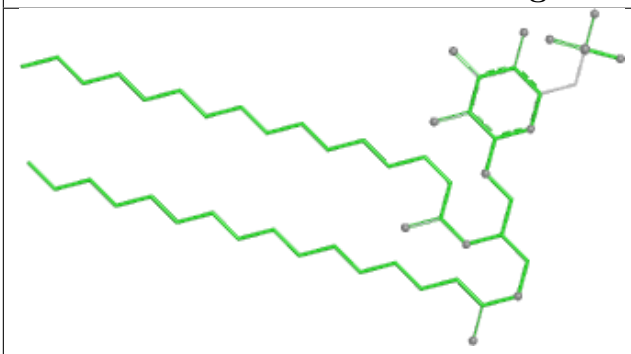


Rings

Ligand SQD c 626



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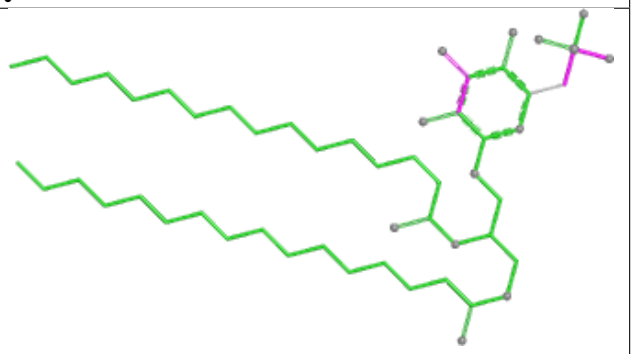
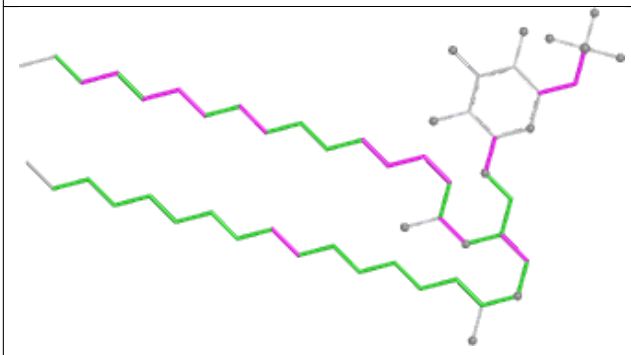


Bond angles



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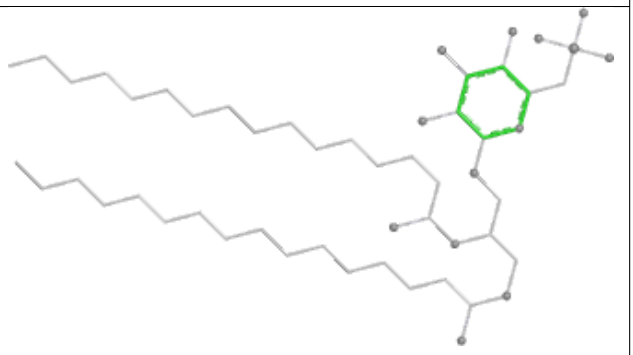
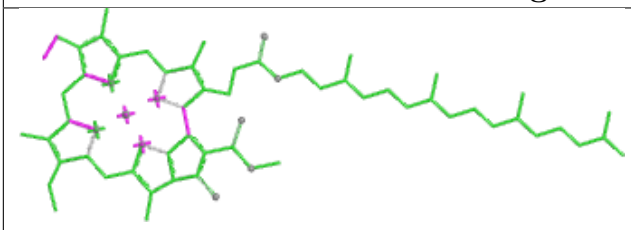
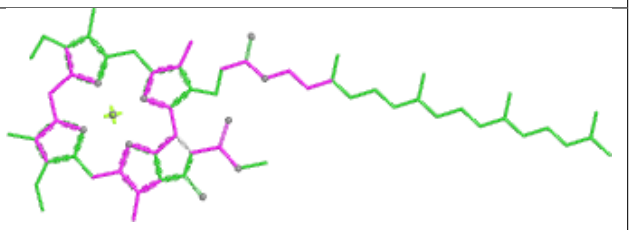
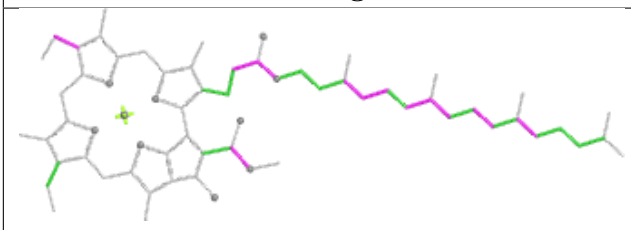
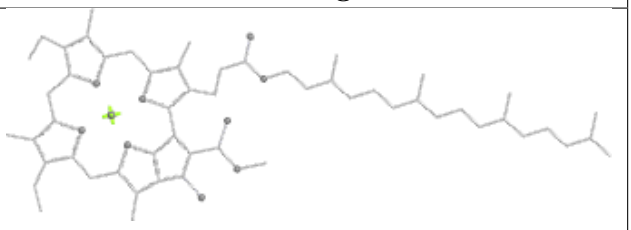
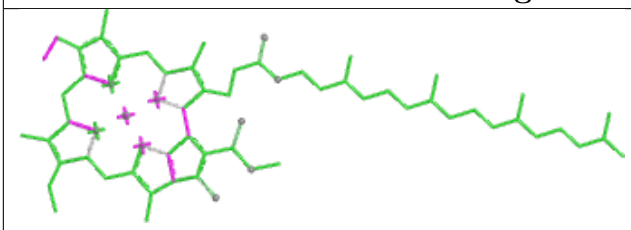
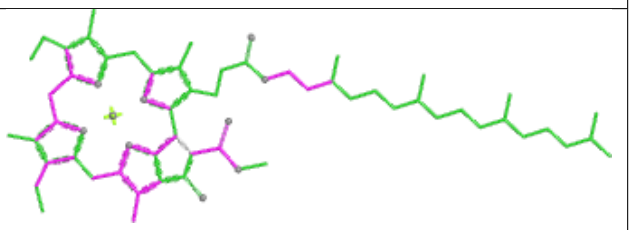
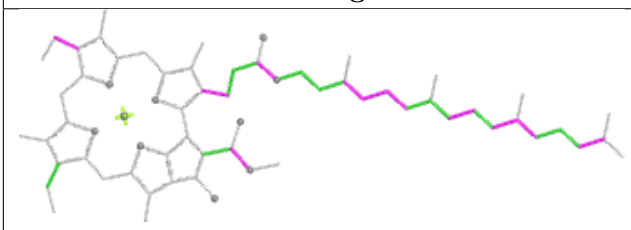
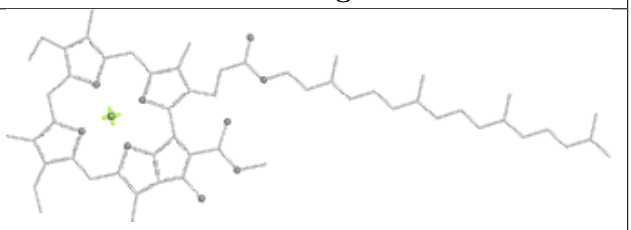
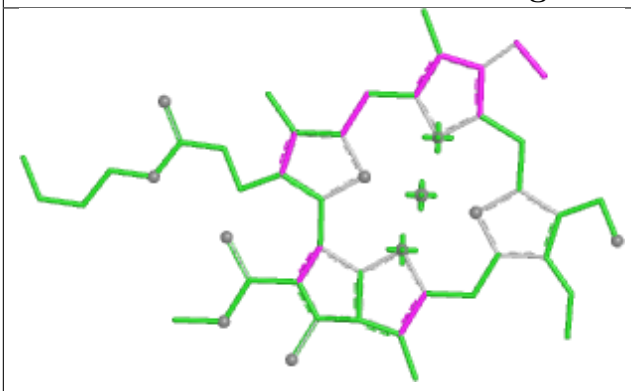


Rings

Ligand CLA s 611	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA N1 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL r 607



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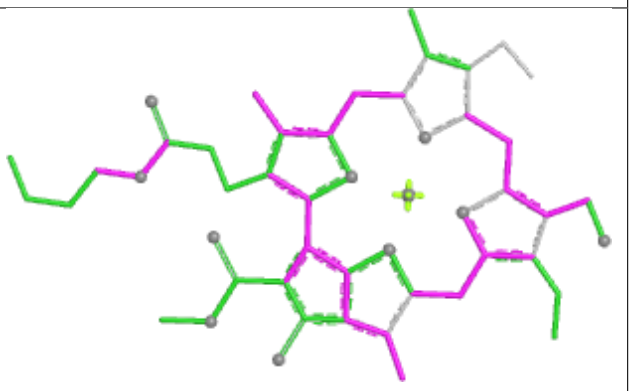
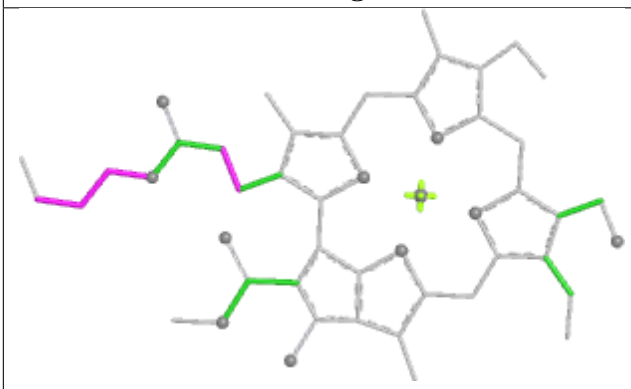
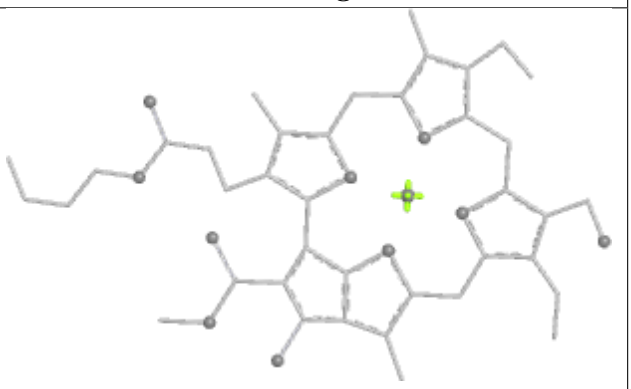


Bond angles

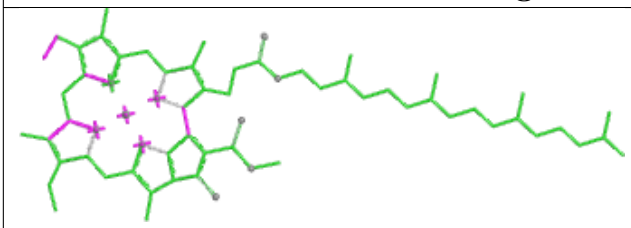


Torsions

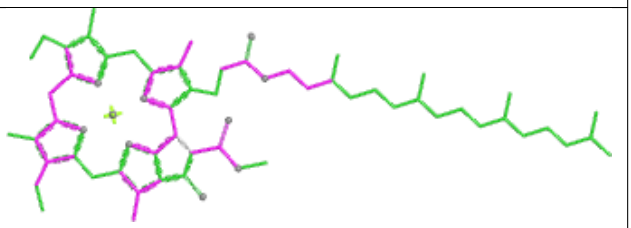


Rings

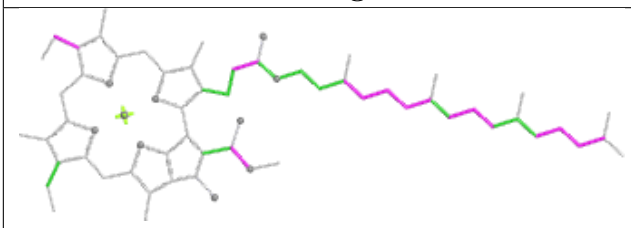
Ligand CLA B1 615



Bond lengths



Bond angles



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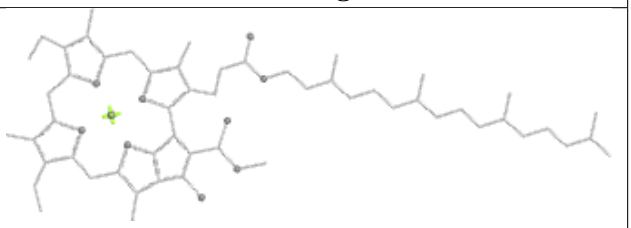
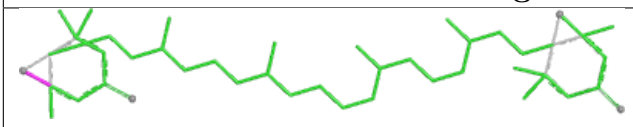


Rings

Ligand XAT N1 622



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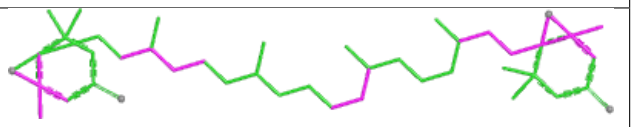
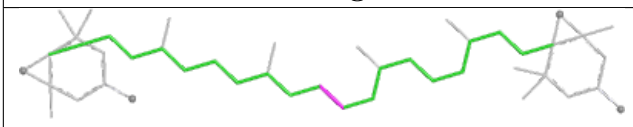


Bond angles



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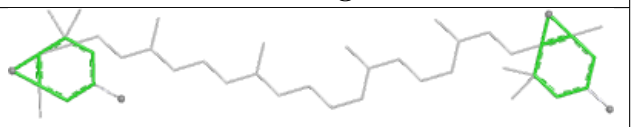
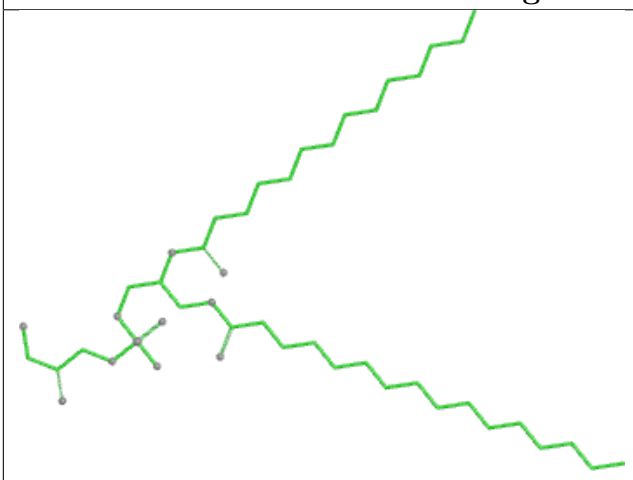


Rings

Ligand LHG C 525



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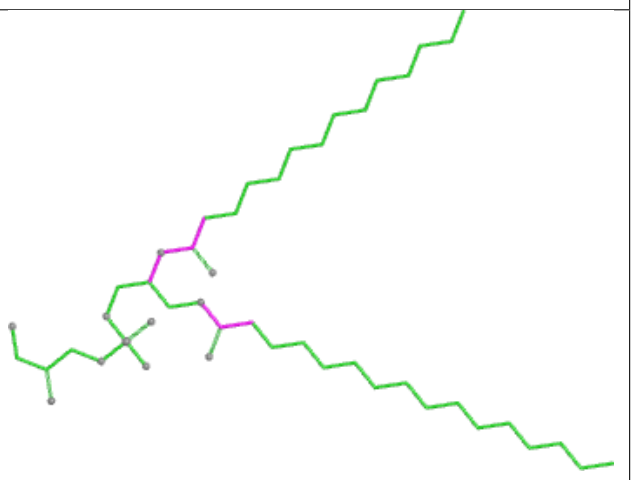
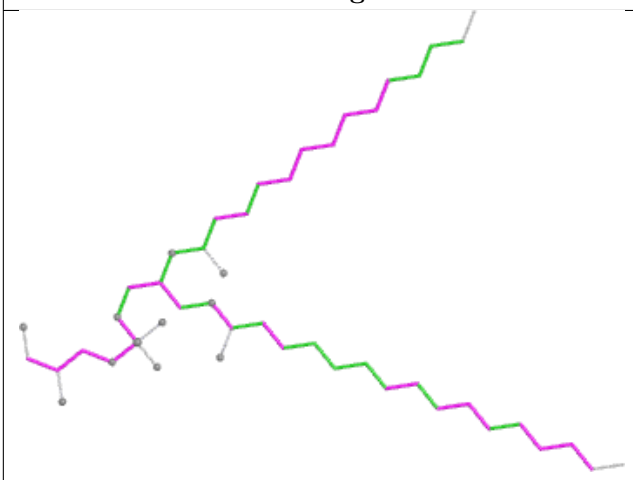
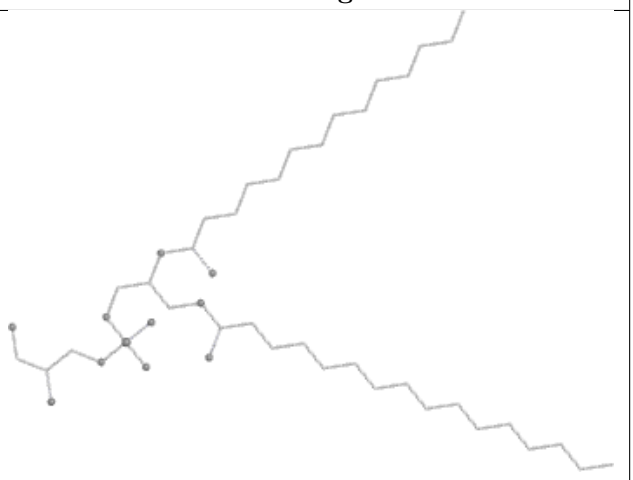


Bond angles

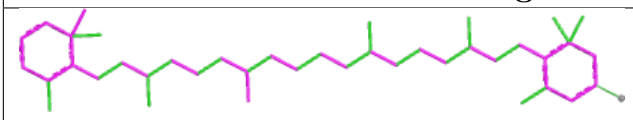


Torsions



Rings

Ligand RRX h1 101



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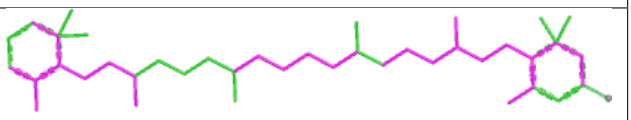
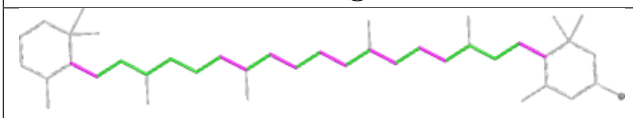
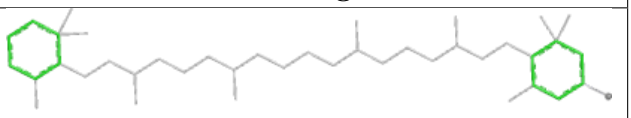


Bond angles

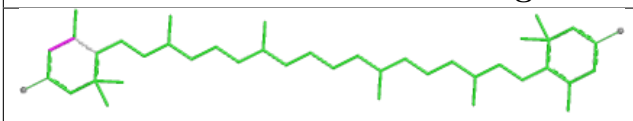


Torsions



Rings

Ligand LUT R1 620



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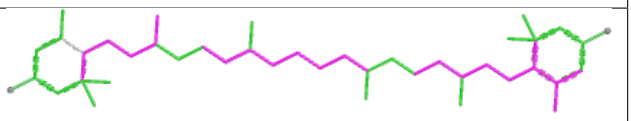
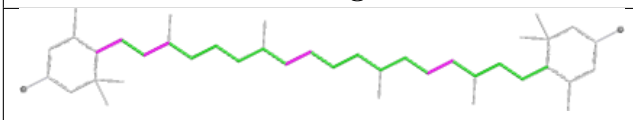
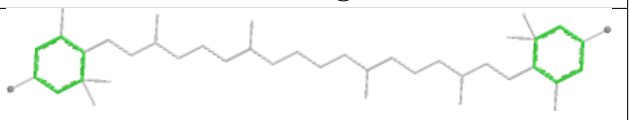


Bond angles

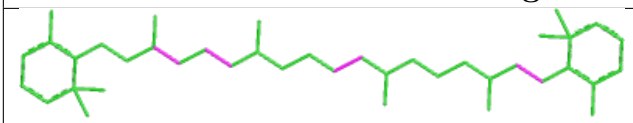


Torsions

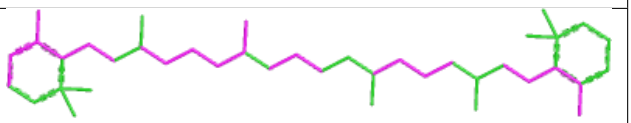


Rings

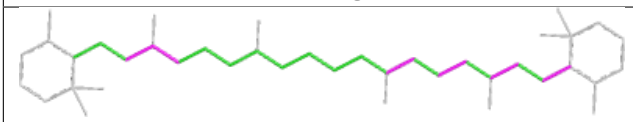
Ligand BCR C 515



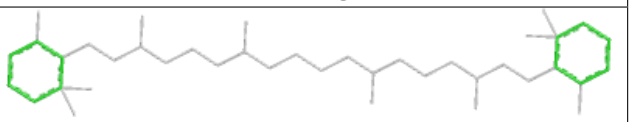
Bond lengths



Bond angles

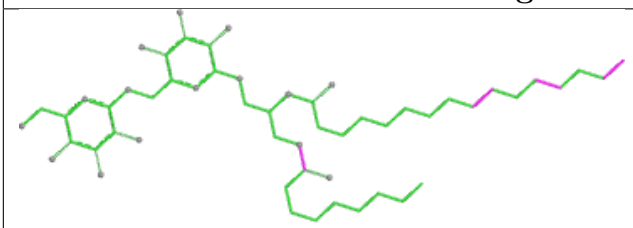


Torsions



Rings

Ligand DGD c1 518



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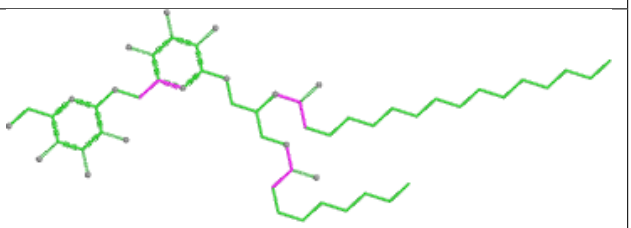
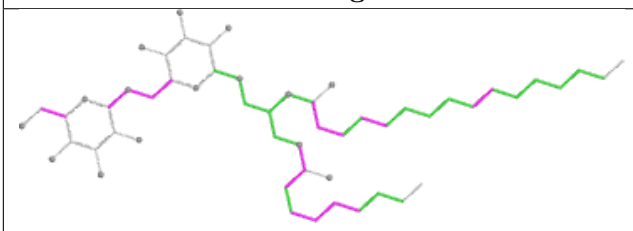


Bond angles



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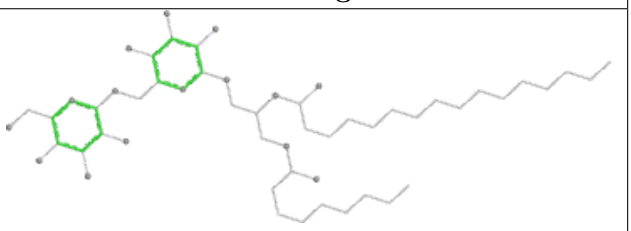
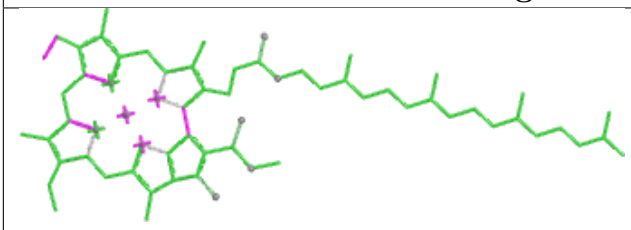
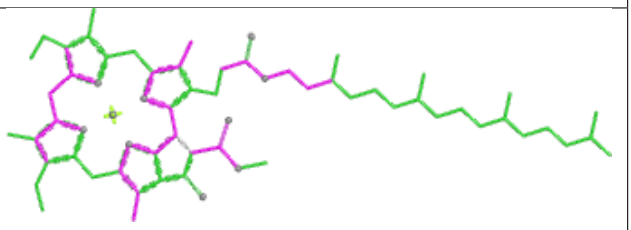


Rings

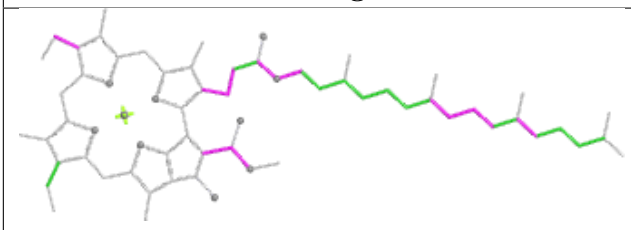
Ligand CLA B1 613



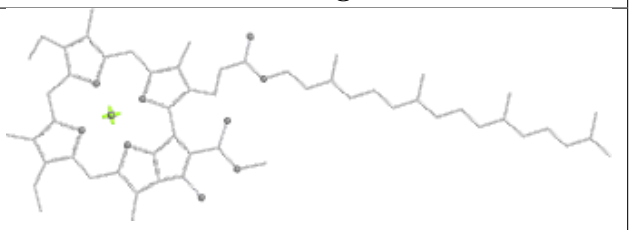
Bond lengths



Bond angles

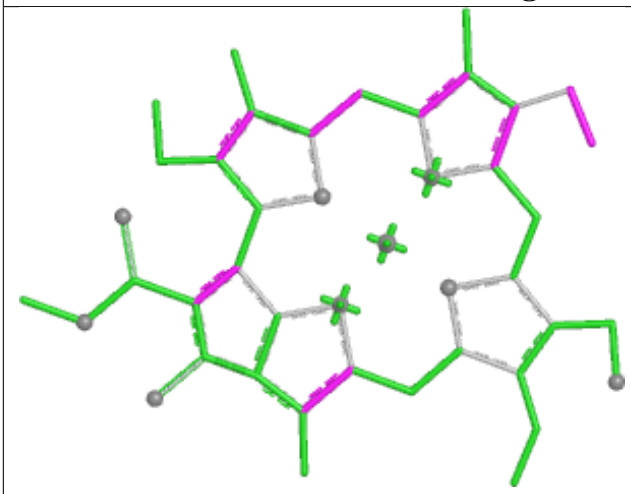


Torsions



Rings

Ligand CHL s1 607



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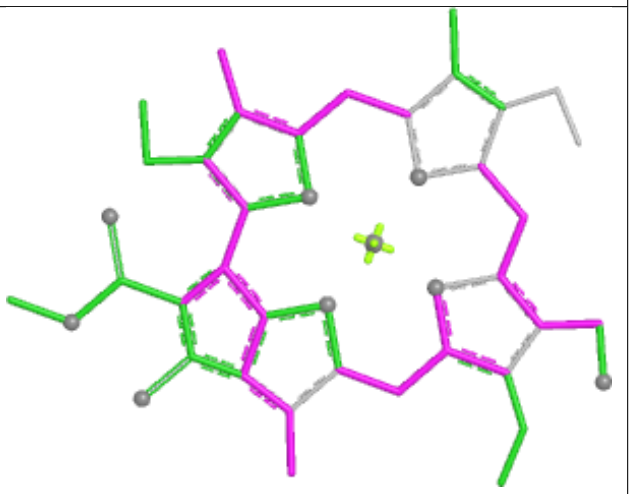
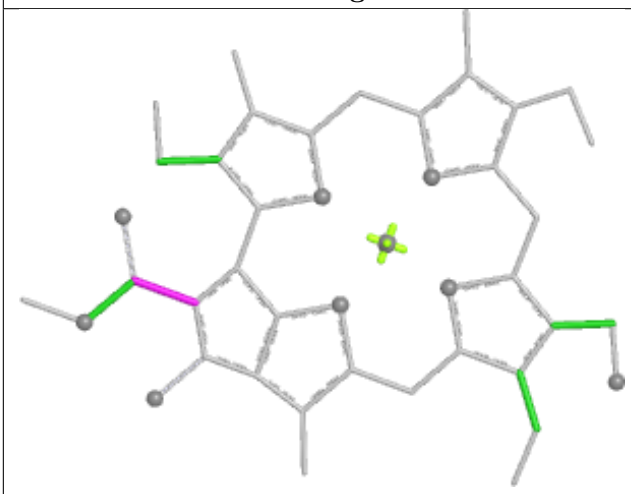
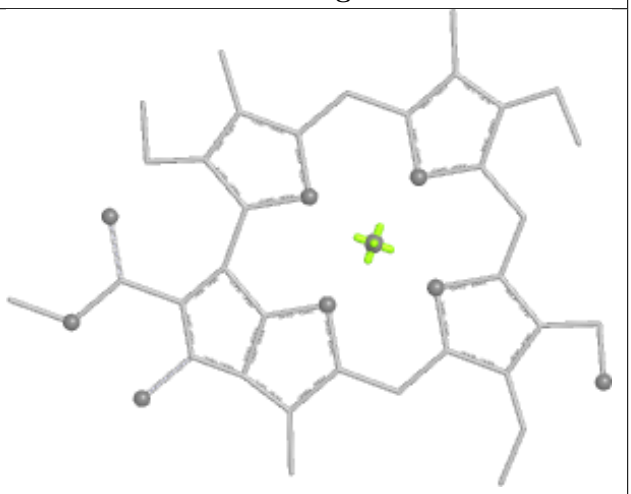


Bond angles

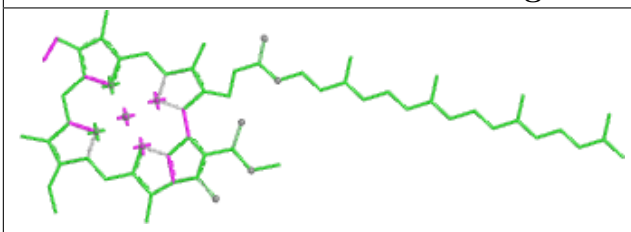


Torsions



Rings

Ligand CLA B 605



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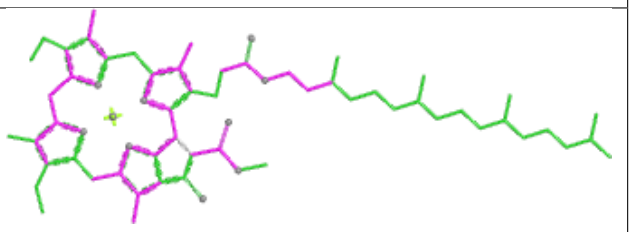
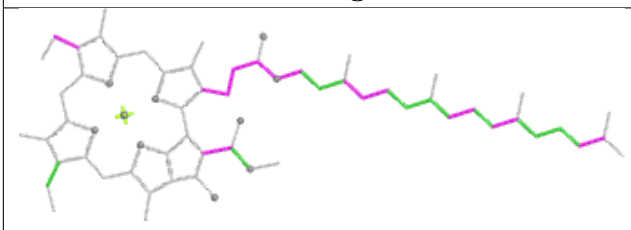


Bond angles



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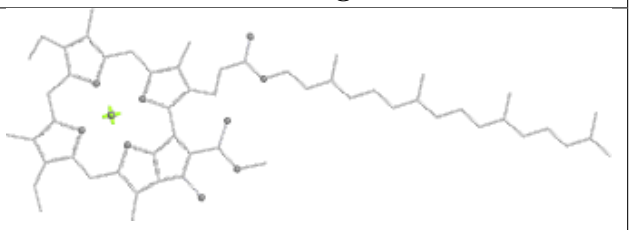
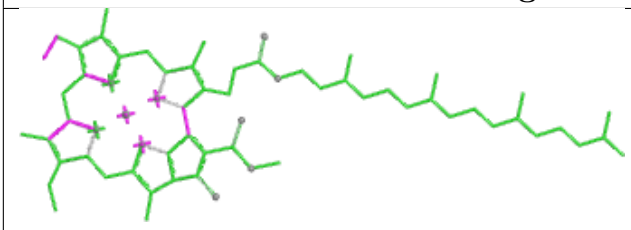


Rings

Ligand CLA y1 602



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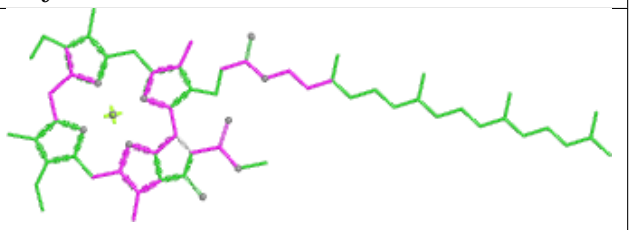
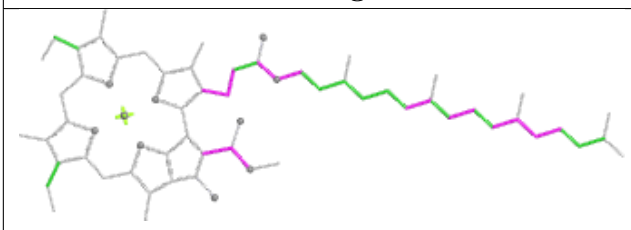


Bond angles



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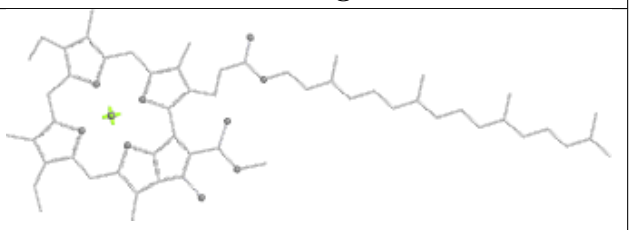
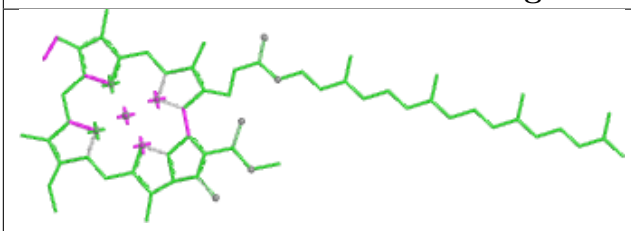


Rings

Ligand CLA B 616



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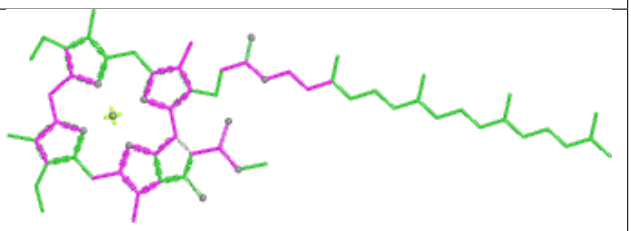
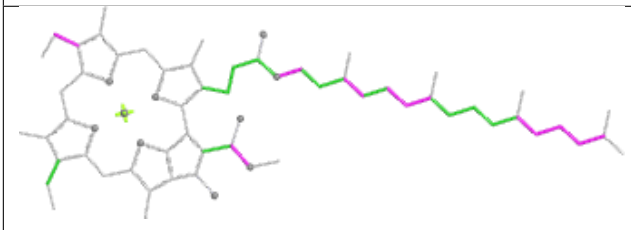
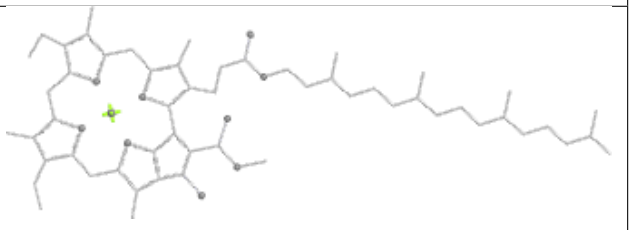


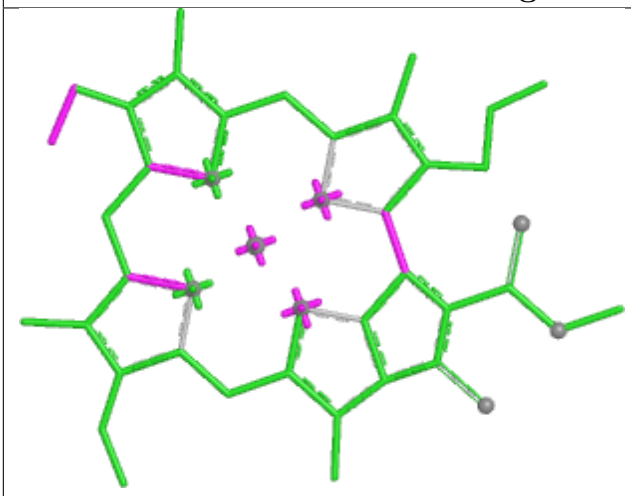
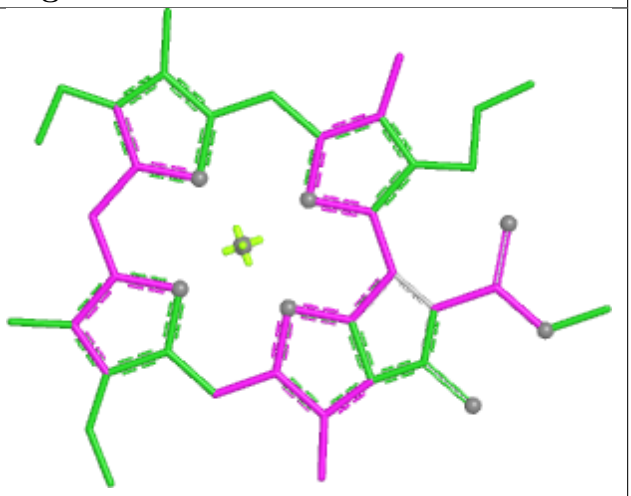
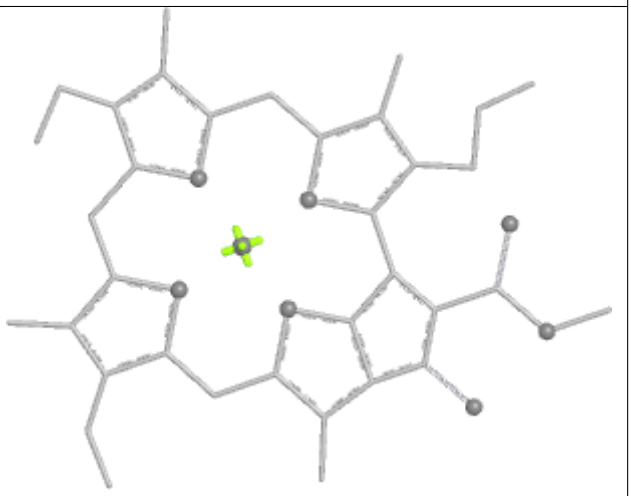
Bond angles

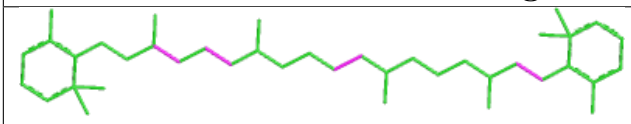
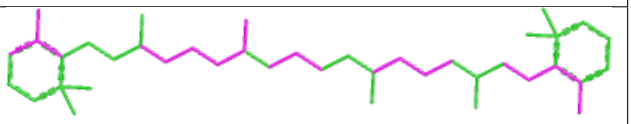
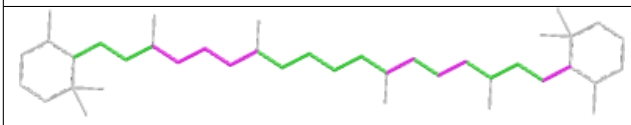
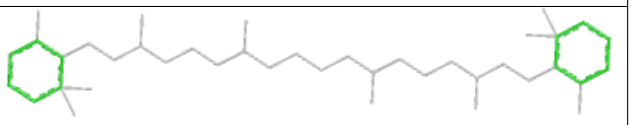


Torsions

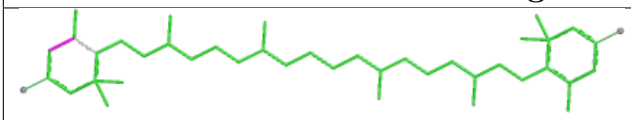


Rings

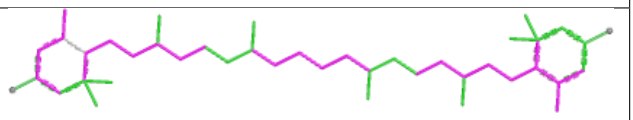
Ligand CLA g1 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand BCR A 411	
	
Bond lengths	Bond angles
	
Torsions	Rings

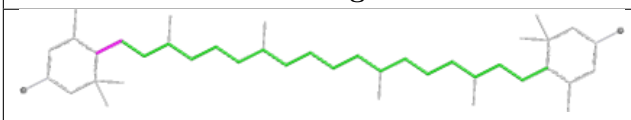
Ligand LUT S 621



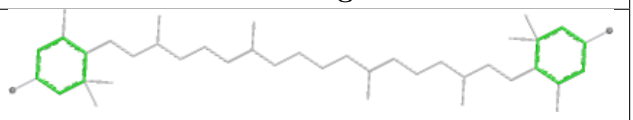
Bond lengths



Bond angles

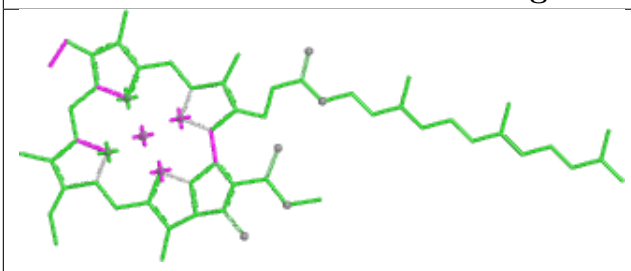


Torsions



Rings

Ligand CLA r 609



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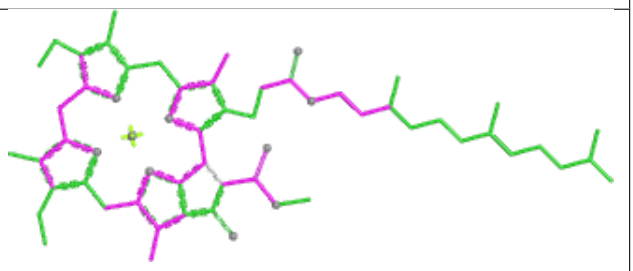
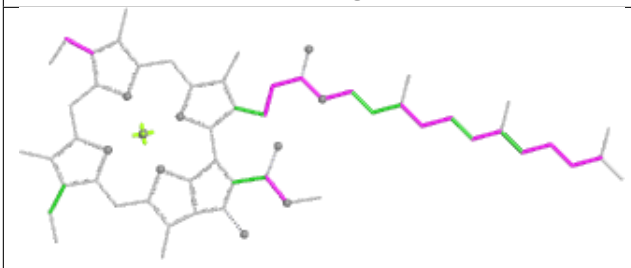


Bond angles



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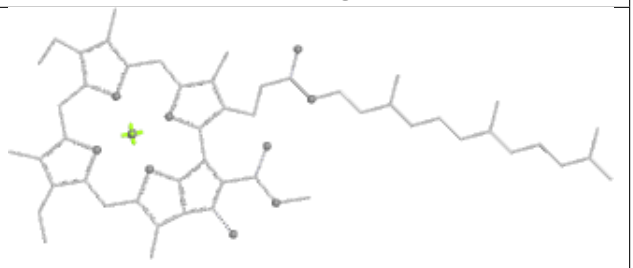
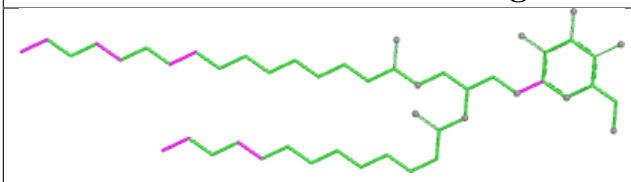
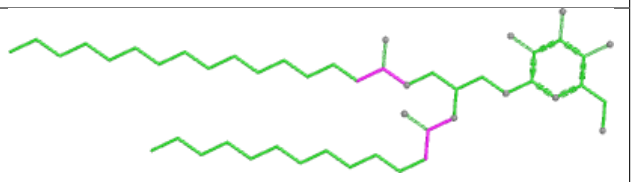


Rings

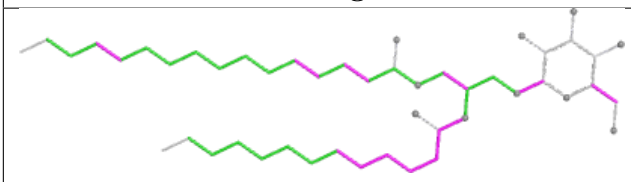
Ligand LMG H1 102



Bond lengths



Bond angles



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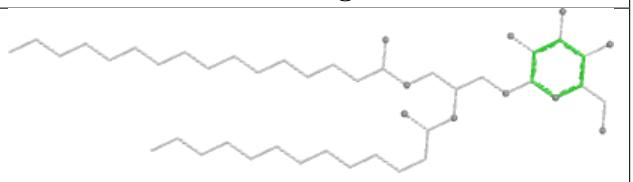
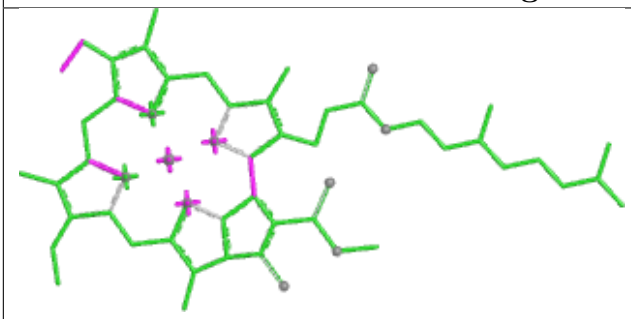
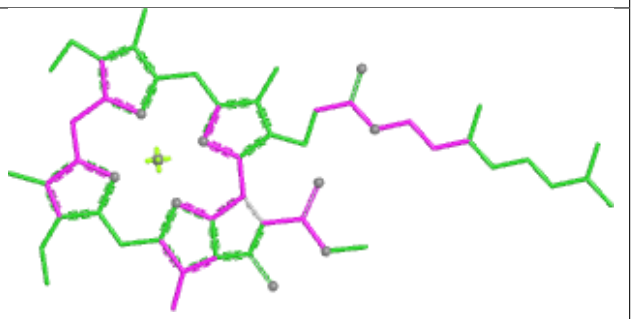


Rings

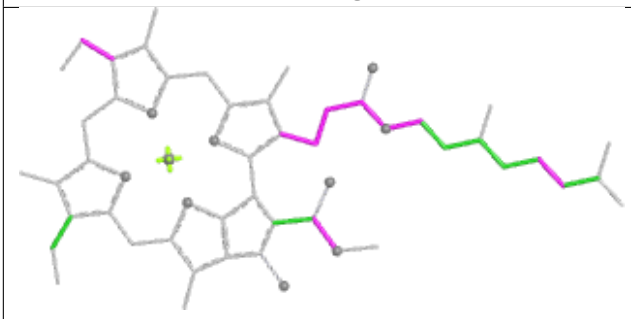
Ligand CLA s1 614



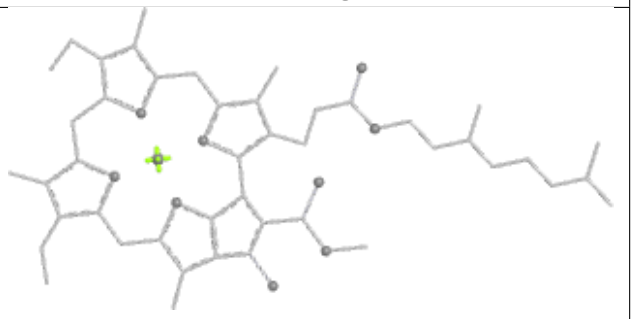
Bond lengths



Bond angles

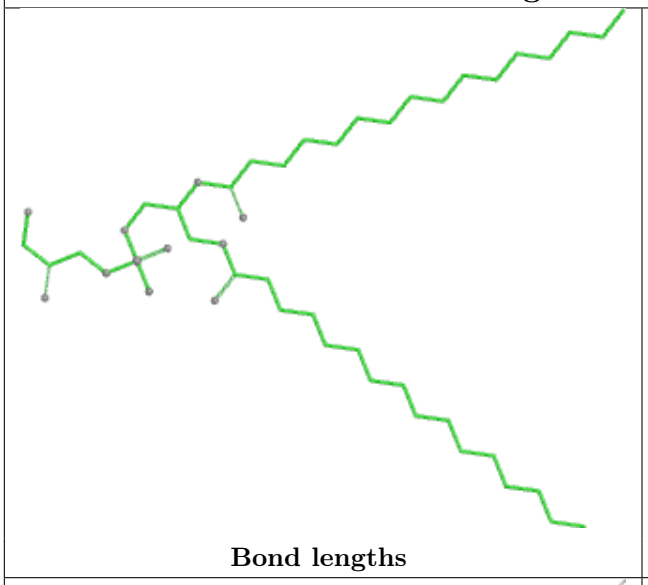


Torsions



Rings

Ligand LHG Y 624



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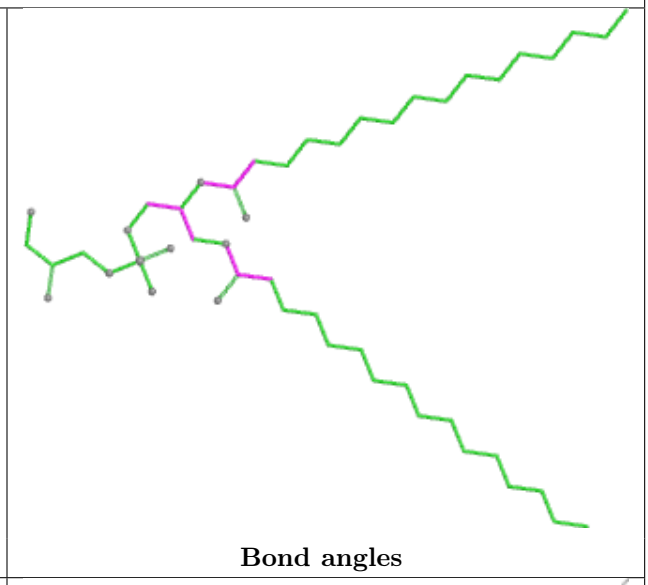
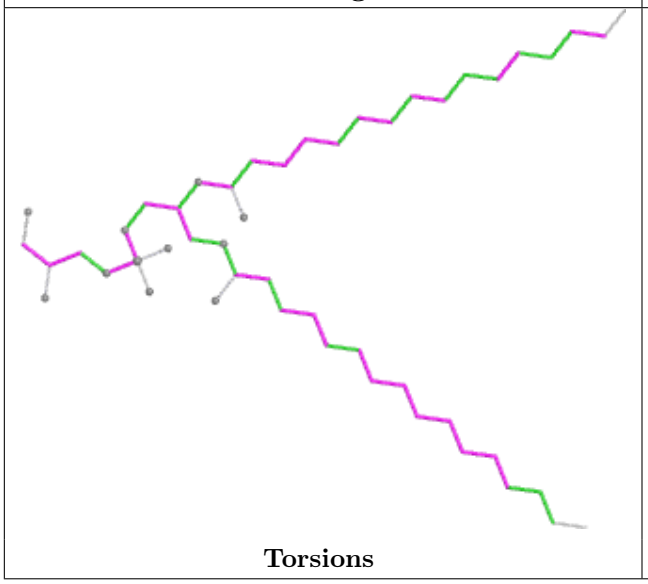


Bond angles



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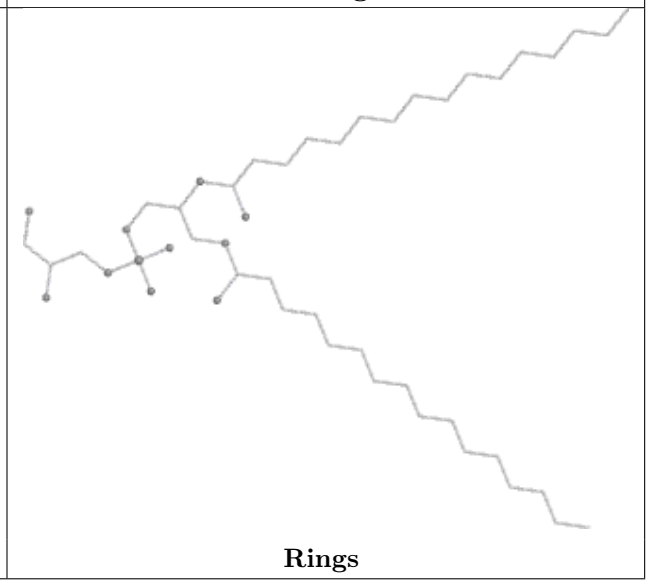
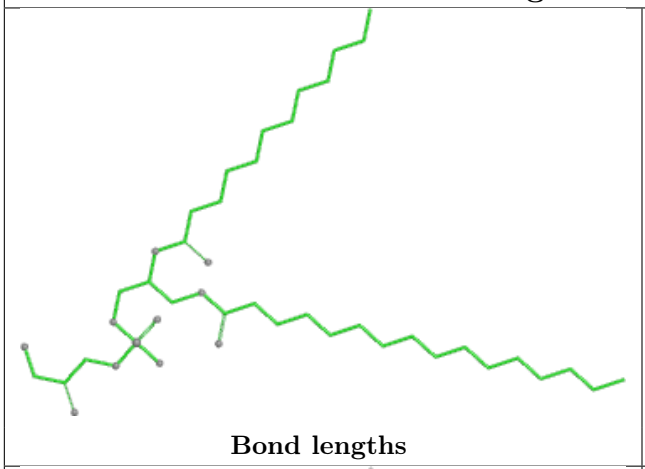


Rings

Ligand LHG S 624



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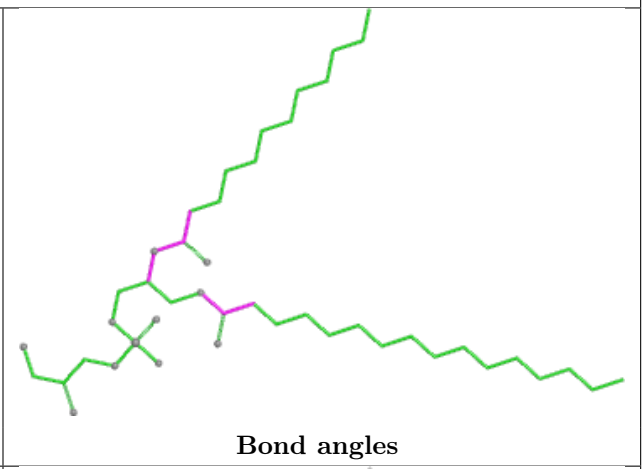
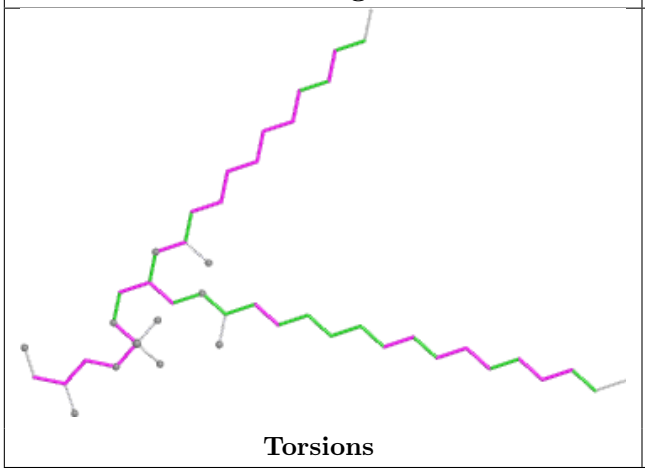
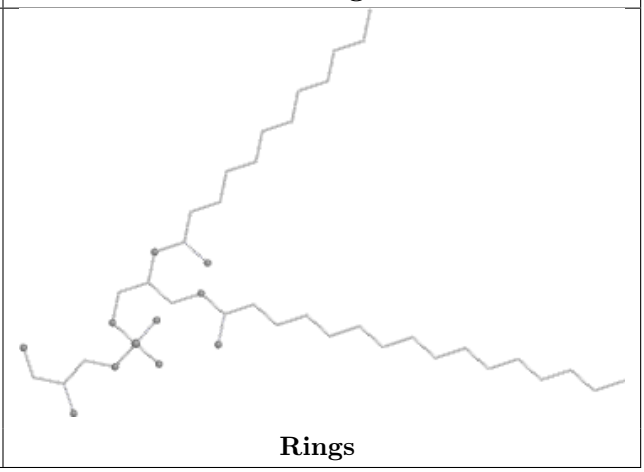


Bond angles

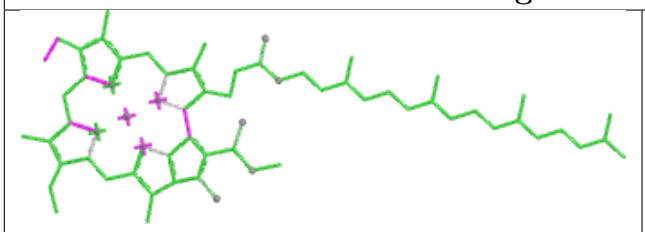


Torsions

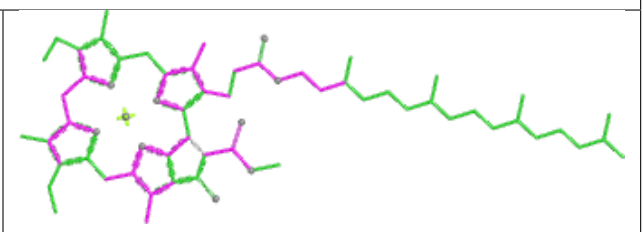


Rings

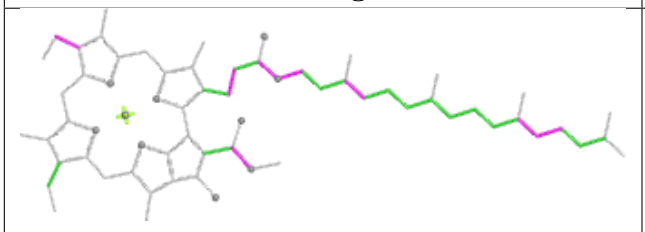
Ligand CLA G1 613



Bond lengths



Bond angles



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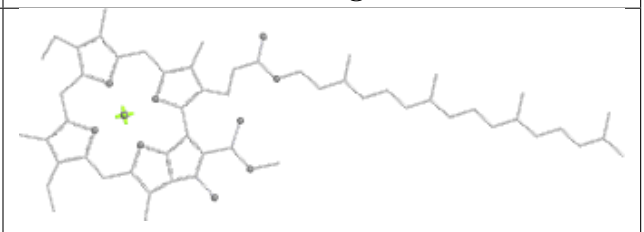
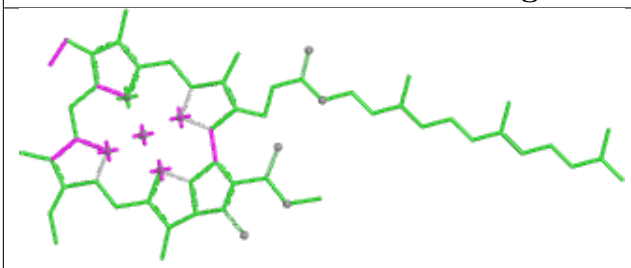


Rings

Ligand CLA s1 609



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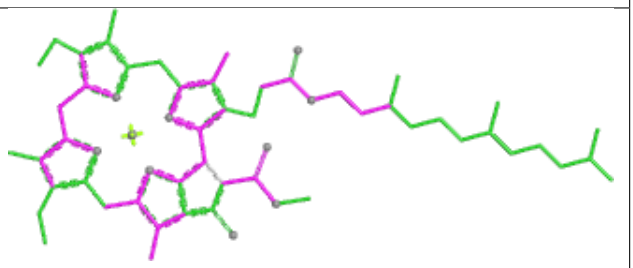
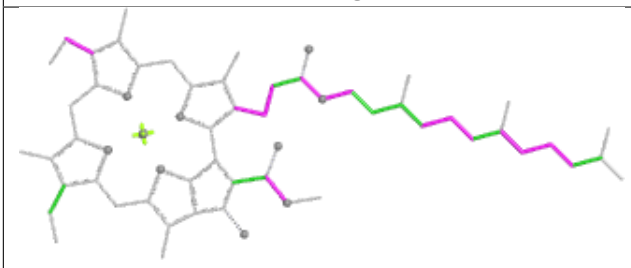


Bond angles



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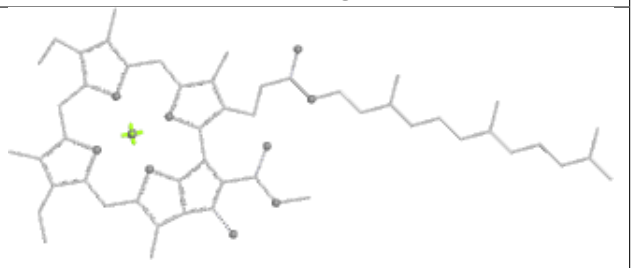
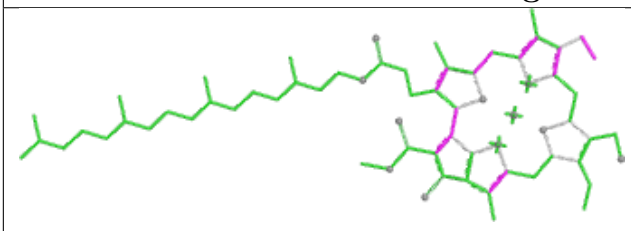


Rings

Ligand CHL N 609



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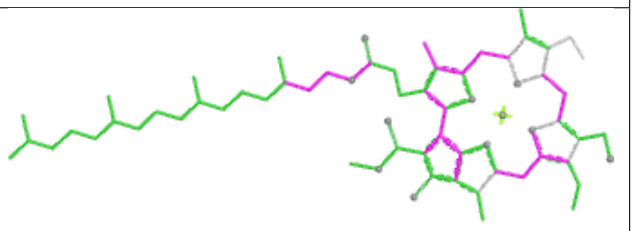
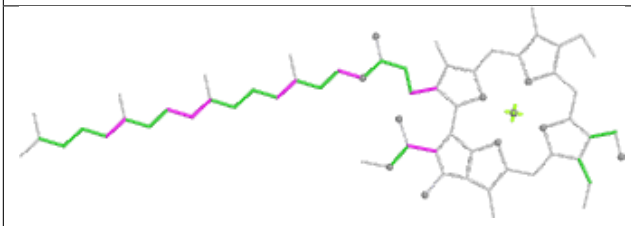


Bond angles



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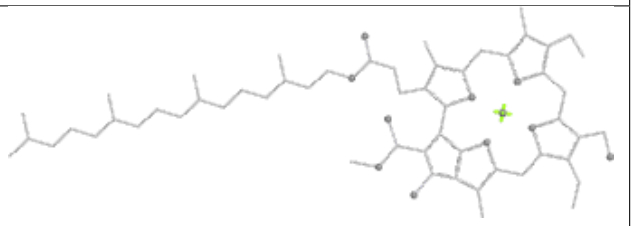
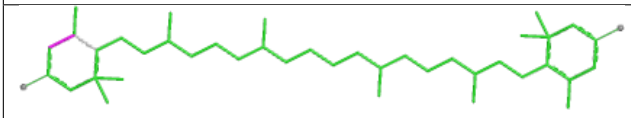
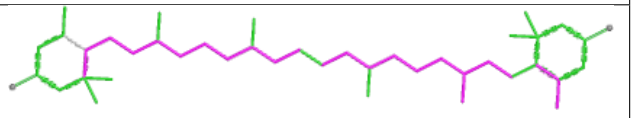


Rings

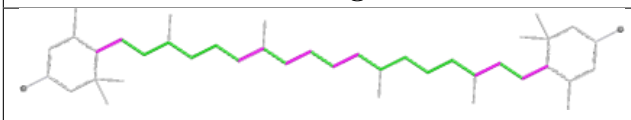
Ligand LUT R 620



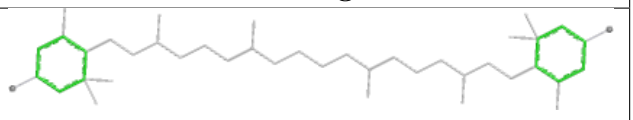
Bond lengths



Bond angles

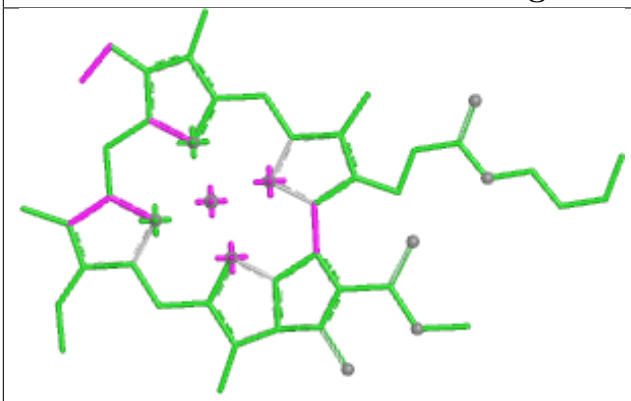


Torsions



Rings

Ligand CLA g 614



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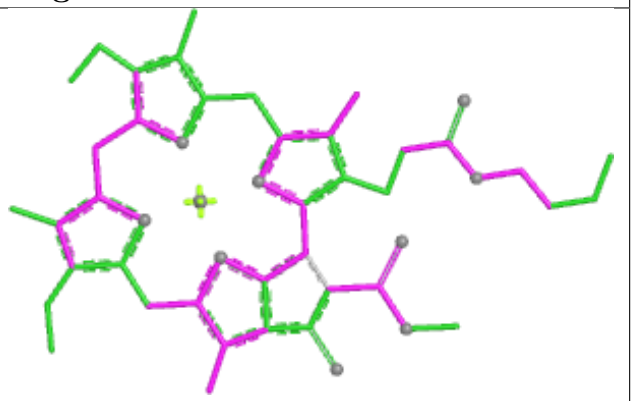
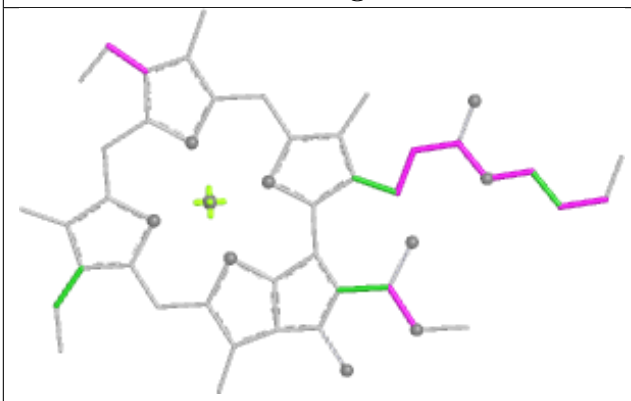


Bond angles



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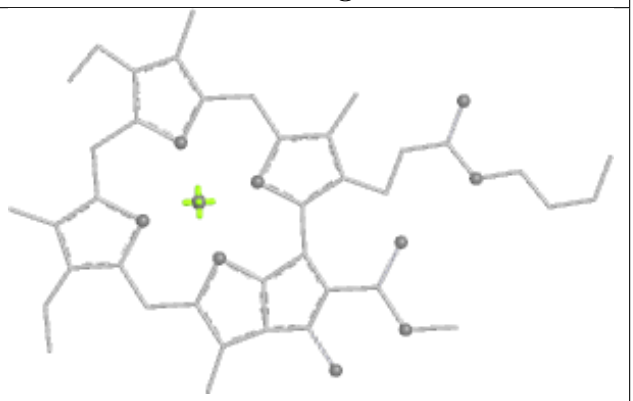
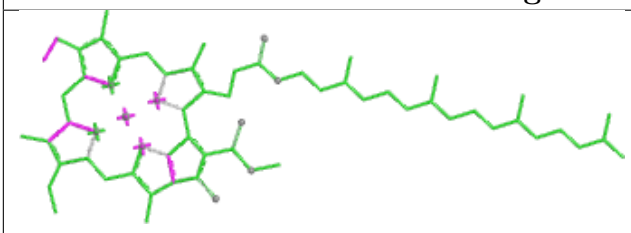


Rings

Ligand CLA Y 602



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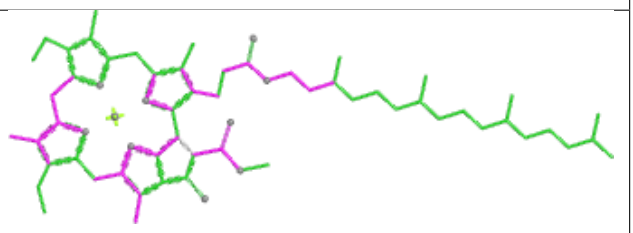
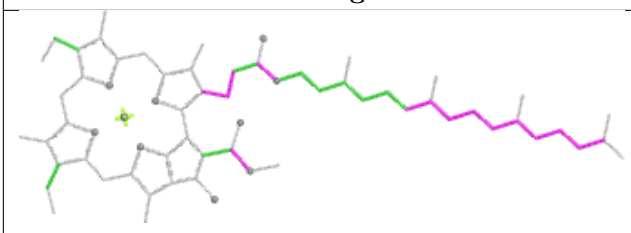


Bond angles



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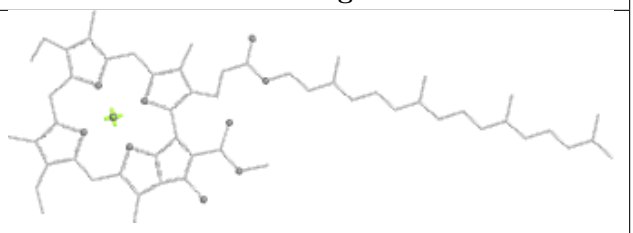
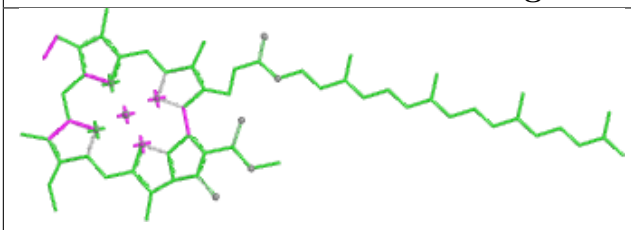
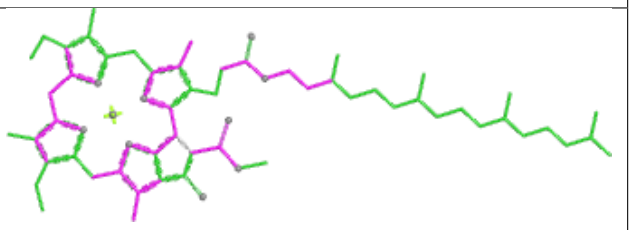
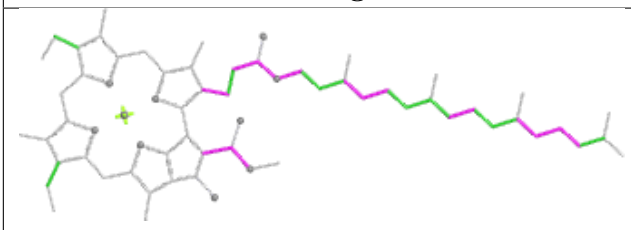
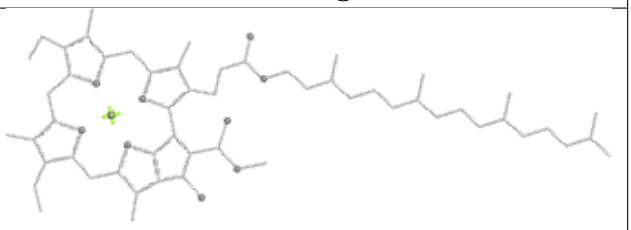
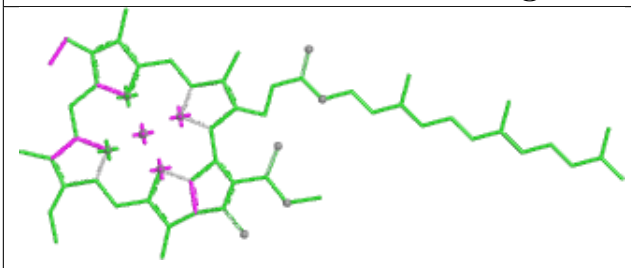
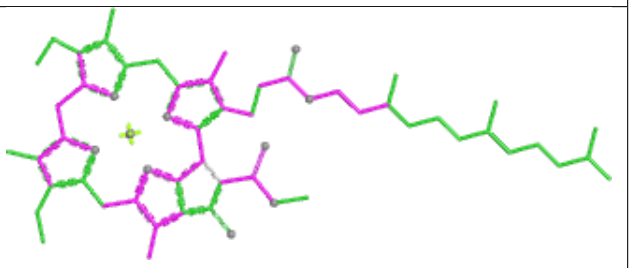
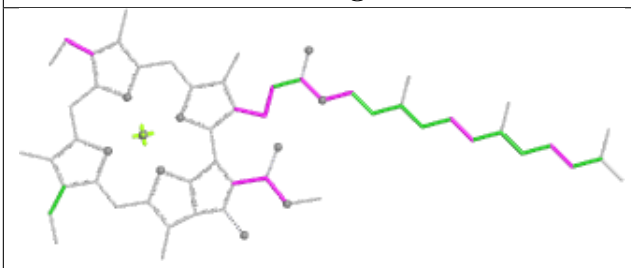
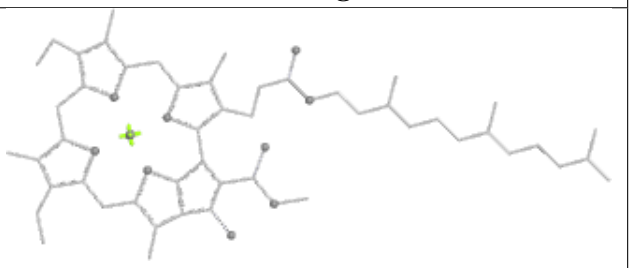
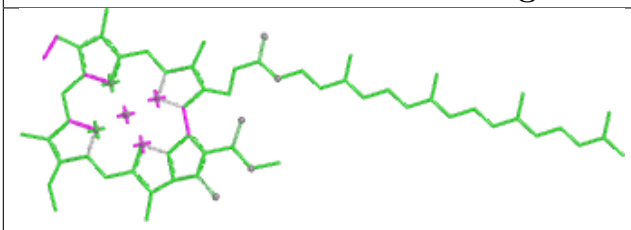


Rings

Ligand CLA B 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA s1 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA y1 610



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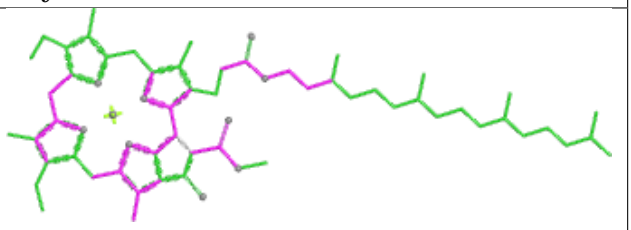
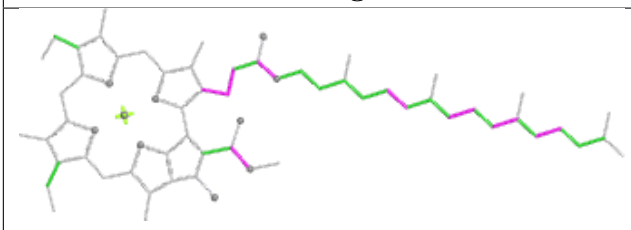
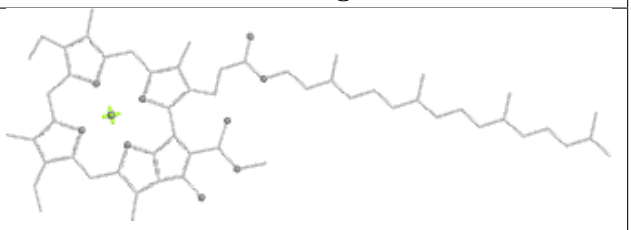


Bond angles

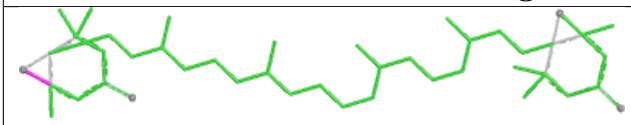


Torsions



Rings

Ligand XAT n1 622



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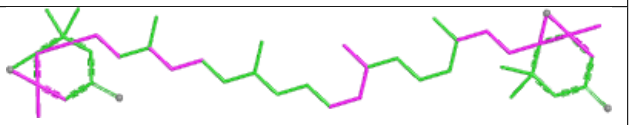
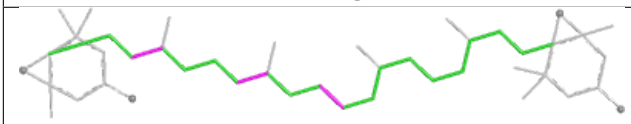
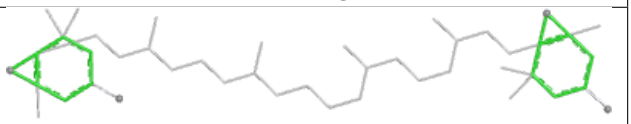


Bond angles

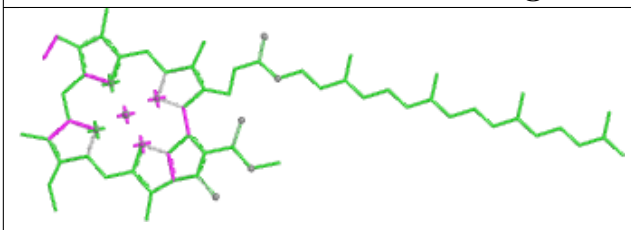


Torsions



Rings

Ligand CLA C 511



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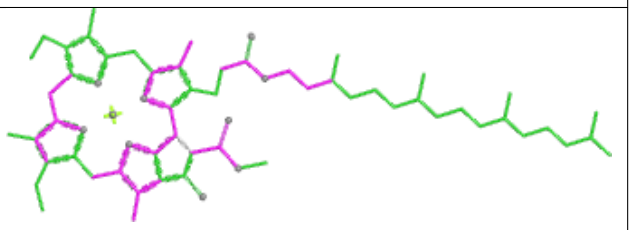
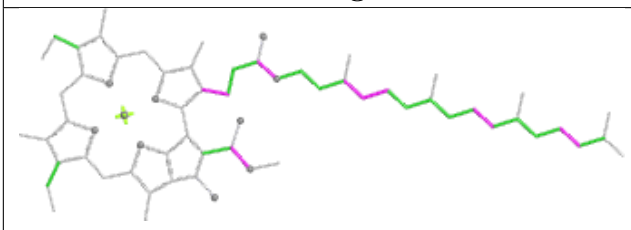
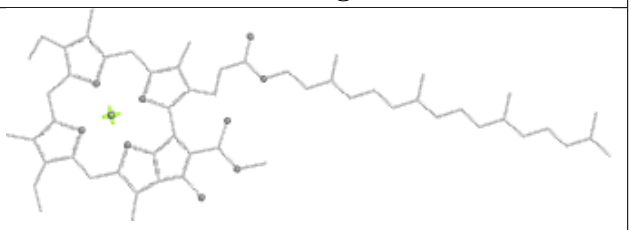


Bond angles

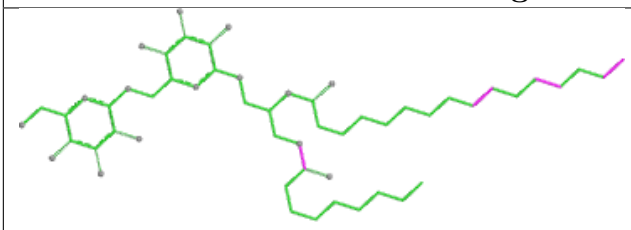


Torsions

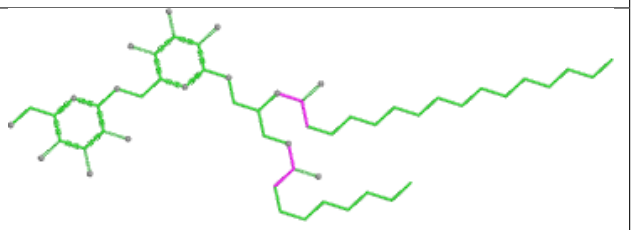


Rings

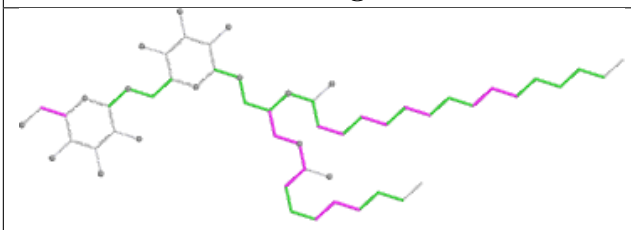
Ligand DGD C1 518



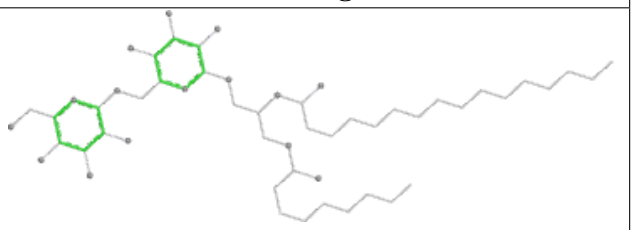
Bond lengths



Bond angles

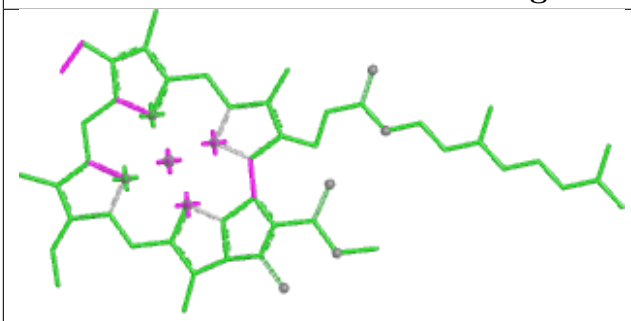


Torsions

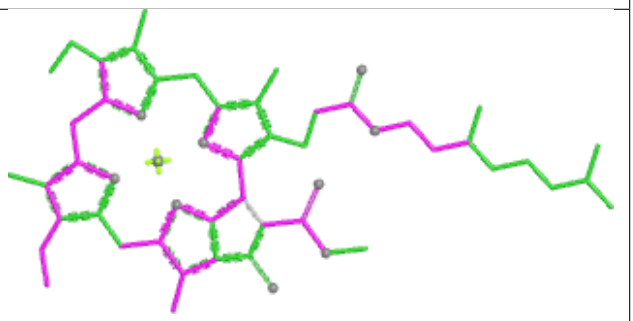


Rings

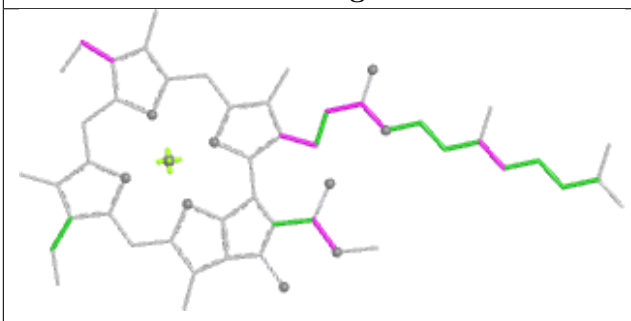
Ligand CLA s 614



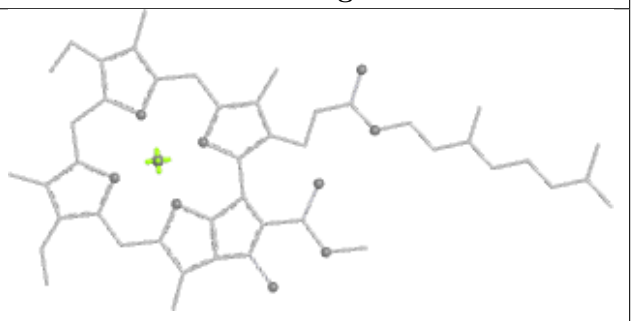
Bond lengths



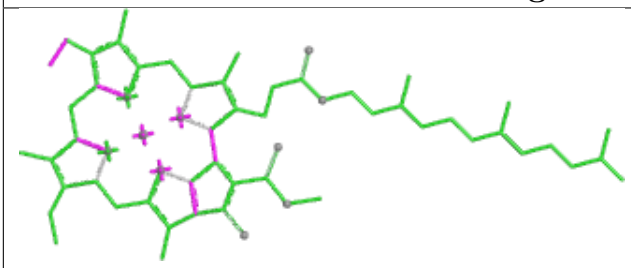
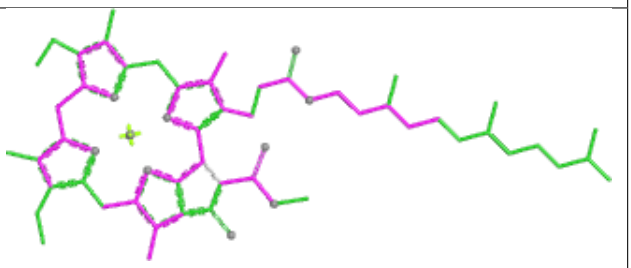
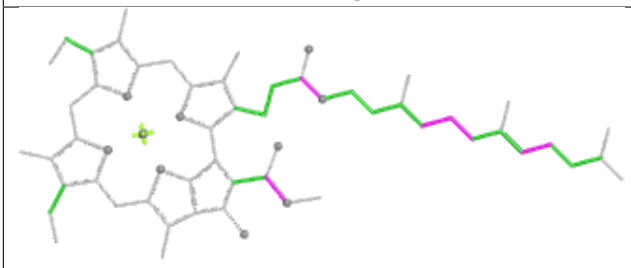
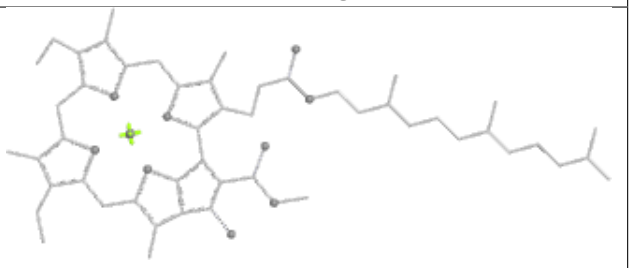
Bond angles

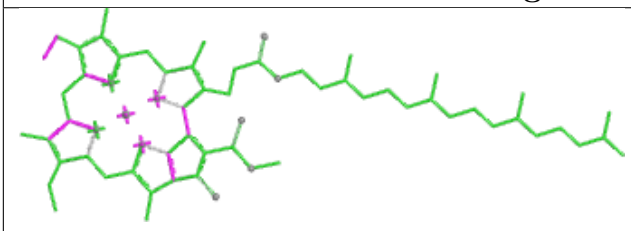
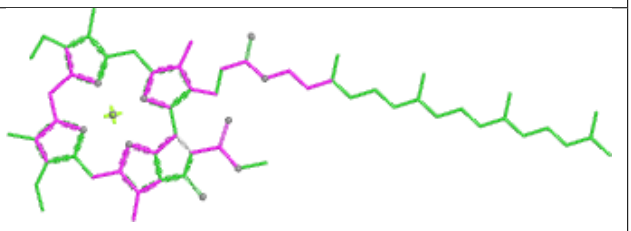
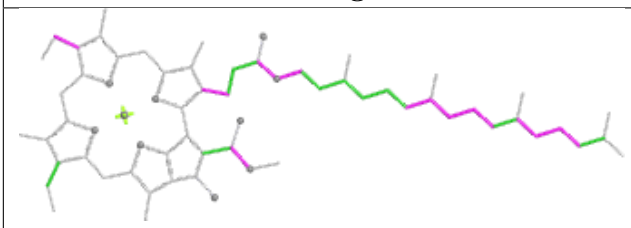
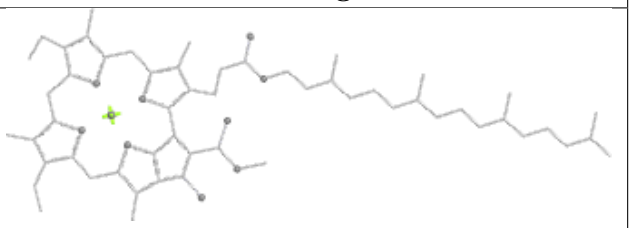


Torsions

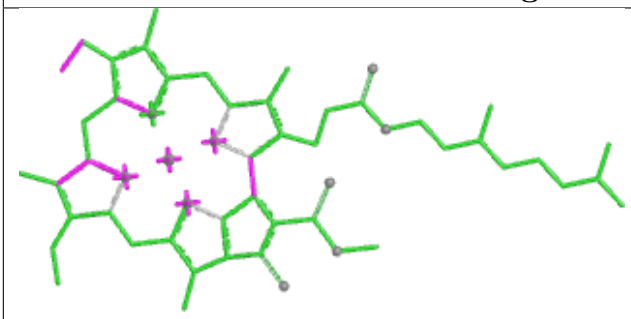


Rings

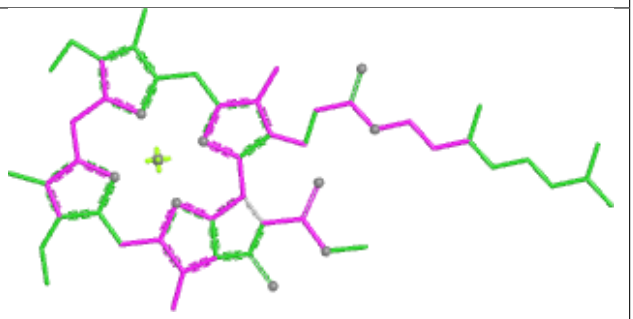
Ligand CLA a 410	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA Y 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

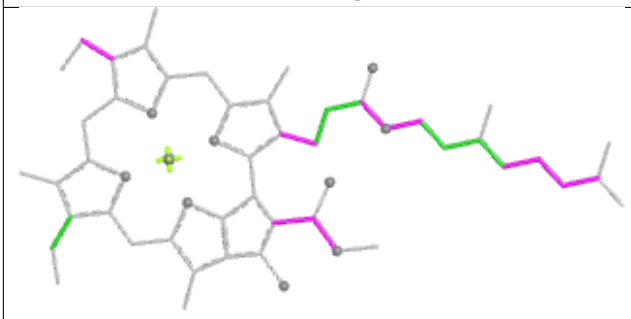
Ligand CLA s1 604



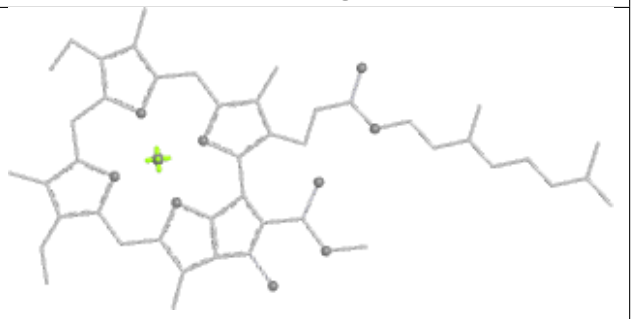
Bond lengths



Bond angles

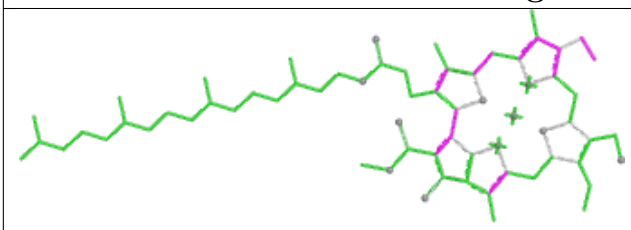


Torsions



Rings

Ligand CHL n 605



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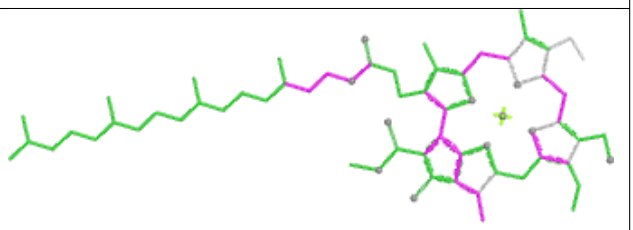
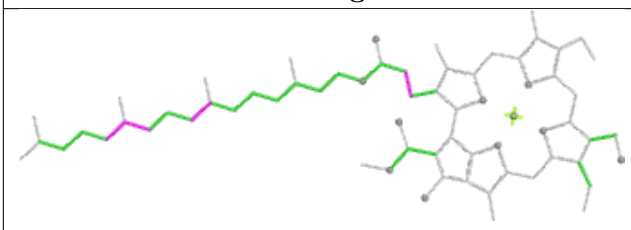


Bond angles



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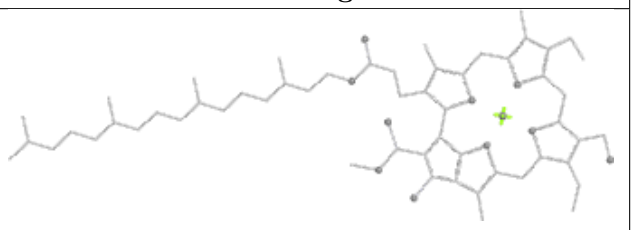
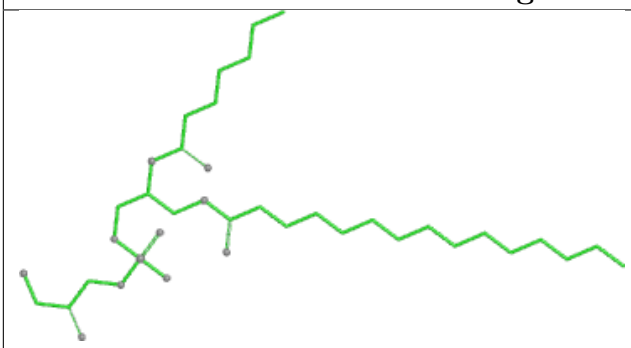


Rings

Ligand LHG d1 410



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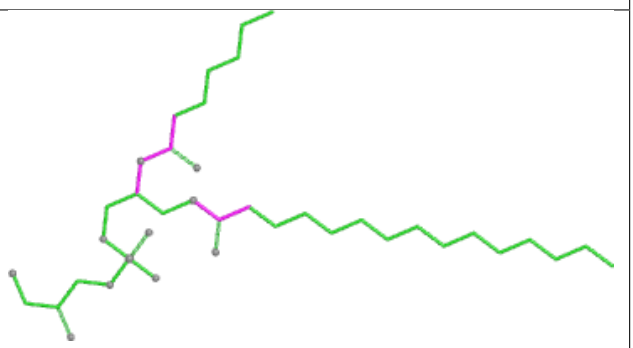
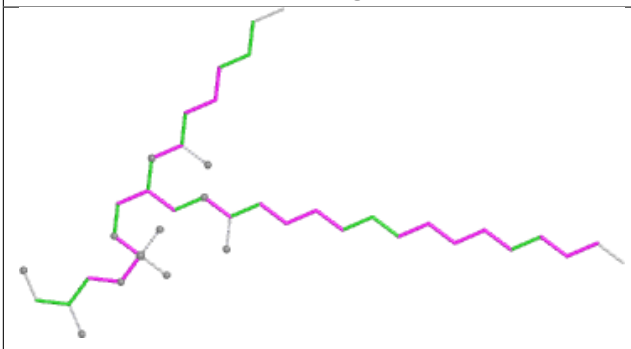


Bond angles



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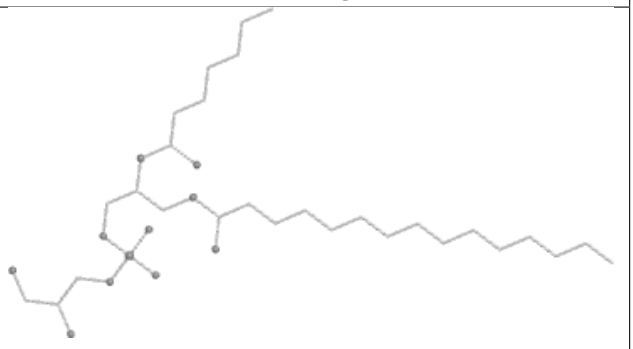
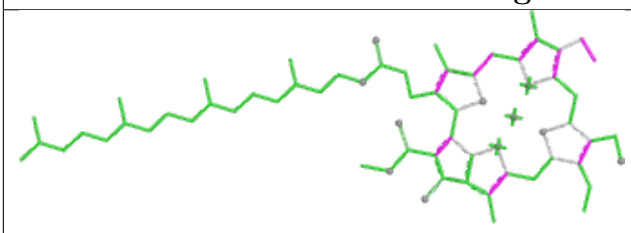


Rings

Ligand CHL N1 609



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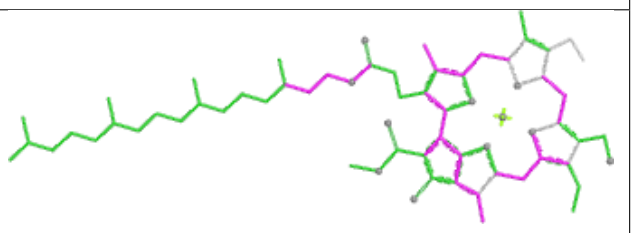
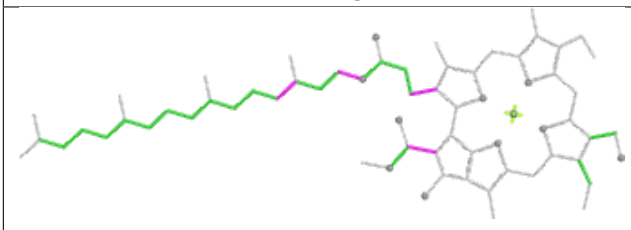


Bond angles



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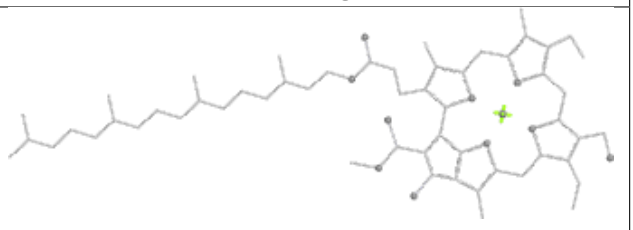
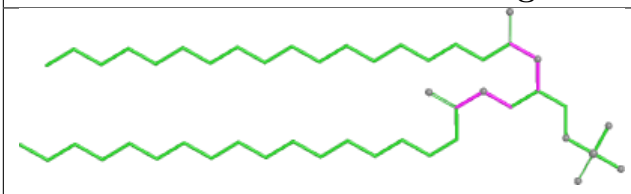
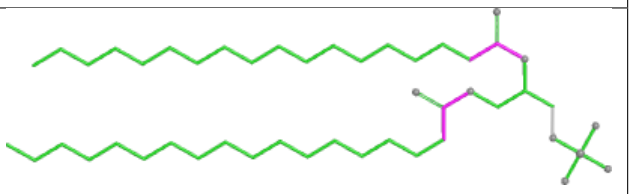
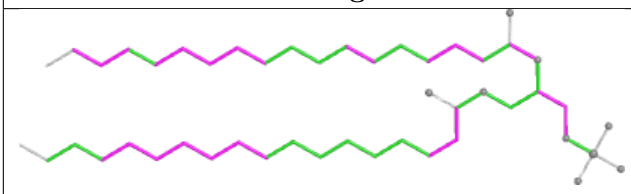
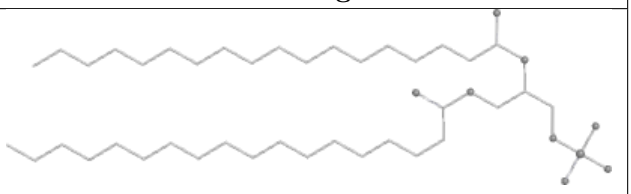


Rings

Ligand 3PH B1 624	
 Bond lengths	 Bond angles
 Torsions	 Rings

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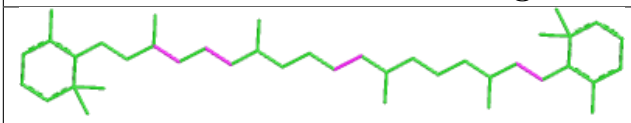
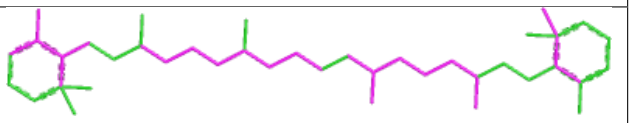
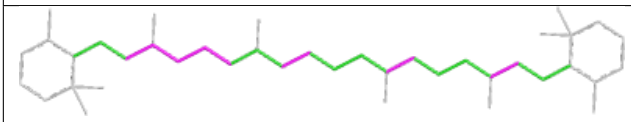
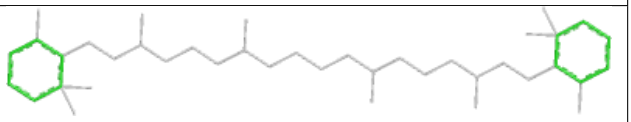
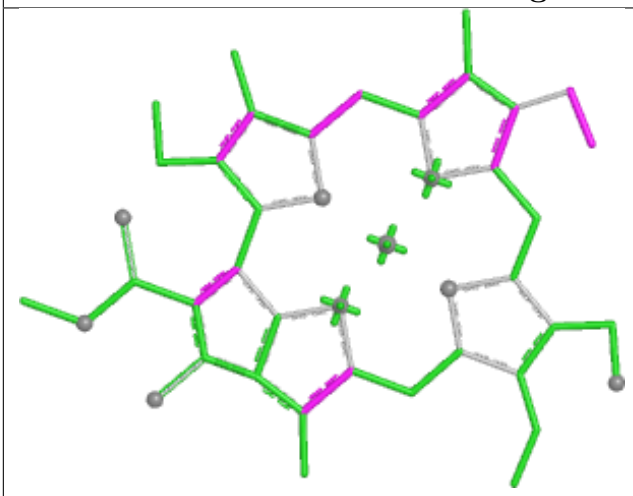
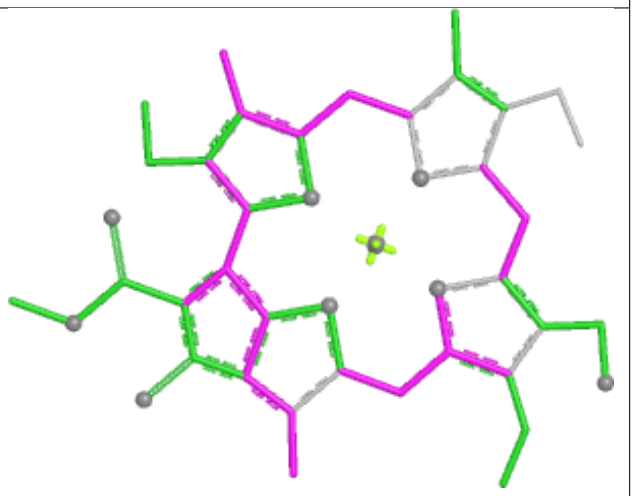
 Bond lengths	 Bond angles
 Torsions	 Rings

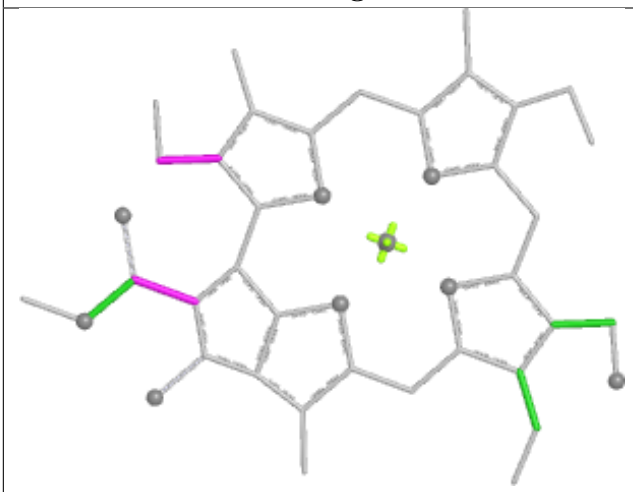
Ligand CHL s 607



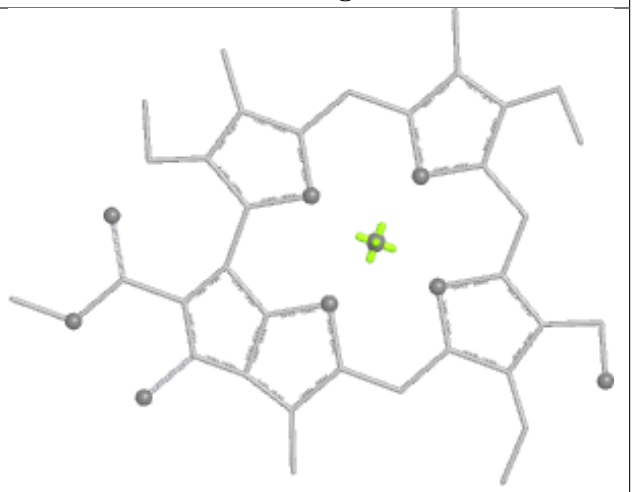
Bond lengths



Bond angles

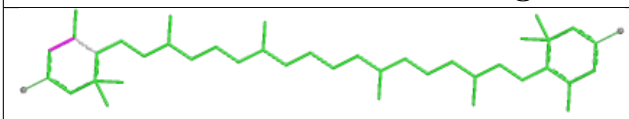


Torsions



Rings

Ligand LUT G1 620



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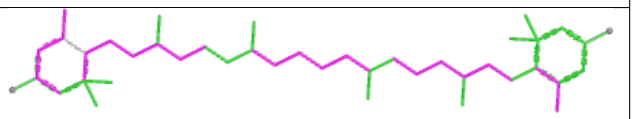
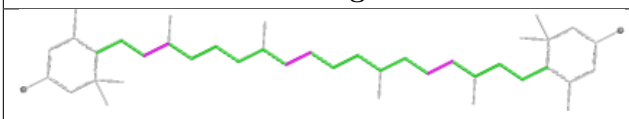


Bond angles



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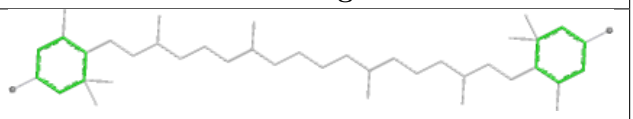
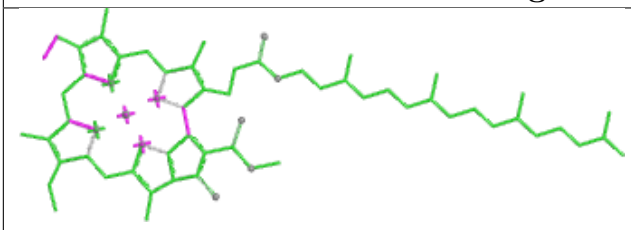


Rings

Ligand CLA a 406



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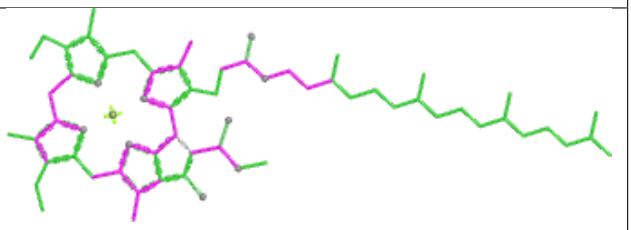
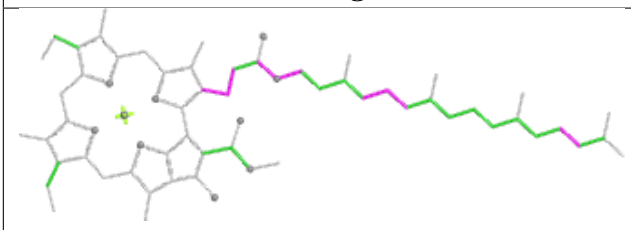


Bond angles



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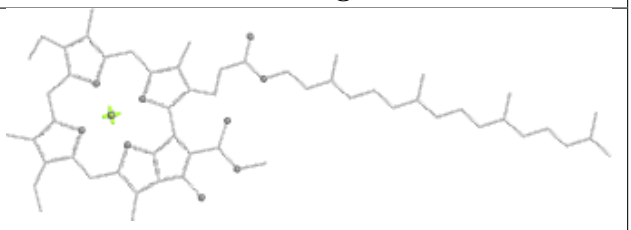
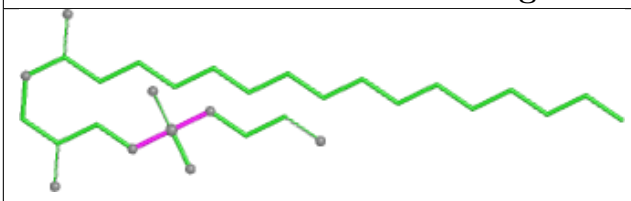


Rings

Ligand LPX S1 625



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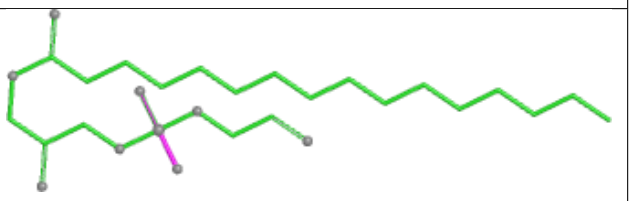
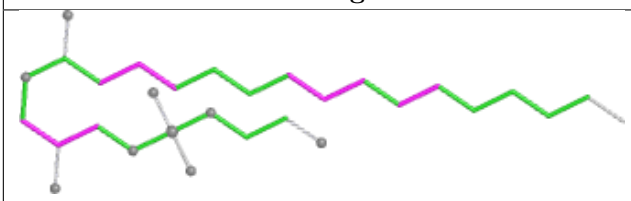


Bond angles



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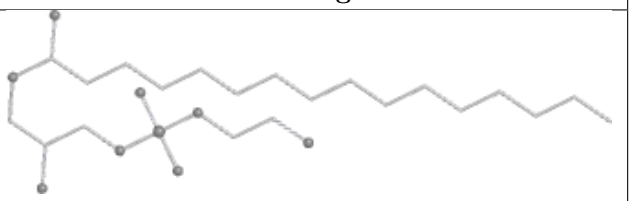
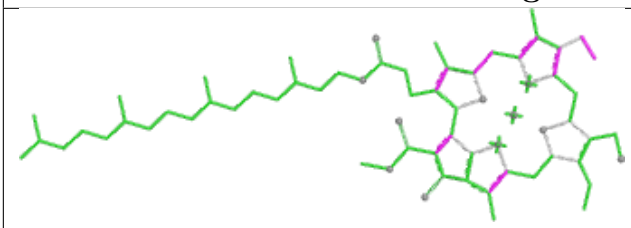


Rings

Ligand CHL N 607



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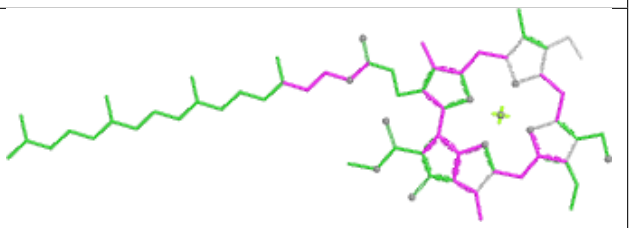
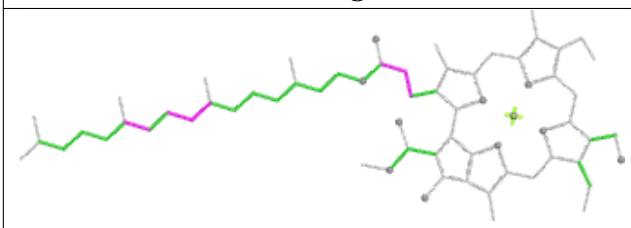
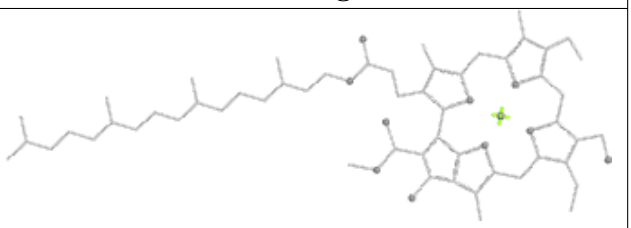


Bond angles

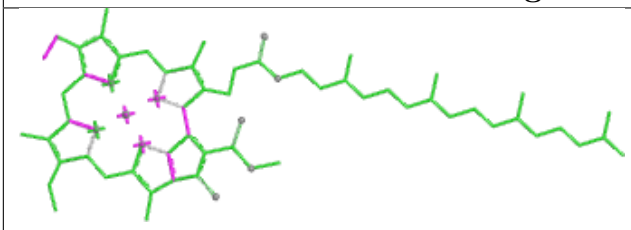


Torsions

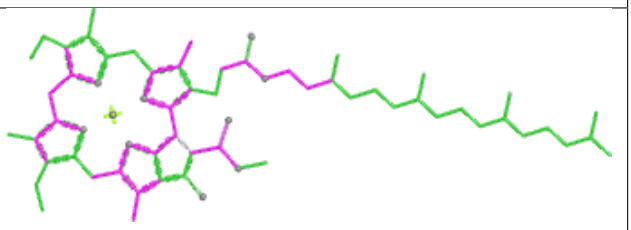


Rings

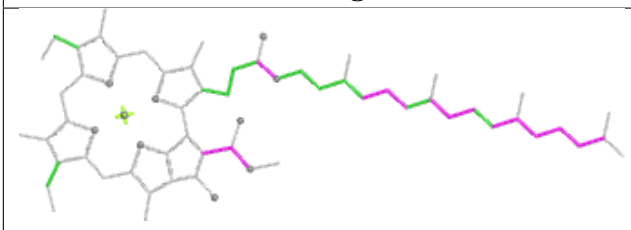
Ligand CLA C 507



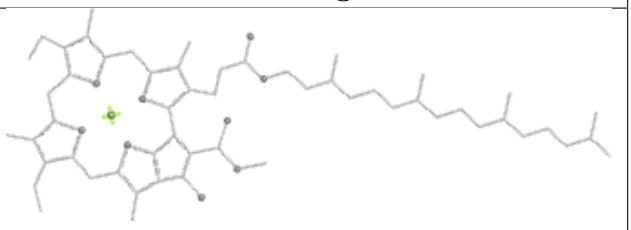
Bond lengths



Bond angles

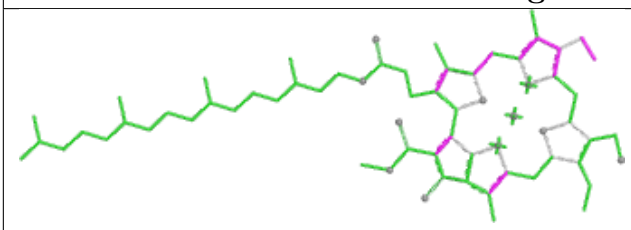


Torsions

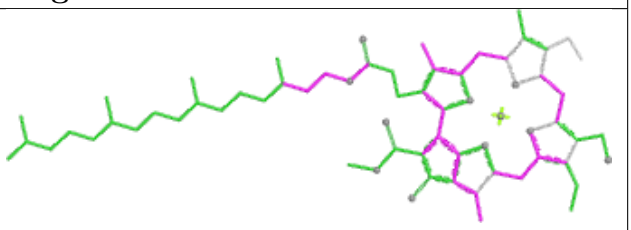


Rings

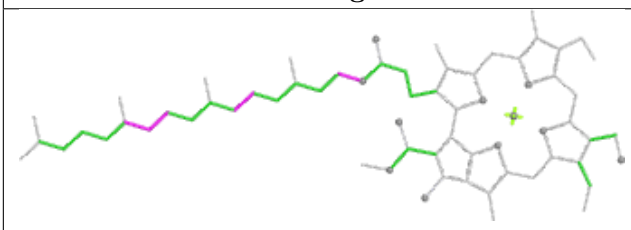
Ligand CHL g 601



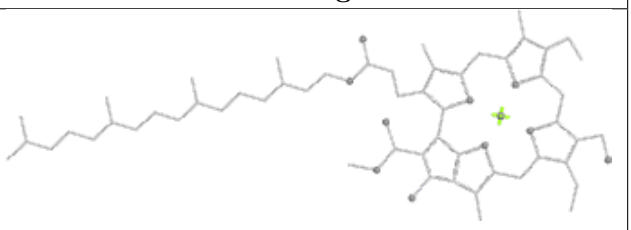
Bond lengths



Bond angles

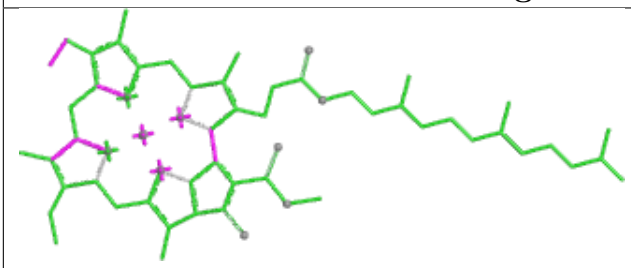


Torsions



Rings

Ligand CLA A1 410



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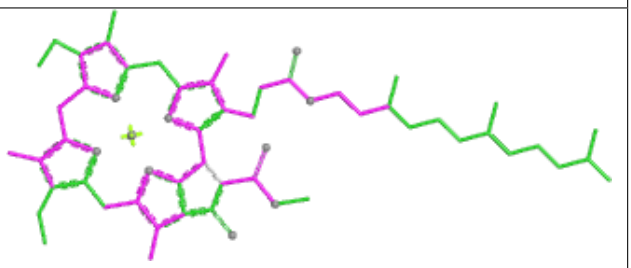
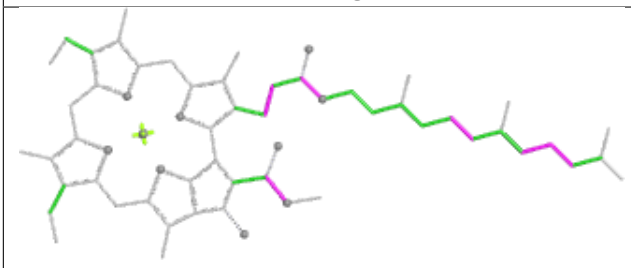


Bond angles



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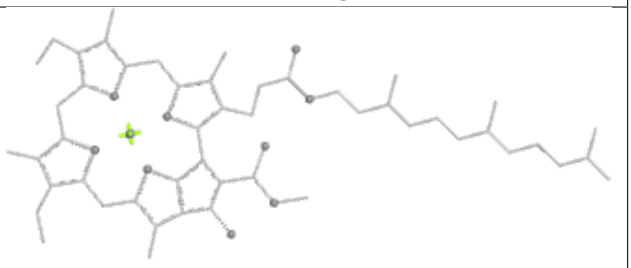
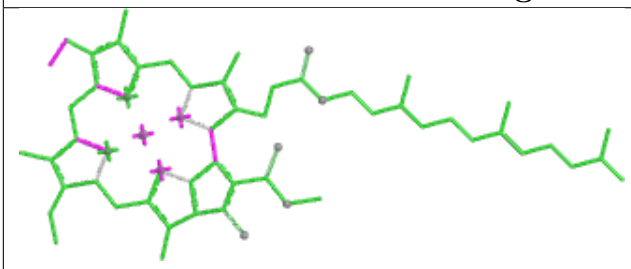


Rings

Ligand CLA R1 602



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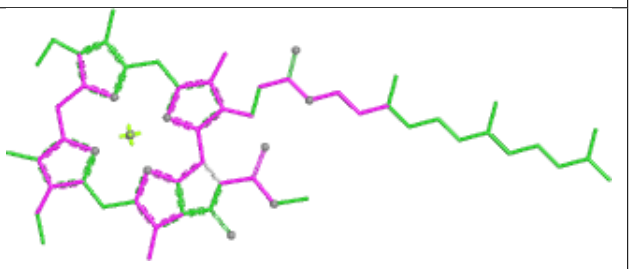
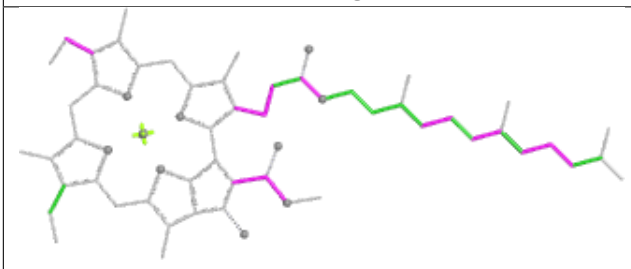


Bond angles



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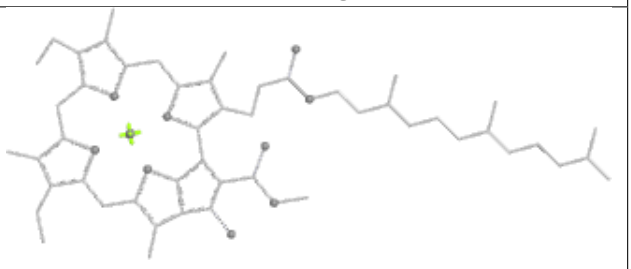
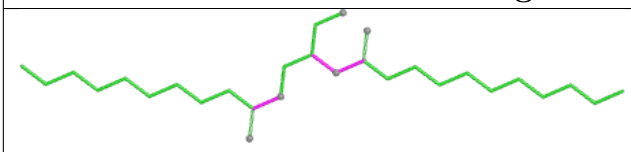


Rings

Ligand DGA J1 101



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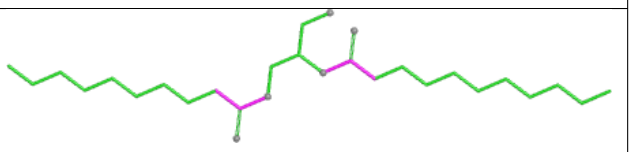
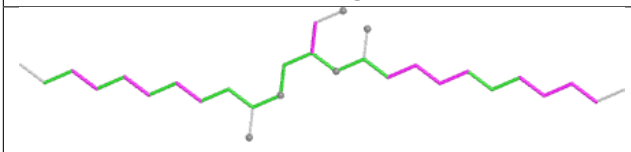


Bond angles



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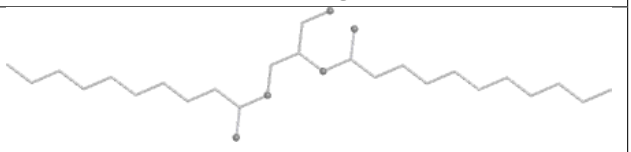
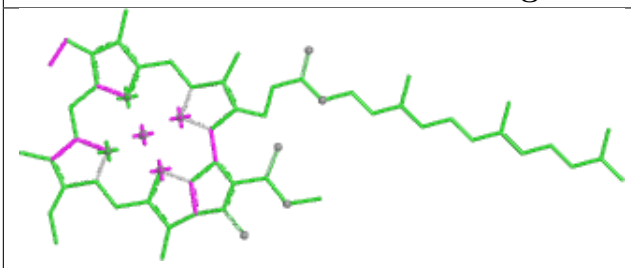


Rings

Ligand CLA r1 610



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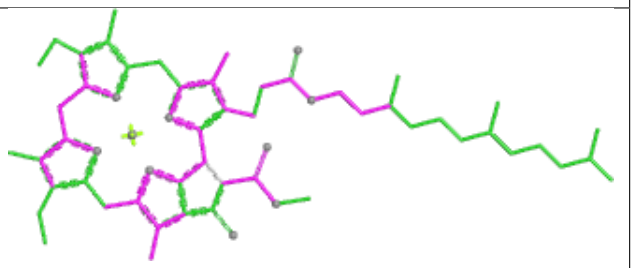

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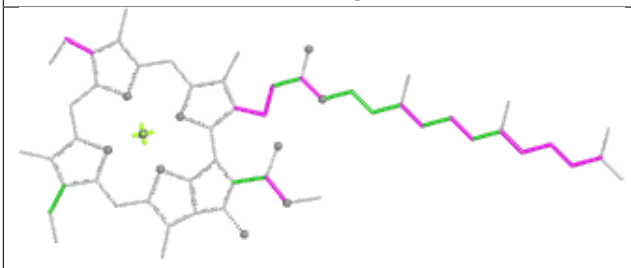

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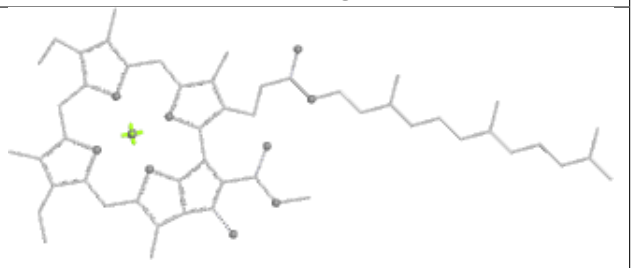
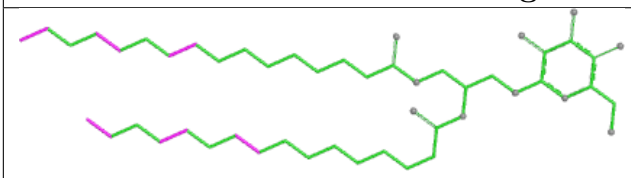


Rings

Ligand LMG C 521



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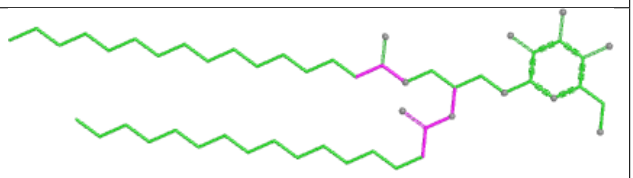
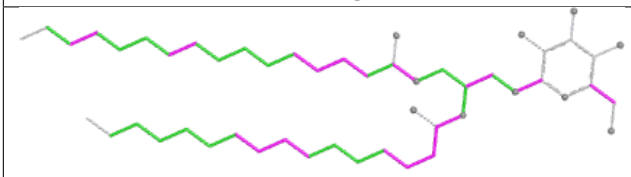


Bond angles



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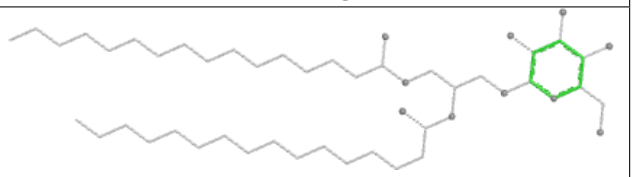
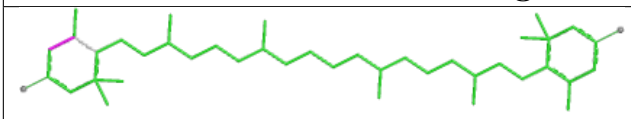


Rings

Ligand LUT G1 621



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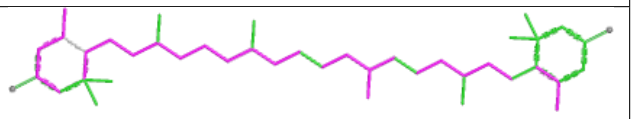
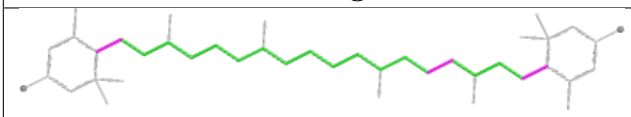


Bond angles



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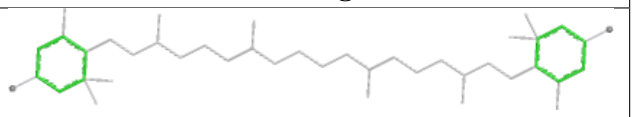
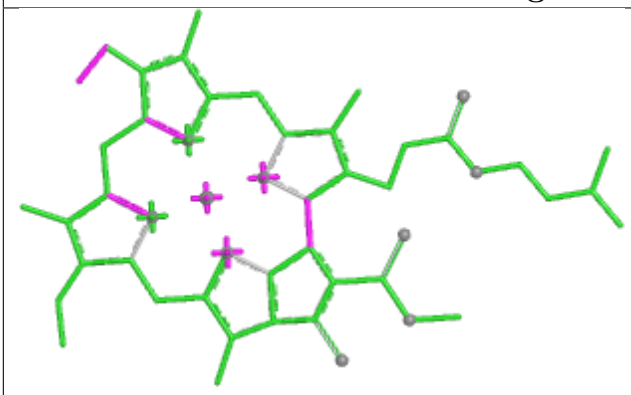


Rings

Ligand CLA S 605



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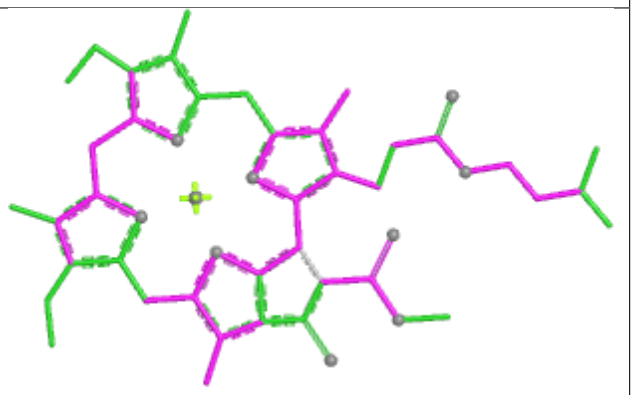

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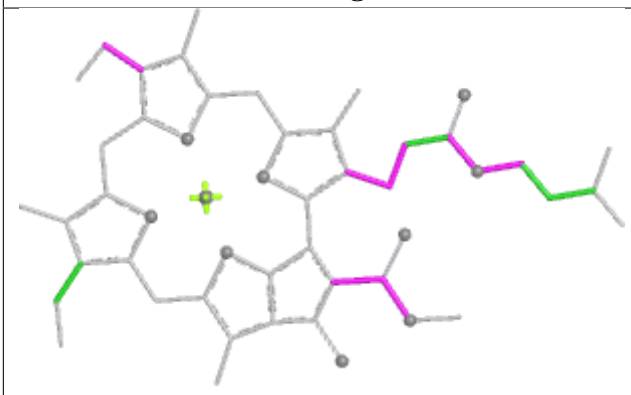

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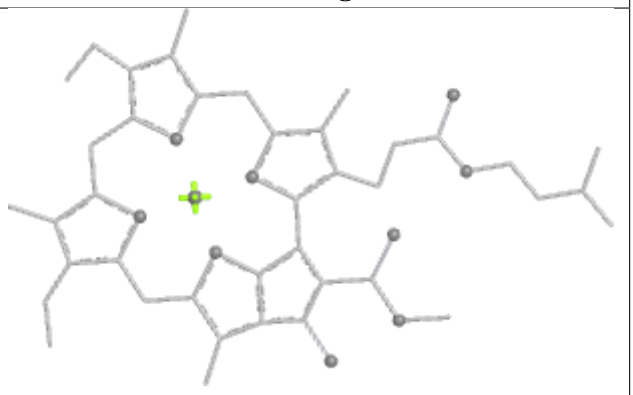
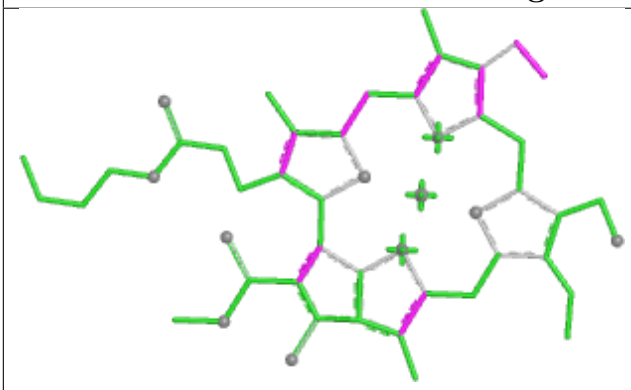


Rings

Ligand CHL g 607



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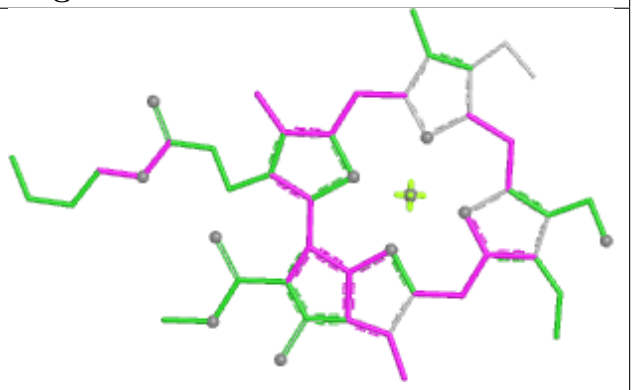
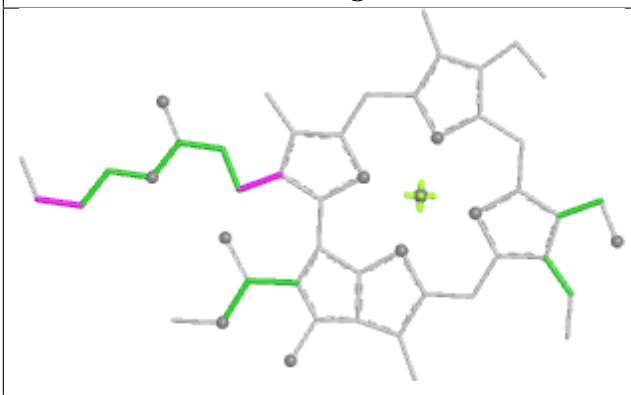


Bond angles



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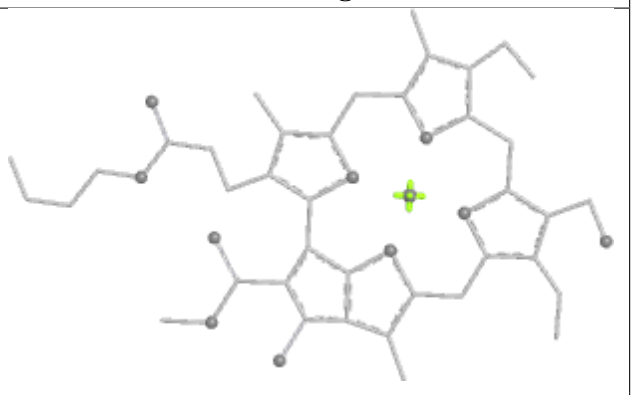
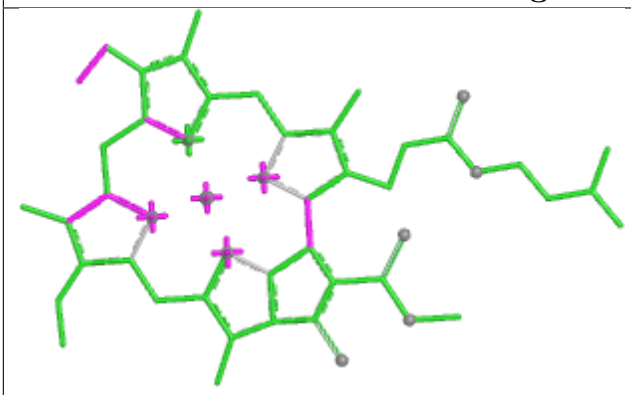


Rings

Ligand CLA s 605



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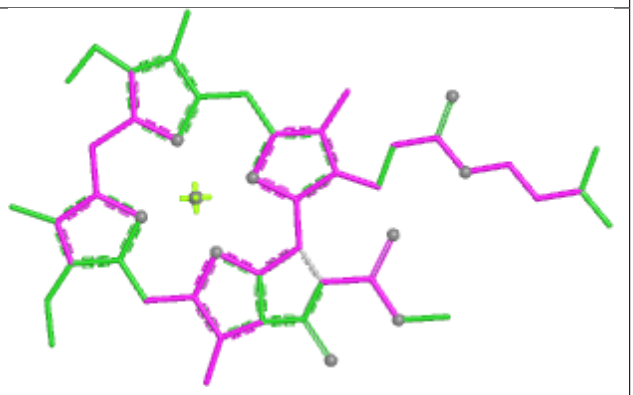

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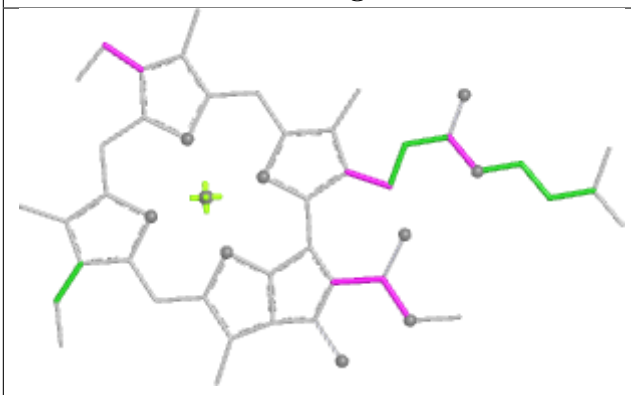
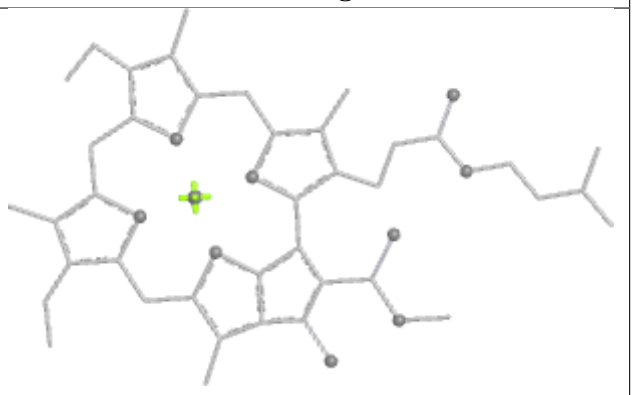
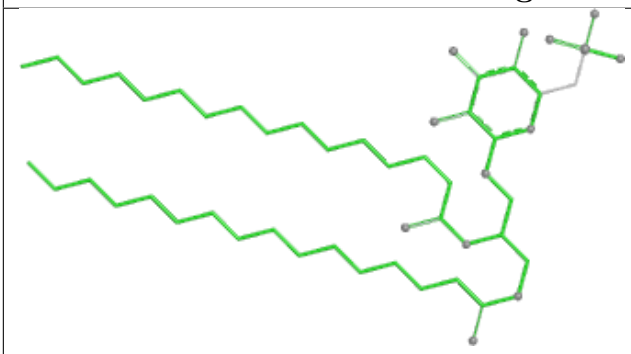


Torsions



Rings

Ligand SQD B1 626



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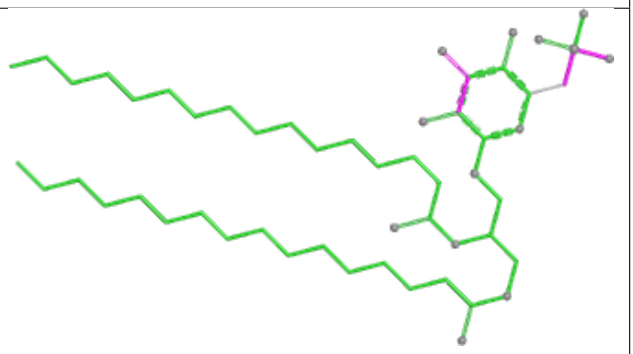

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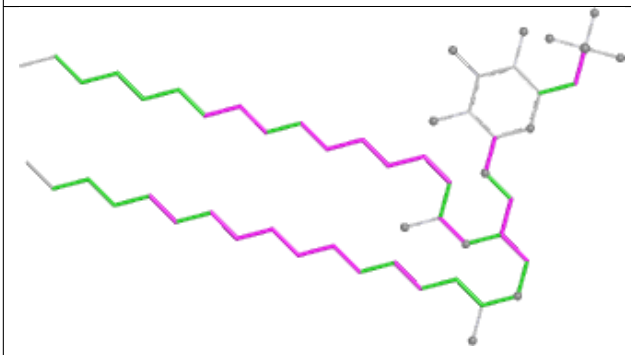

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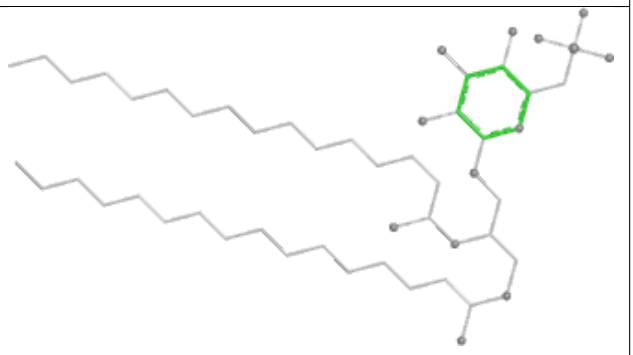
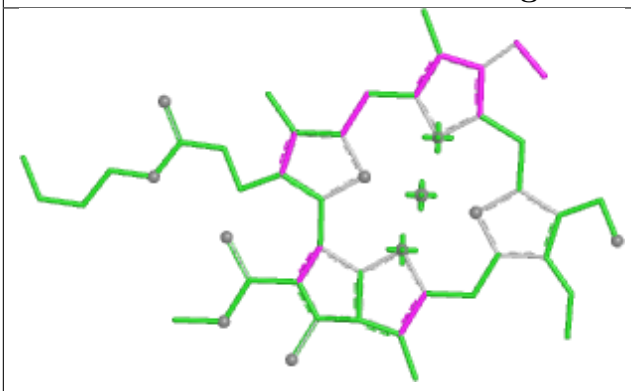


Rings

Ligand CHL r1 607



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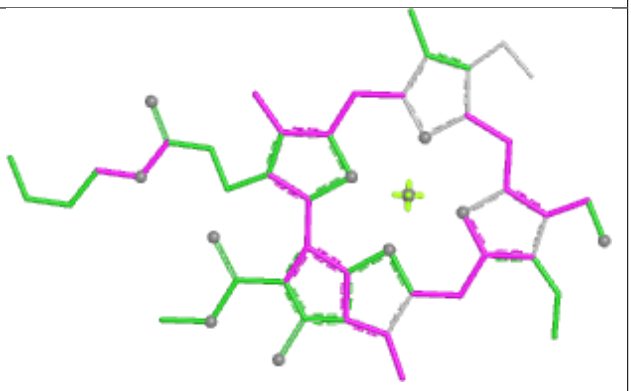
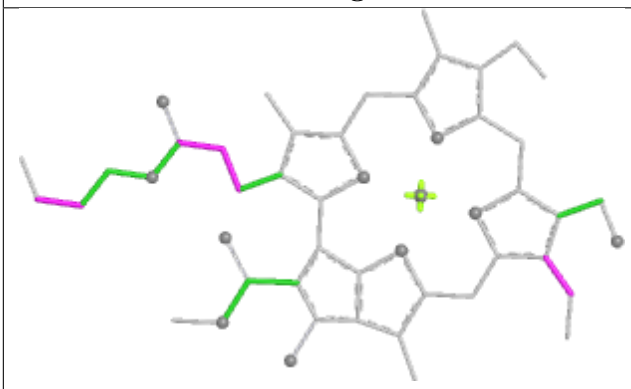
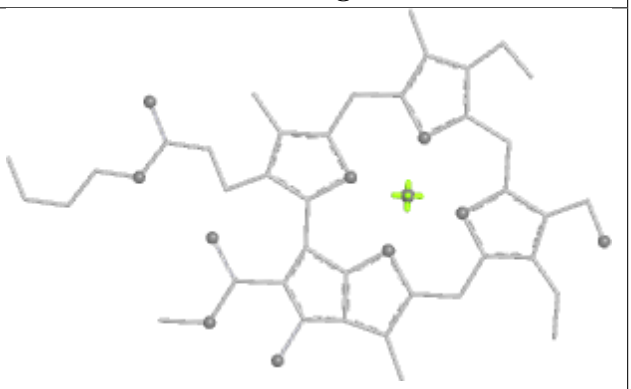


Bond angles

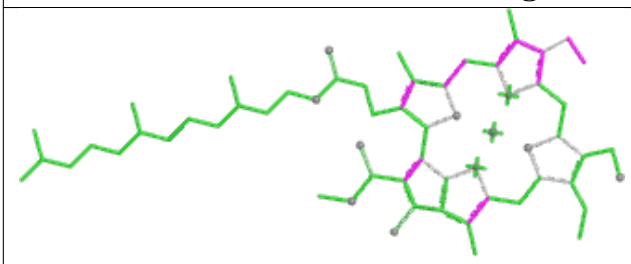


Torsions



Rings

Ligand CHL s1 608



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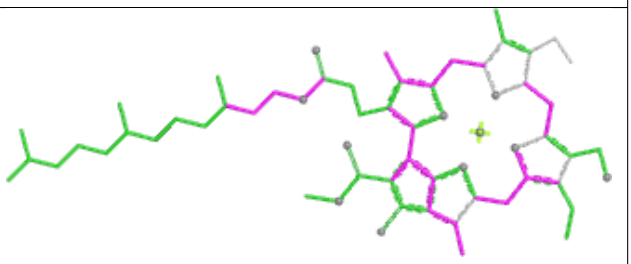
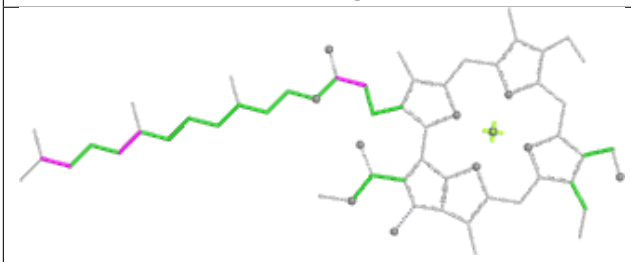
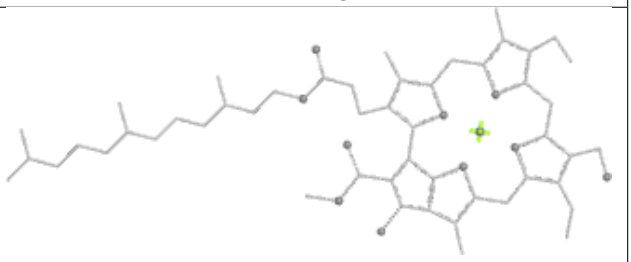


Bond angles

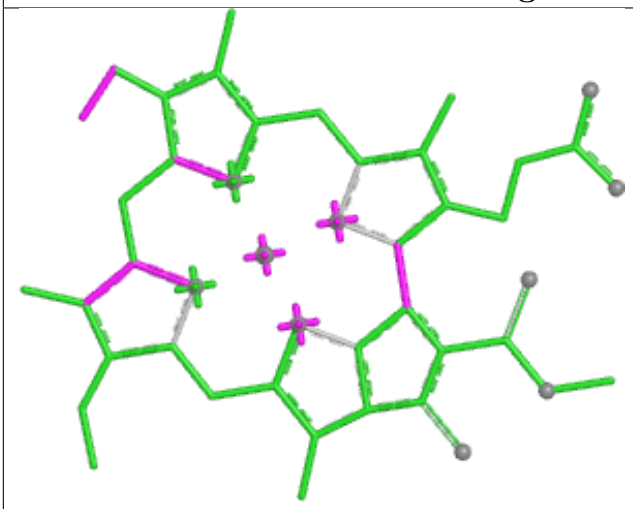


Torsions



Rings

Ligand CLA n1 612



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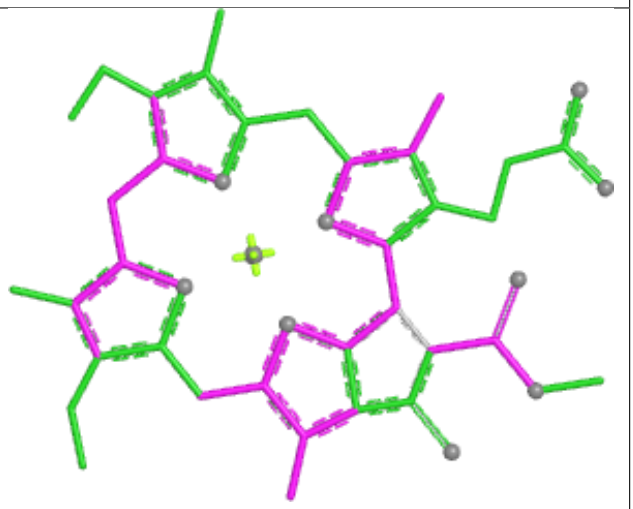
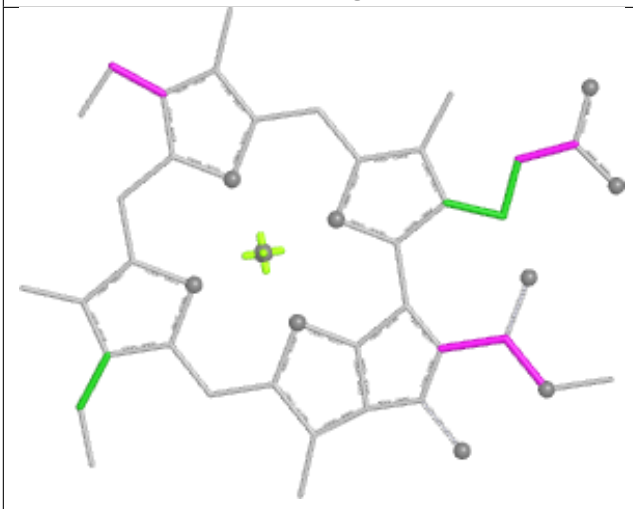


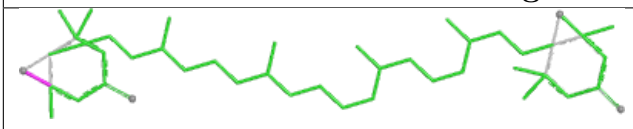
Bond angles



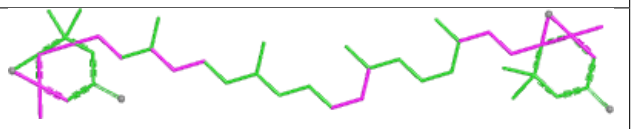
Torsions

Rings

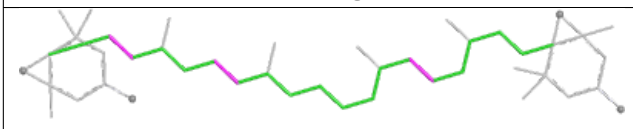
Ligand XAT N 622



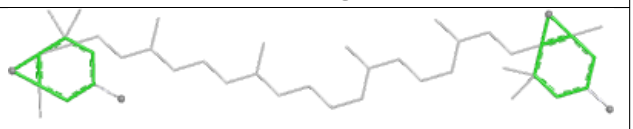
Bond lengths



Bond angles

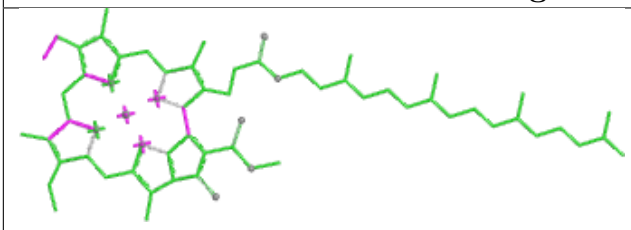


Torsions



Rings

Ligand CLA c 513



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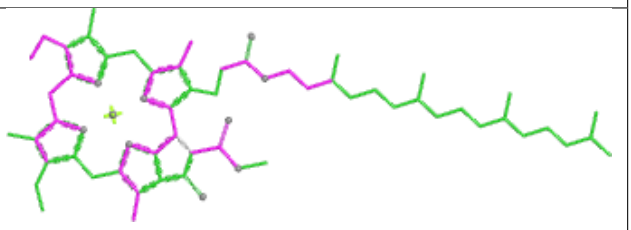

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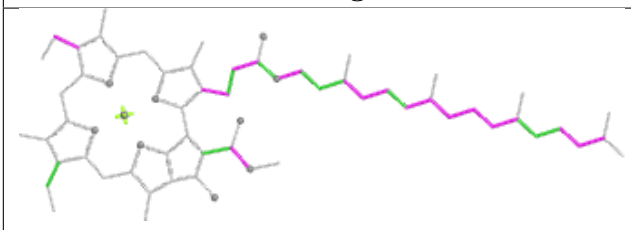

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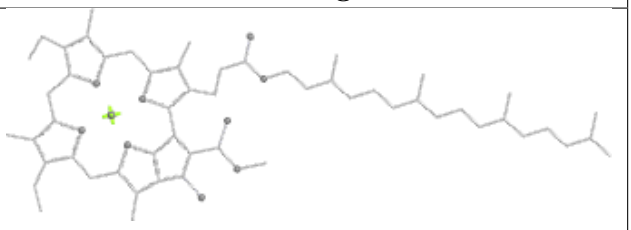
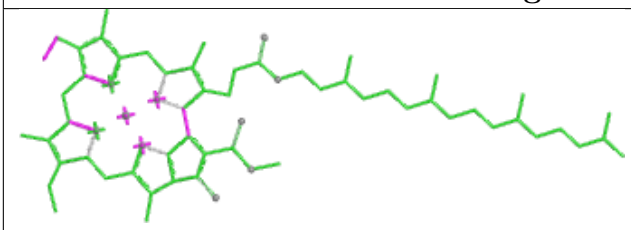


Rings

Ligand CLA Y 614



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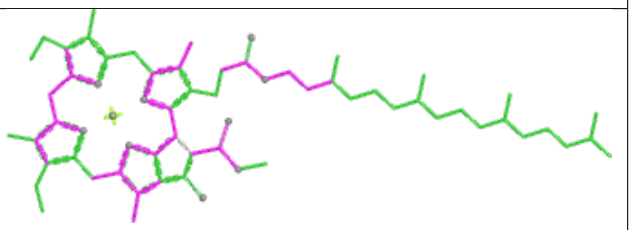

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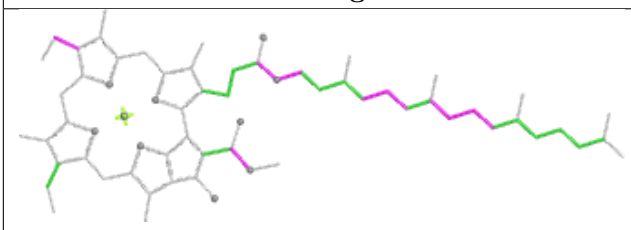

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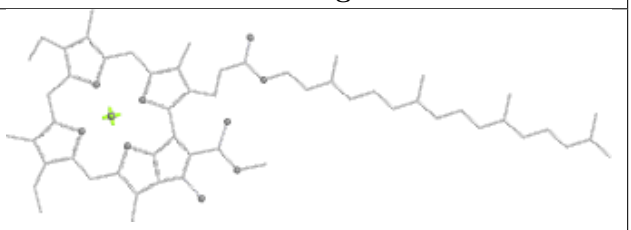
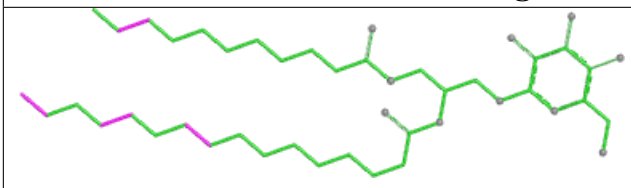


Rings

Ligand LMG d1 411



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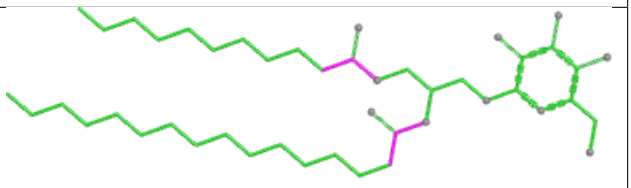
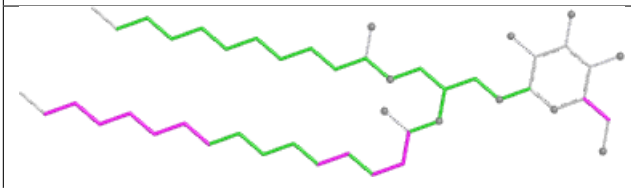


Bond angles



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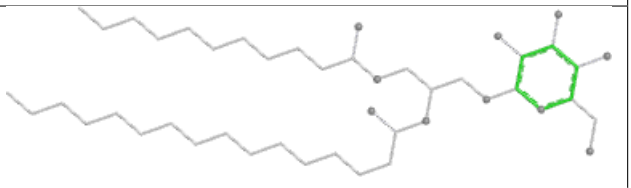
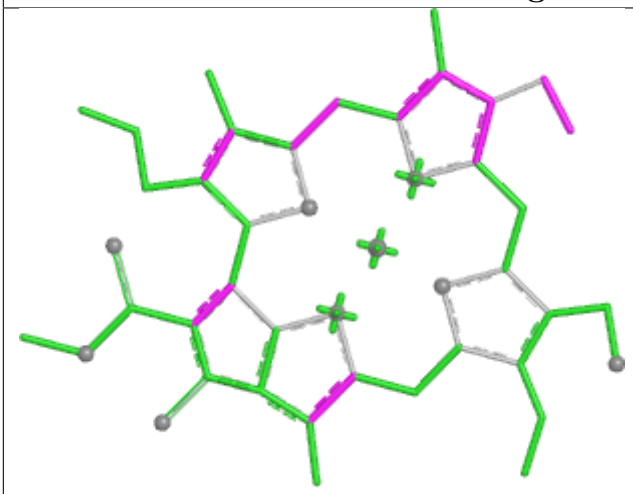


Rings

Ligand CHL g 608



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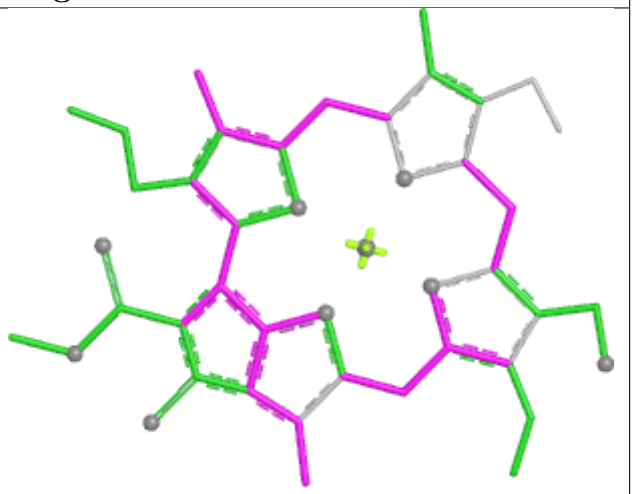

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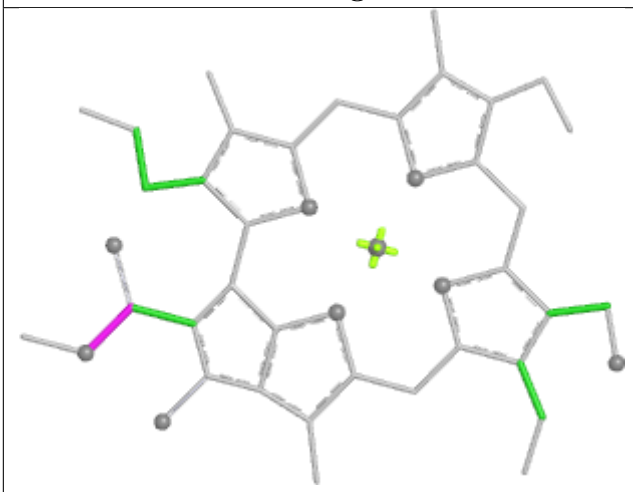

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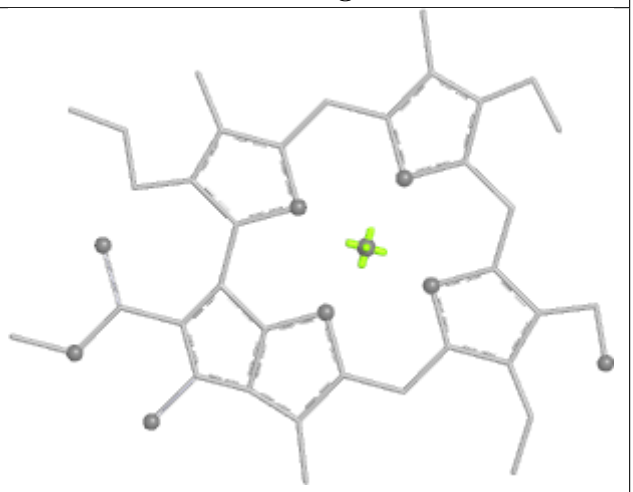
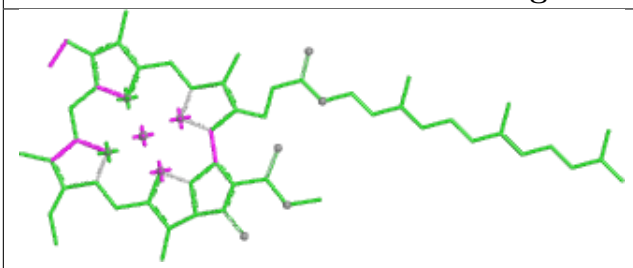


Rings

Ligand CLA r 603



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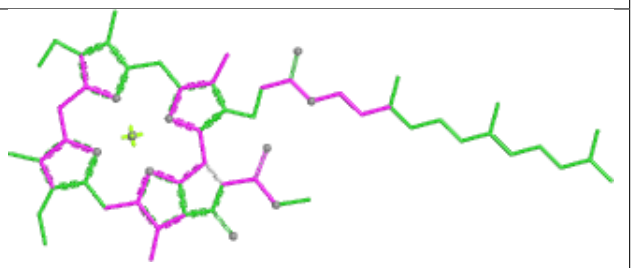
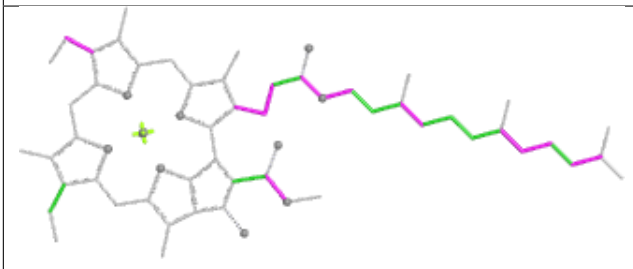


Bond angles



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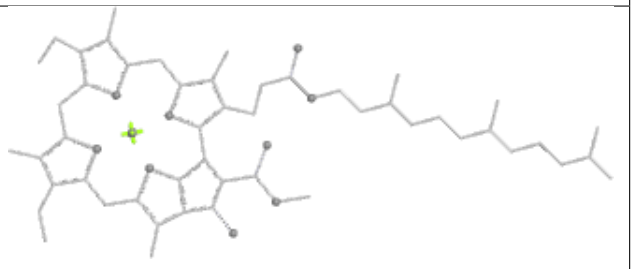
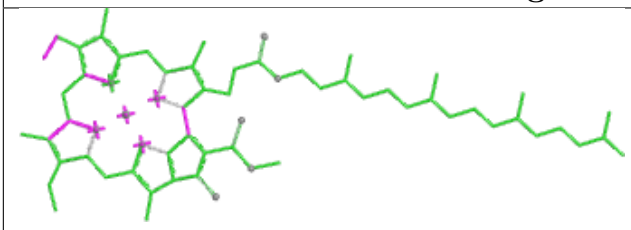


Rings

Ligand CLA S 603



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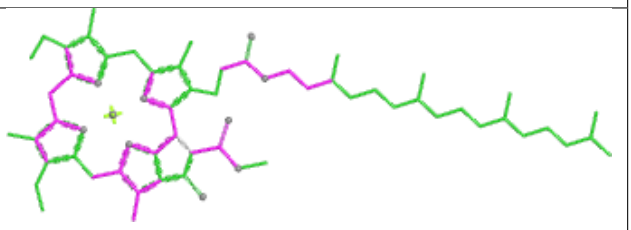

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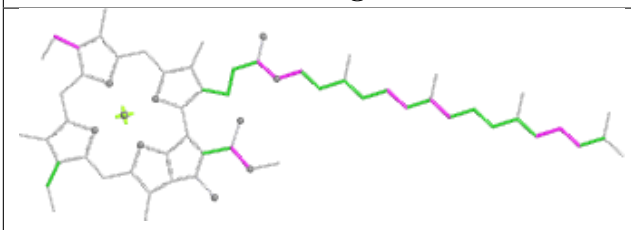

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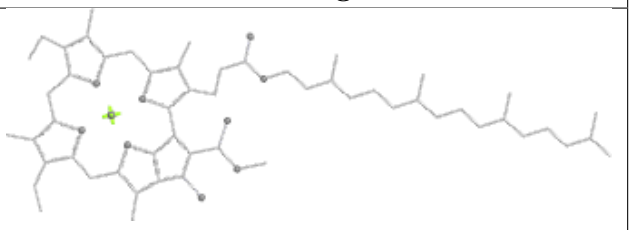
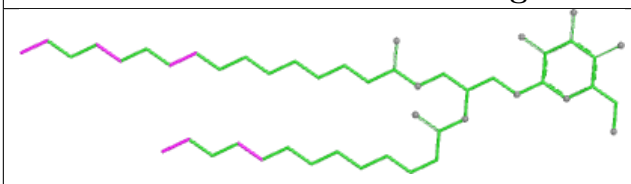


Rings

Ligand LMG A1 413



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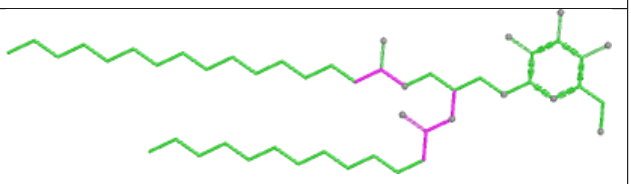

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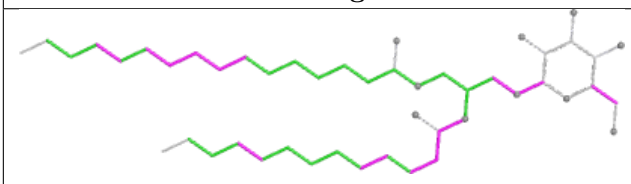

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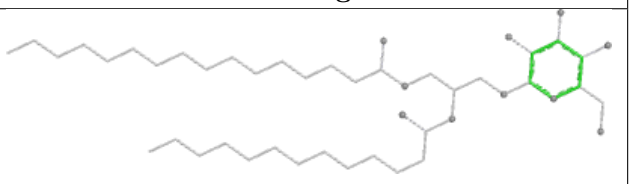
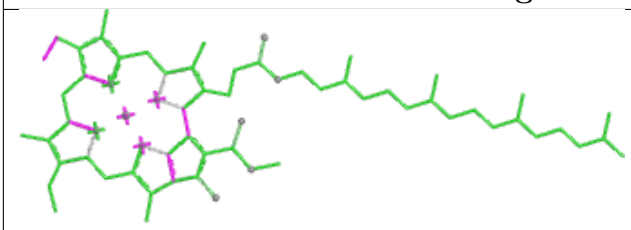


Rings

Ligand CLA B1 617



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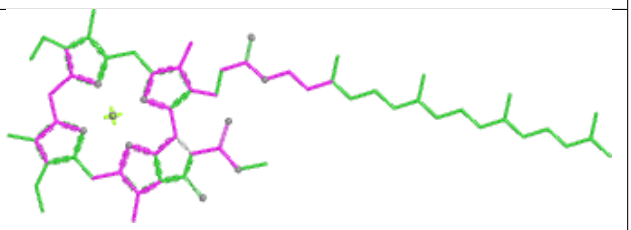

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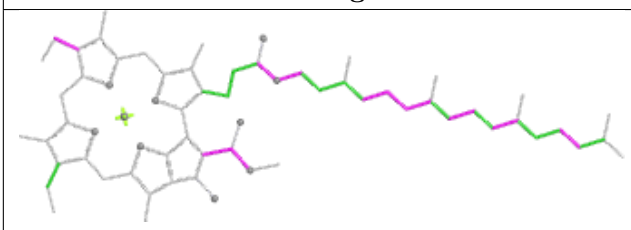

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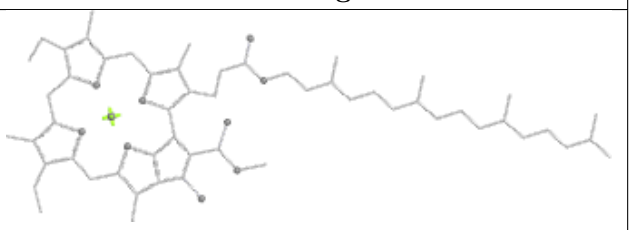
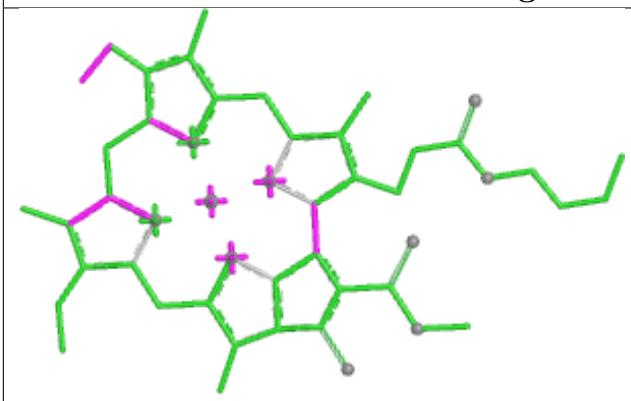


Rings

Ligand CLA n1 614



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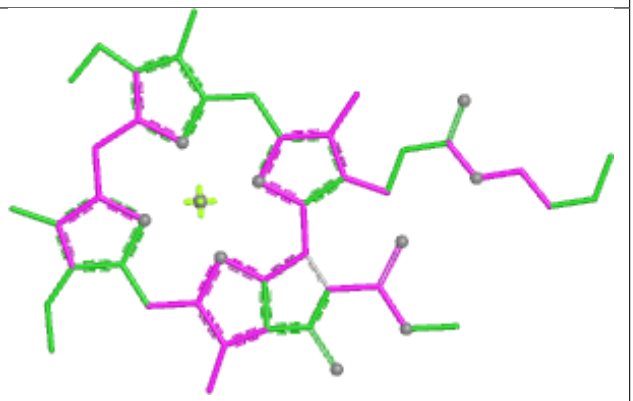

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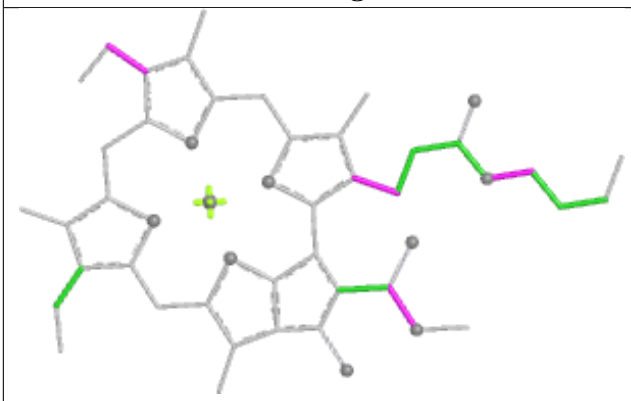

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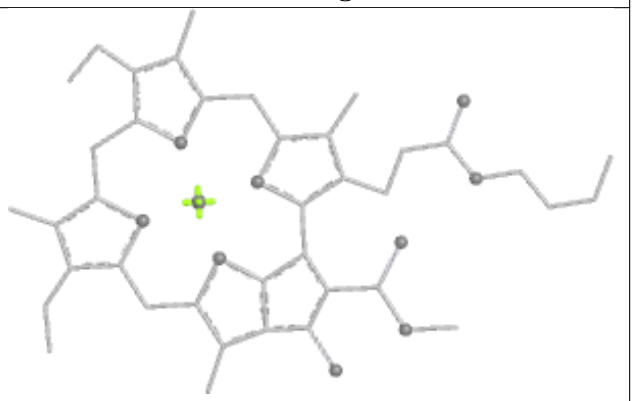
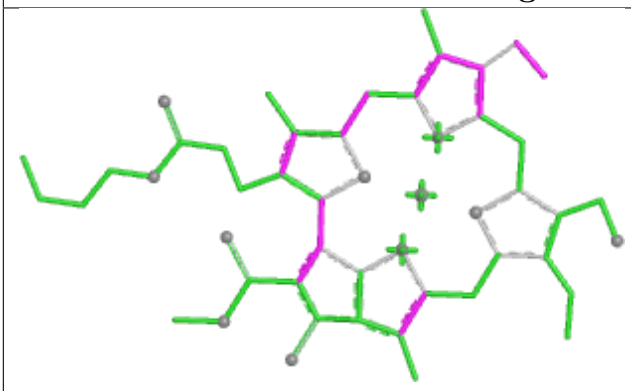


Rings

Ligand CHL g1 606



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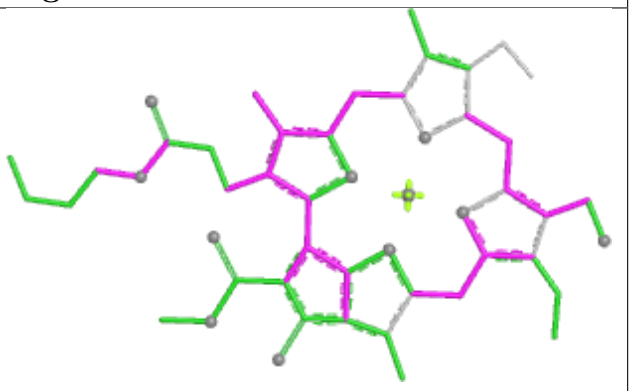

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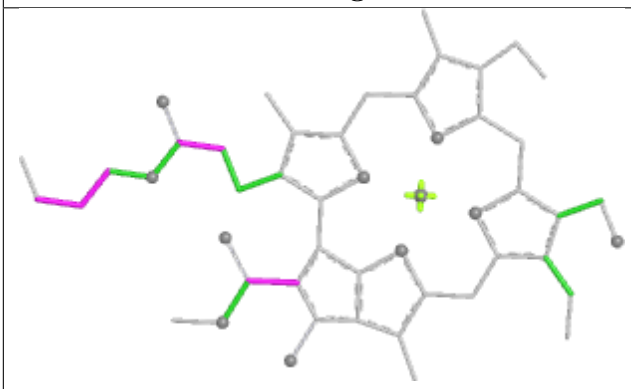

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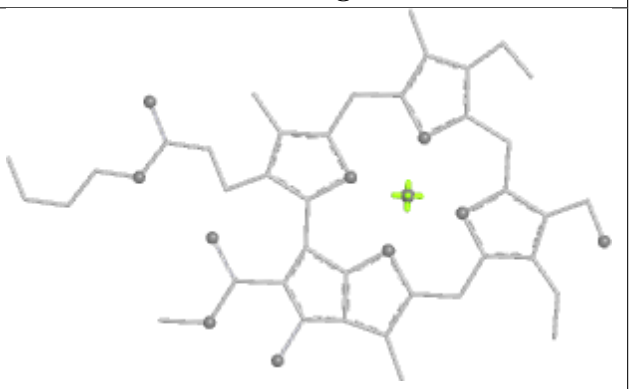
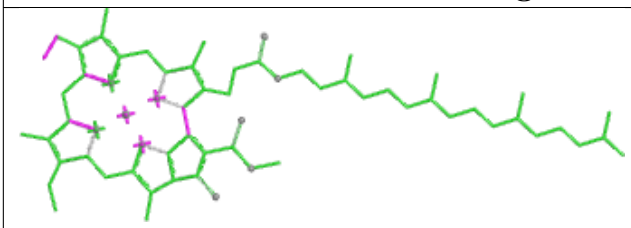


Rings

Ligand CLA B1 611



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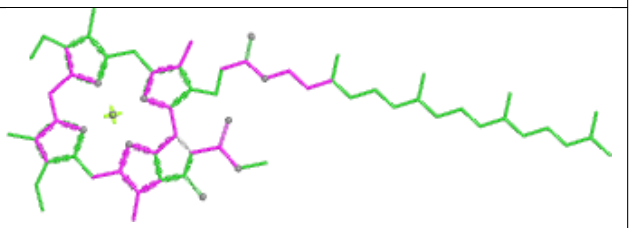
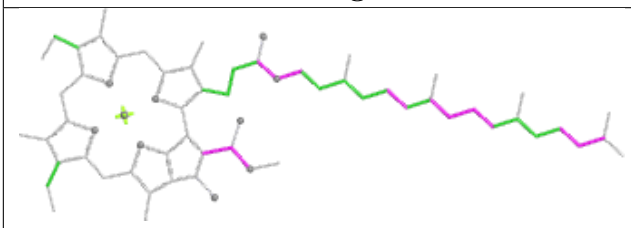


Bond angles



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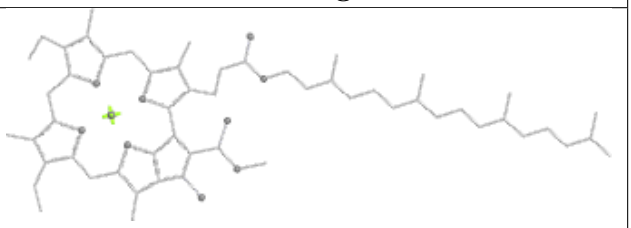
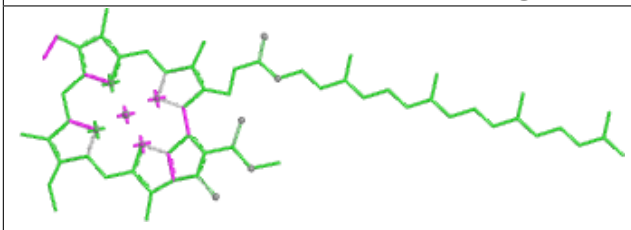


Rings

Ligand CLA C1 502



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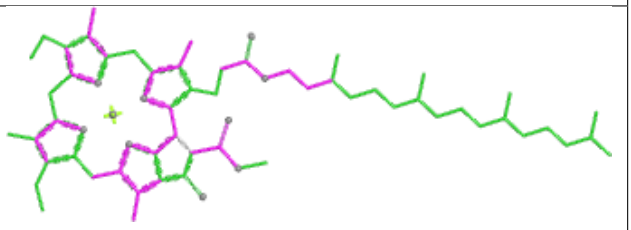
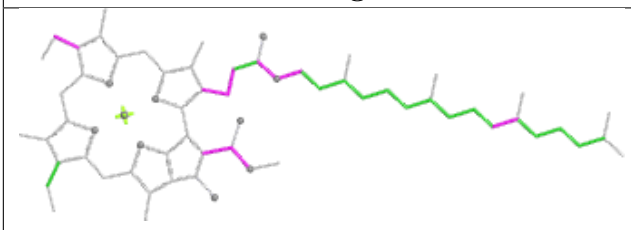
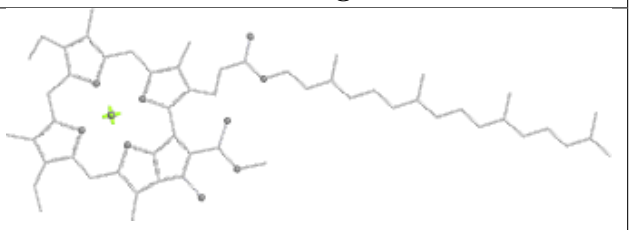


Bond angles

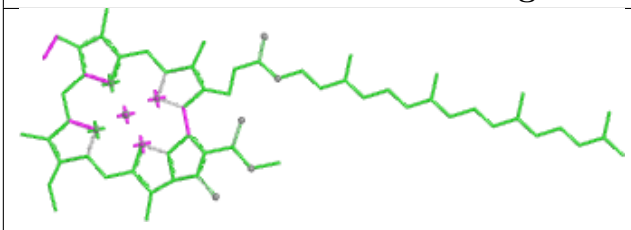


Torsions



Rings

Ligand CLA b1 604



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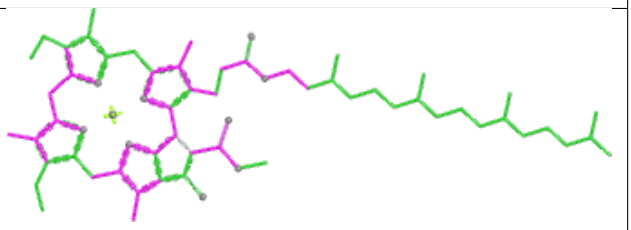
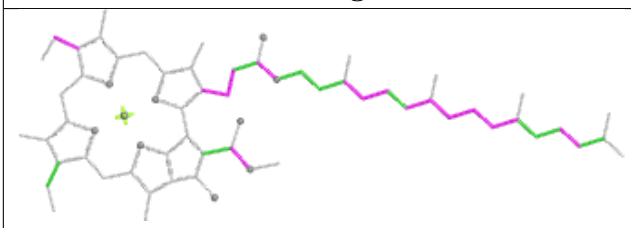


Bond angles



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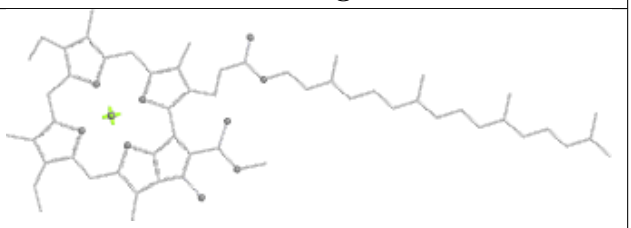
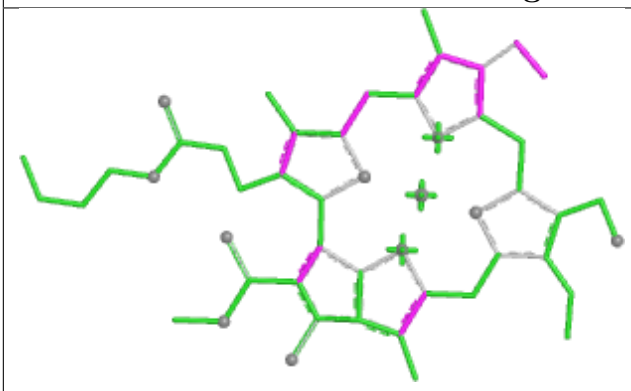
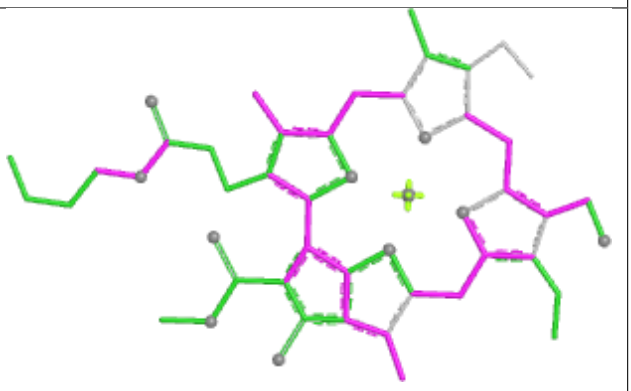


Rings

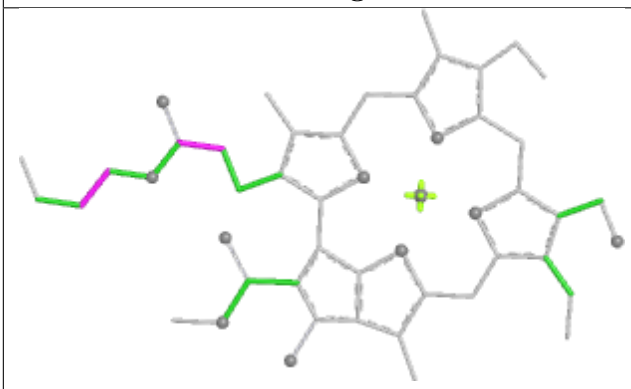
Ligand CHL R 607



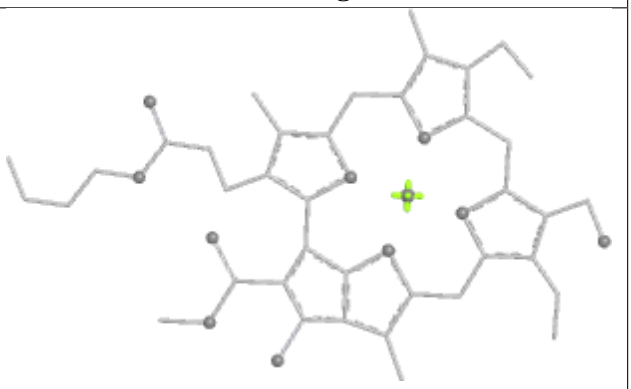
Bond lengths



Bond angles

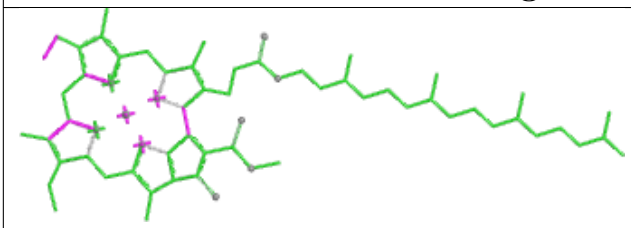


Torsions



Rings

Ligand CLA c1 513



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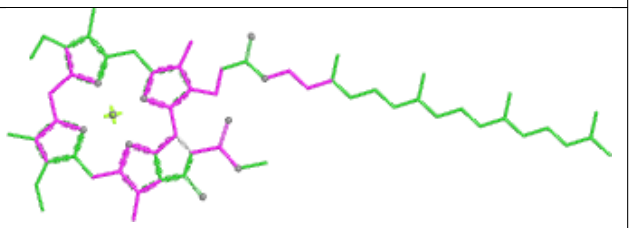

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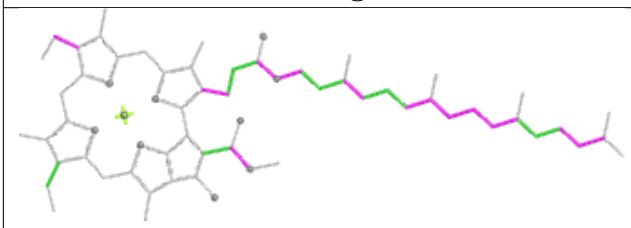

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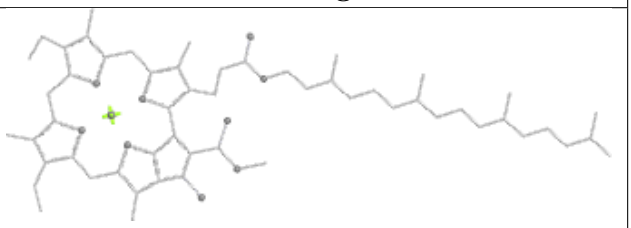
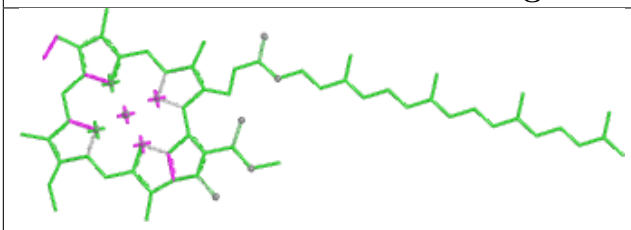
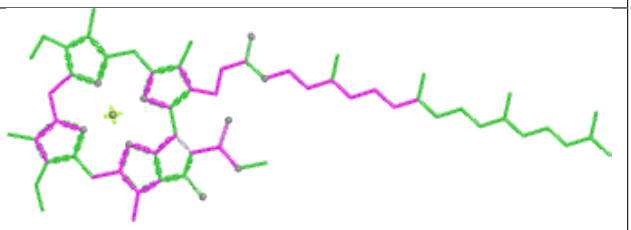
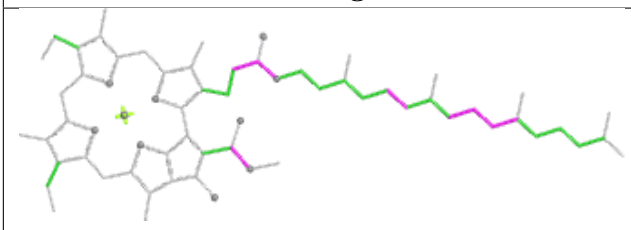
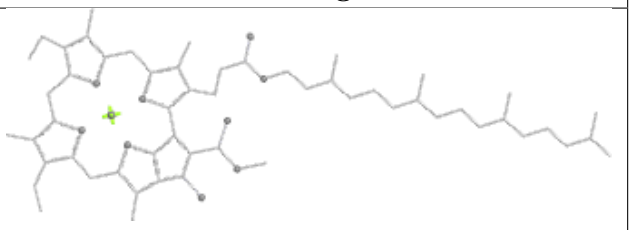
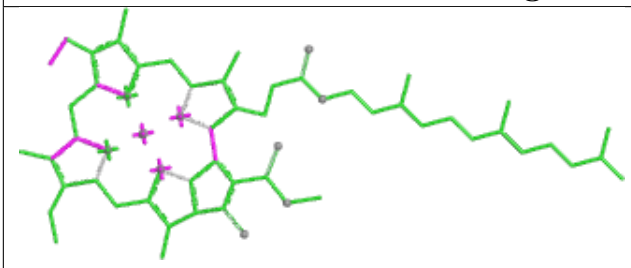
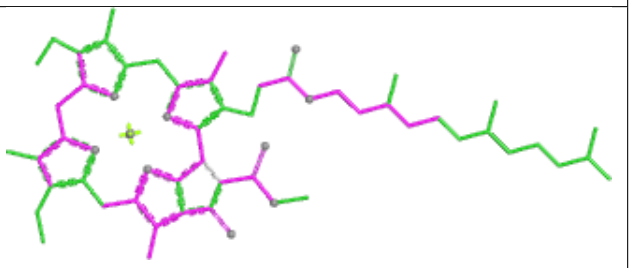
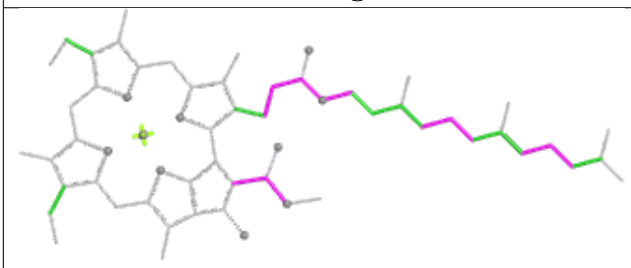
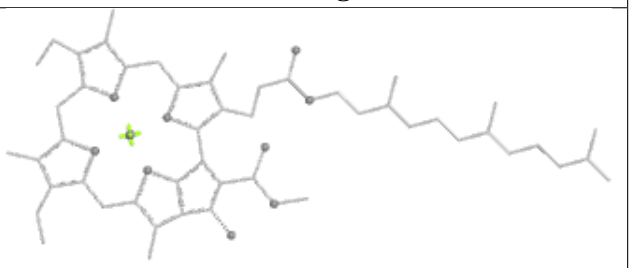
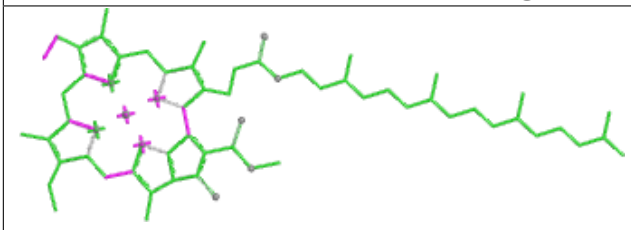


Rings

Ligand CLA A 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA R 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA b1 609



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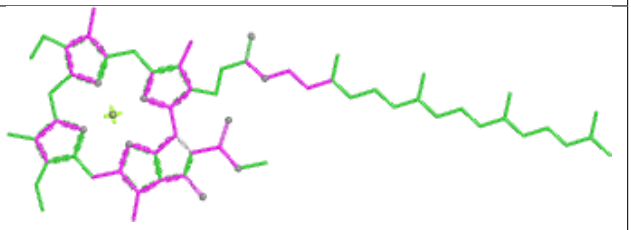
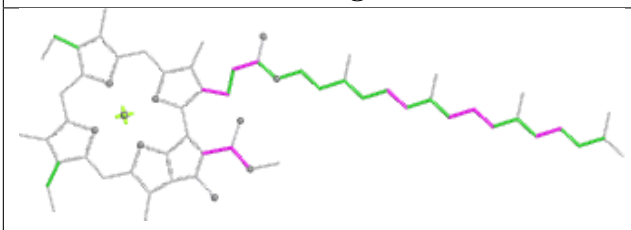
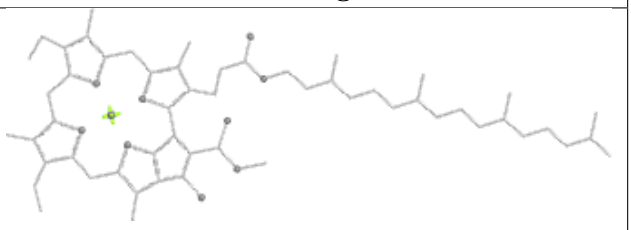


Bond angles

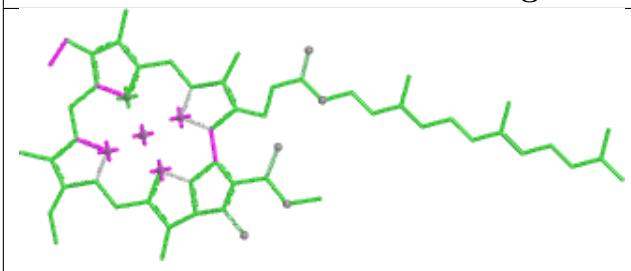


Torsions



Rings

Ligand CLA r1 608



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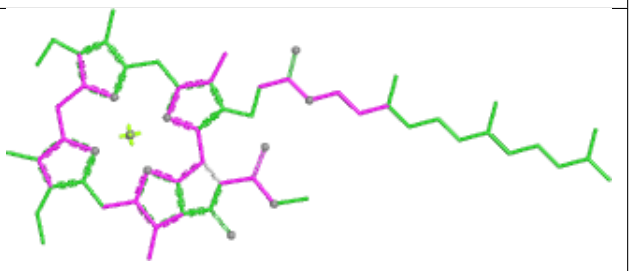
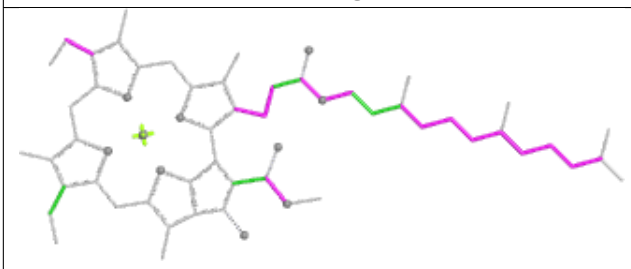


Bond angles



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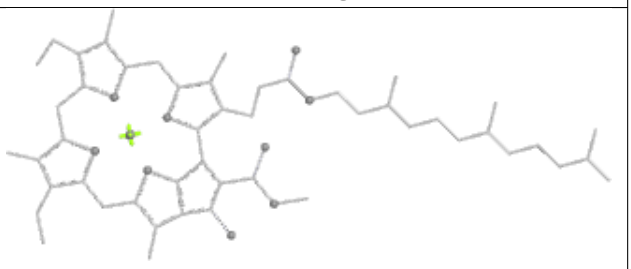
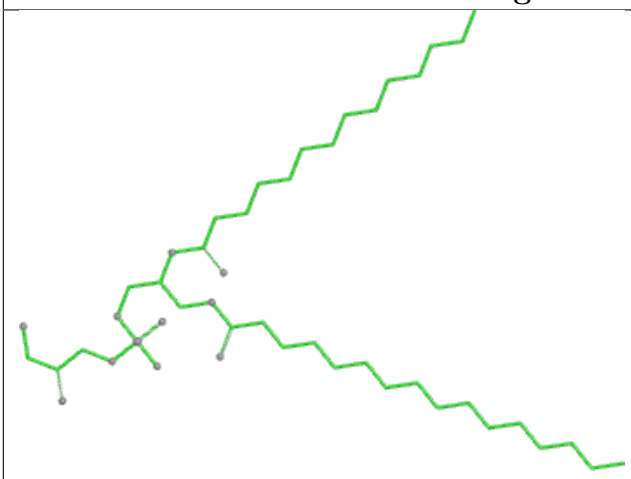


Rings

Ligand LHG C1 525



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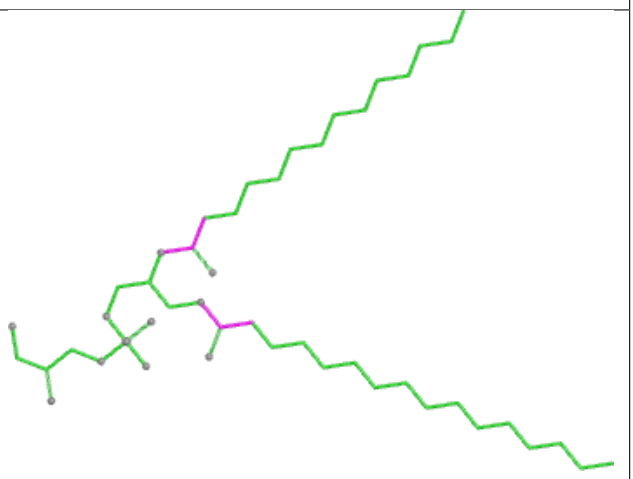
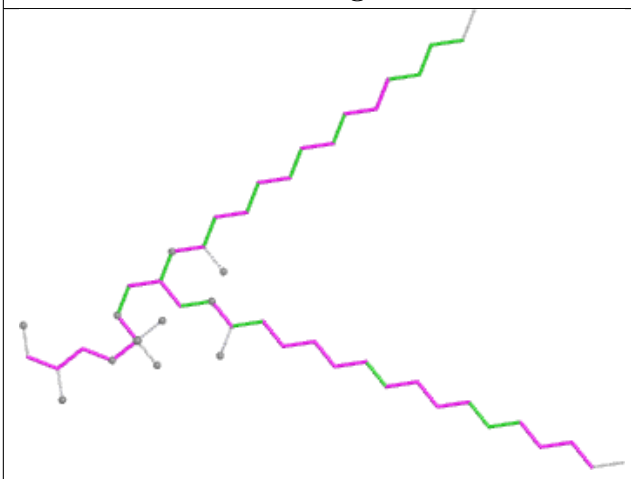


Bond angles



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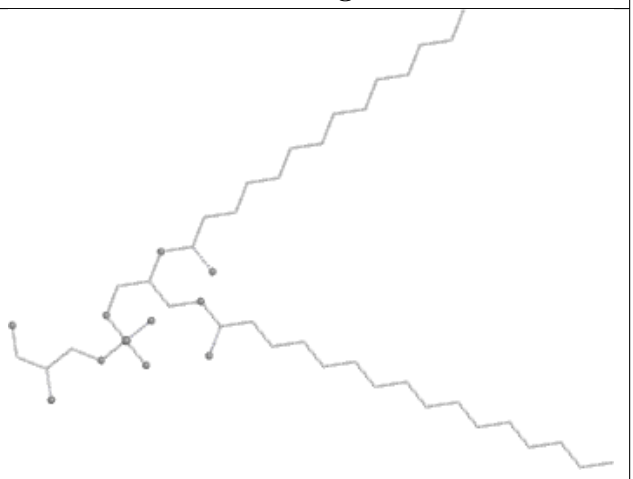
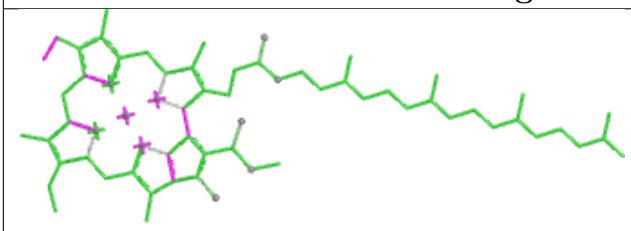


Rings

Ligand CLA C1 505



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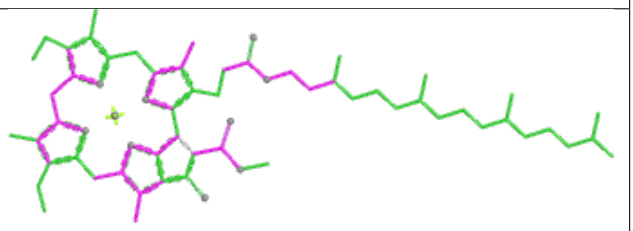
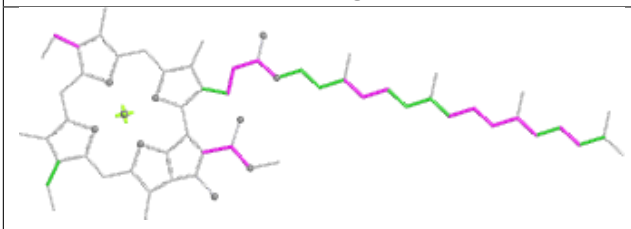


Bond angles



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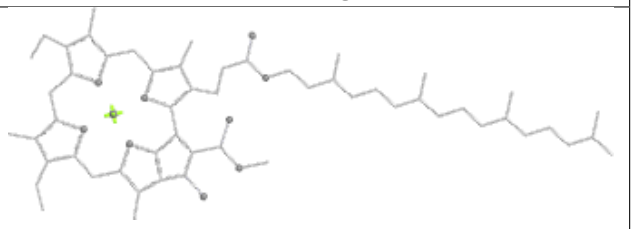
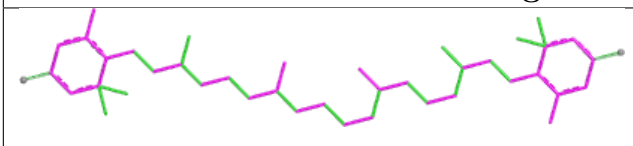


Rings

Ligand C7Z b1 620



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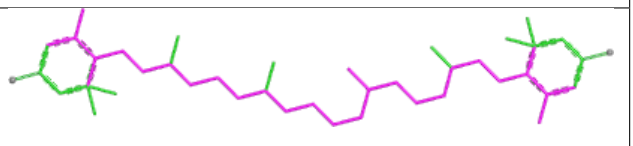
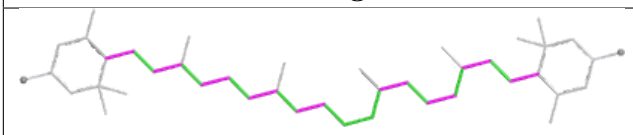


Bond angles



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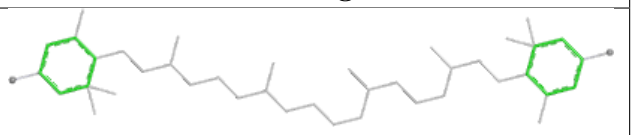
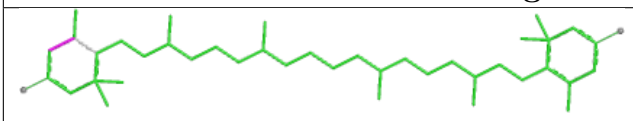


Rings

Ligand LUT G 620



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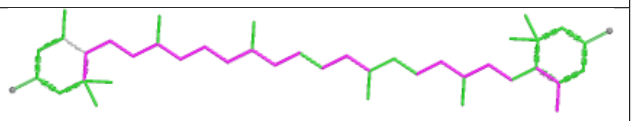
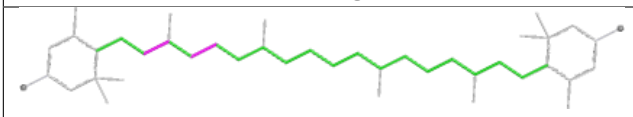


Bond angles



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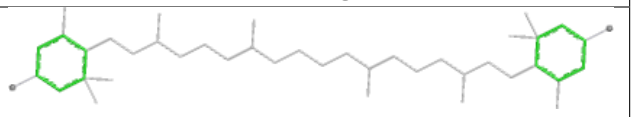
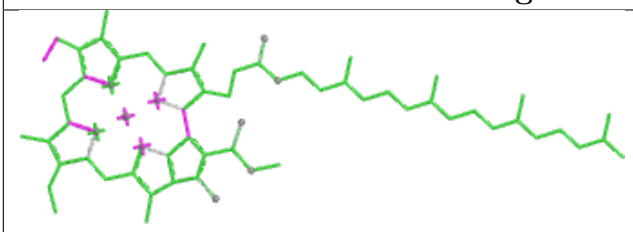


Rings

Ligand CLA B1 609



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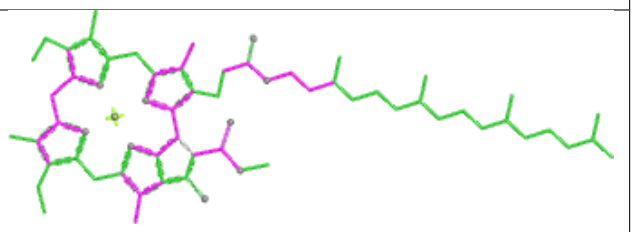

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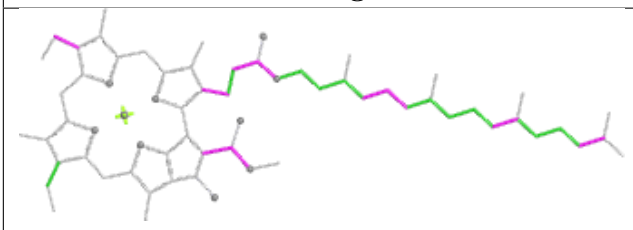

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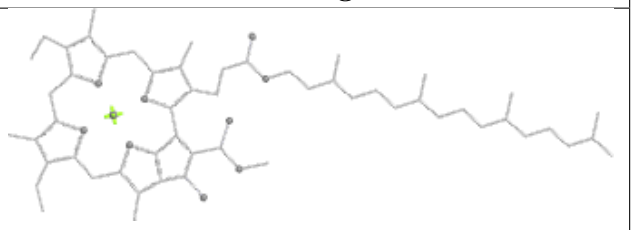
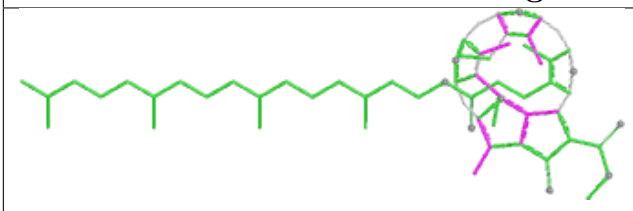


Rings

Ligand PHO a 408



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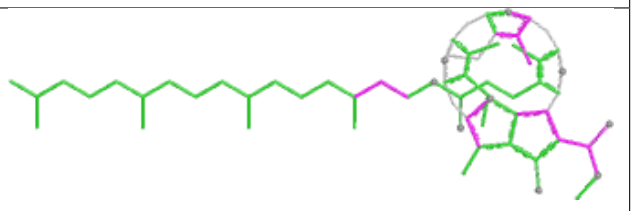
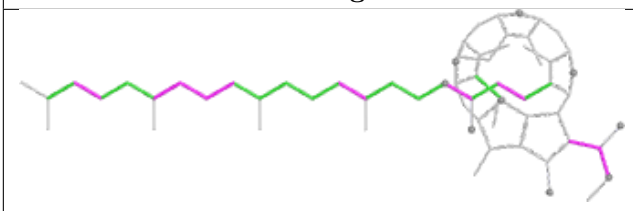
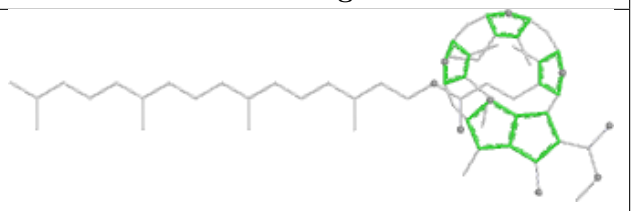


Bond angles

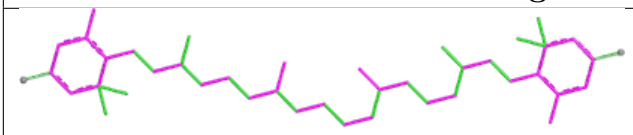


Torsions



Rings

Ligand C7Z B 620



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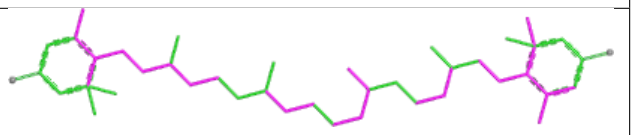
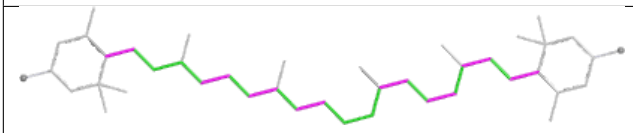
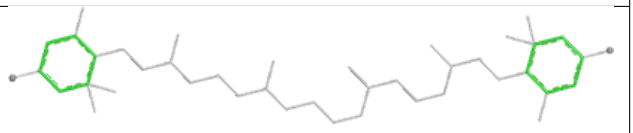


Bond angles

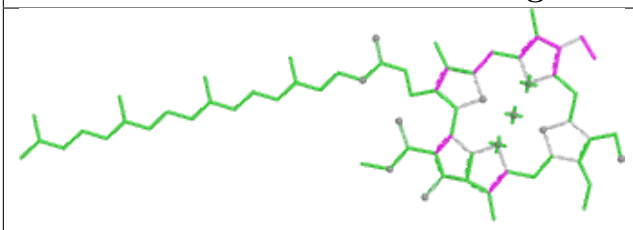


Torsions

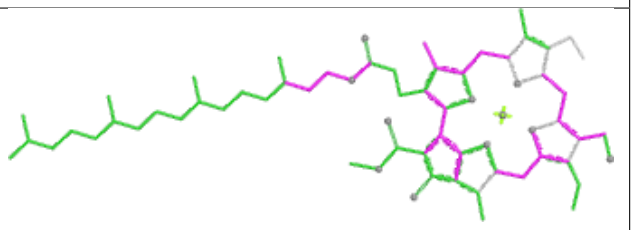


Rings

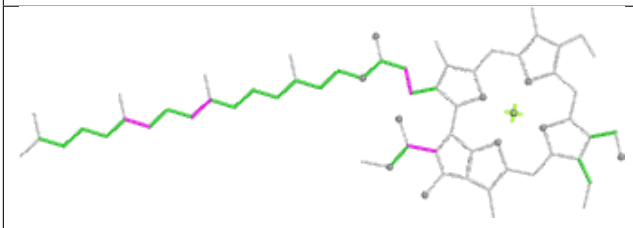
Ligand CHL n 606



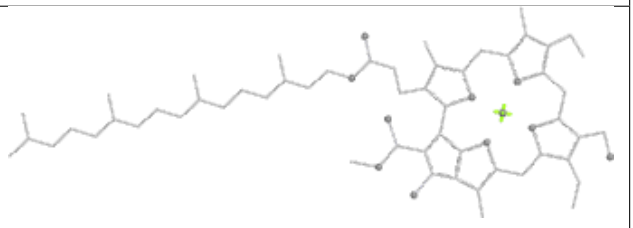
Bond lengths



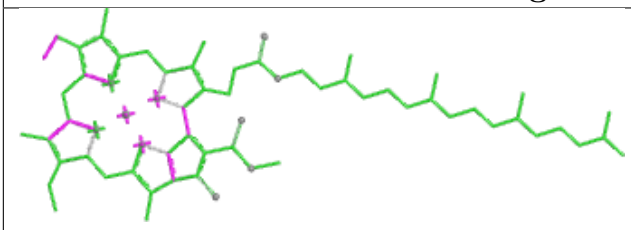
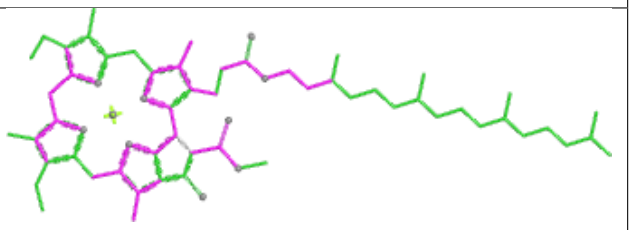
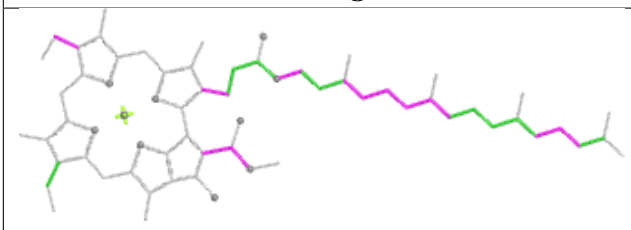
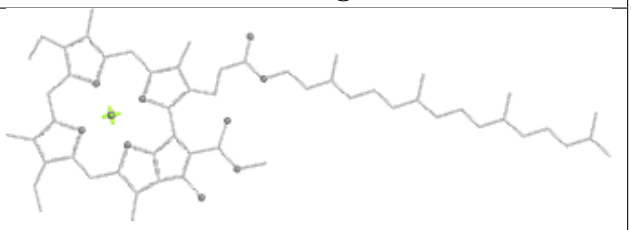
Bond angles

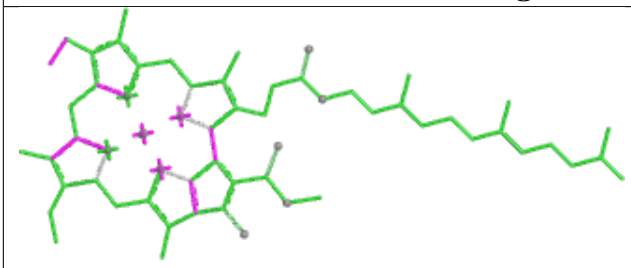
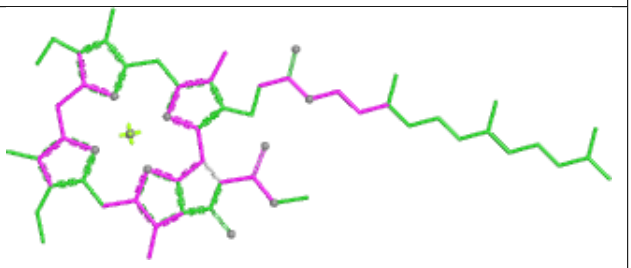
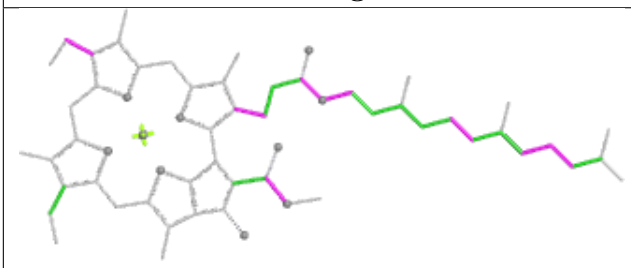
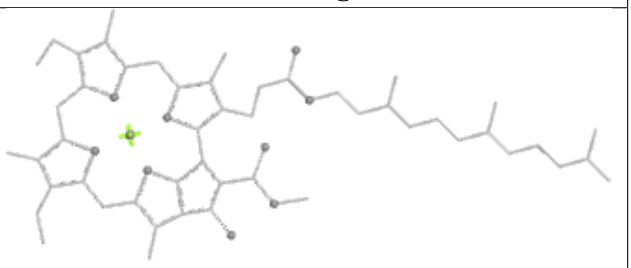


Torsions

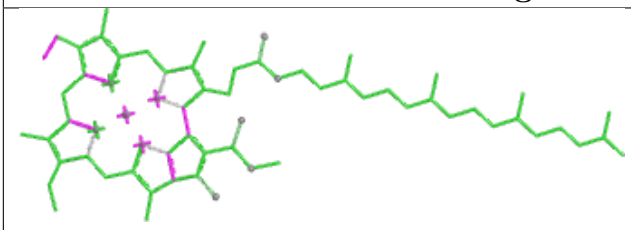


Rings

Ligand CLA c 501	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA R1 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA Y1 603



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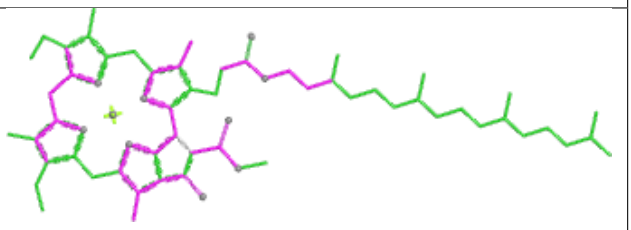

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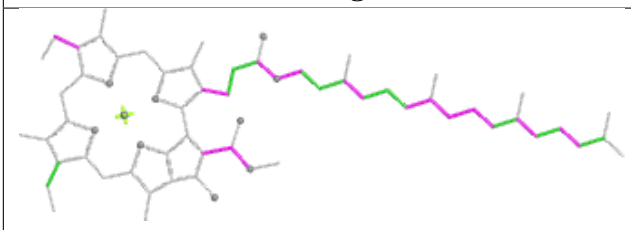
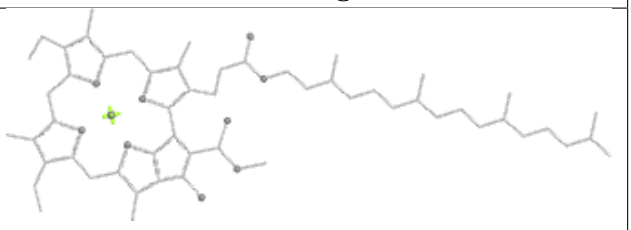
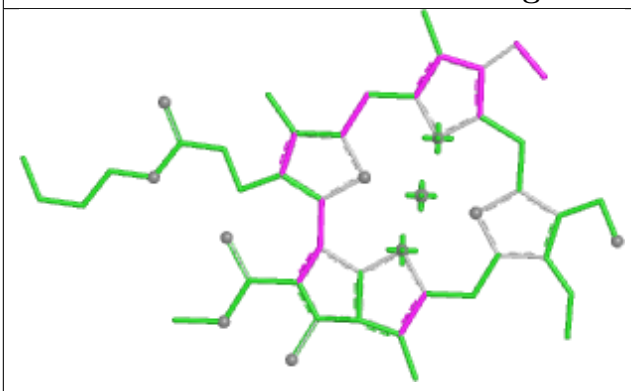


Torsions



Rings

Ligand CHL G 606



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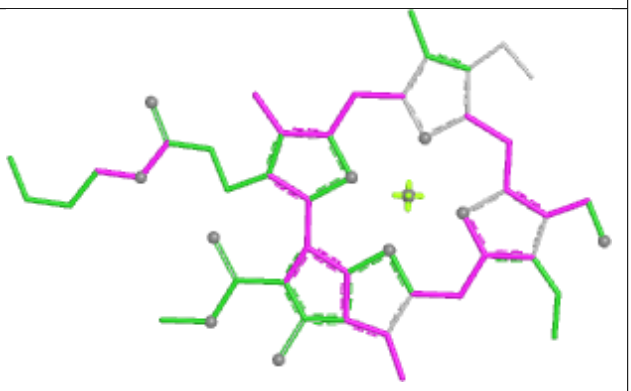

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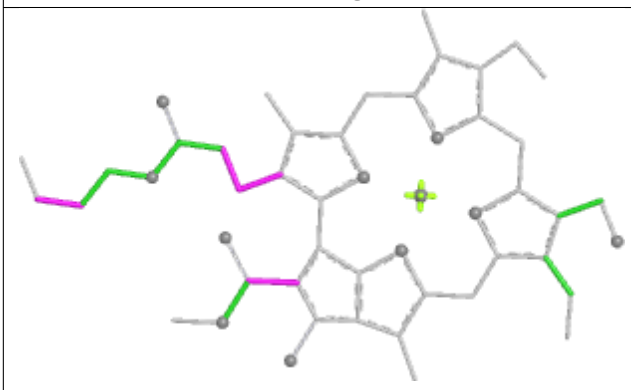
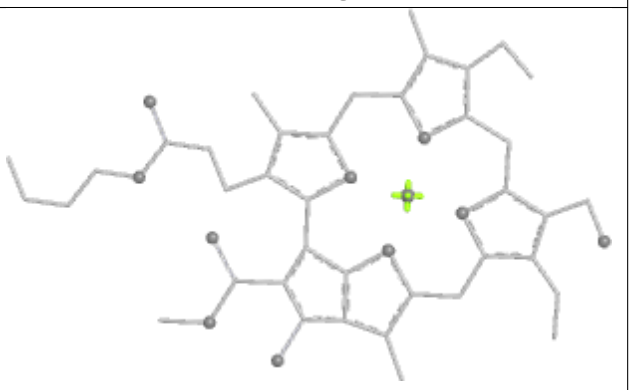
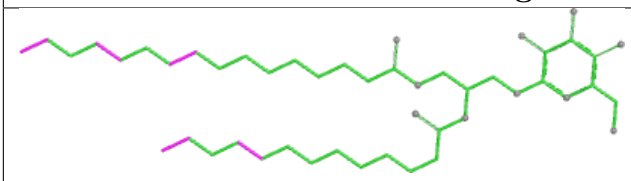
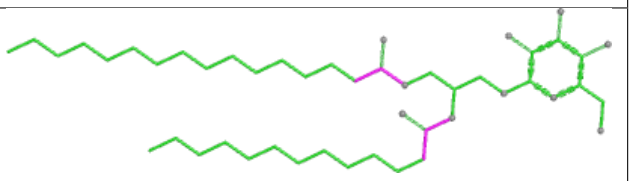
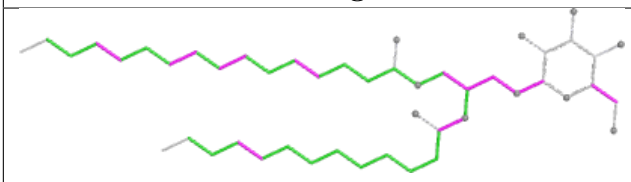
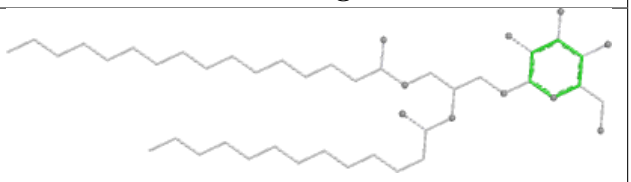
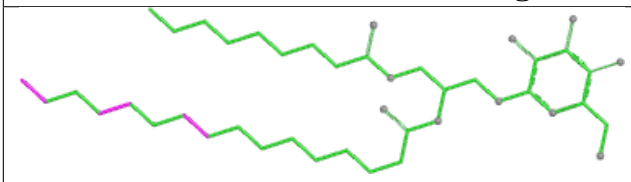
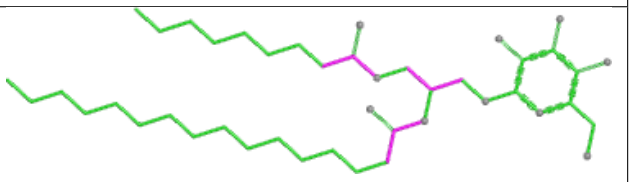
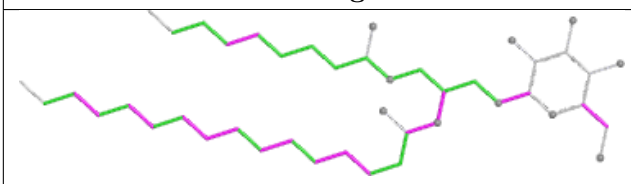
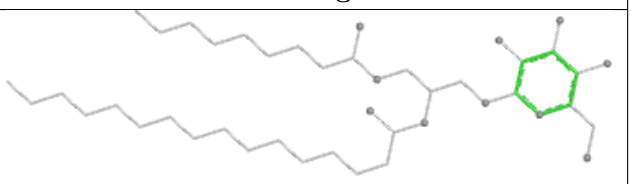


Torsions

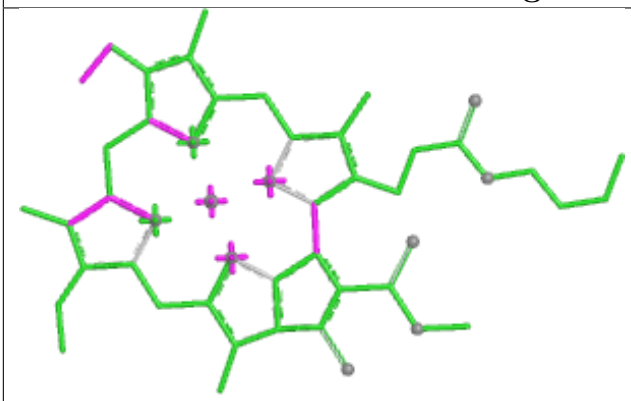


Rings

Ligand LMG a1 413	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LMG b1 622	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA N 614



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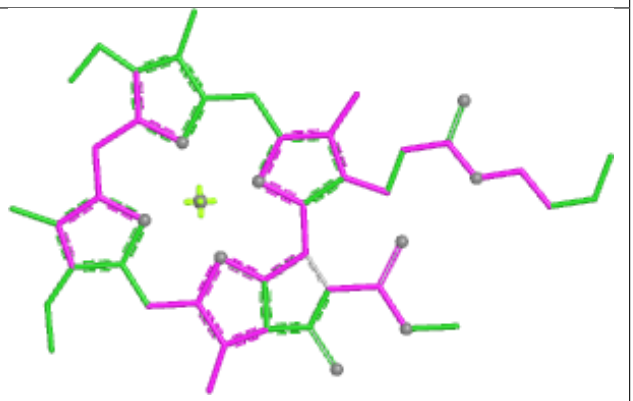
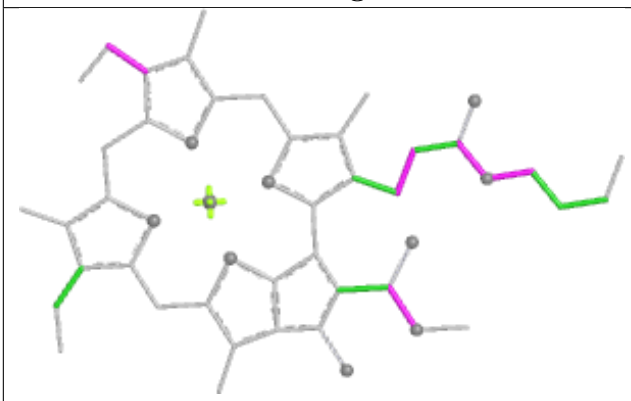
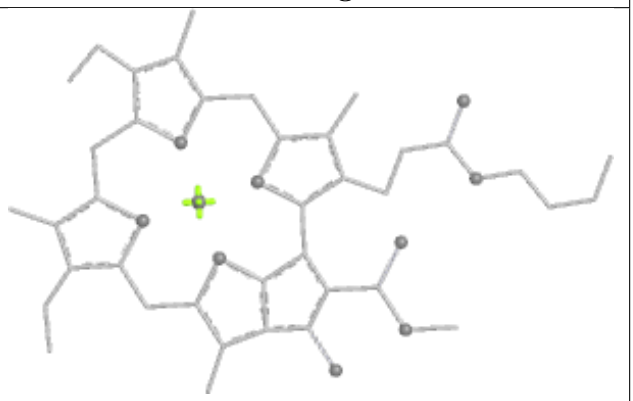


Bond angles

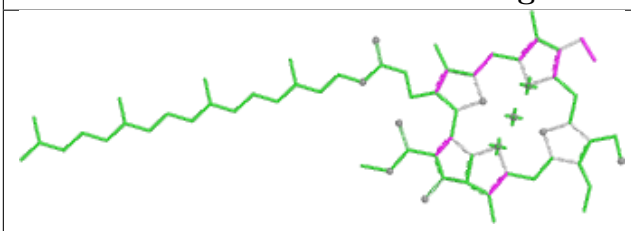


Torsions



Rings

Ligand CHL n1 607



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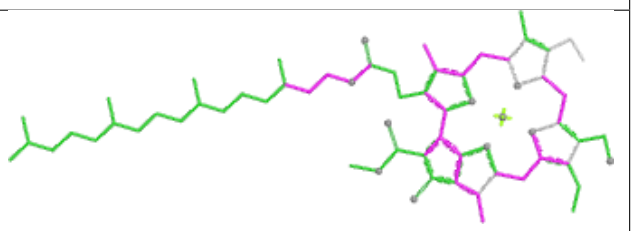
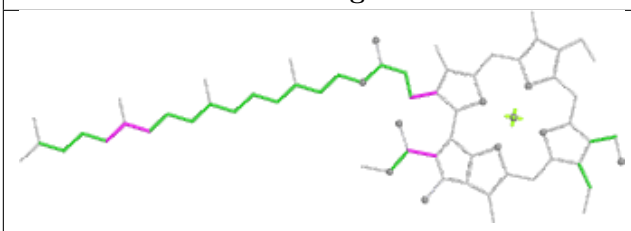


Bond angles



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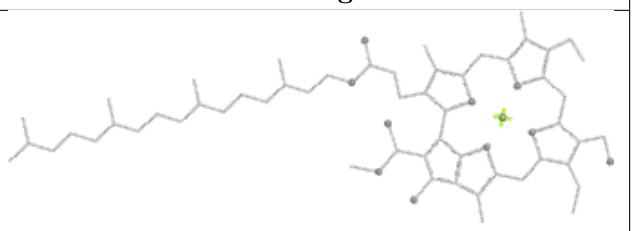
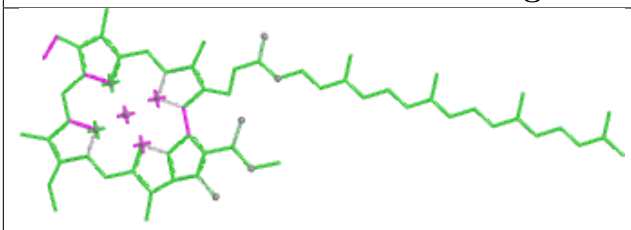


Rings

Ligand CLA Y 611



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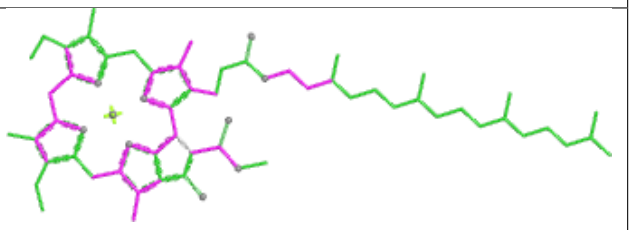
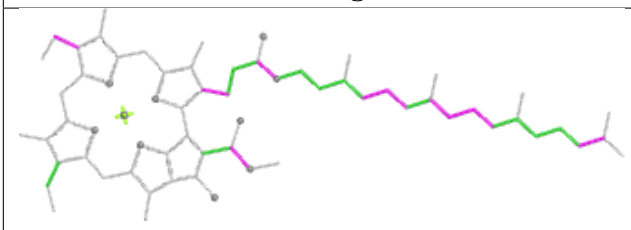
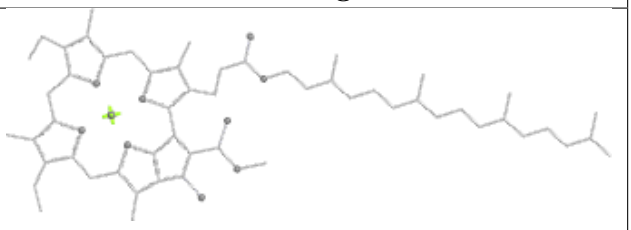


Bond angles

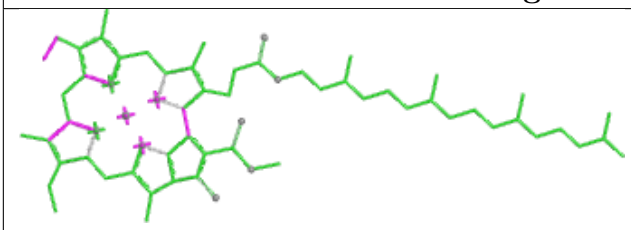


Torsions



Rings

Ligand CLA D 403



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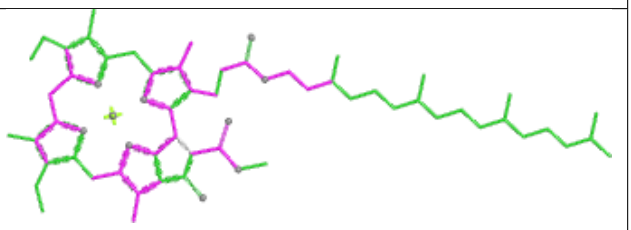
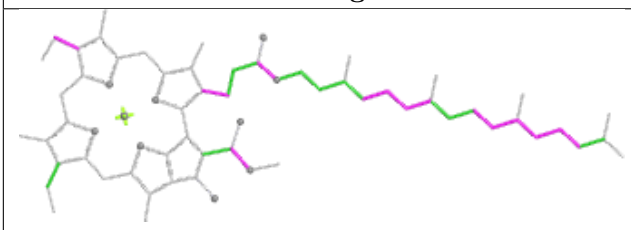


Bond angles



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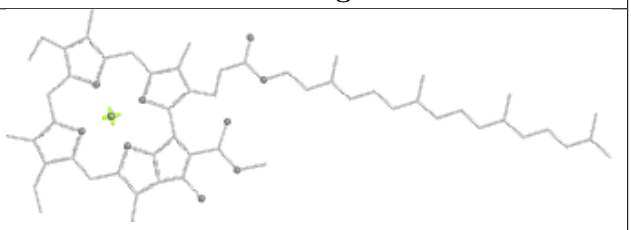
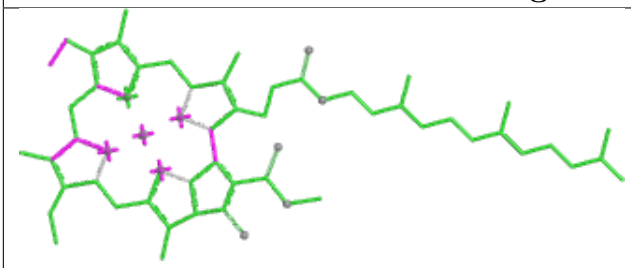


Rings

Ligand CLA s 609



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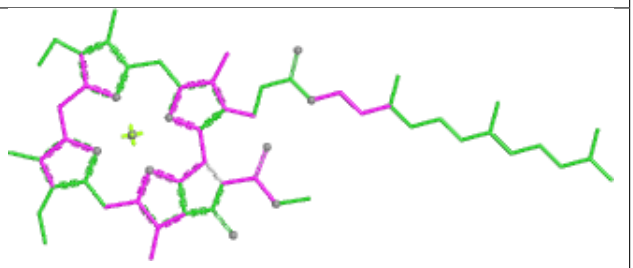
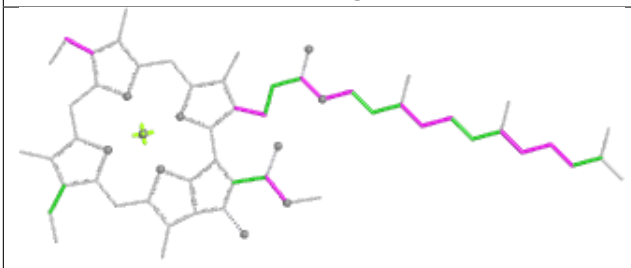
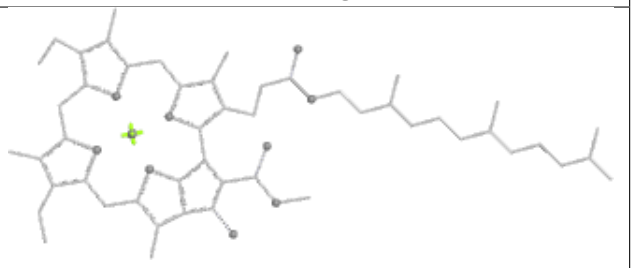


Bond angles

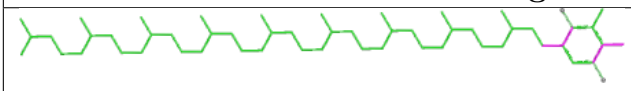


Torsions



Rings

Ligand PL9 D 405



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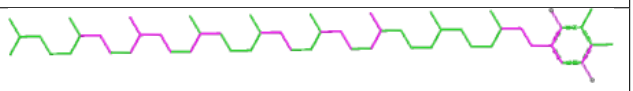
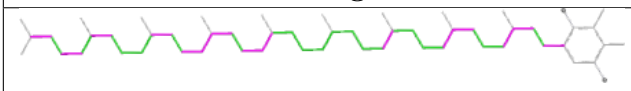
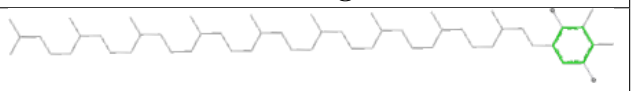


Bond angles

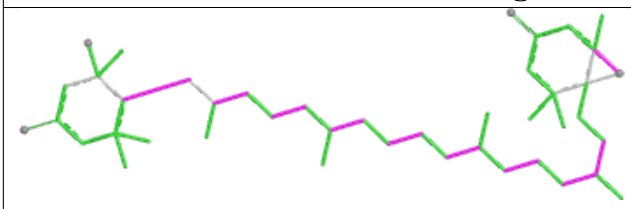


Torsions



Rings

Ligand NEX N1 623



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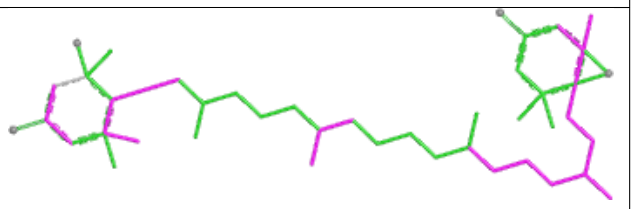
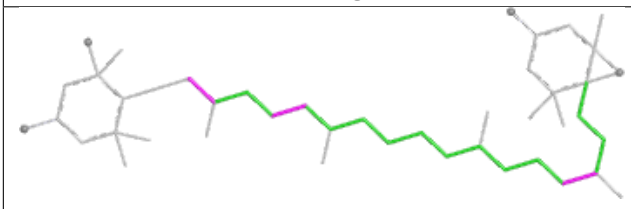
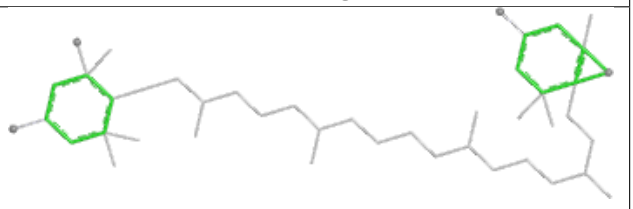


Bond angles

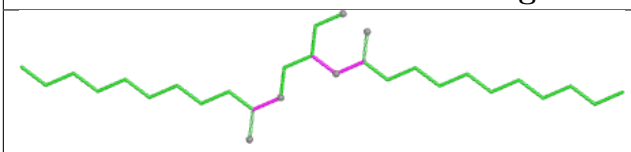


Torsions

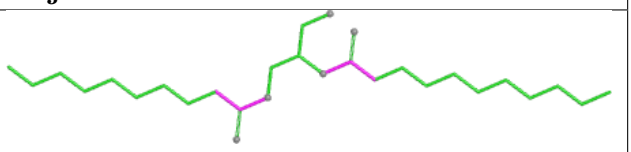


Rings

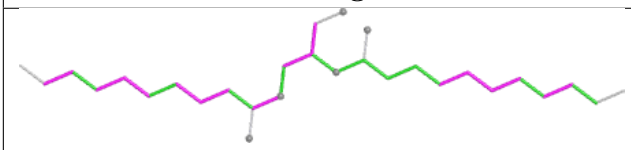
Ligand DGA j1 101



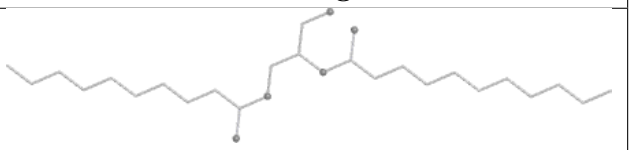
Bond lengths



Bond angles

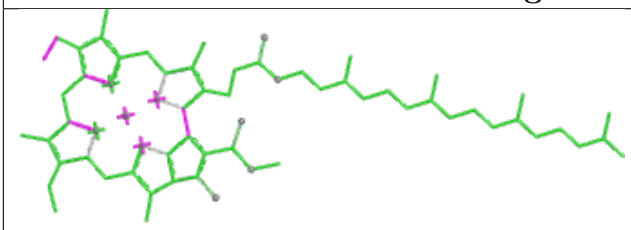


Torsions

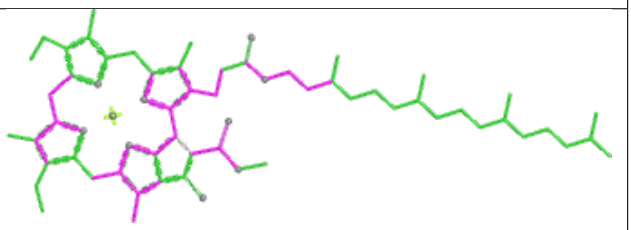


Rings

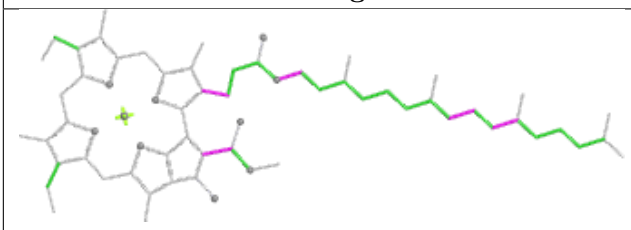
Ligand CLA B 615



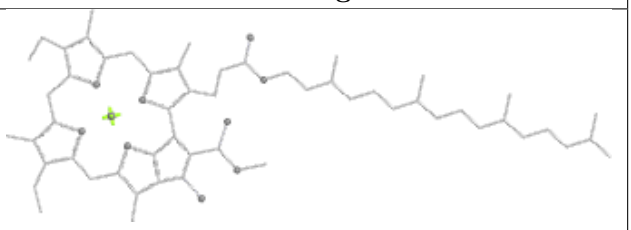
Bond lengths



Bond angles

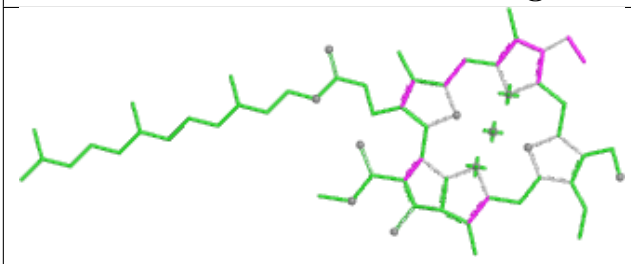


Torsions



Rings

Ligand CHL S 608



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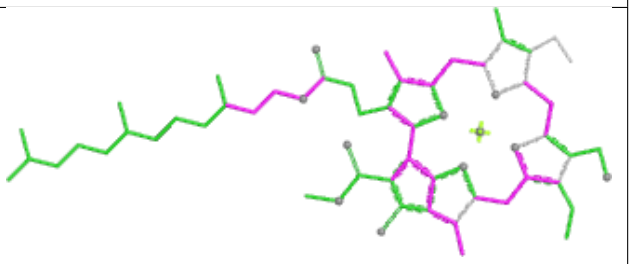
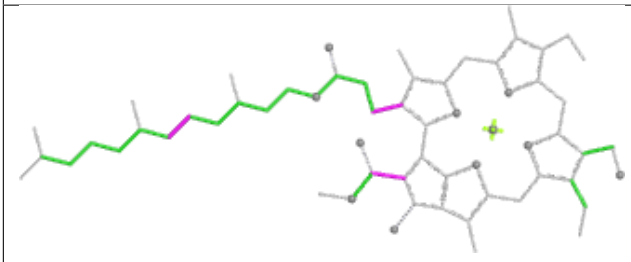
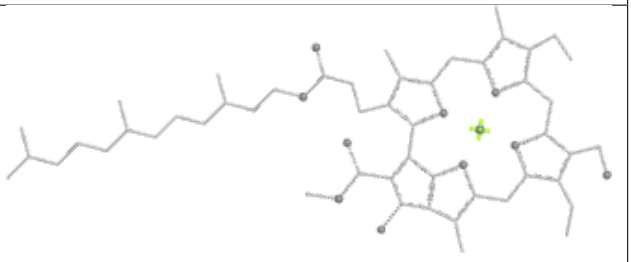


Bond angles

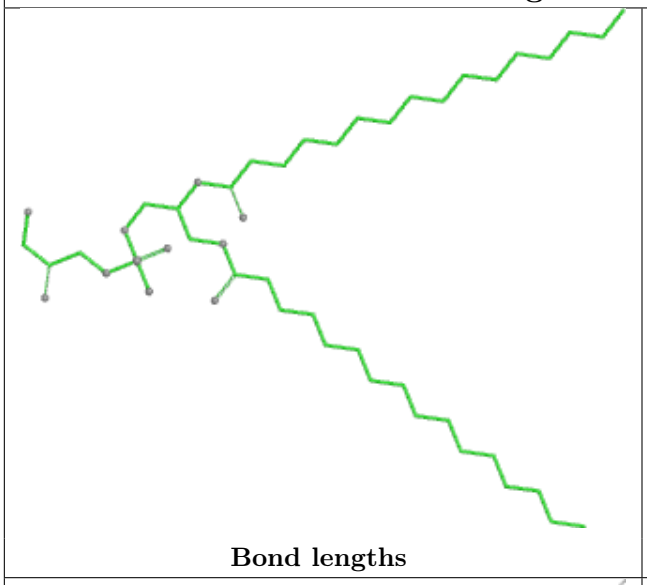


Torsions



Rings

Ligand LHG L 101



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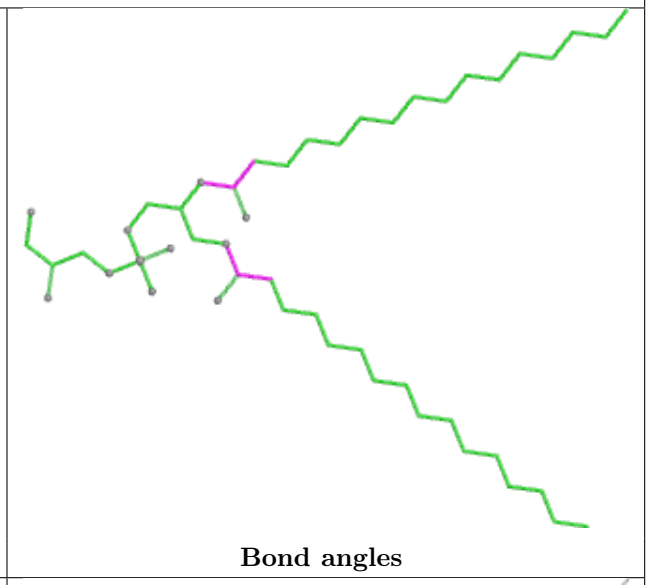
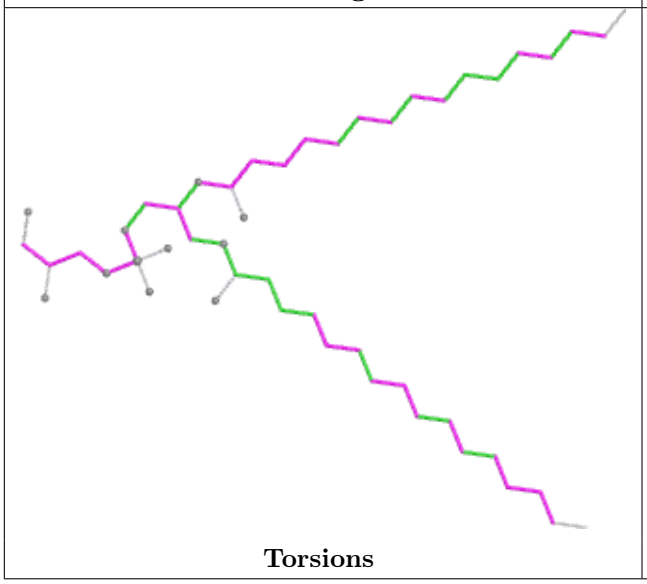


Bond angles



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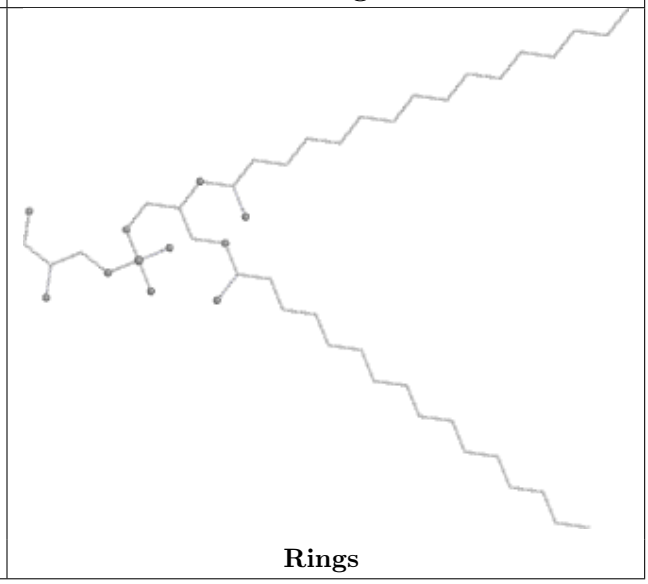
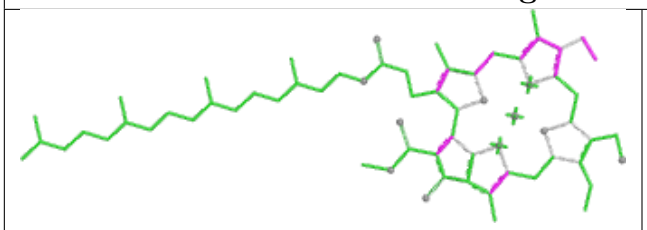


Rings

Ligand CHL y1 609



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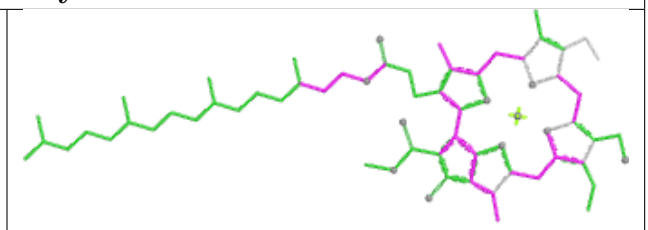
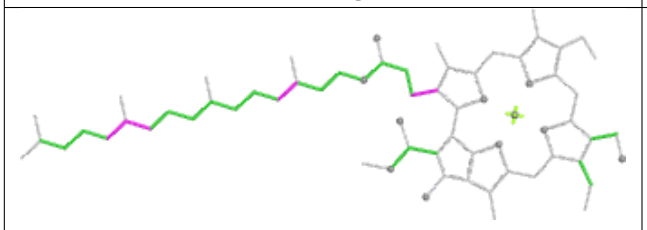


Bond angles



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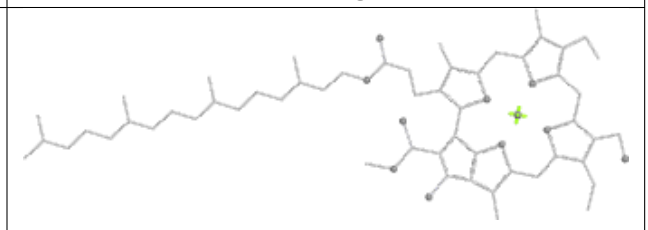
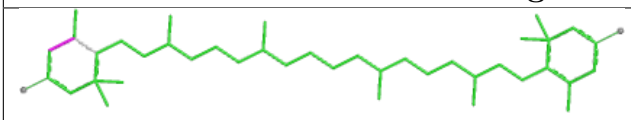


Rings

Ligand LUT n 620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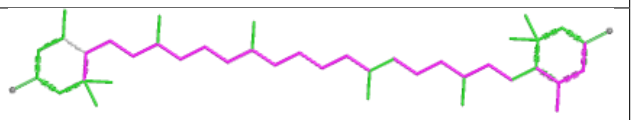
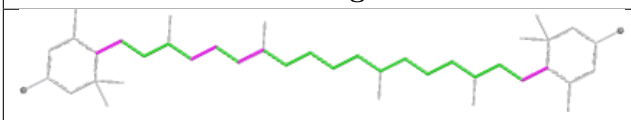

Bond angles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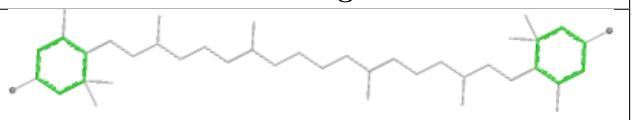
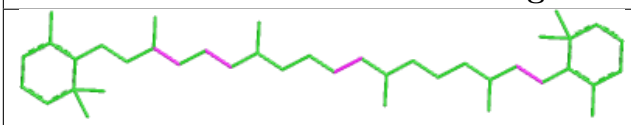

Rings

Ligand BCR c 514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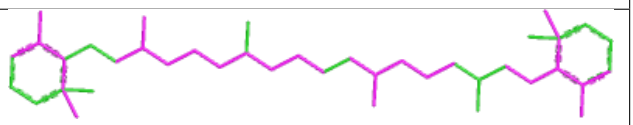
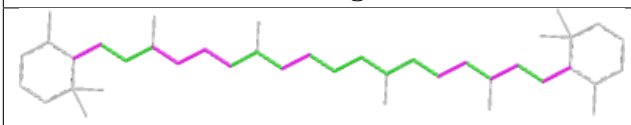
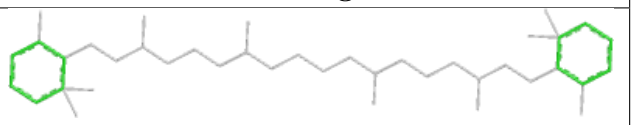
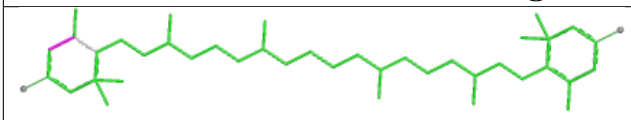

Bond angles


Torsions


Rings

Ligand LUT n 621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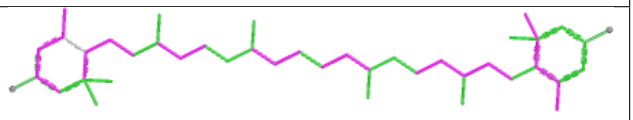
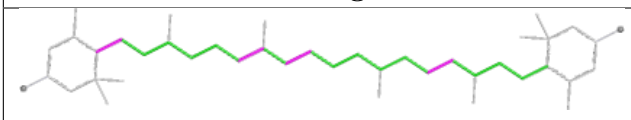
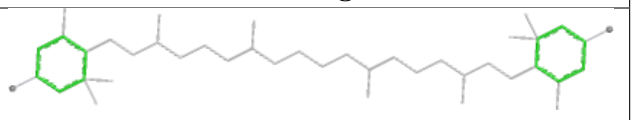
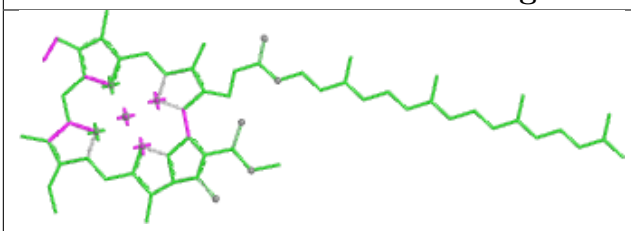

Bond angles


Torsions


Rings

Ligand CLA g1 602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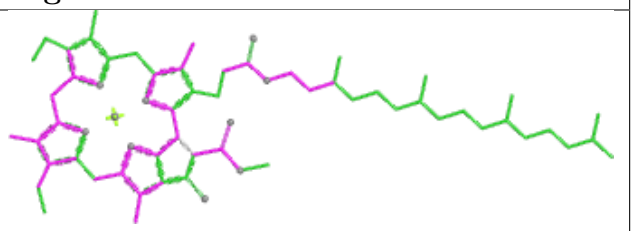
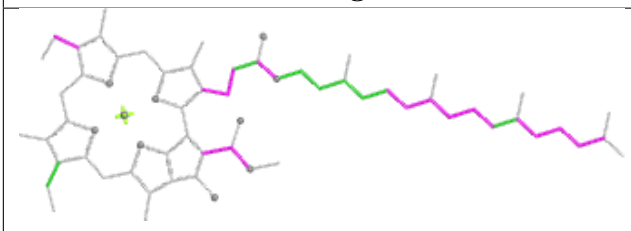
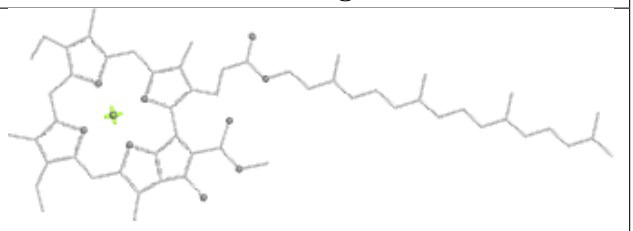
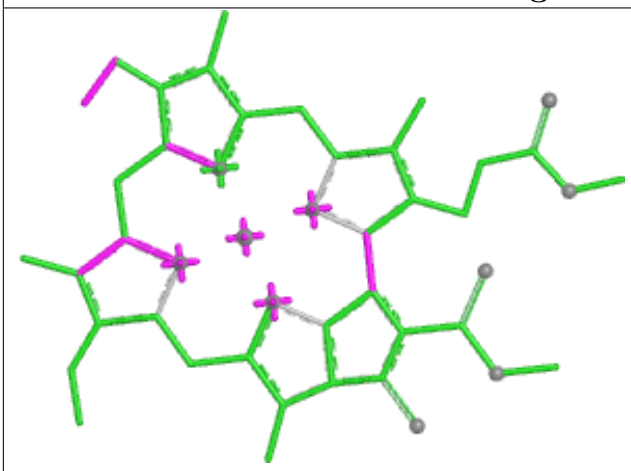

Bond angles

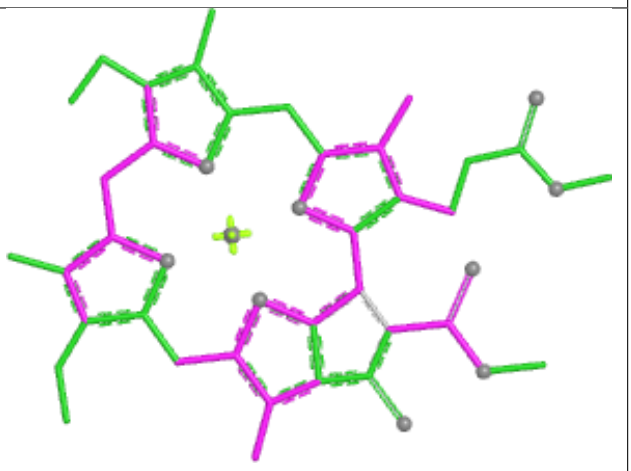

Torsions


Rings

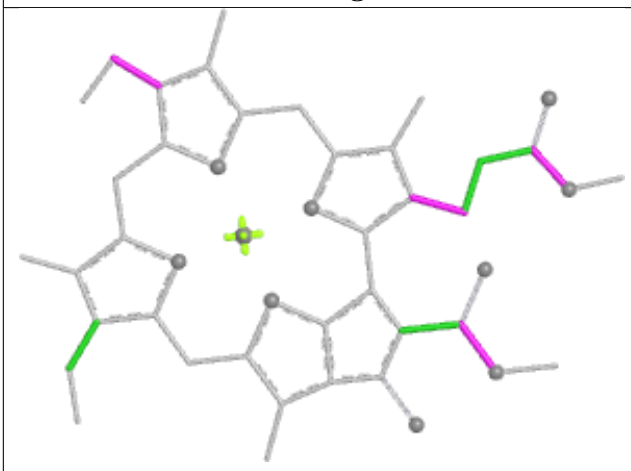
Ligand CLA r 611



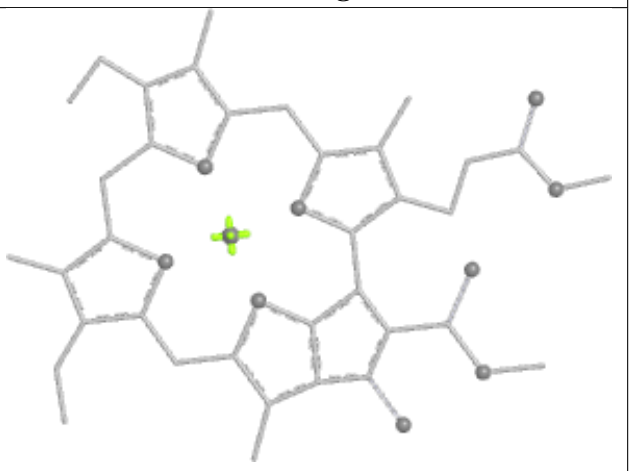
Bond lengths



Bond angles

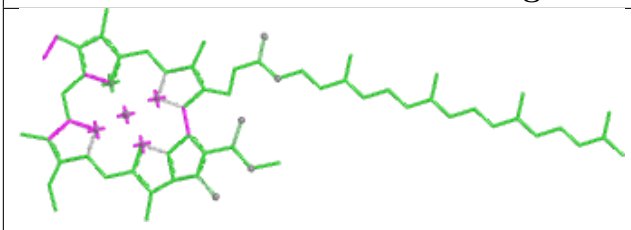


Torsions



Rings

Ligand CLA G 613



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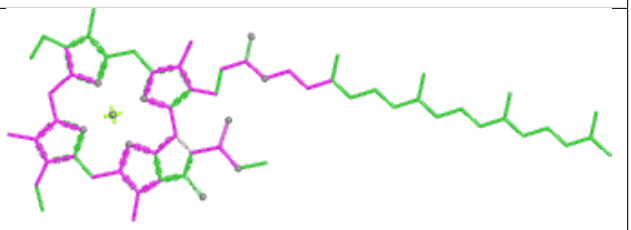
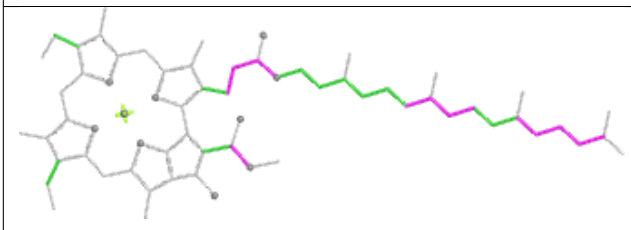


Bond angles



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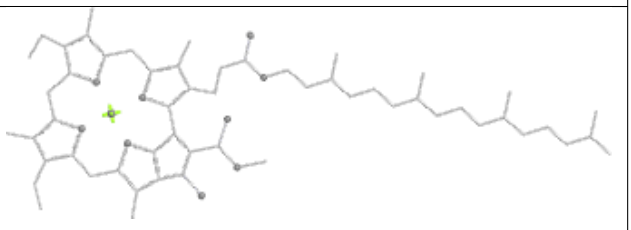
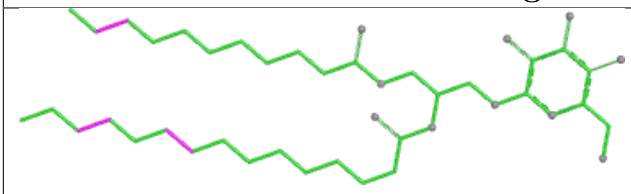


Rings

Ligand LMG J 101



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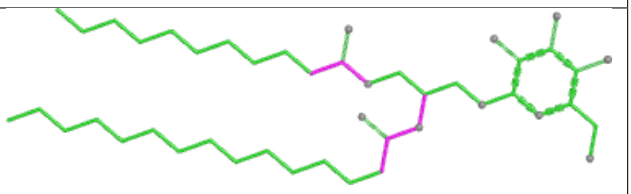

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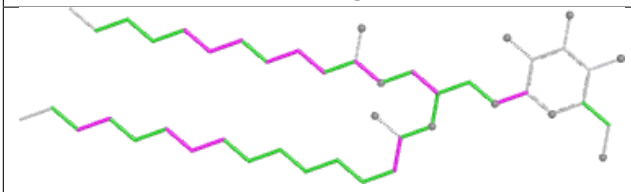

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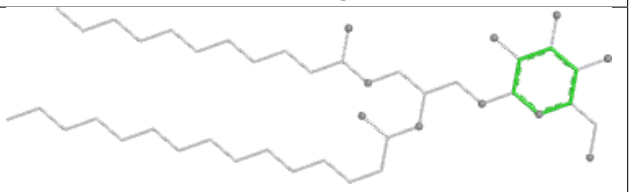
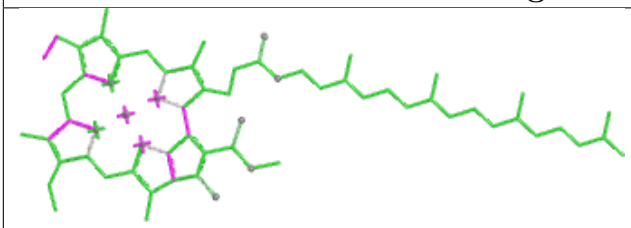


Rings

Ligand CLA S 610



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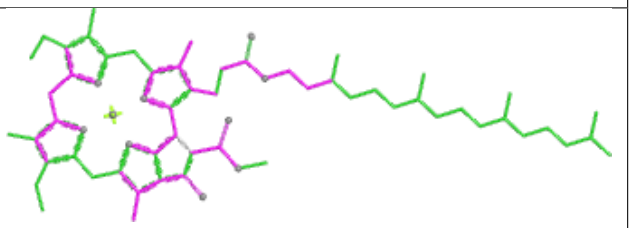
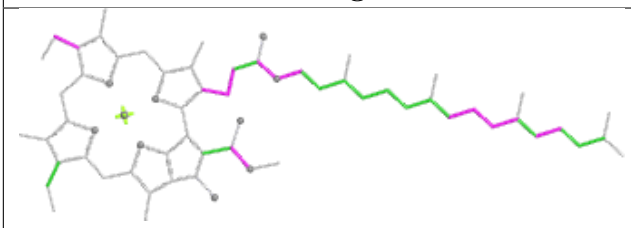
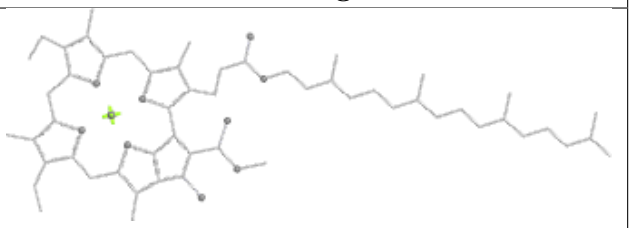


Bond angles

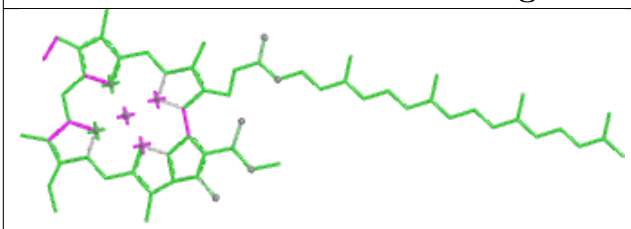


Torsions



Rings

Ligand CLA y1 604



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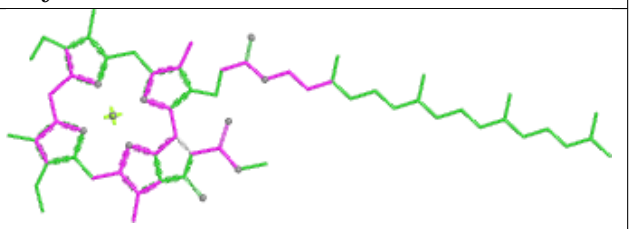
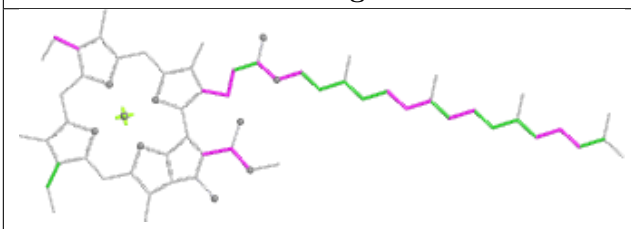
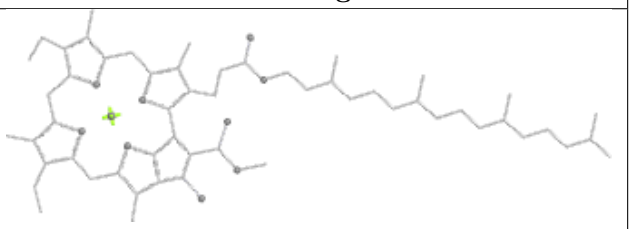


Bond angles

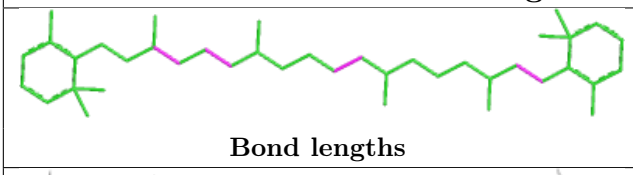


Torsions



Rings

Ligand BCR b 618



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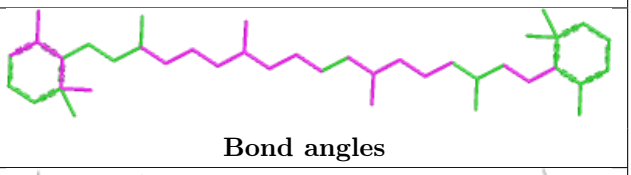
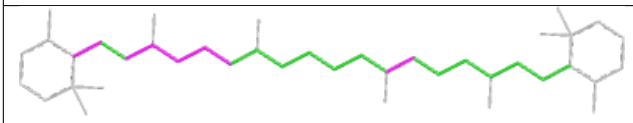
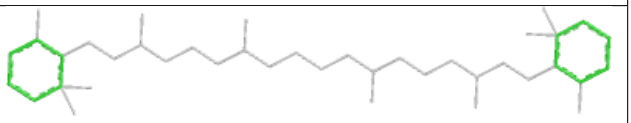


Bond angles

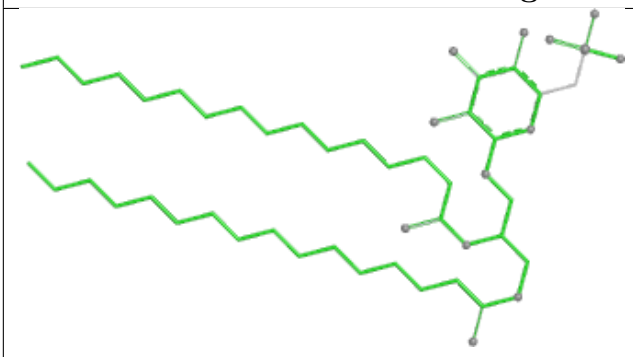


Torsions



Rings

Ligand SQD c1 526



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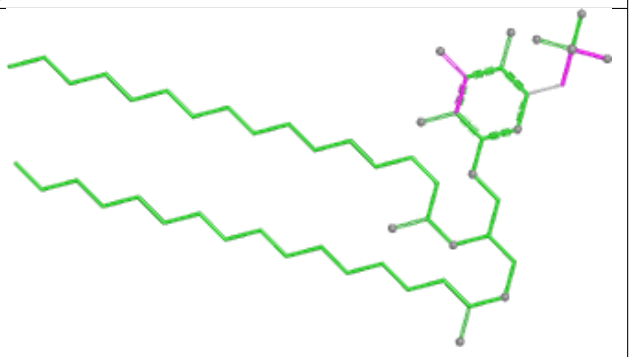
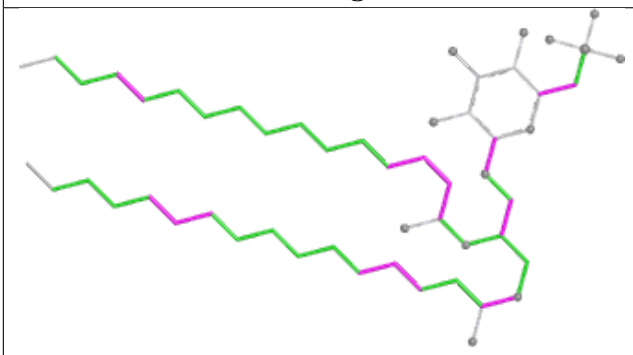
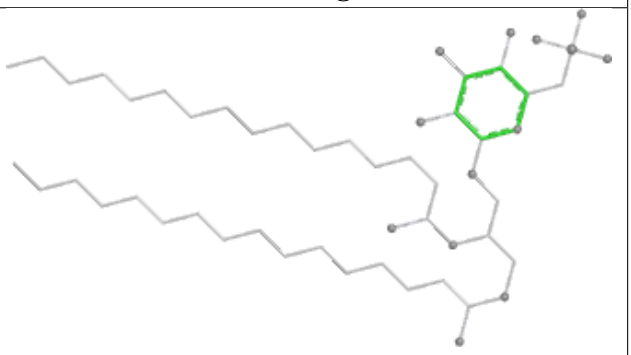


Bond angles

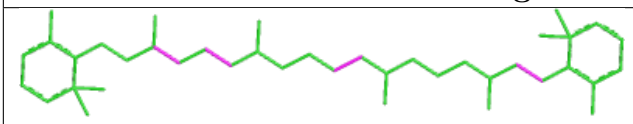


Torsions



Rings

Ligand BCR C1 515



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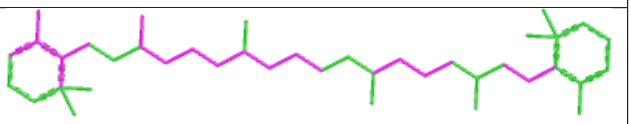
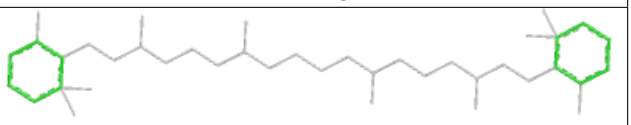


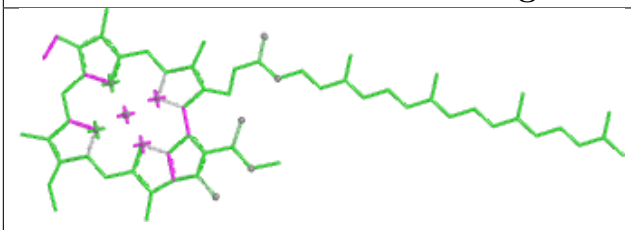
Bond angles

Torsions



Rings

Ligand CLA y1 611



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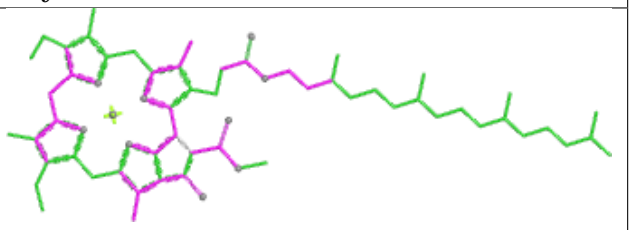

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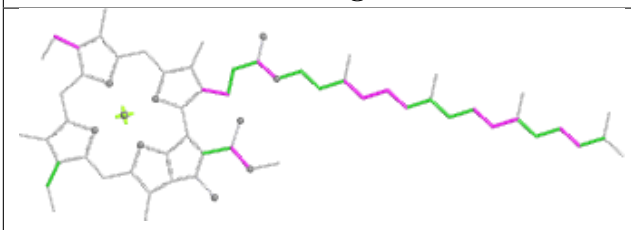

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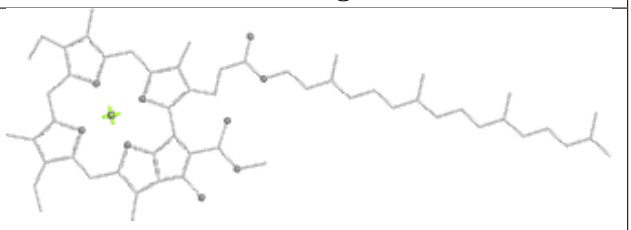
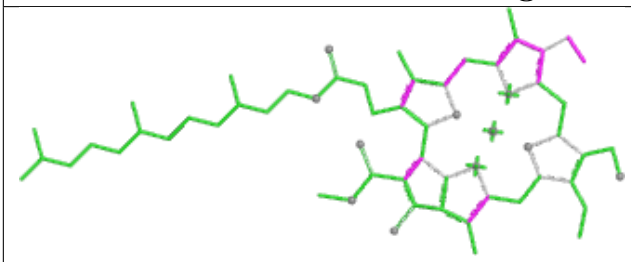


Rings

Ligand CHL S1 608



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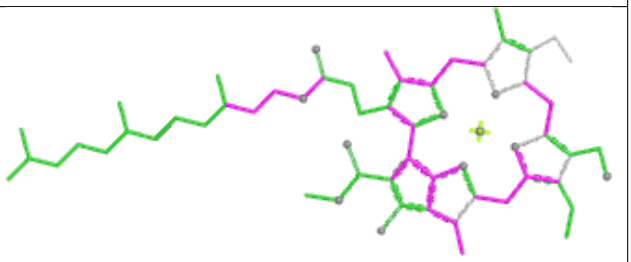

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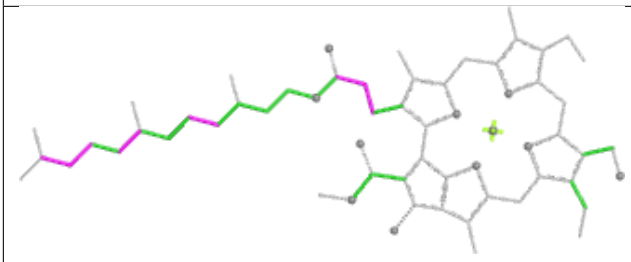

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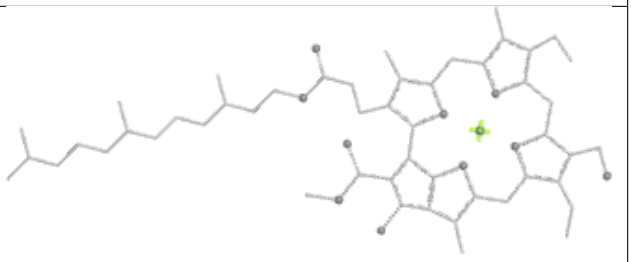
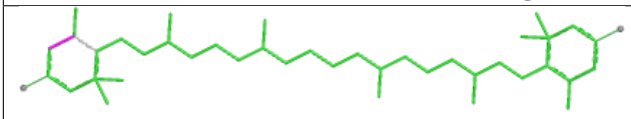


Rings

Ligand LUT y1 620



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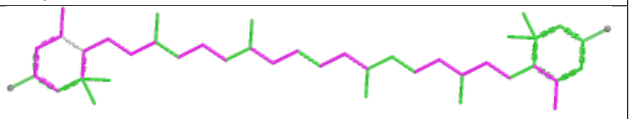

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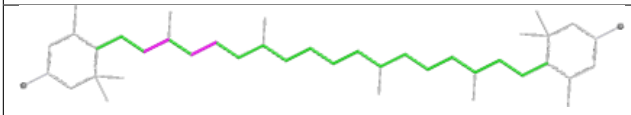

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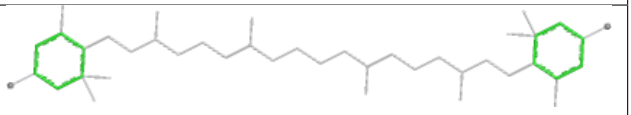
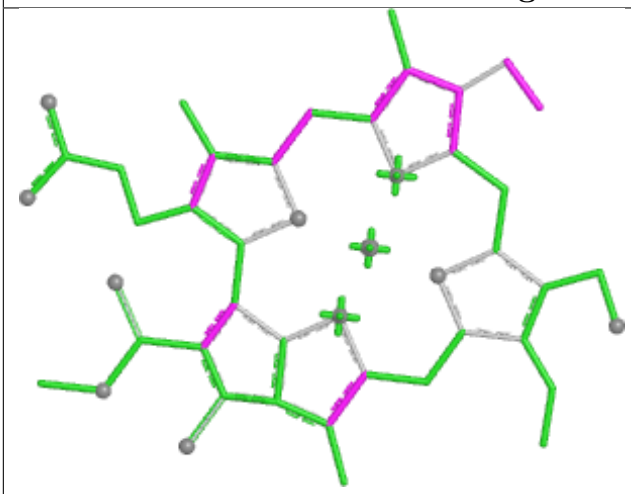


Rings

Ligand CHL y1 605



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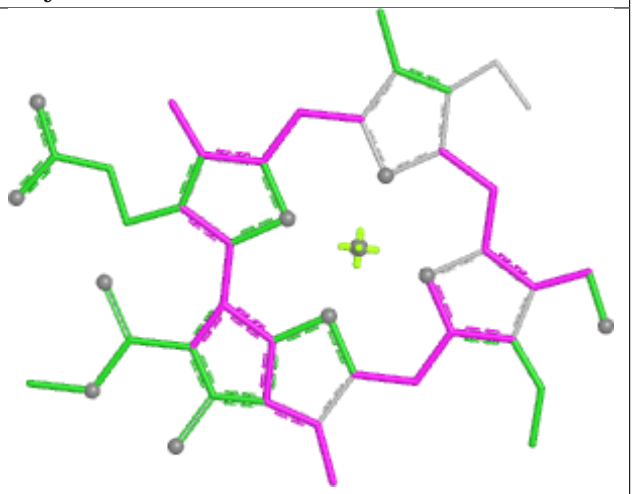

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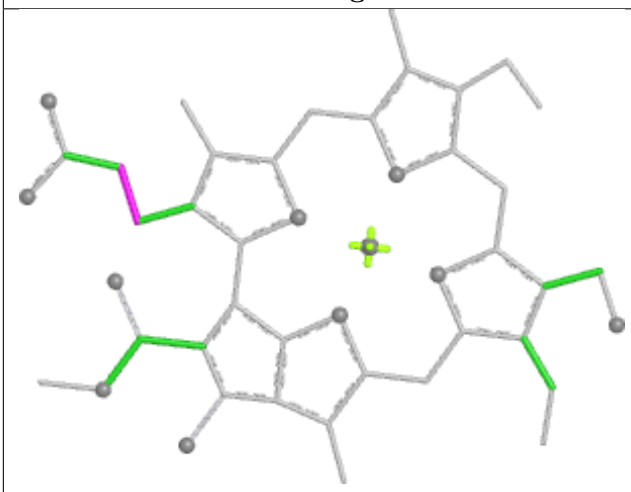

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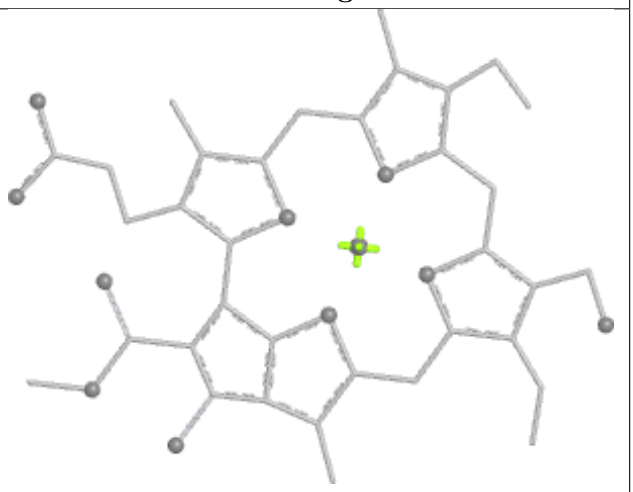
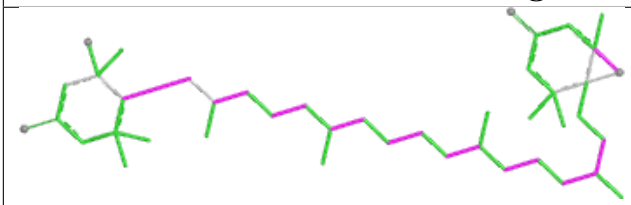


Rings

Ligand NEX r 623



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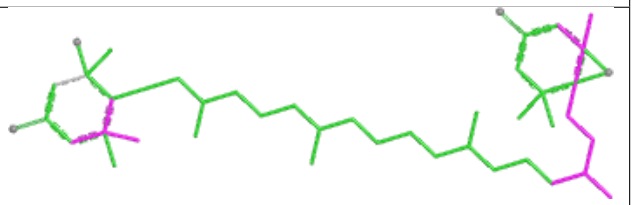

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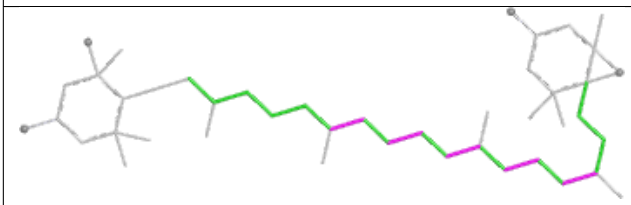

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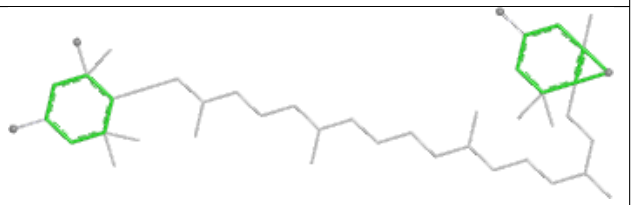
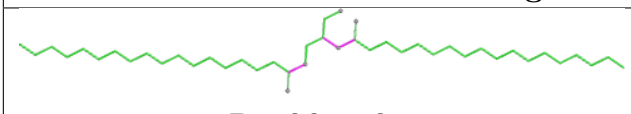


Rings

Ligand DGA c 524



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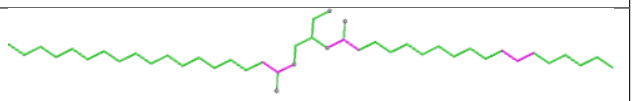
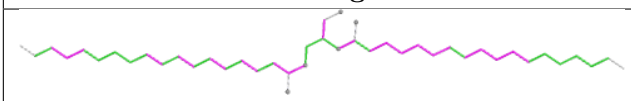


Bond angles



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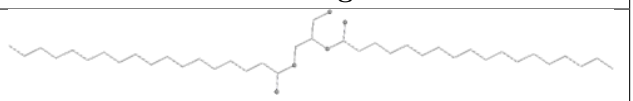
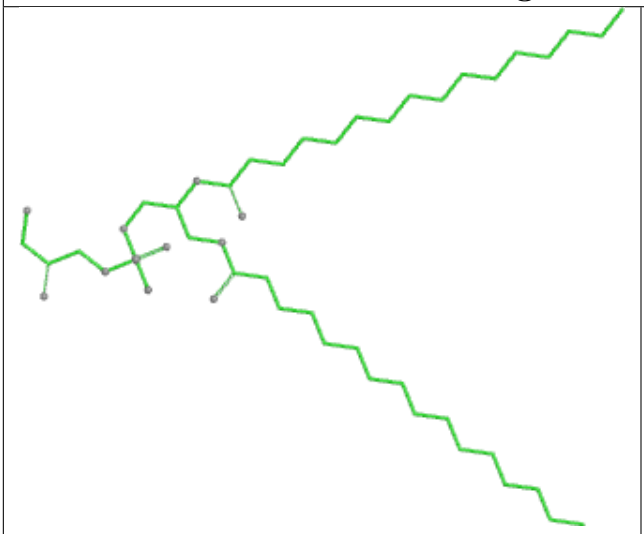


Rings

Ligand LHG L1 101



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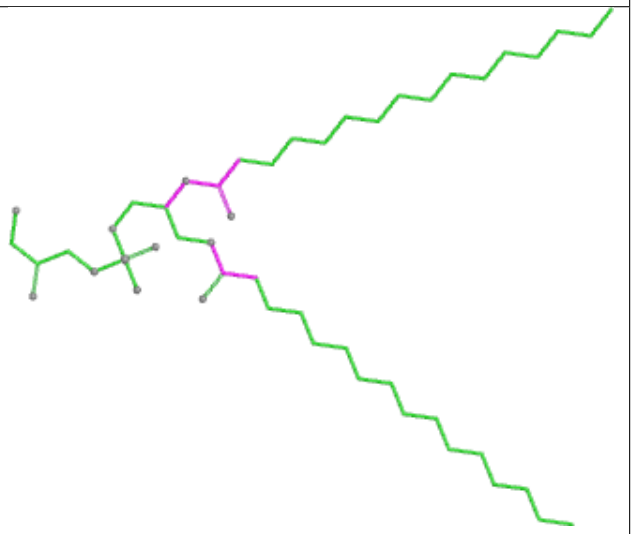

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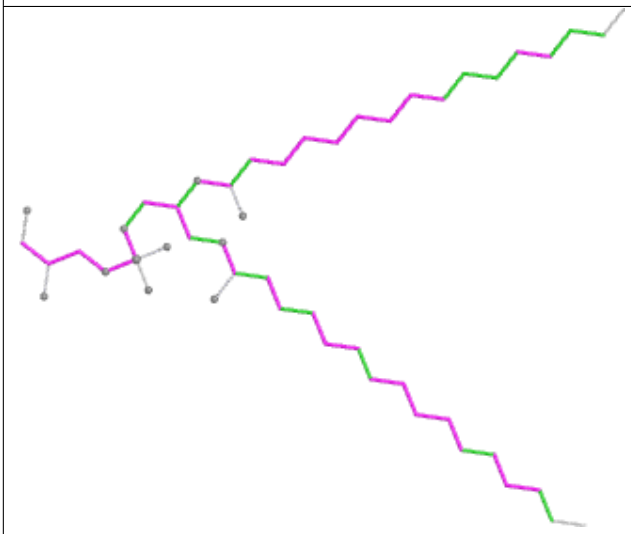

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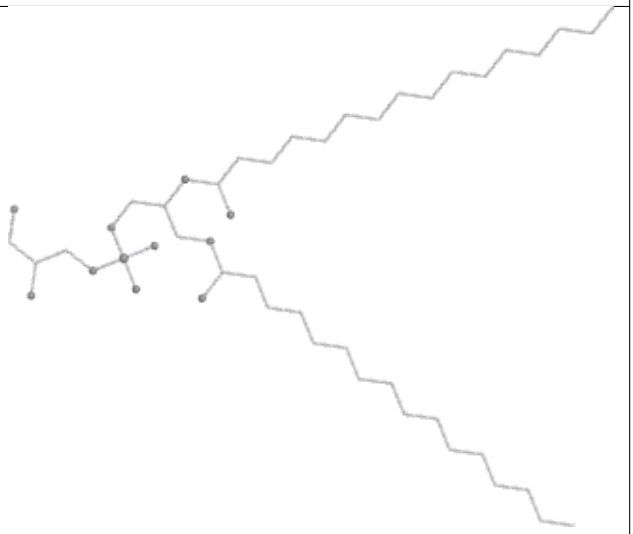
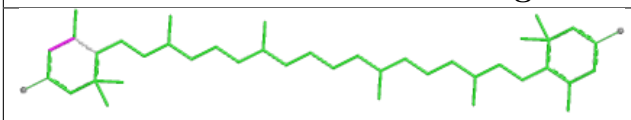


Rings

Ligand LUT N1 620



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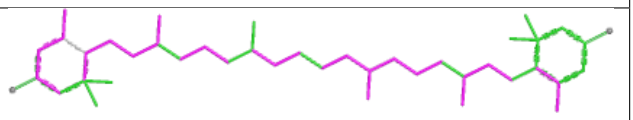

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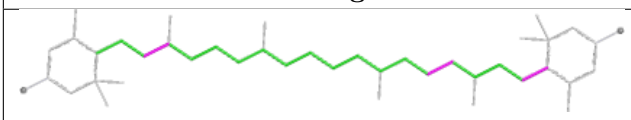

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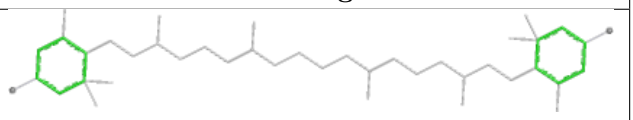
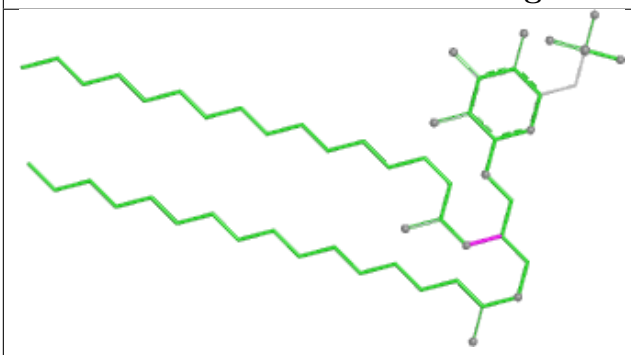


Rings

Ligand SQD C 526



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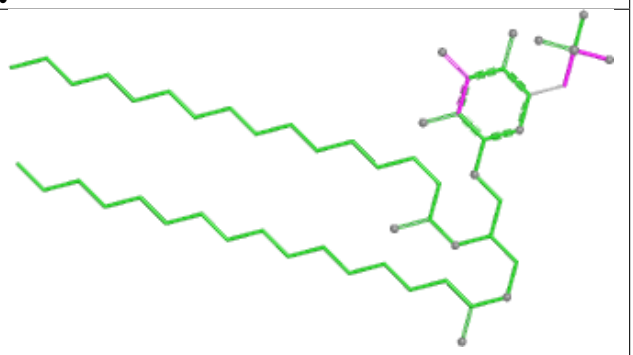

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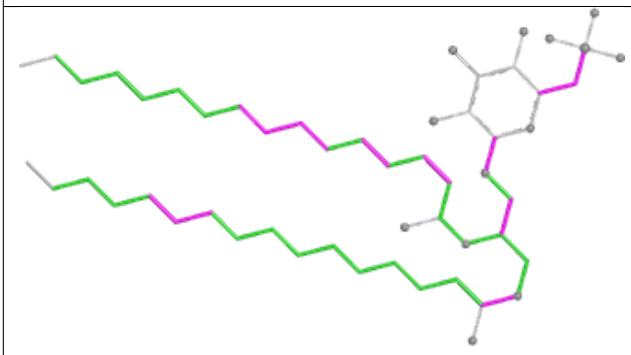

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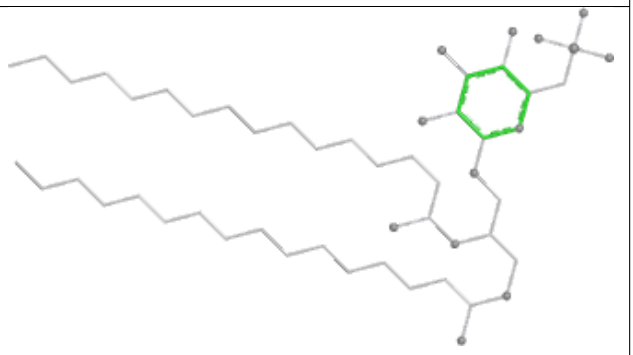
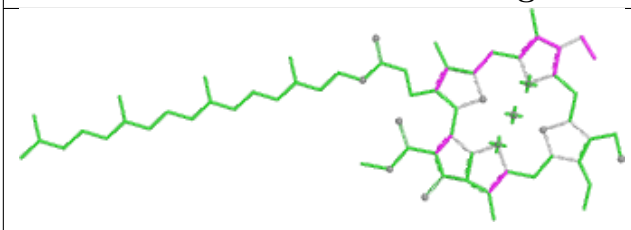


Rings

Ligand CHL n1 601



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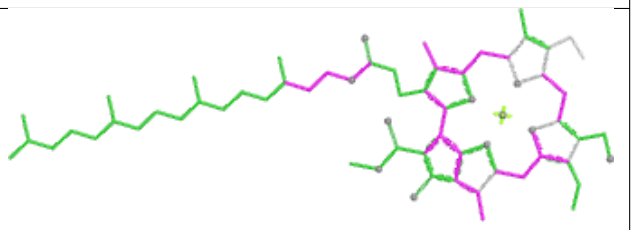
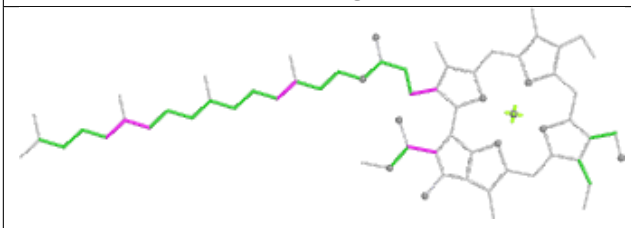
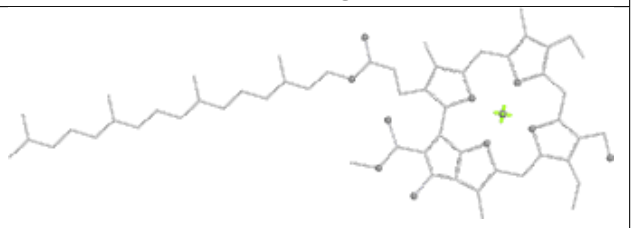


Bond angles

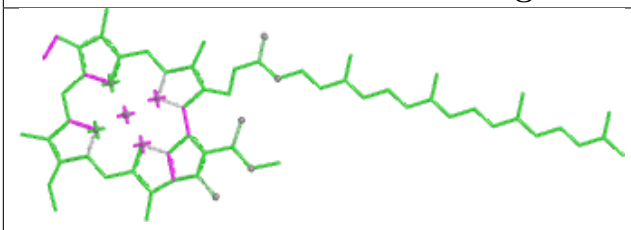


Torsions



Rings

Ligand CLA C1 507



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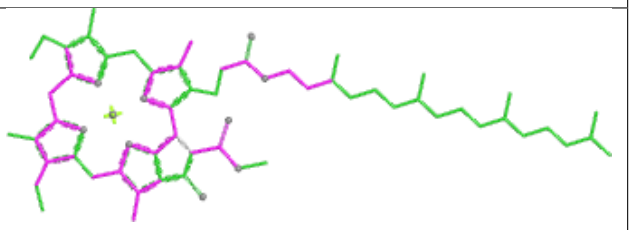
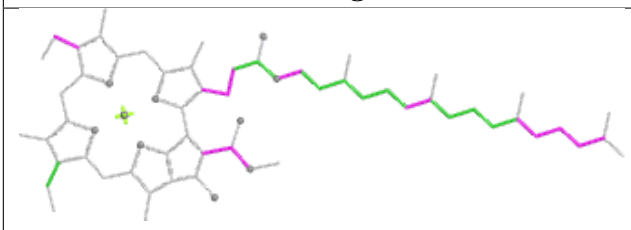
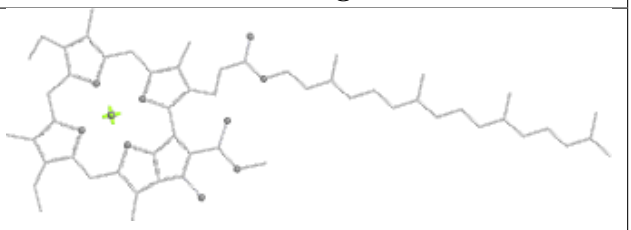


Bond angles

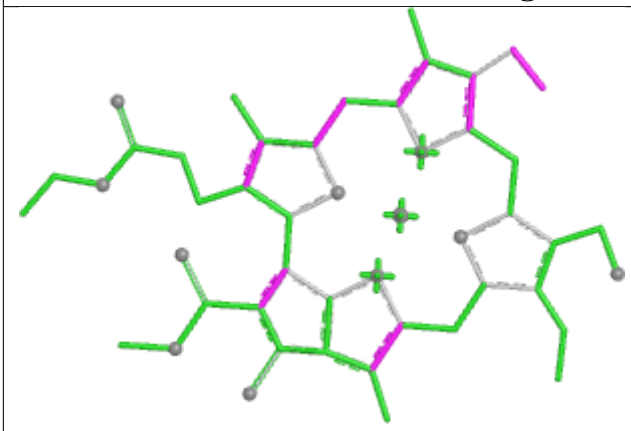


Torsions



Rings

Ligand CHL g1 605



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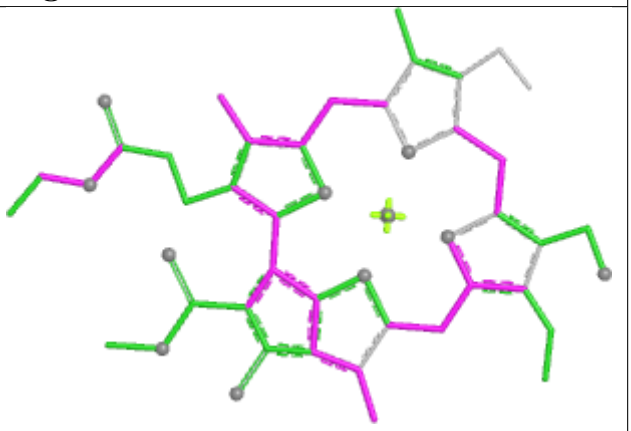
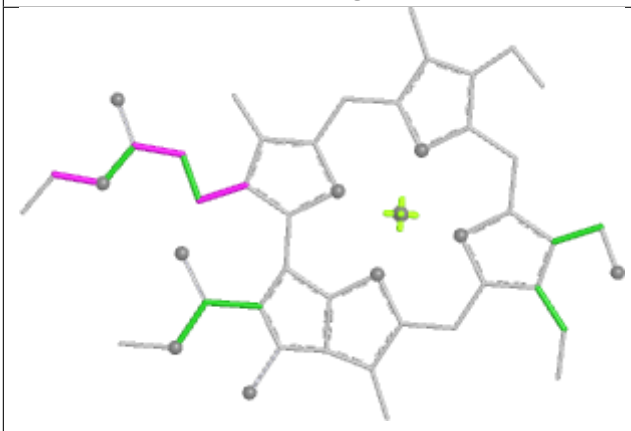


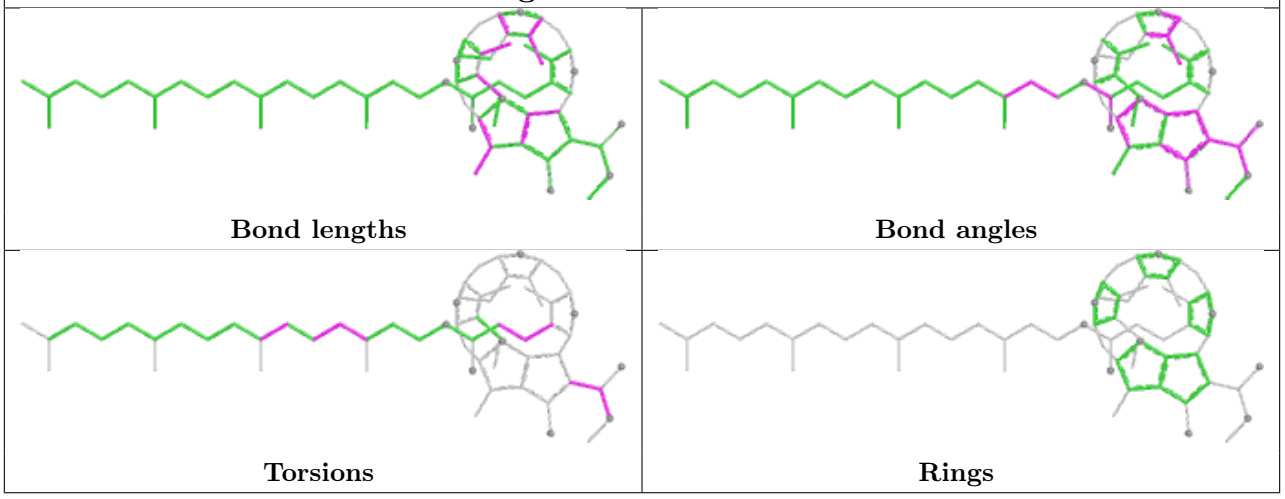
Bond angles



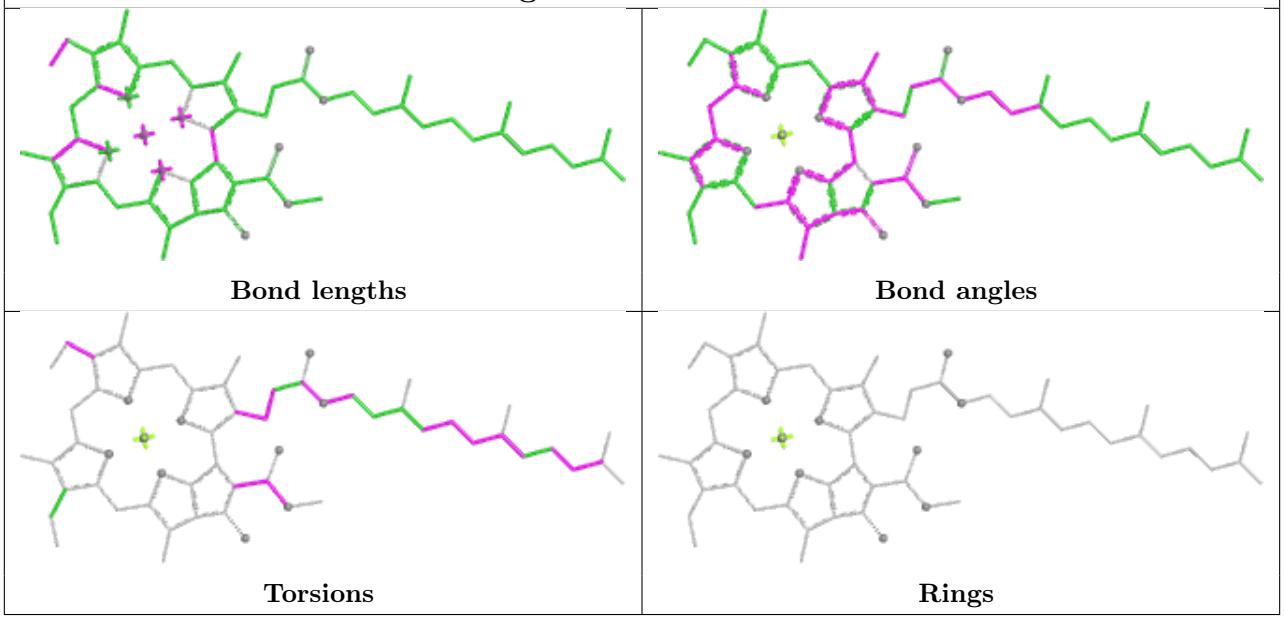
Torsions

Rings

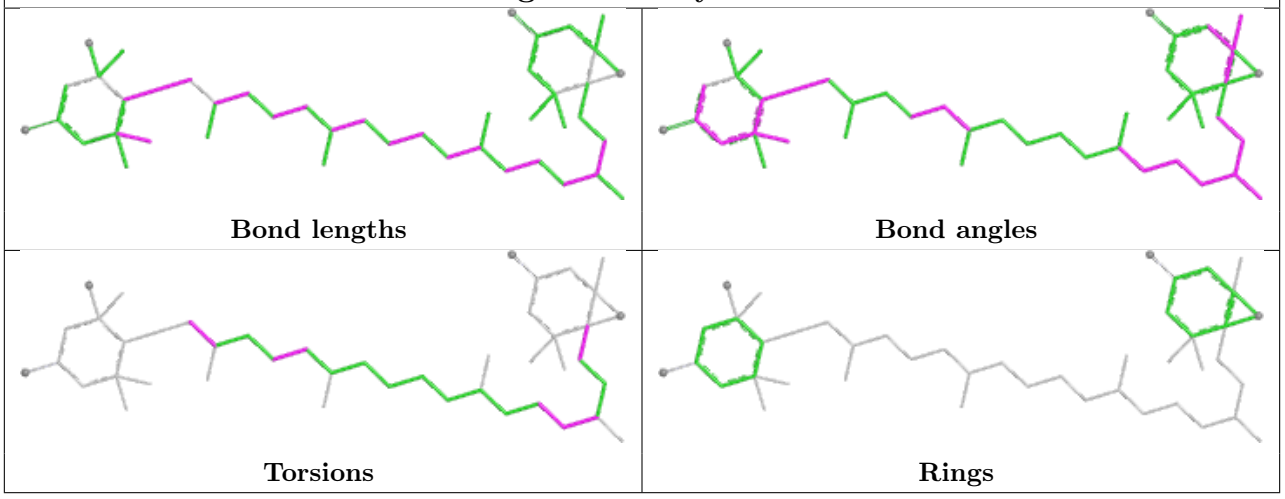
Ligand PHO a1 409



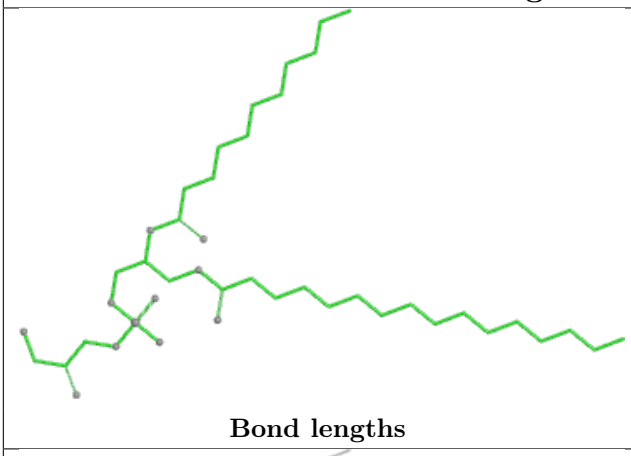
Ligand CLA S1 602



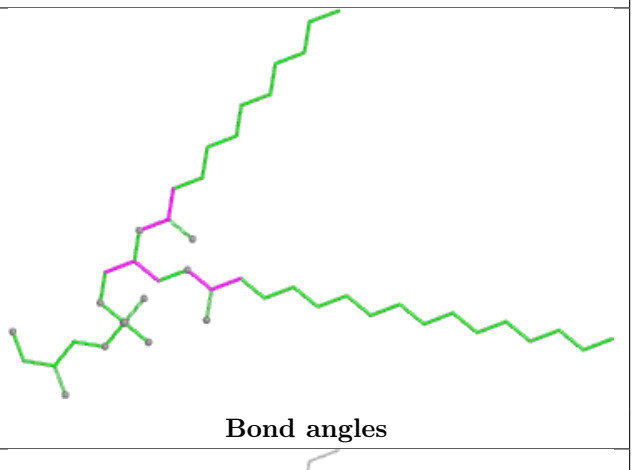
Ligand NEX y1 623



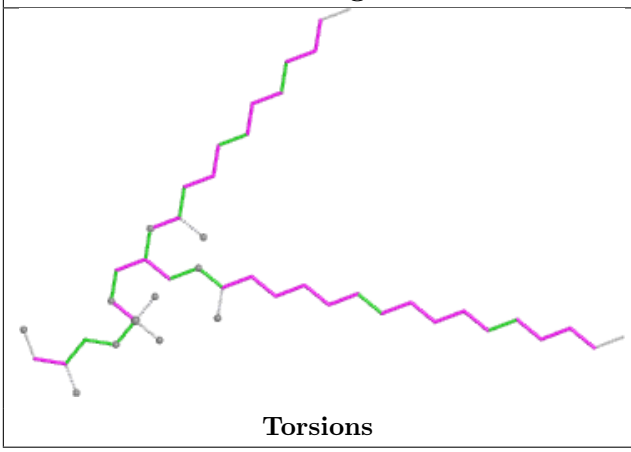
Ligand LHG d 408



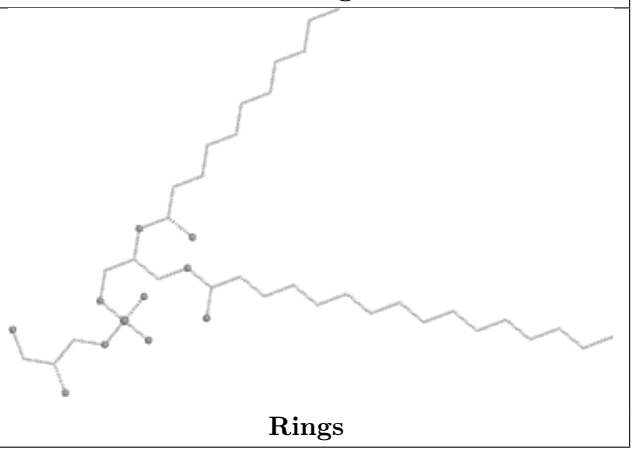
Bond lengths



Bond angles

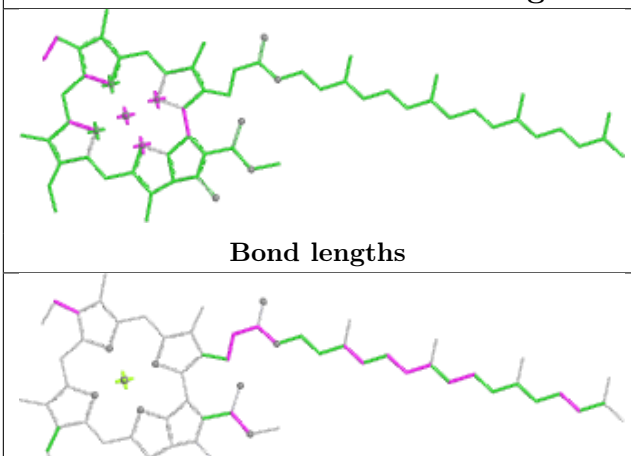


Torsions

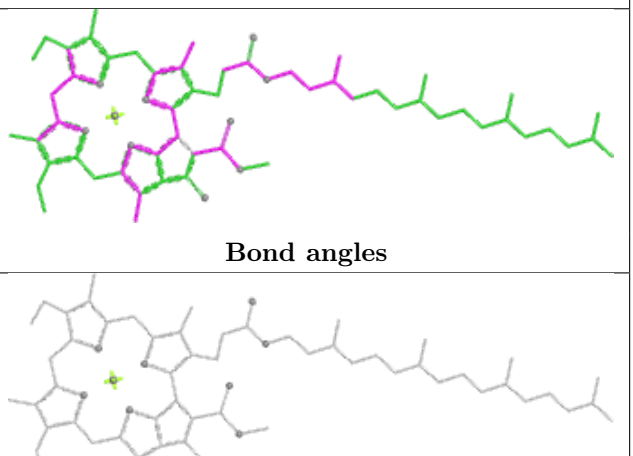


Rings

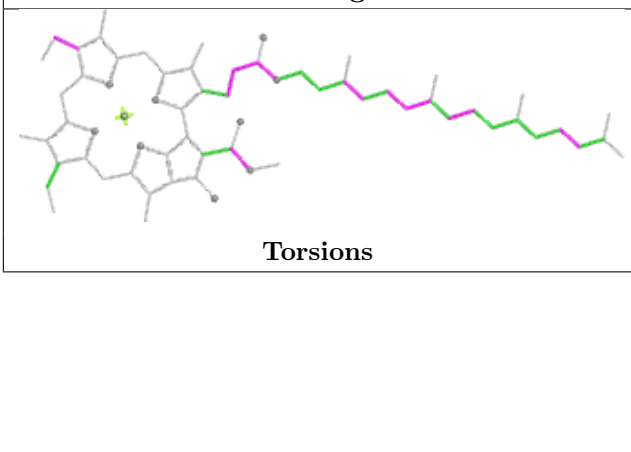
Ligand CLA b 617



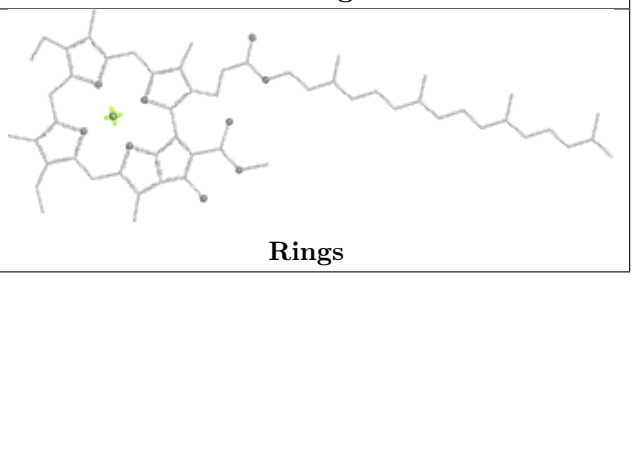
Bond lengths



Bond angles

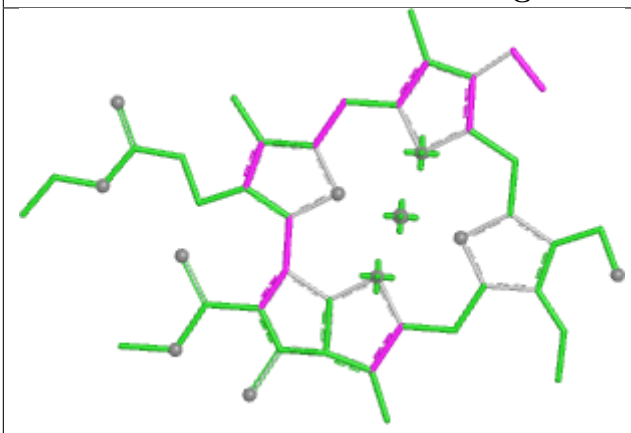


Torsions



Rings

Ligand CHL G1 605



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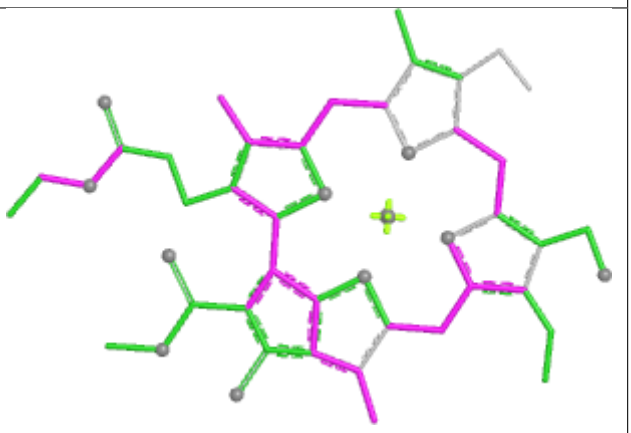
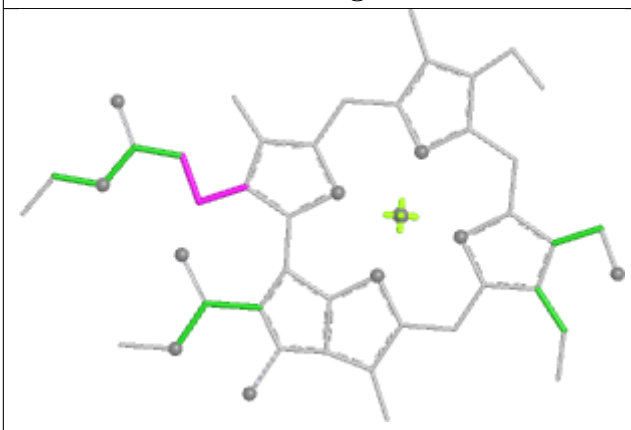


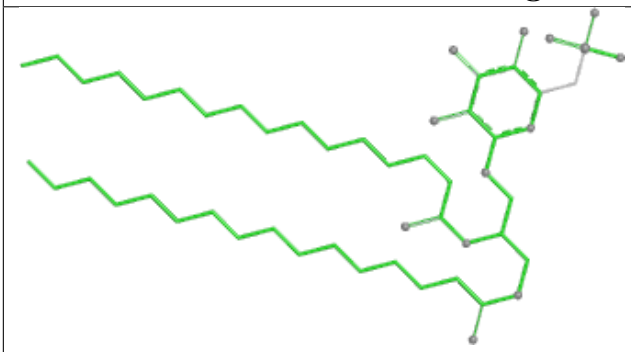
Bond angles



Torsions

Rings

Ligand SQD B 621



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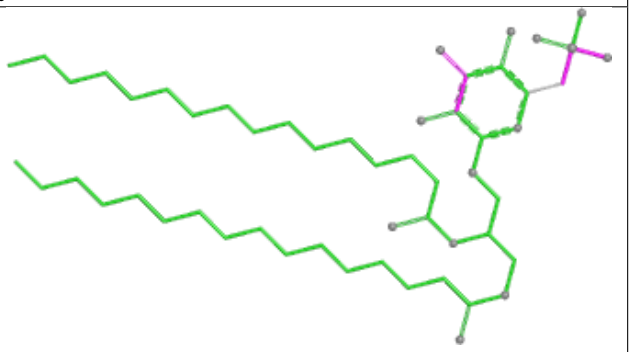
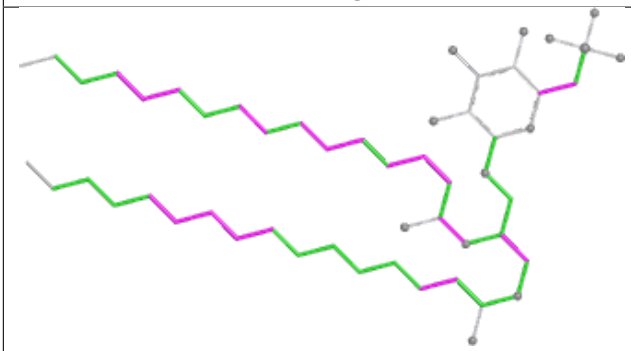
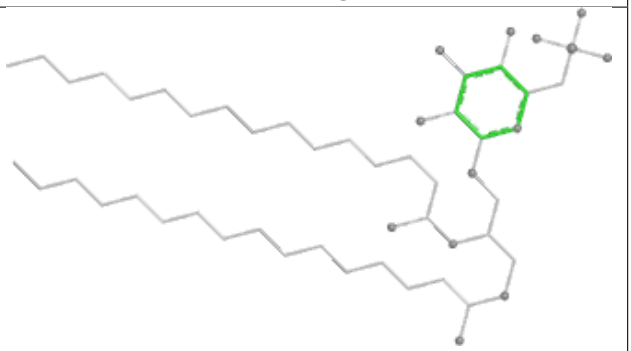


Bond angles

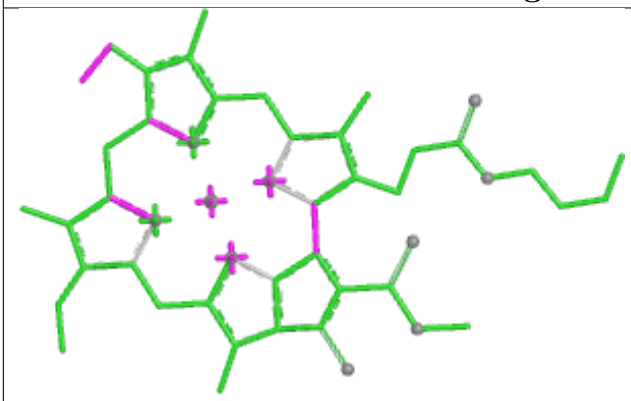


Torsions



Rings

Ligand CLA R 604



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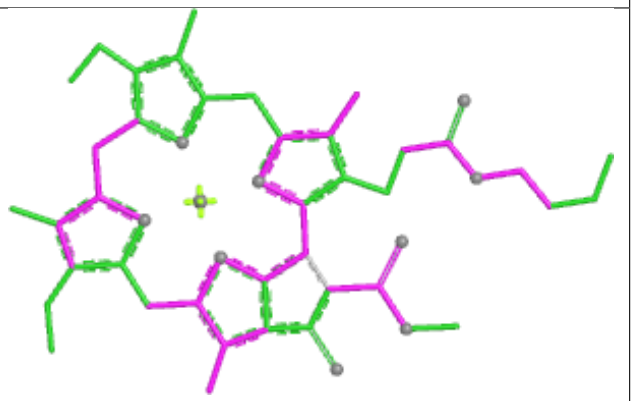
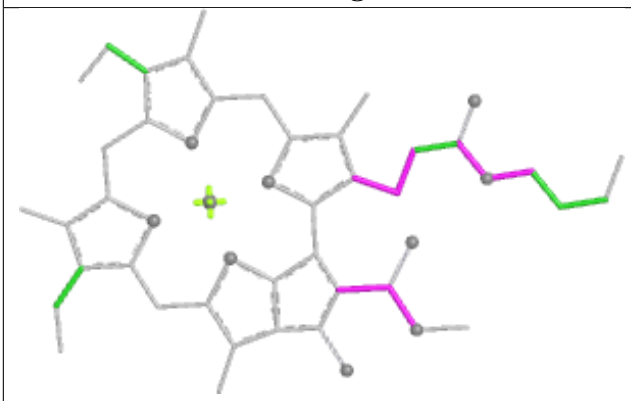


Bond angles



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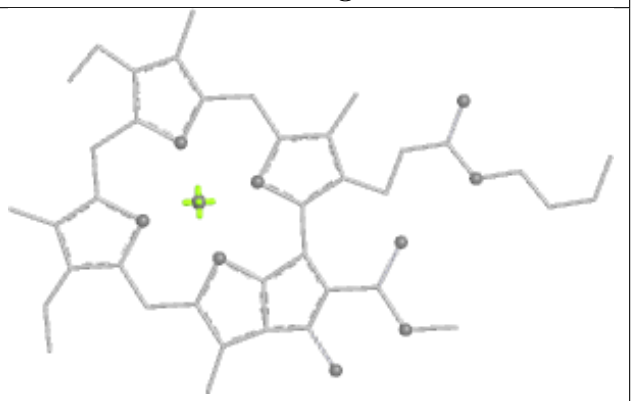
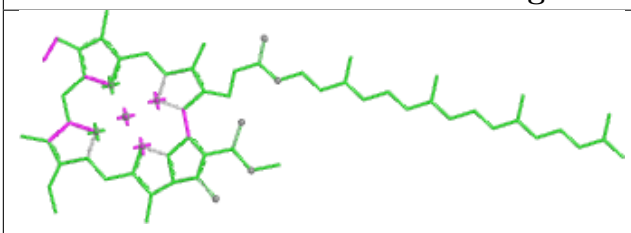


Rings

Ligand CLA y 610



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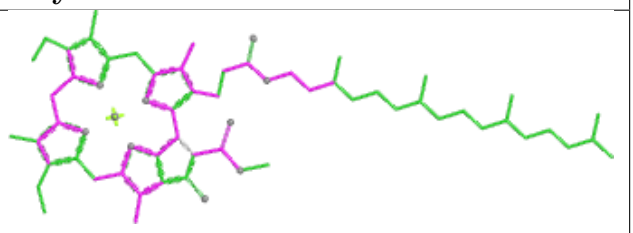
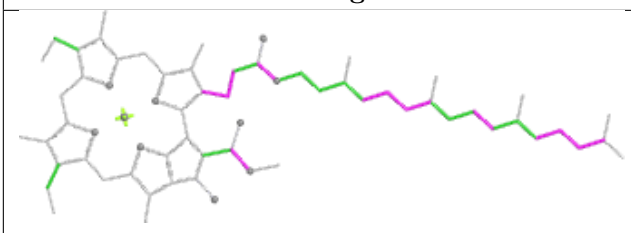
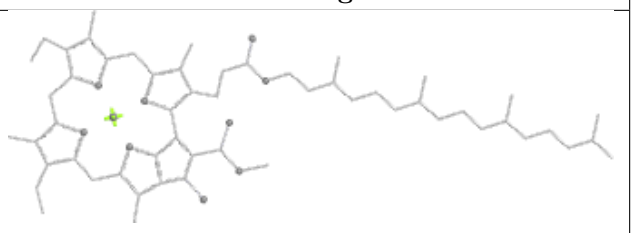


Bond angles

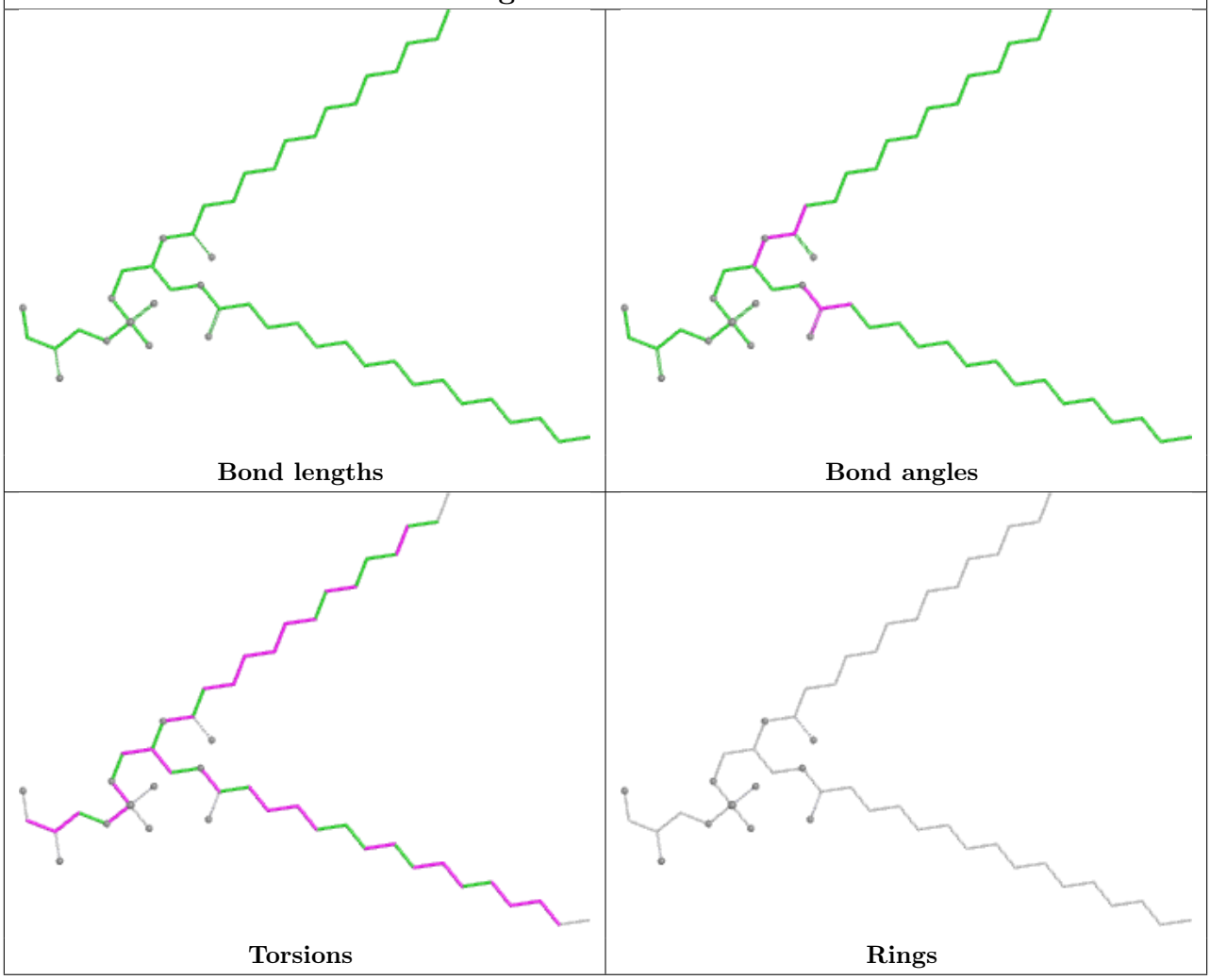


Torsions

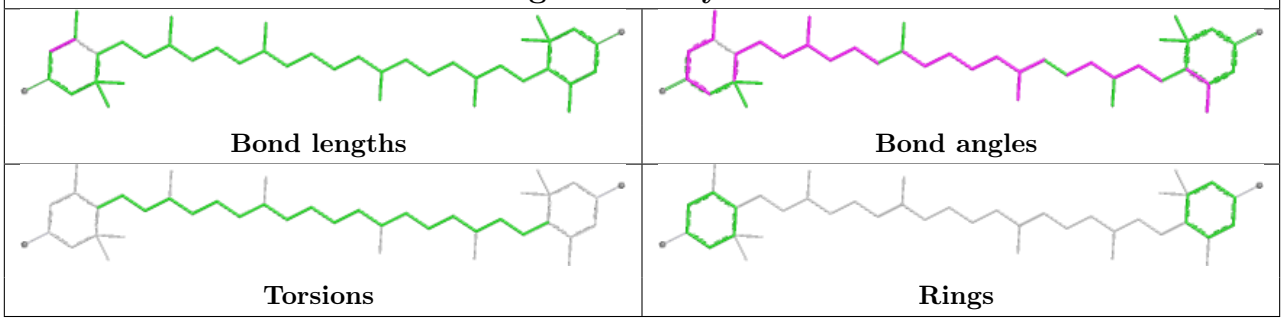


Rings

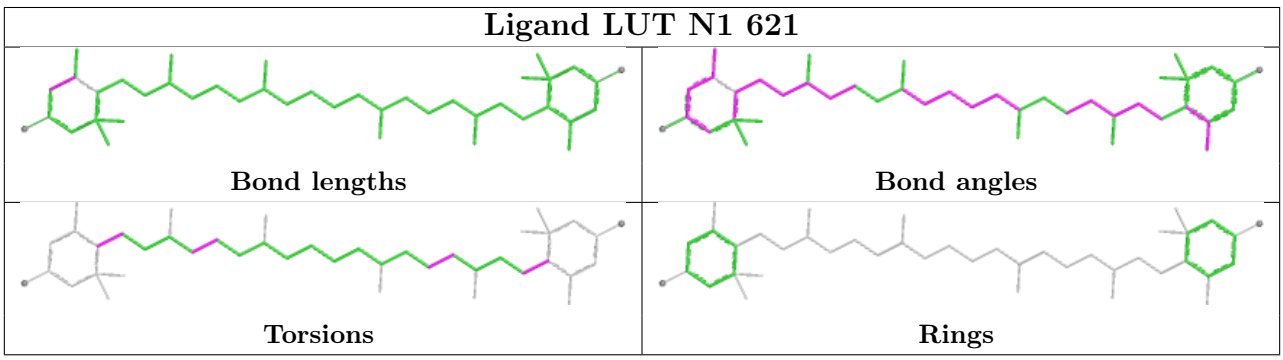
Ligand LHG c 625



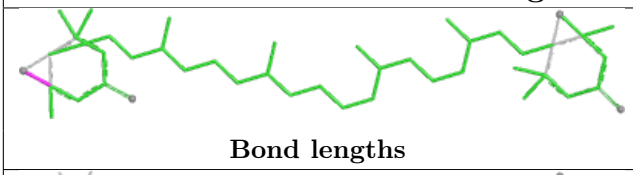
Ligand LUT y 620



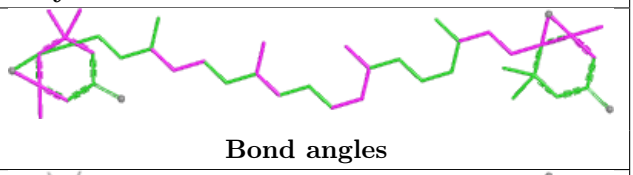
Ligand LUT N1 621



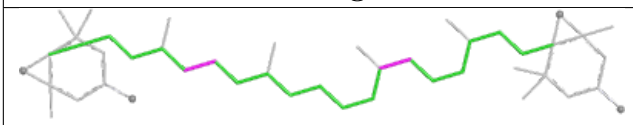
Ligand XAT y 622



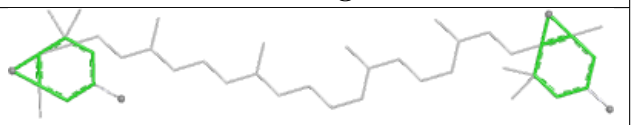
Bond lengths



Bond angles

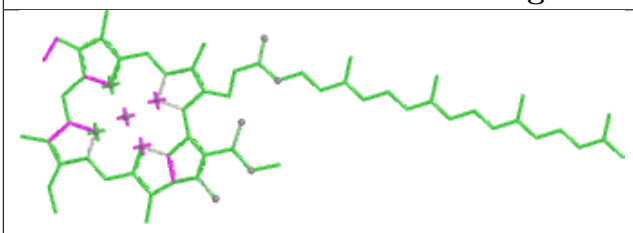


Torsions

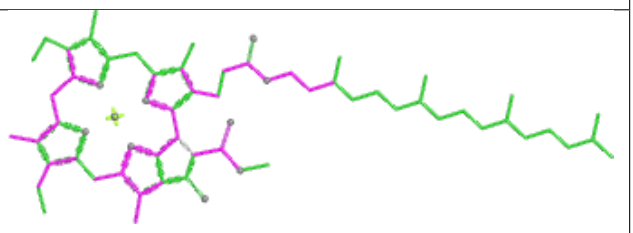


Rings

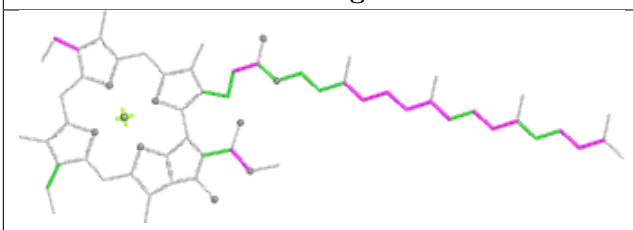
Ligand CLA d 402



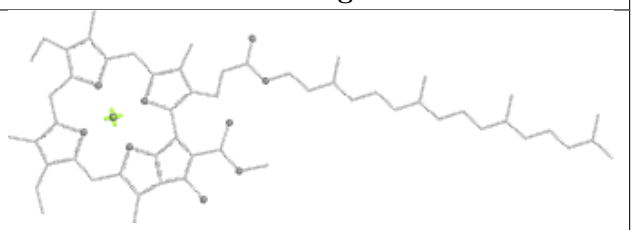
Bond lengths



Bond angles

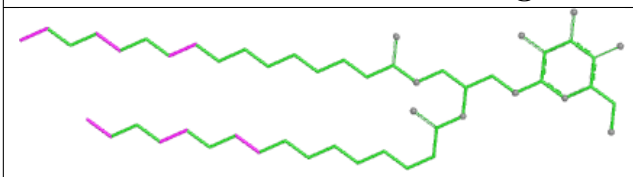


Torsions

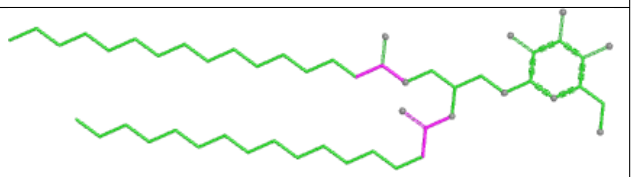


Rings

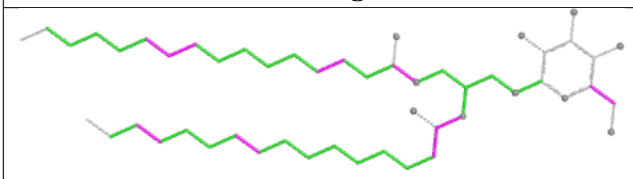
Ligand LMG c1 521



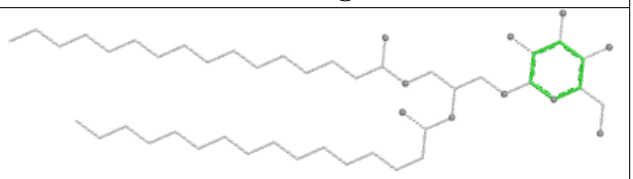
Bond lengths



Bond angles

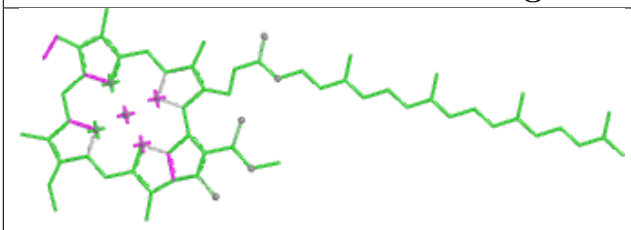


Torsions



Rings

Ligand CLA C 508



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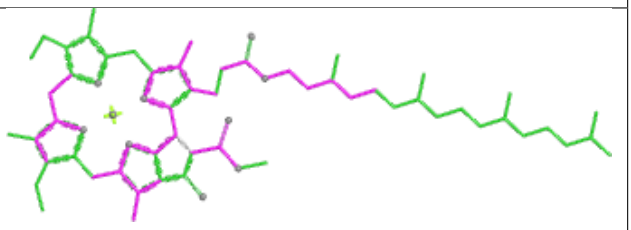
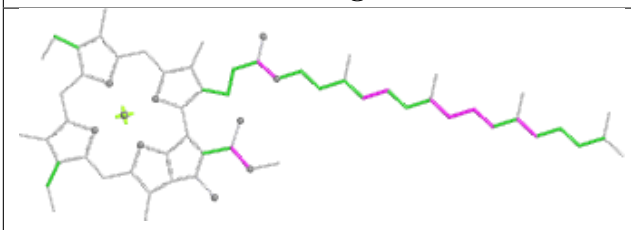


Bond angles



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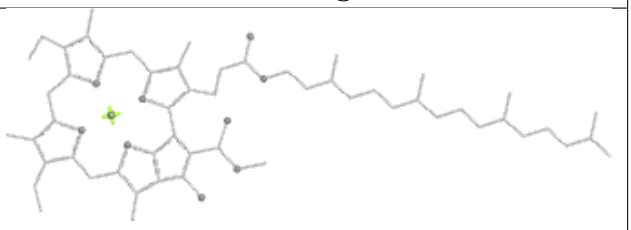
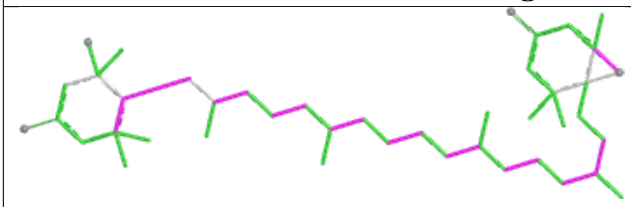


Rings

Ligand NEX r1 622



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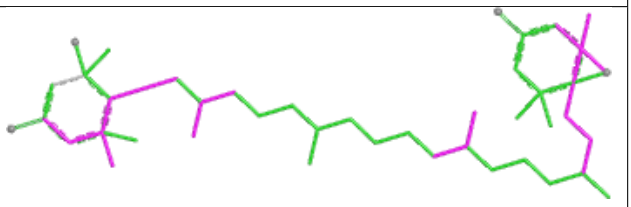
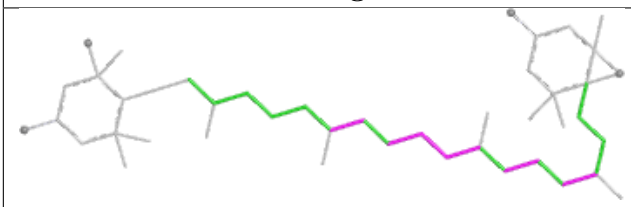


Bond angles



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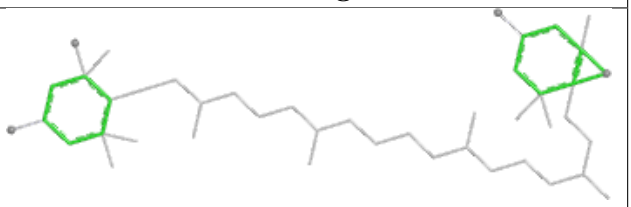
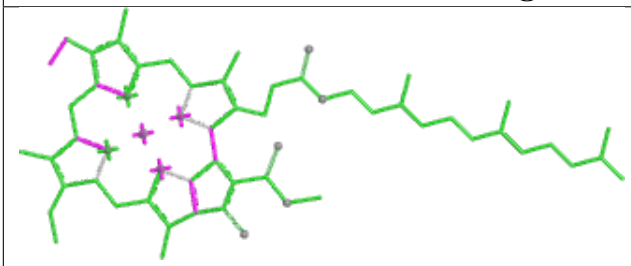


Rings

Ligand CLA S1 609



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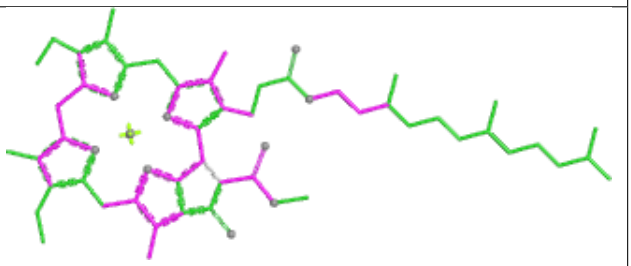
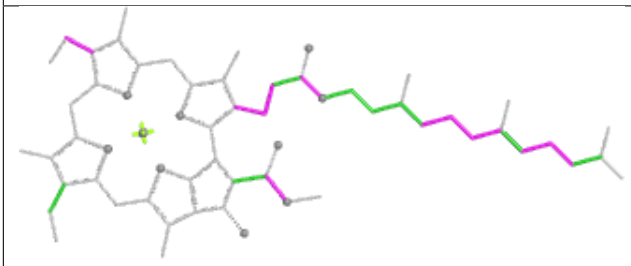
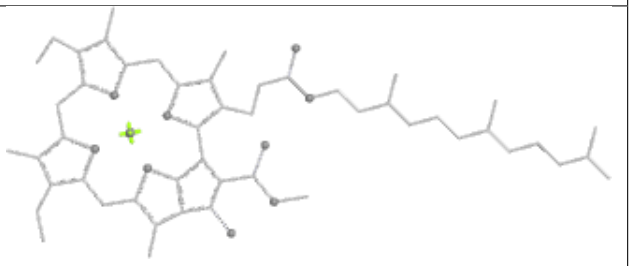


Bond angles

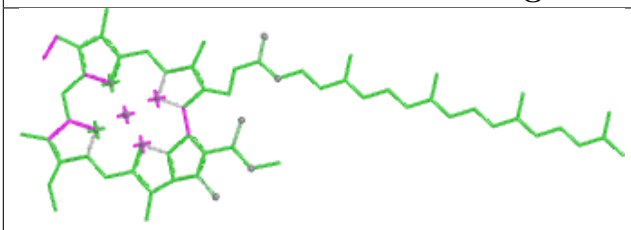


Torsions

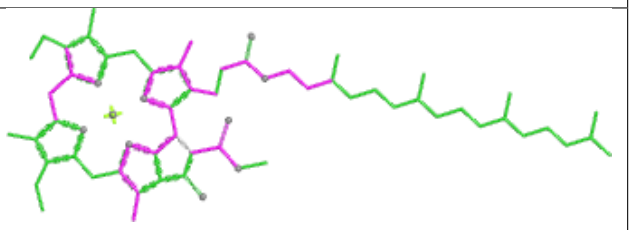


Rings

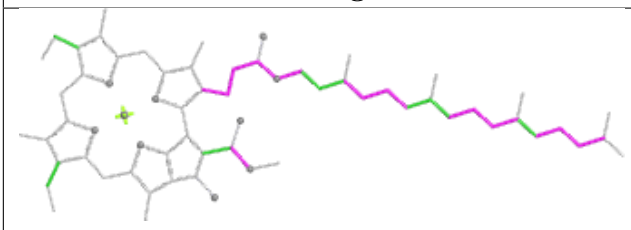
Ligand CLA B 612



Bond lengths



Bond angles



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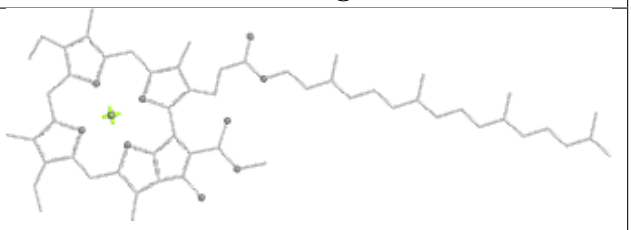
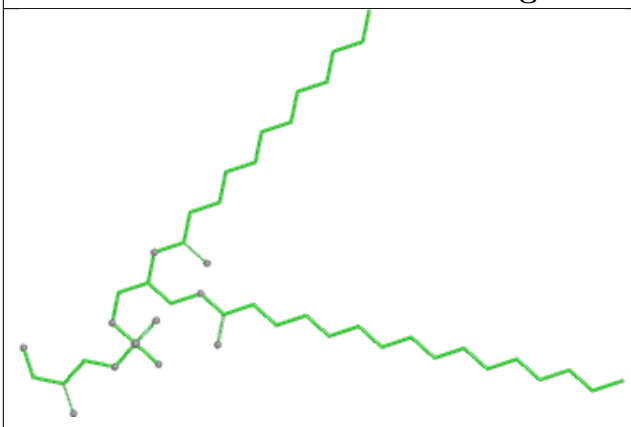
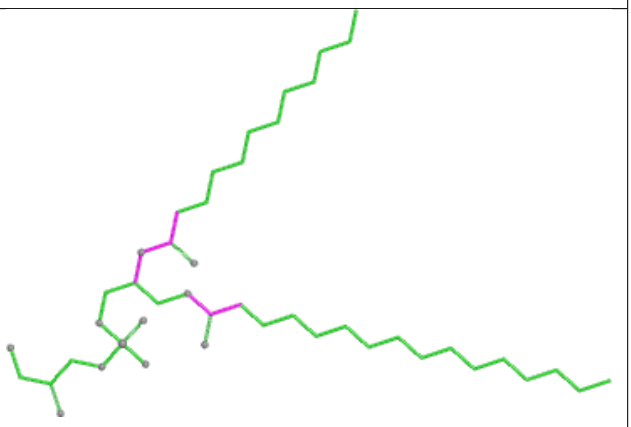


Rings

Ligand LHG s1 624



Bond lengths



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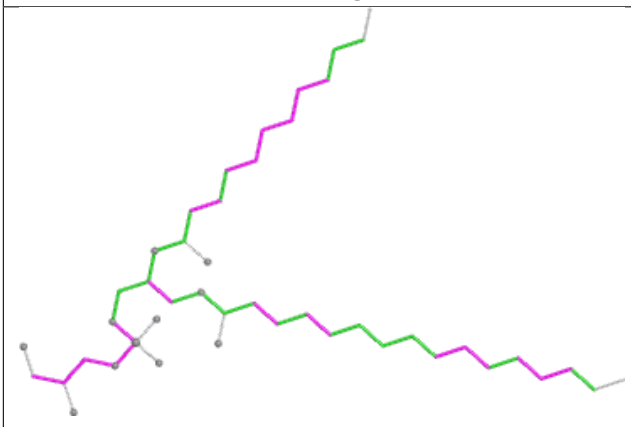
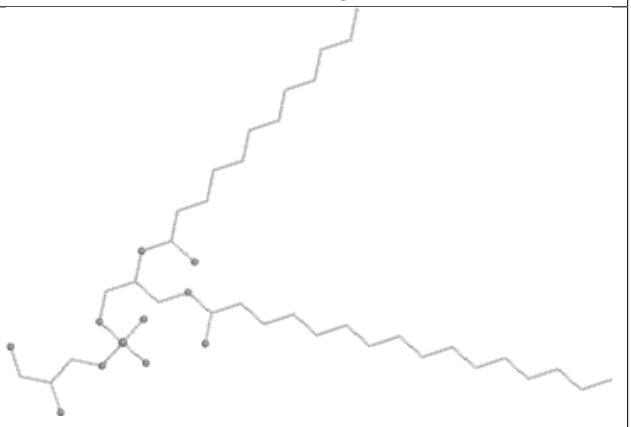
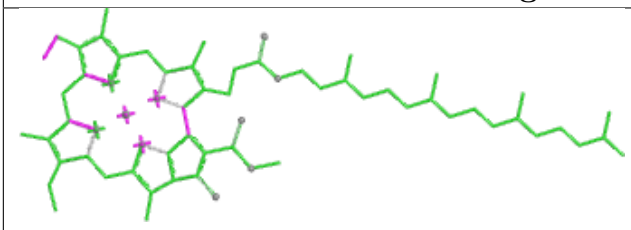


Torsions



Rings

Ligand CLA a1 406



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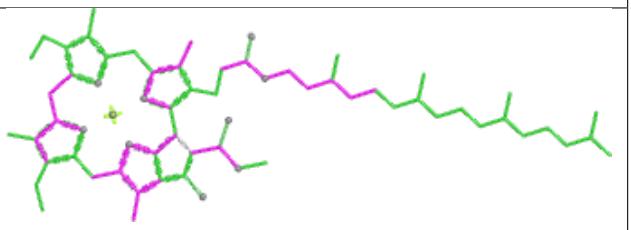

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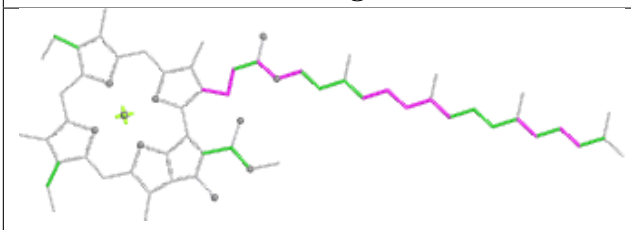

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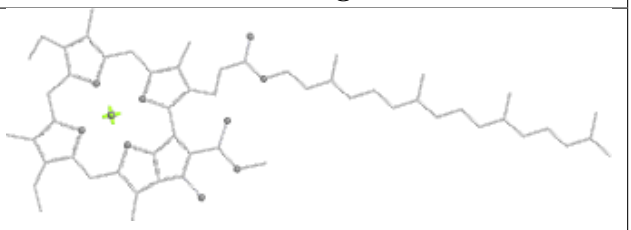
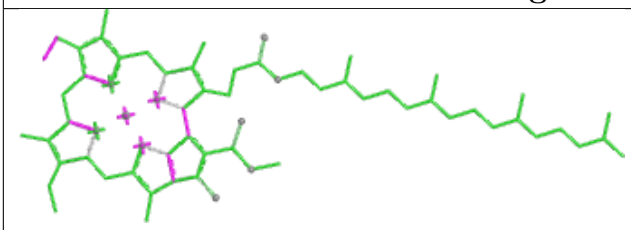


Rings

Ligand CLA c 506



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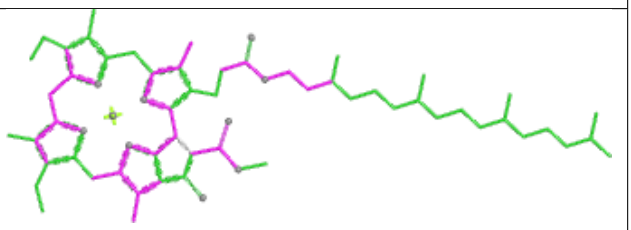

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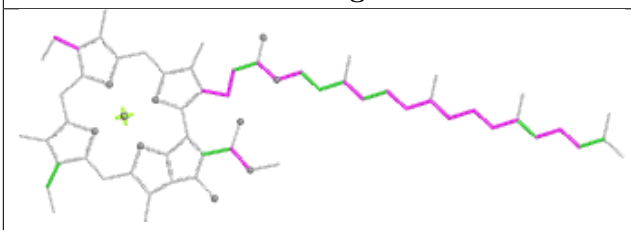

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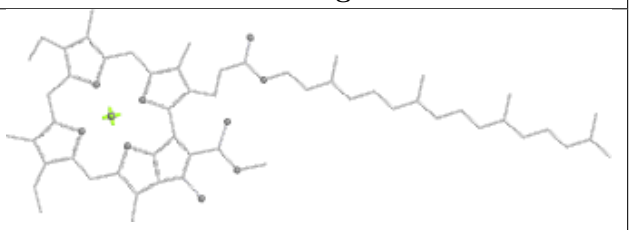
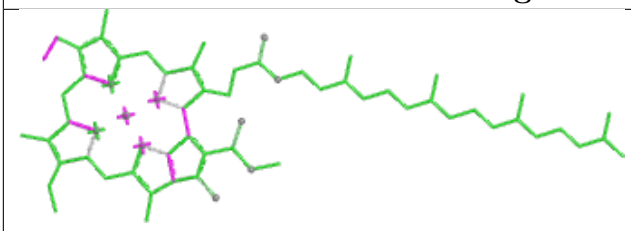


Rings

Ligand CLA G1 603



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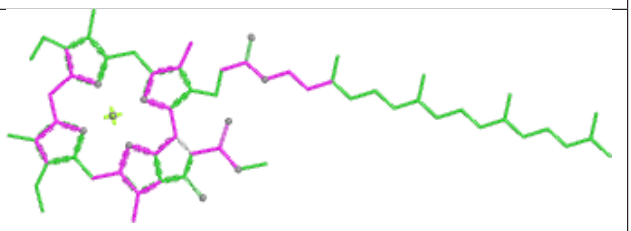

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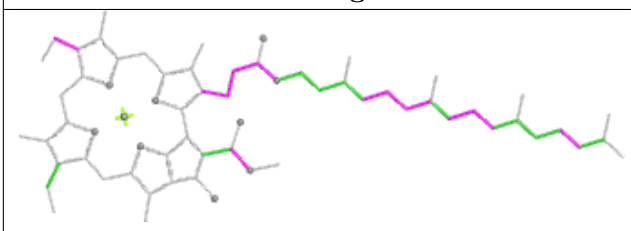

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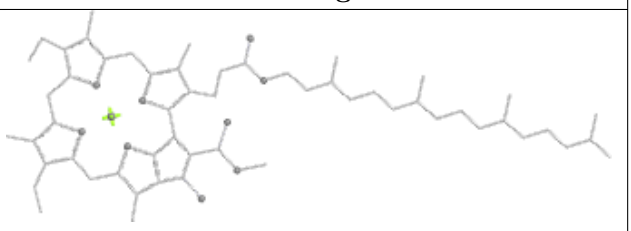
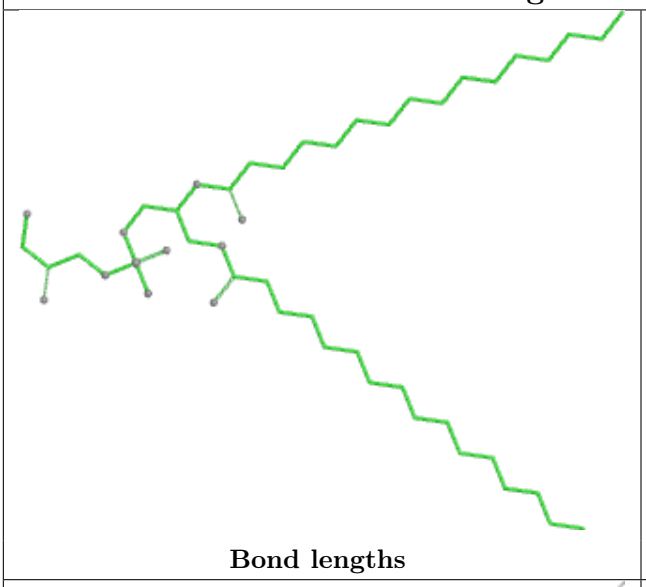


Rings

Ligand LHG g 624



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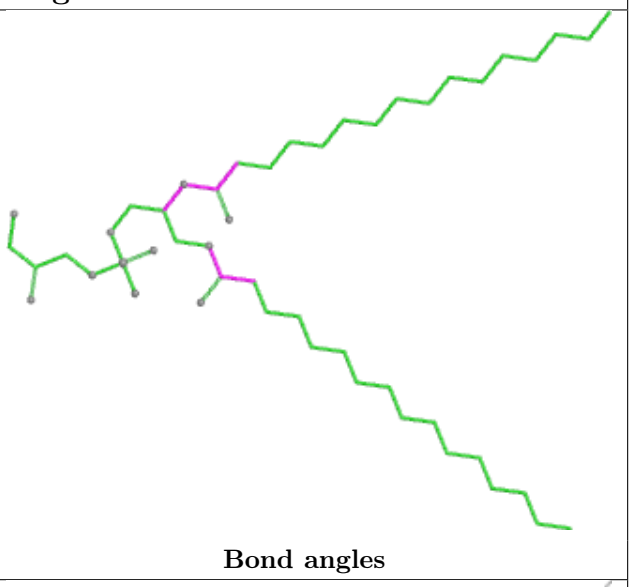
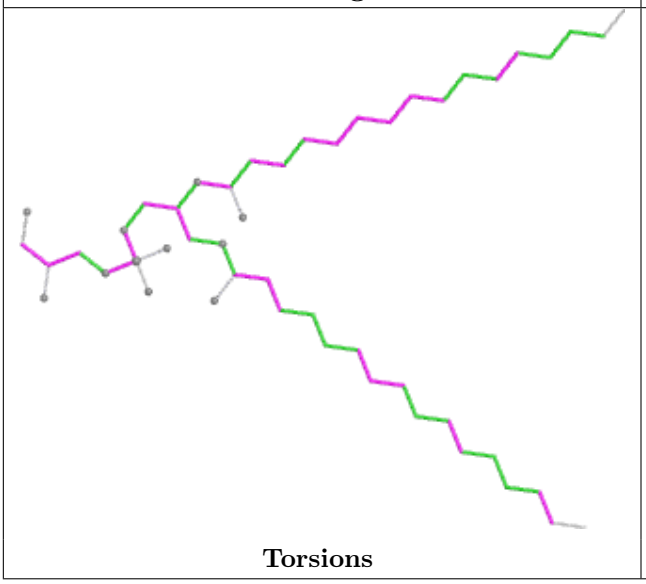


Bond angles



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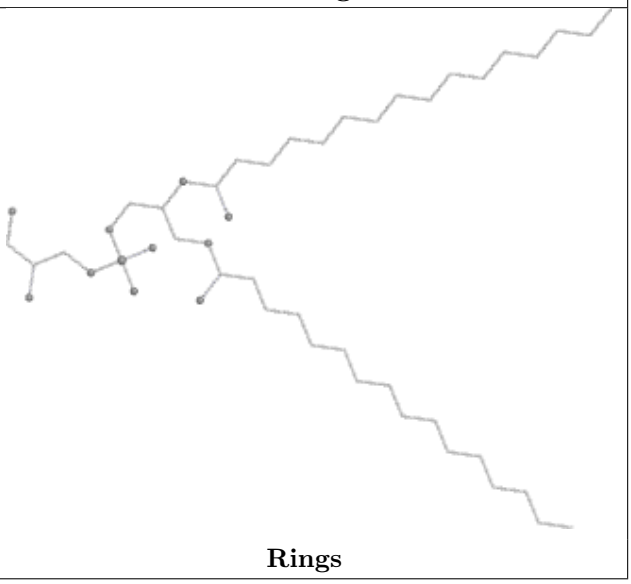
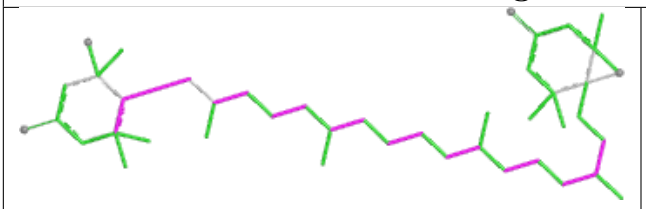


Rings

Ligand NEX Y1 623



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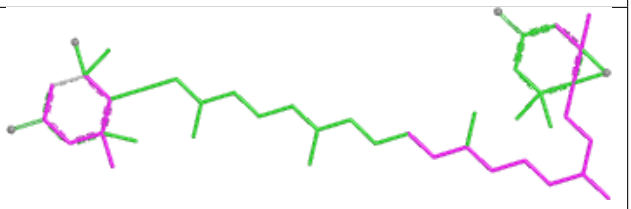

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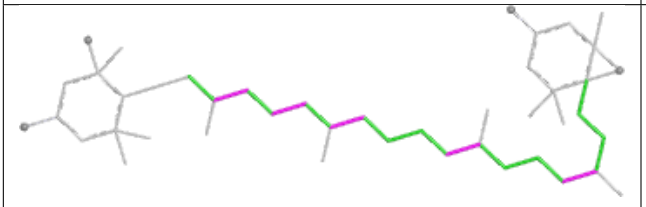

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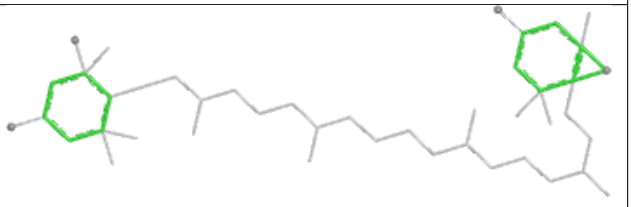
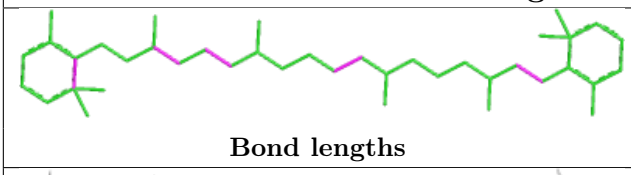


Rings

Ligand BCR c 515



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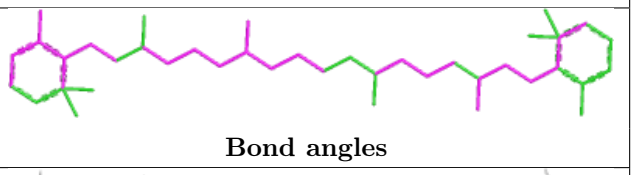
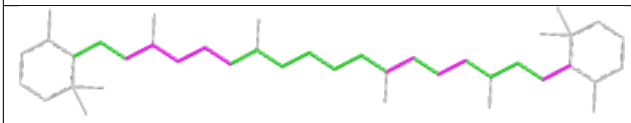


Bond angles



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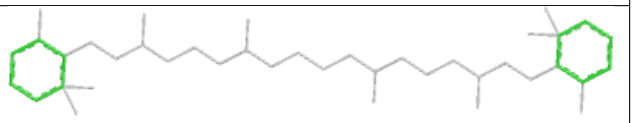
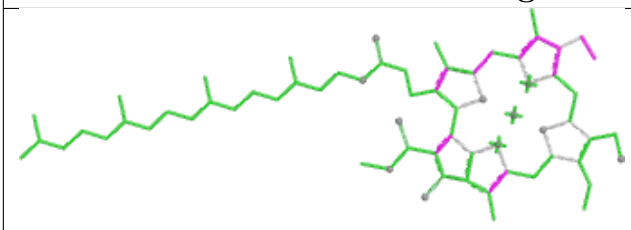


Rings

Ligand CHL n1 605



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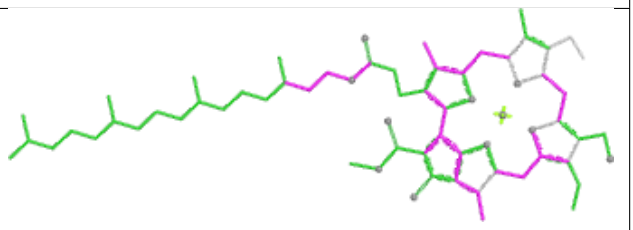

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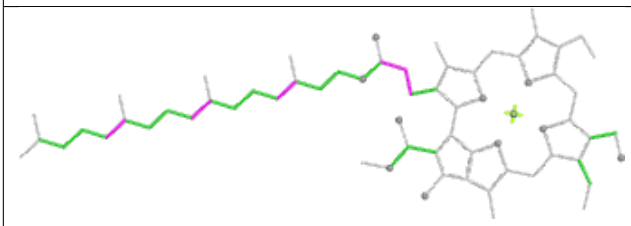

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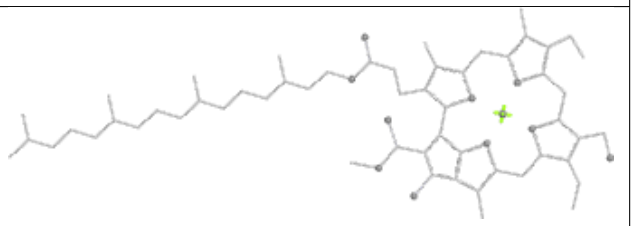
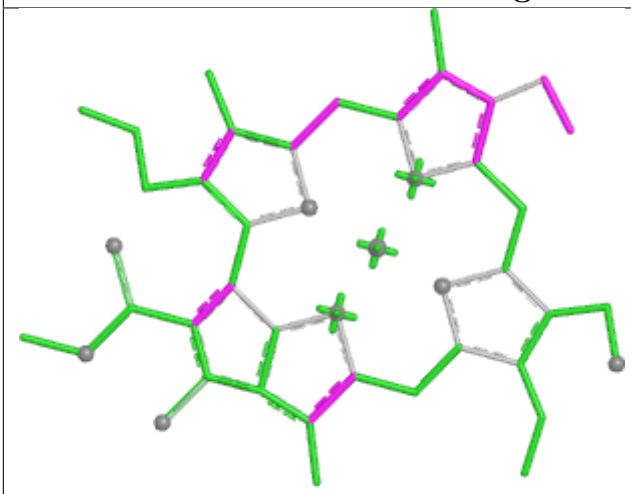


Rings

Ligand CHL G1 608



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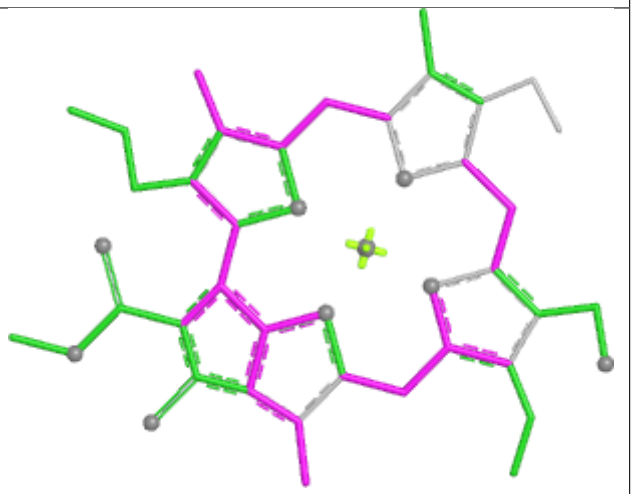

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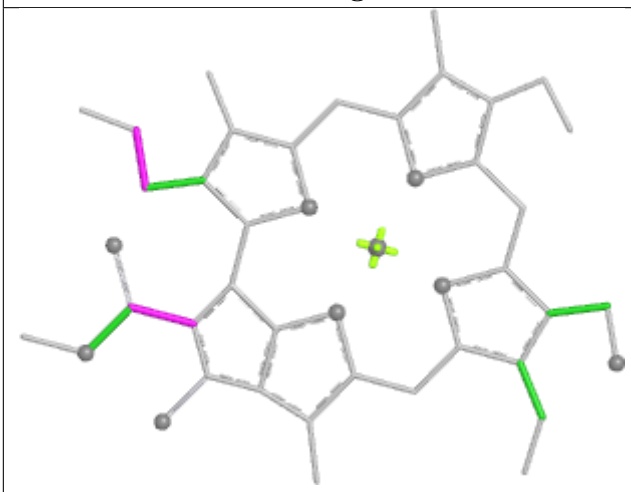

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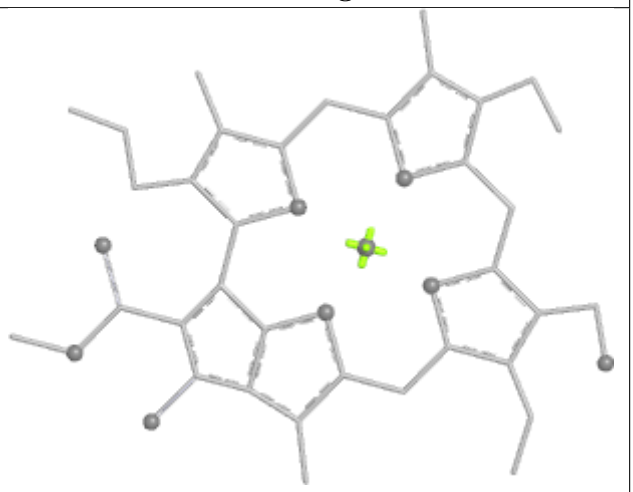
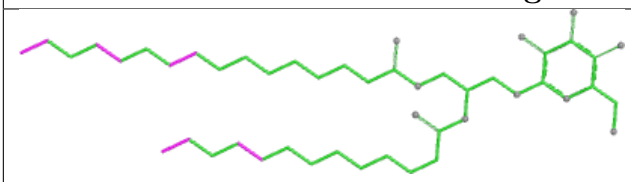


Rings

Ligand LMG a 413



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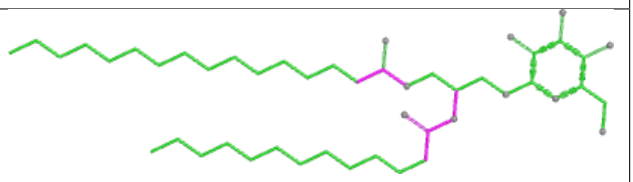
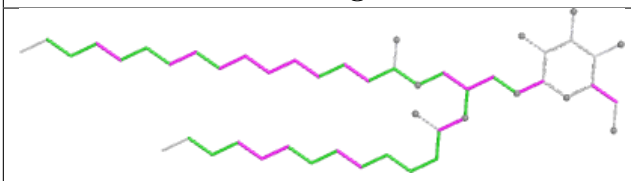


Bond angles



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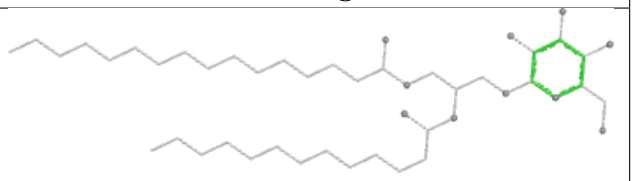
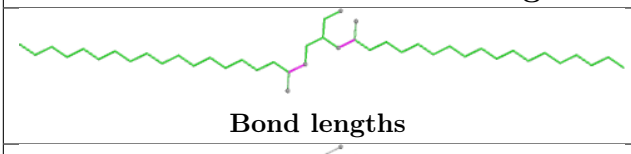


Rings

Ligand DGA b 623



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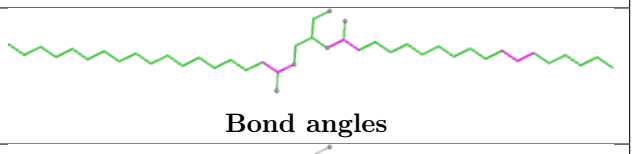

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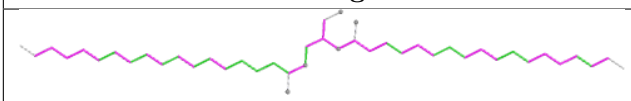

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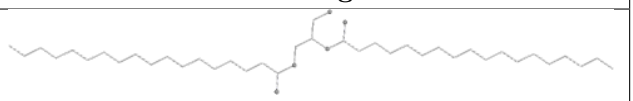
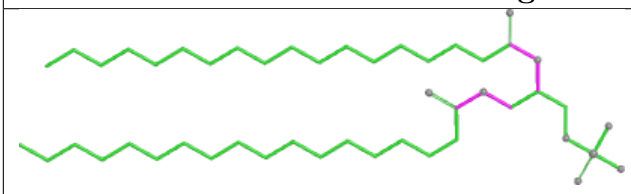


Rings

Ligand 3PH T1 101



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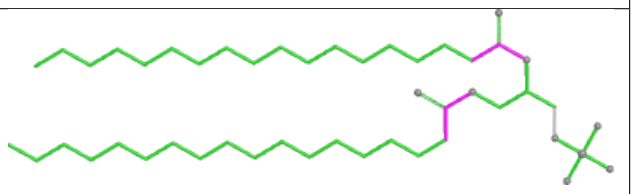
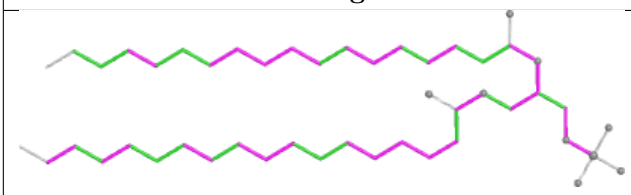
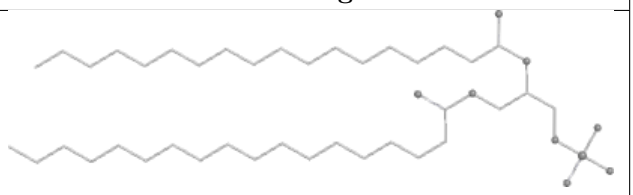


Bond angles

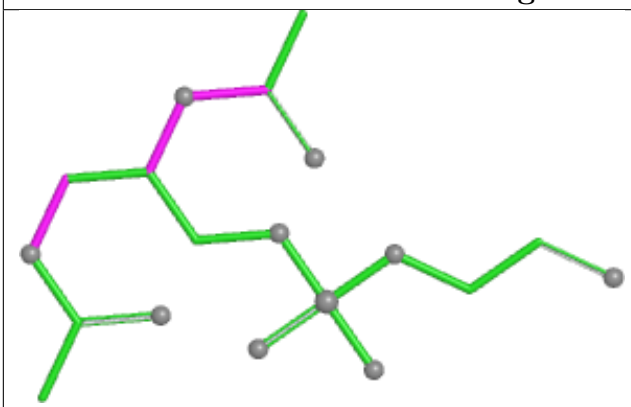


Torsions



Rings

Ligand PTY y1 627



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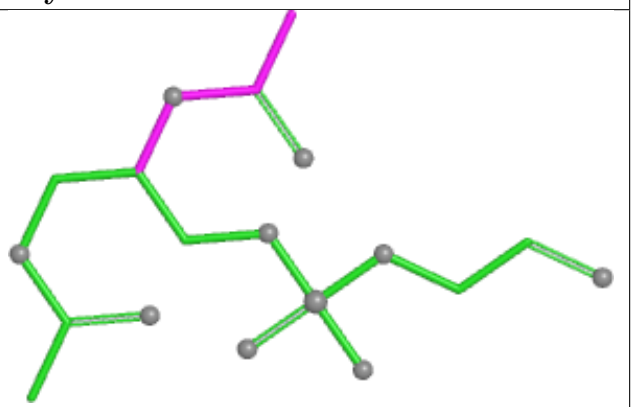
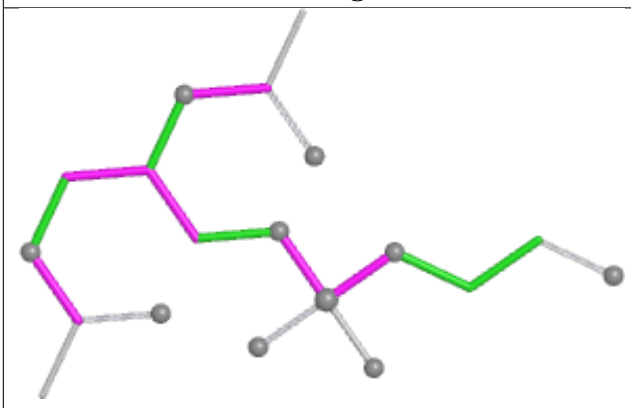
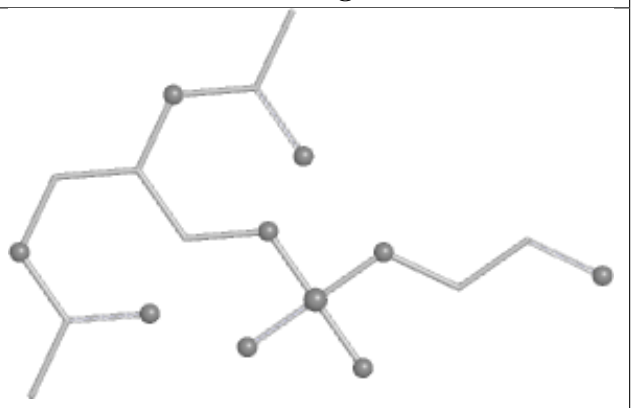


Bond angles

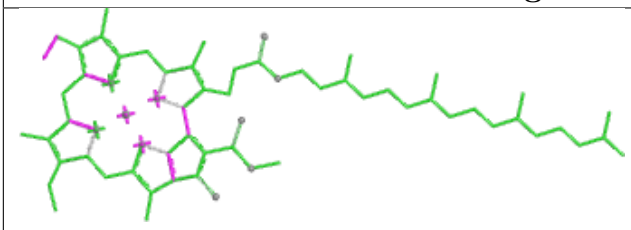


Torsions

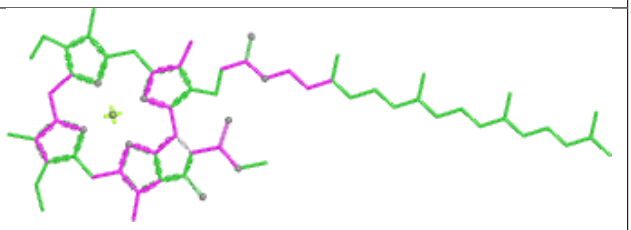


Rings

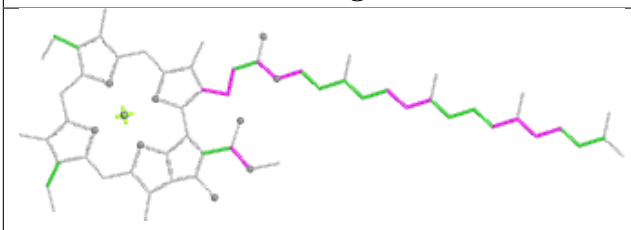
Ligand CLA B 613



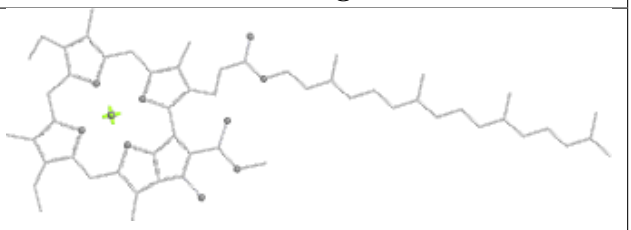
Bond lengths



Bond angles

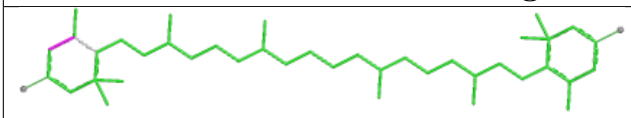


Torsions

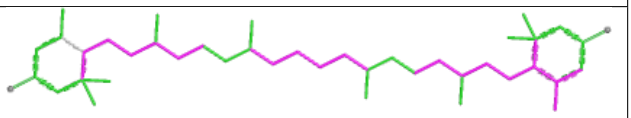


Rings

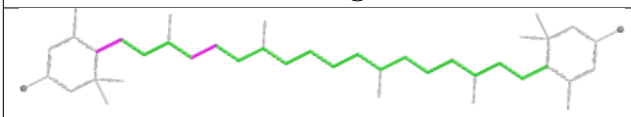
Ligand LUT s1 621



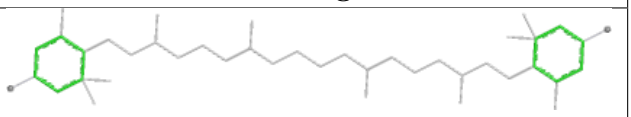
Bond lengths



Bond angles

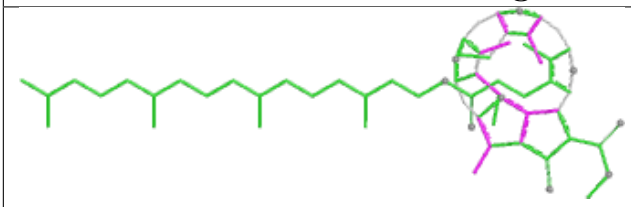


Torsions



Rings

Ligand PHO A1 408



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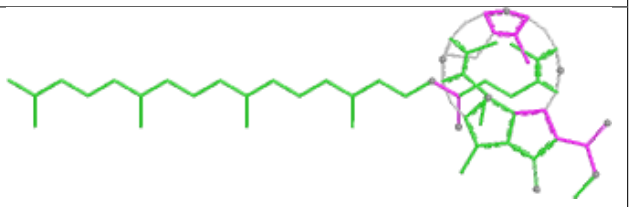
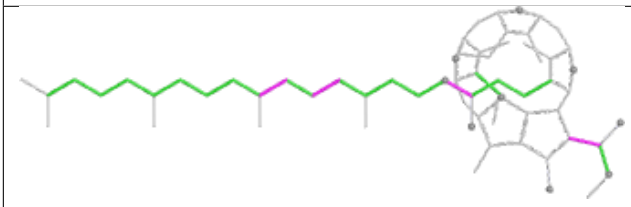
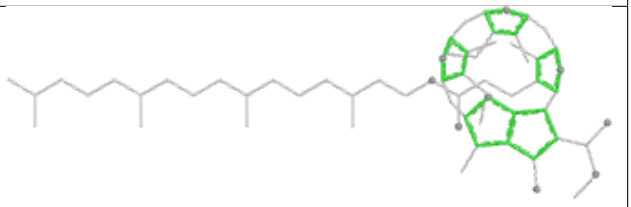


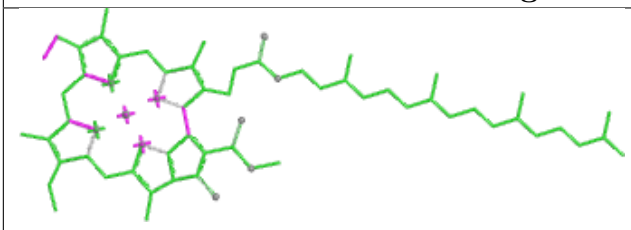
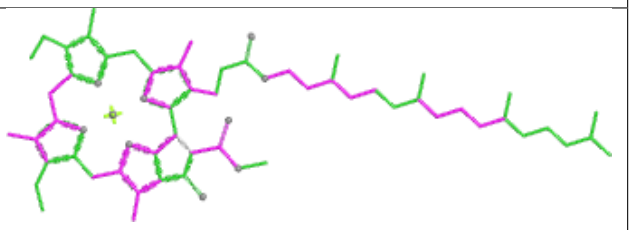
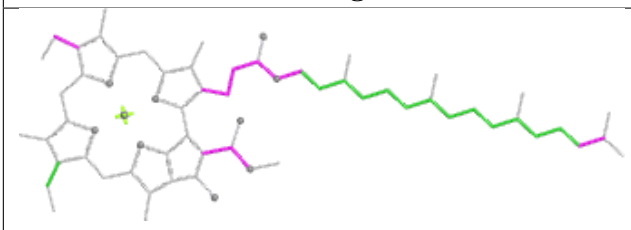
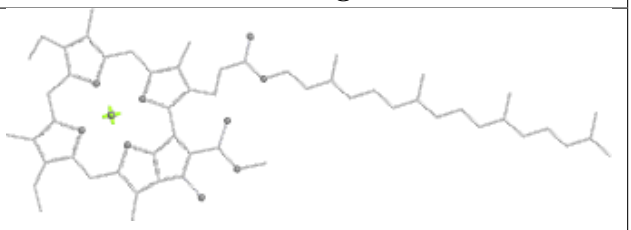
Bond angles

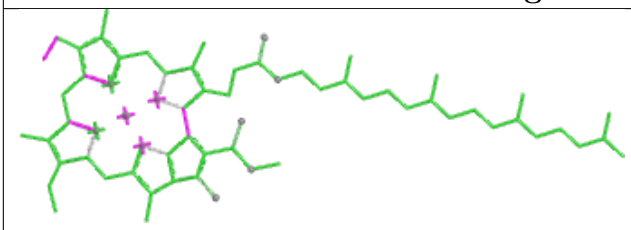
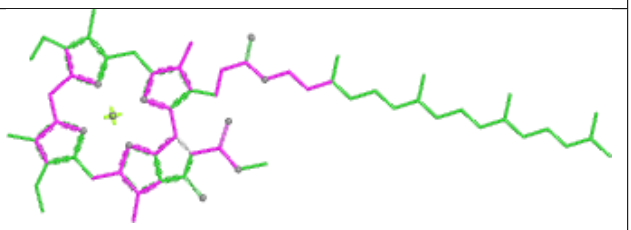
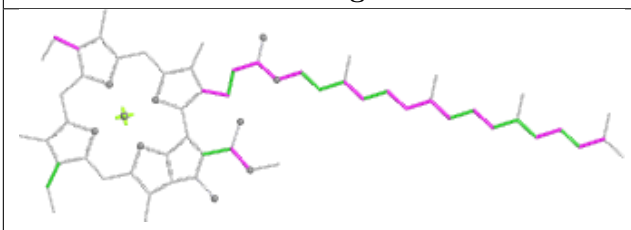
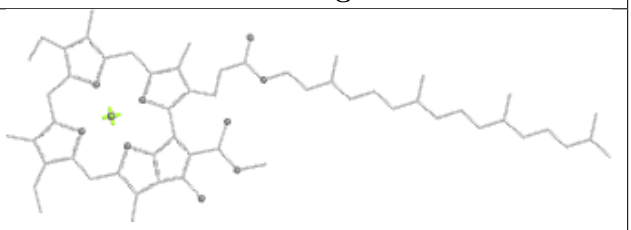


Torsions

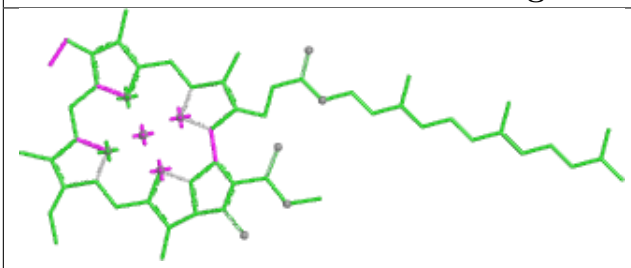


Rings

Ligand CLA c1 502	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA S 602



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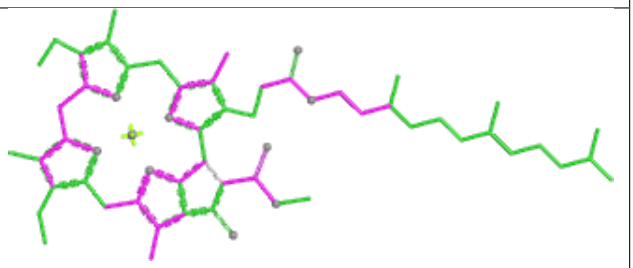
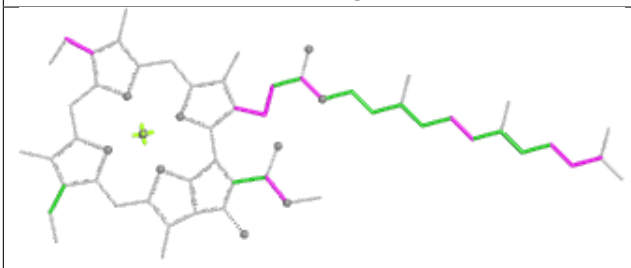
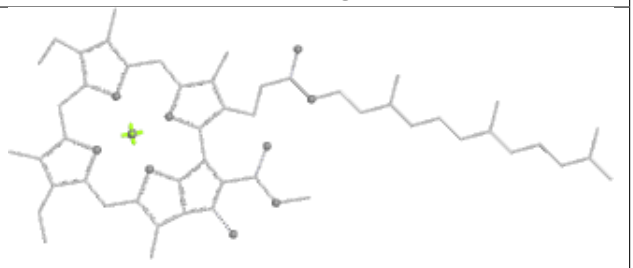


Bond angles

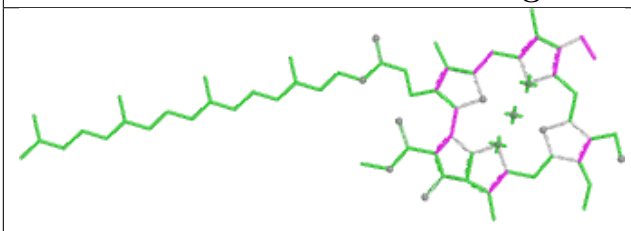


Torsions

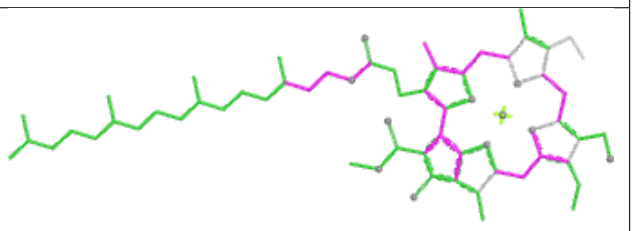


Rings

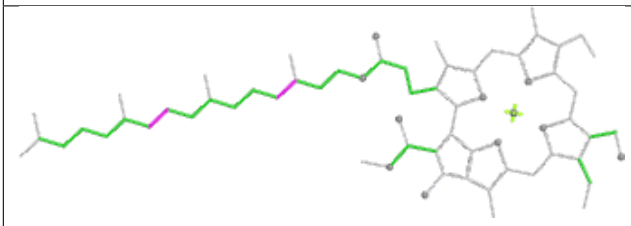
Ligand CHL G 601



Bond lengths



Bond angles



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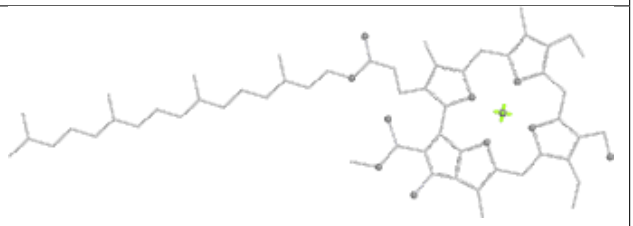
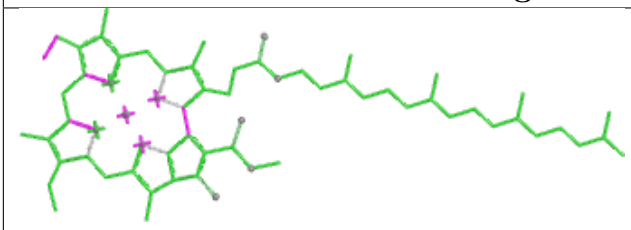


Rings

Ligand CLA G1 610



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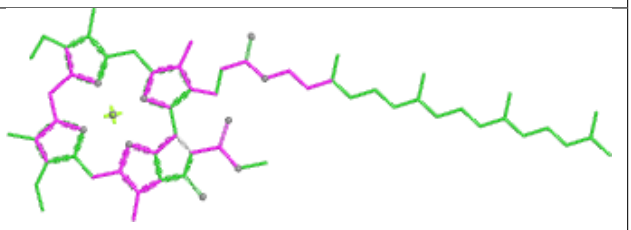
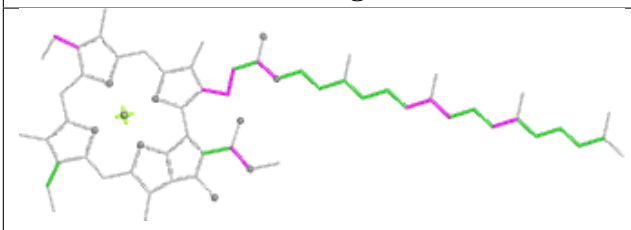


Bond angles



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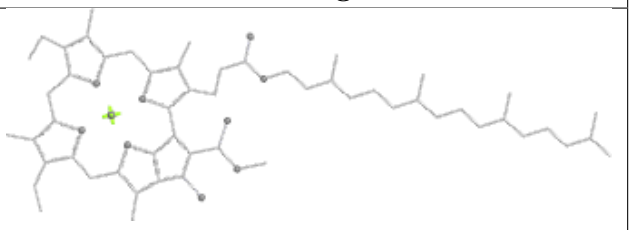

Rings

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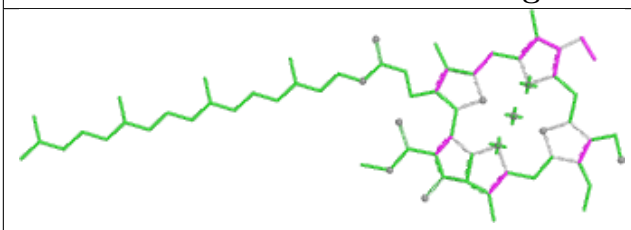

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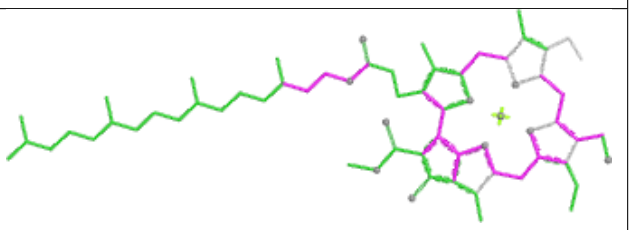
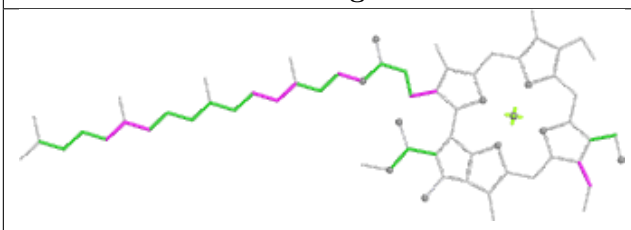


Bond angles



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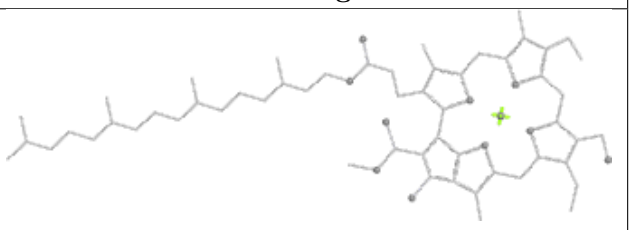
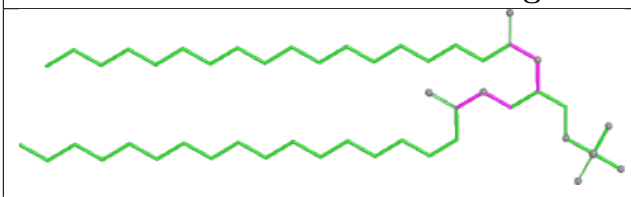


Rings

Ligand 3PH s1 626



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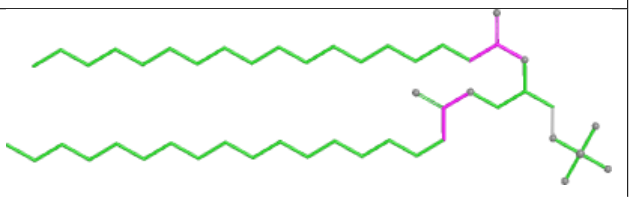
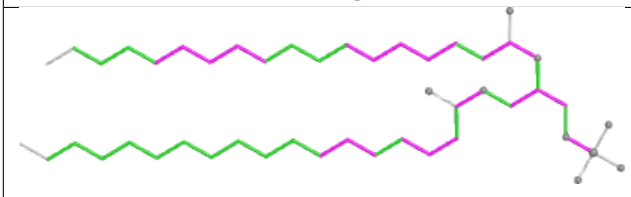


Bond angles



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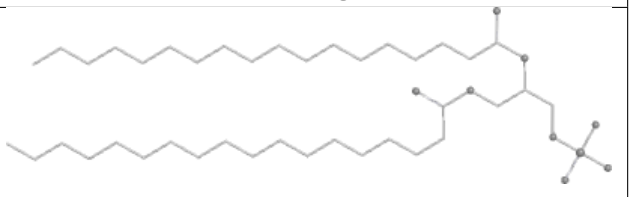
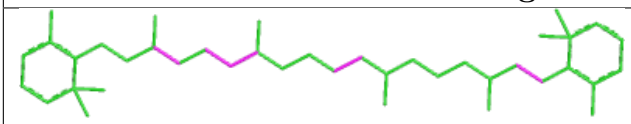
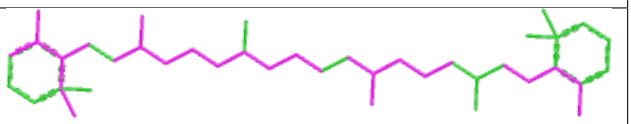
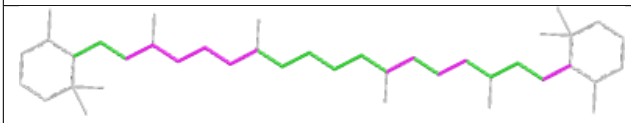
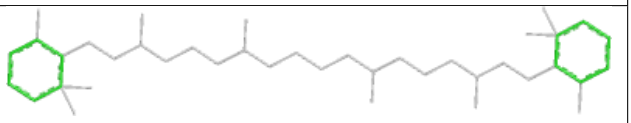
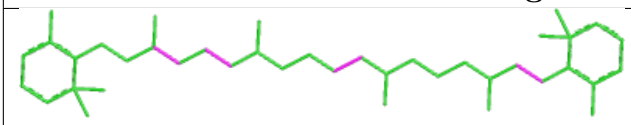
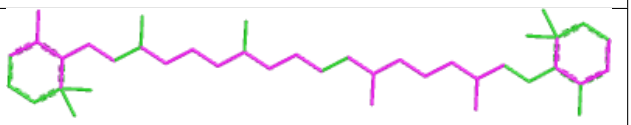
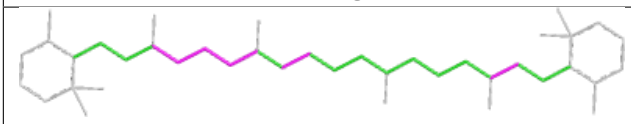
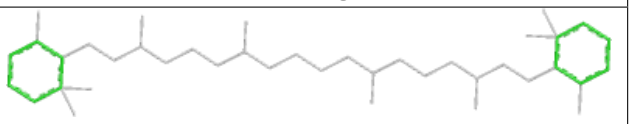
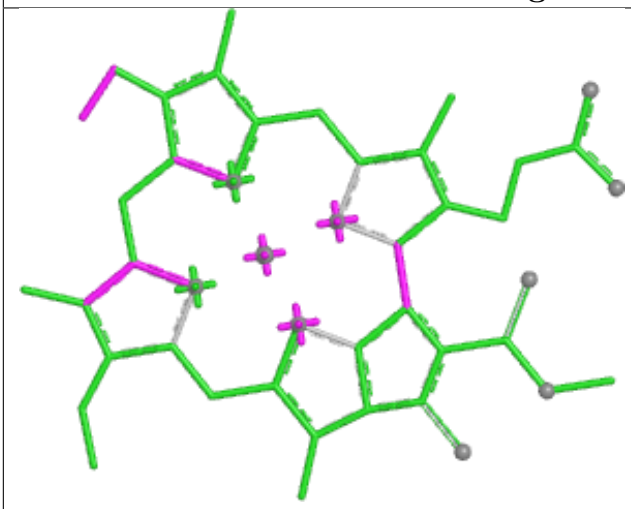


Rings

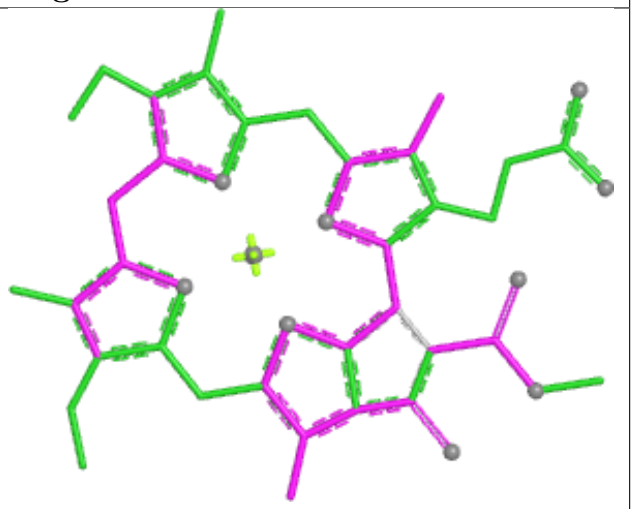
Ligand BCR c1 515	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand BCR b 619	
 Bond lengths	 Bond angles
 Torsions	 Rings

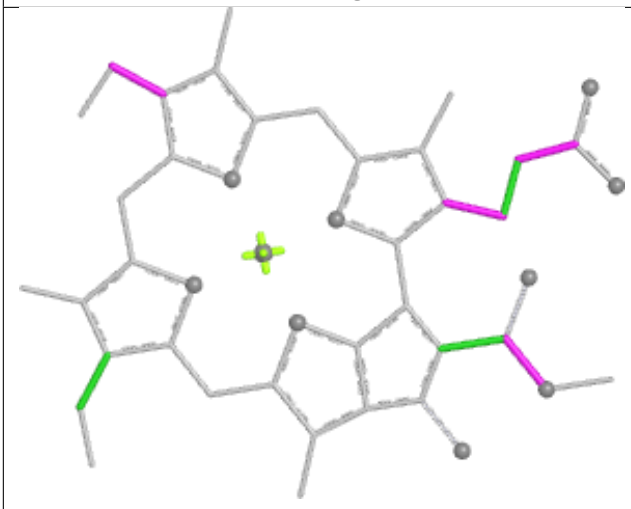
Ligand CLA g 611



Bond lengths



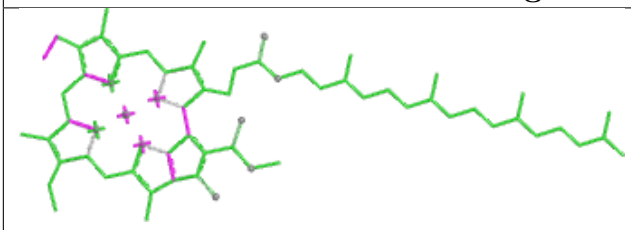
Bond angles



Torsions

Rings

Ligand CLA C 502



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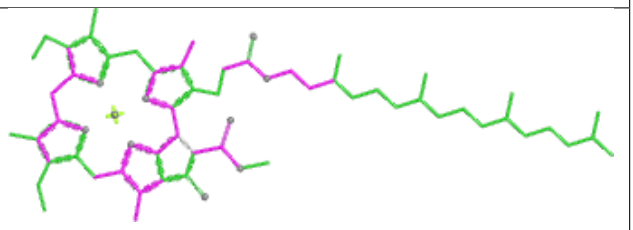
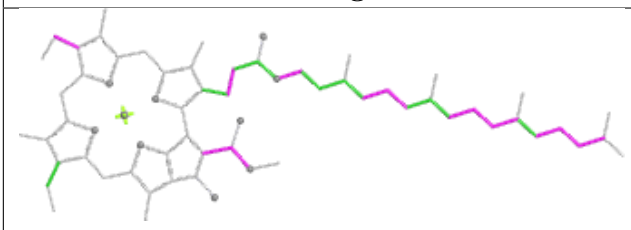
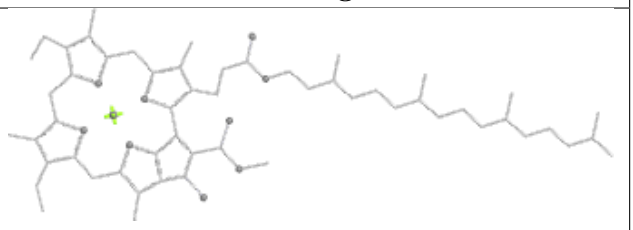


Bond angles

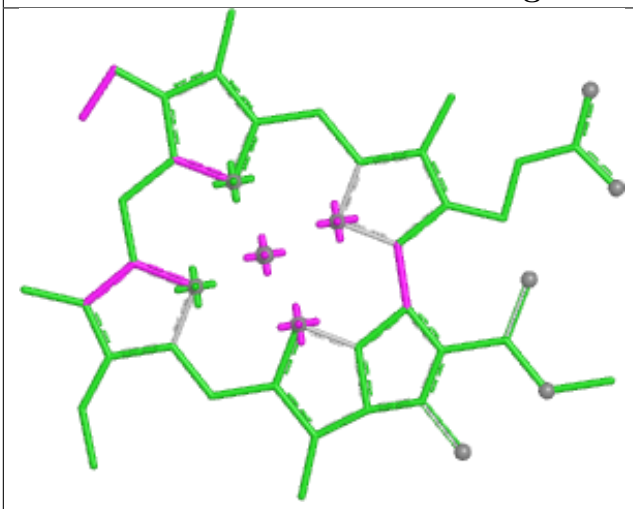


Torsions



Rings

Ligand CLA N 612



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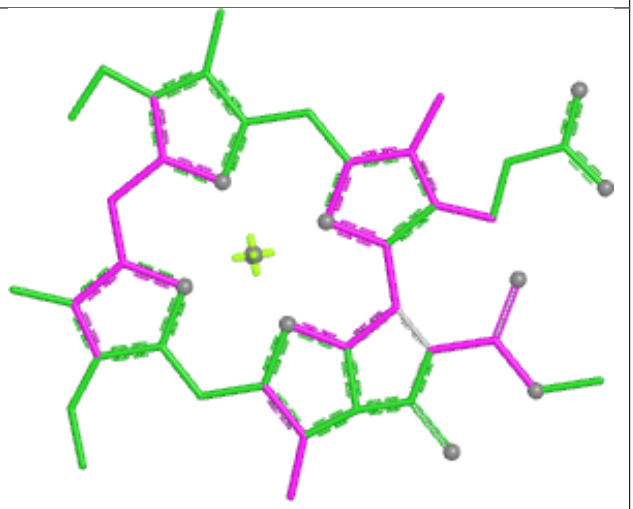
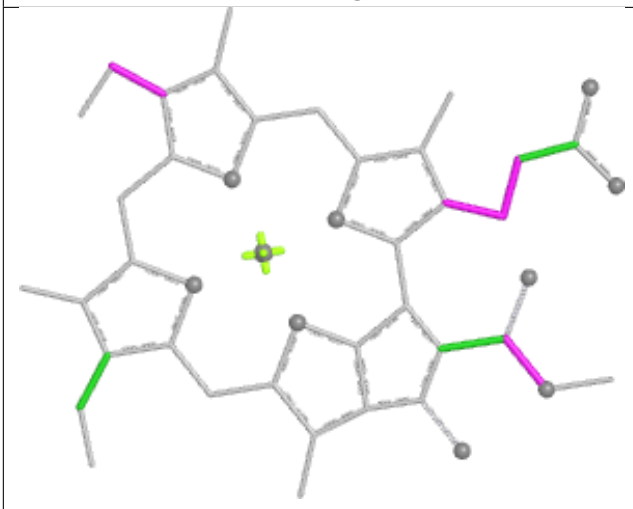


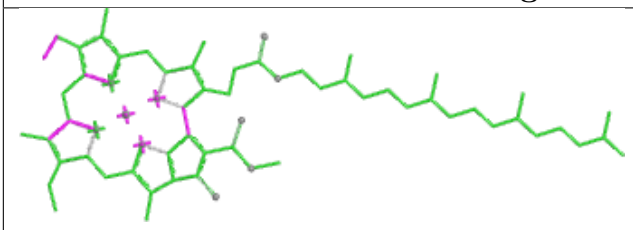
Bond angles



Torsions

Rings

Ligand CLA c1 508



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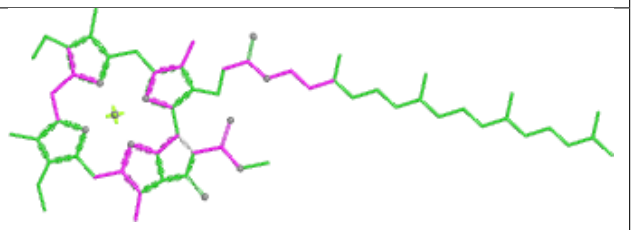
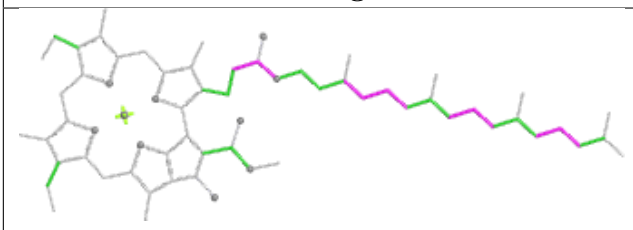
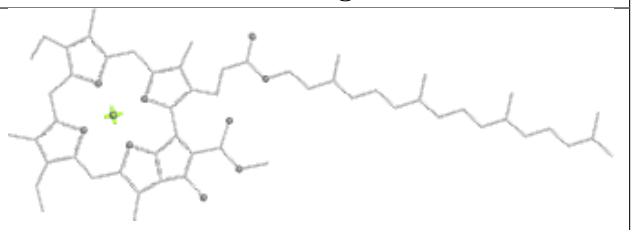


Bond angles

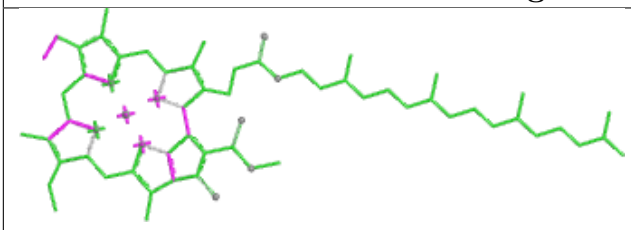


Torsions



Rings

Ligand CLA b 603



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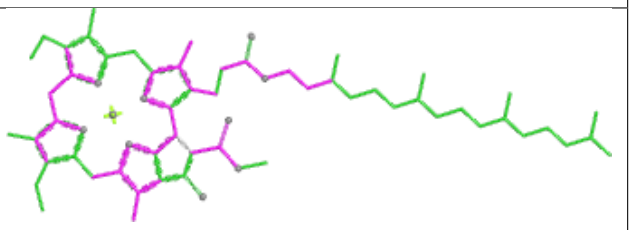

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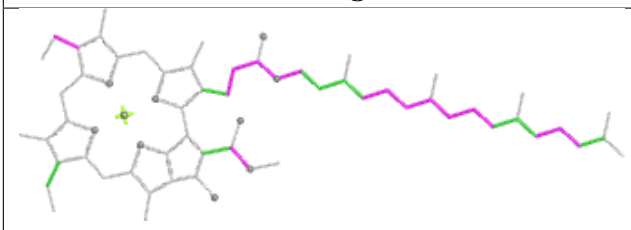

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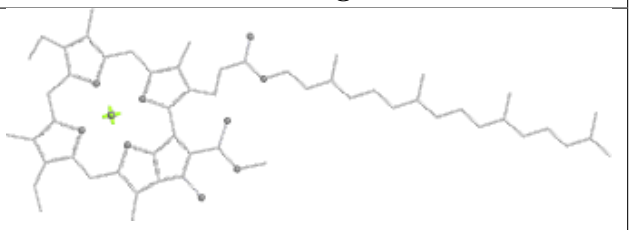
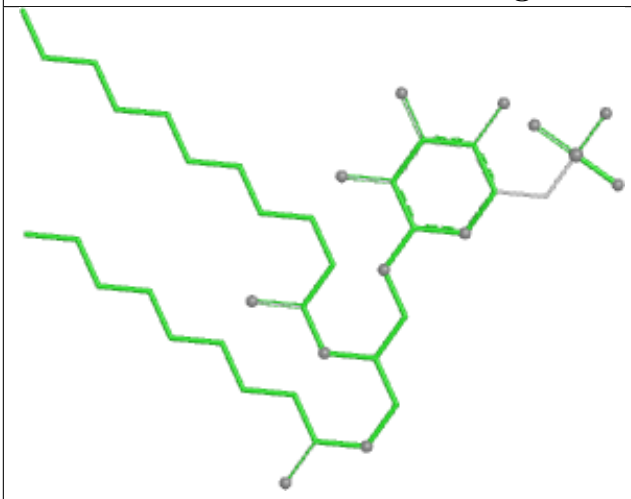


Rings

Ligand SQD m1 101



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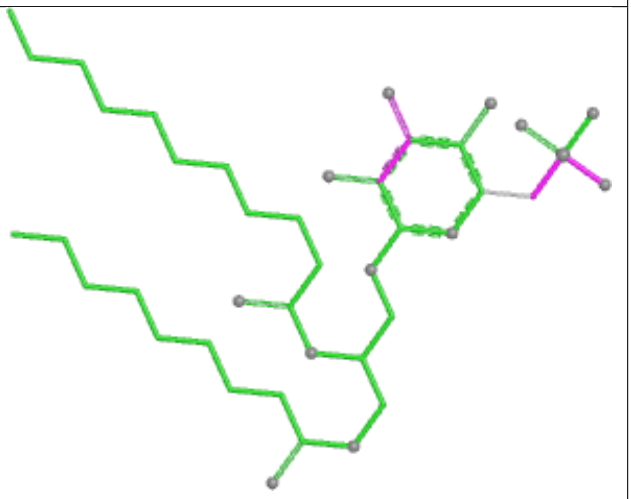
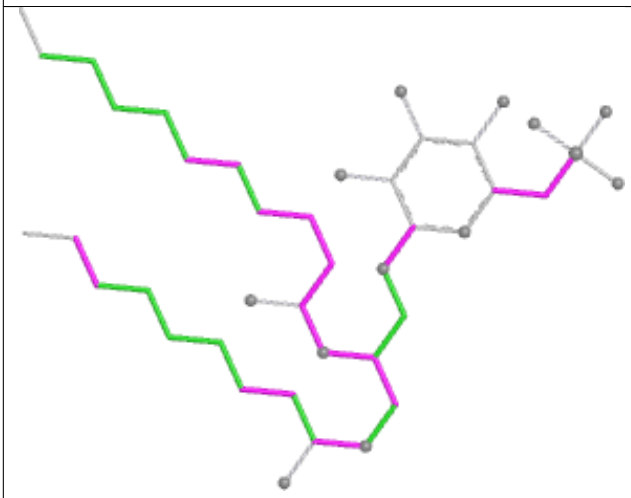
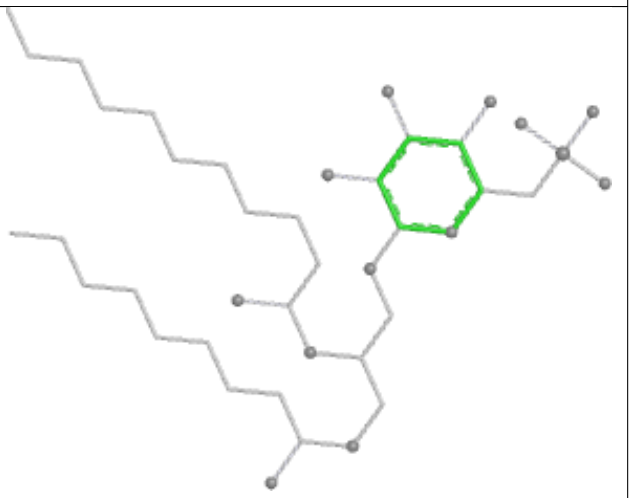


Bond angles

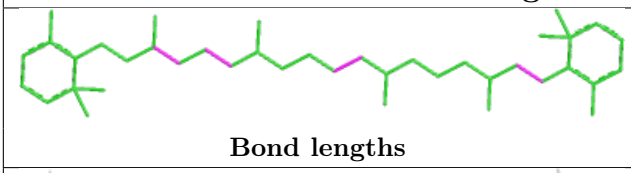


Torsions



Rings

Ligand BCR C 517



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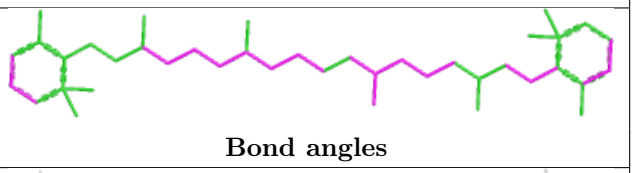

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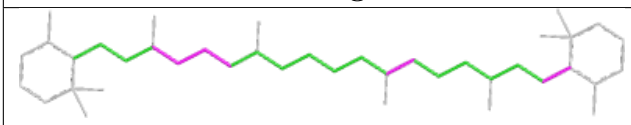

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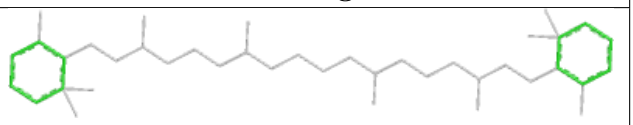
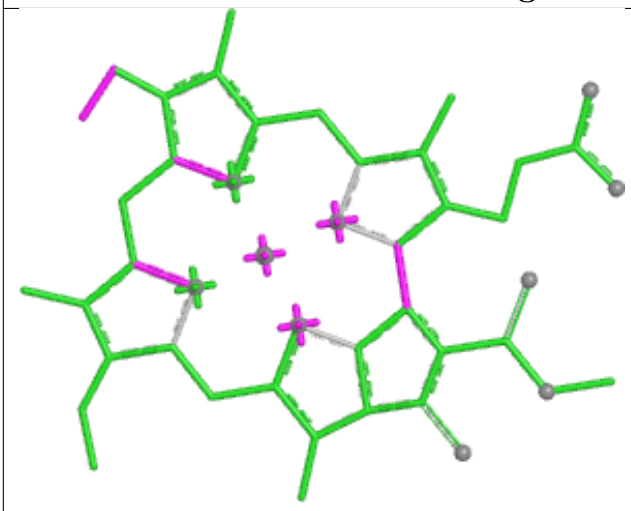


Rings

Ligand CLA S1 612



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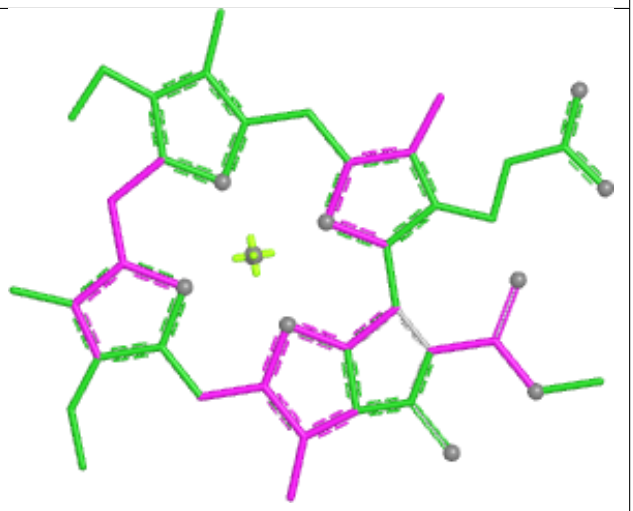

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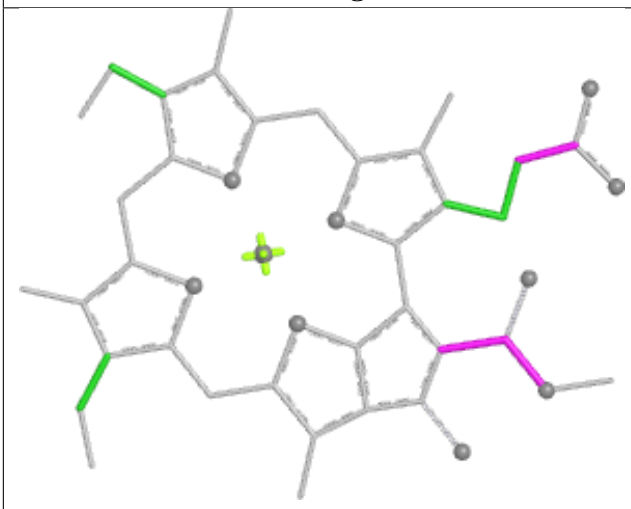
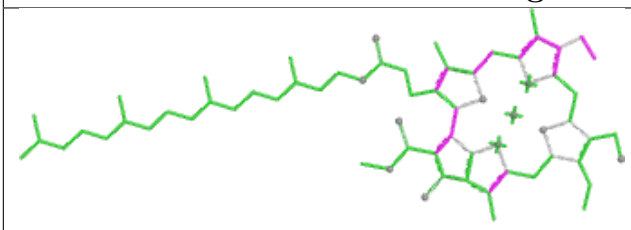


Torsions

Rings

Ligand CHL n 601



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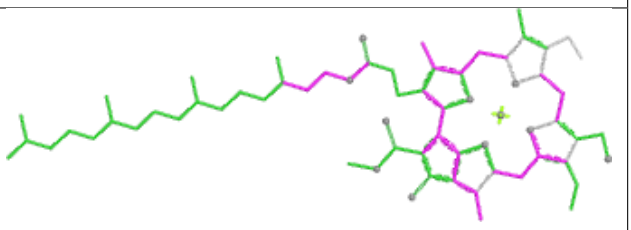
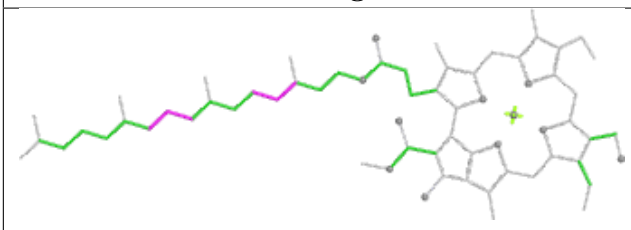


Bond angles



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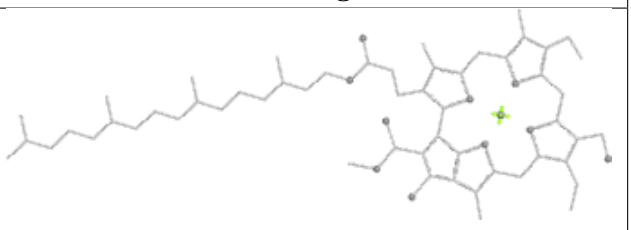
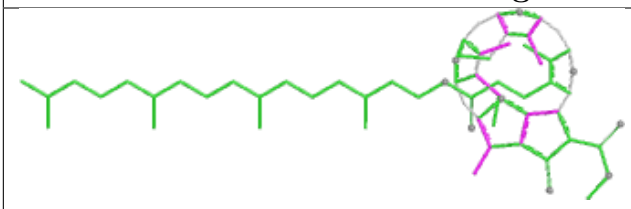


Rings

Ligand PHO A1 409



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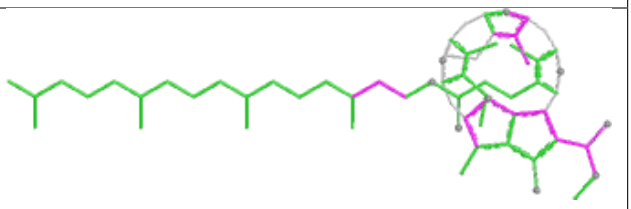
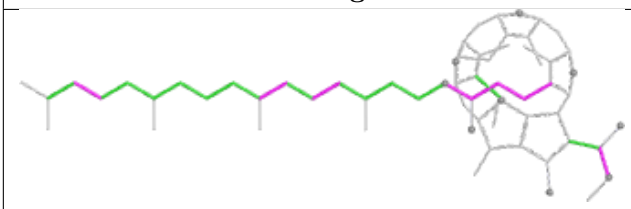


Bond angles



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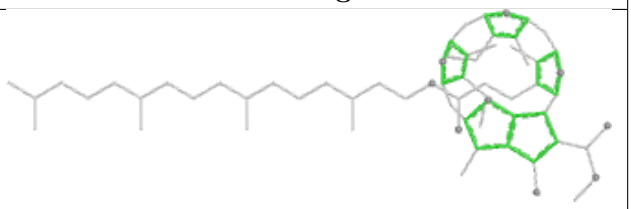
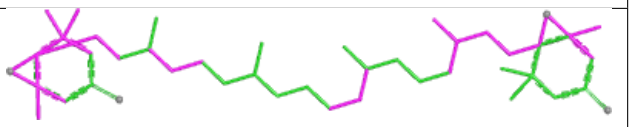


Rings

Ligand XAT Y1 622

Bond lengths



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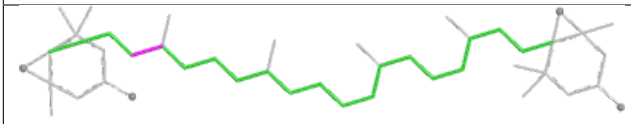

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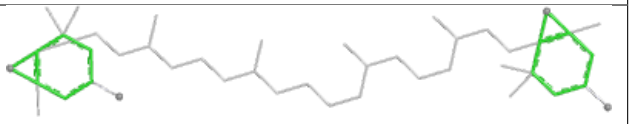
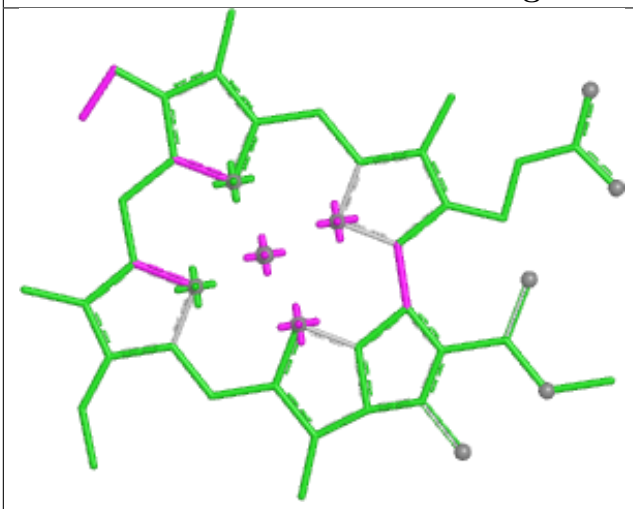


Rings

Ligand CLA G 611



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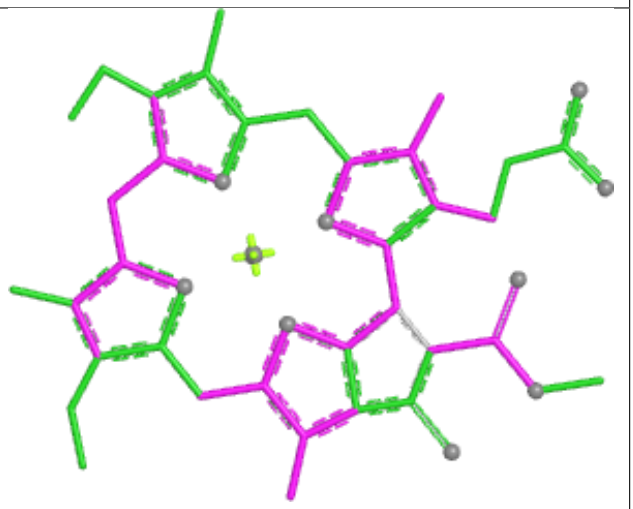
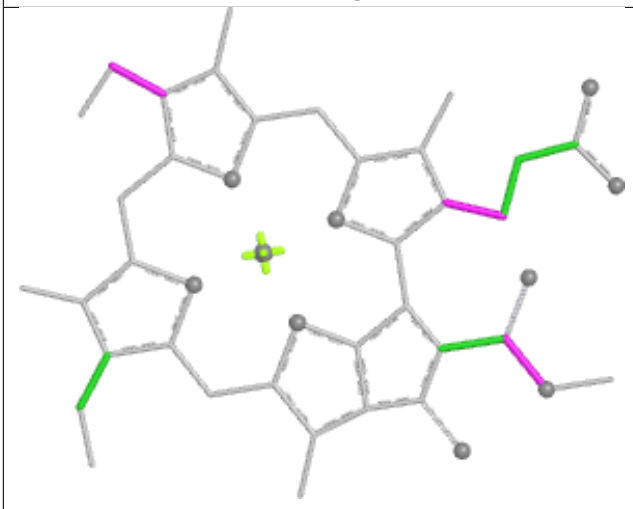


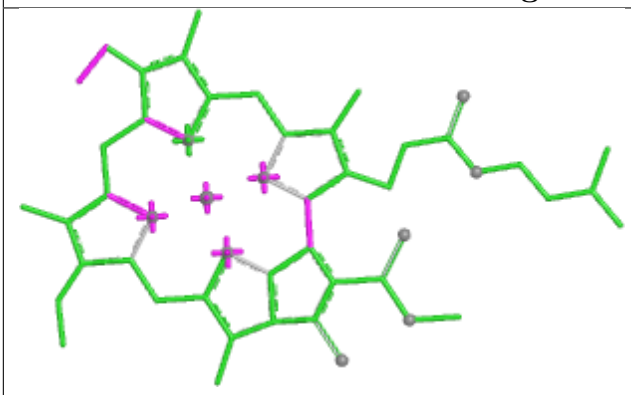
Bond angles



Torsions

Rings

Ligand CLA s1 605



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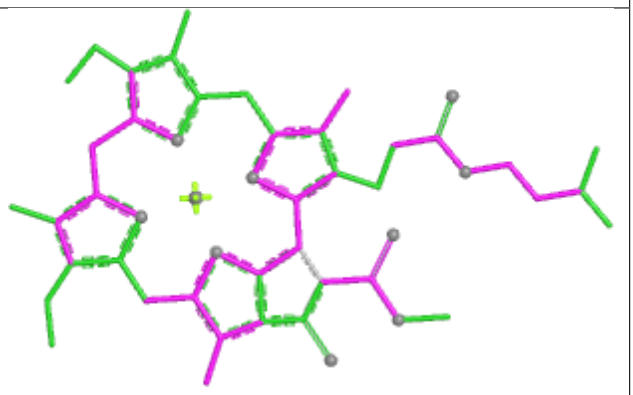
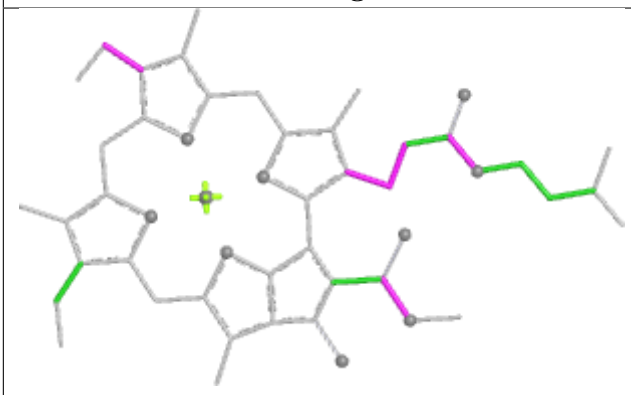


Bond angles



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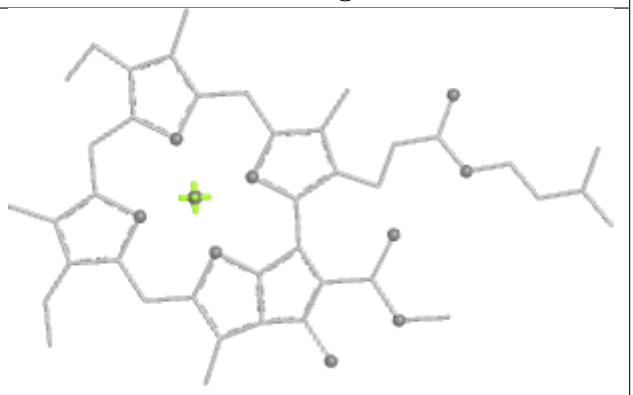
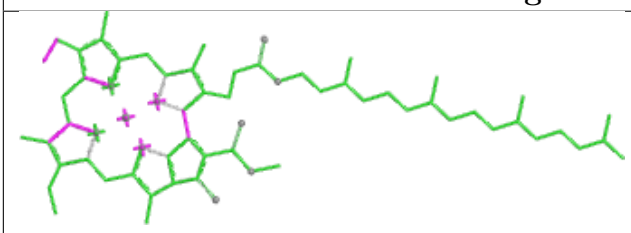


Rings

Ligand CLA B 611



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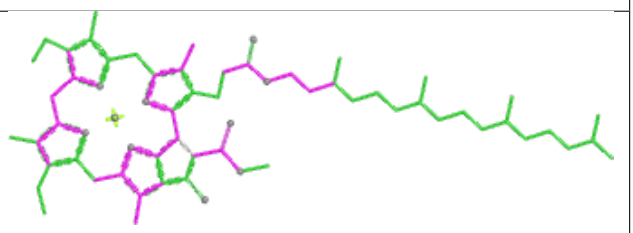
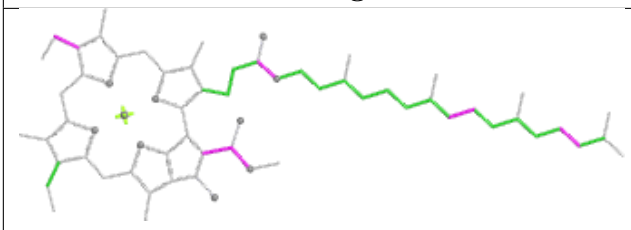


Bond angles



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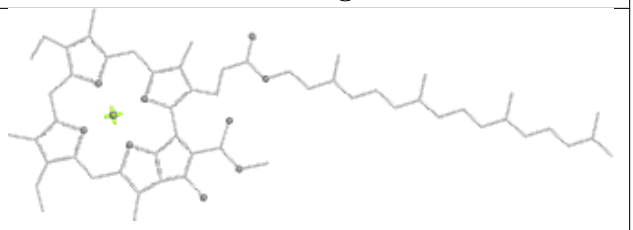
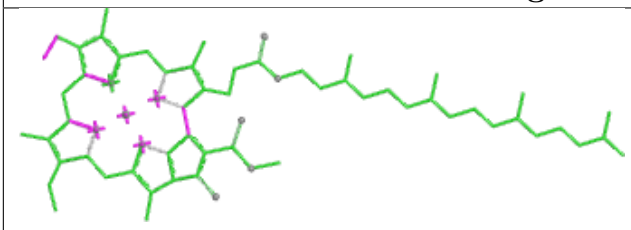


Rings

Ligand CLA S 611



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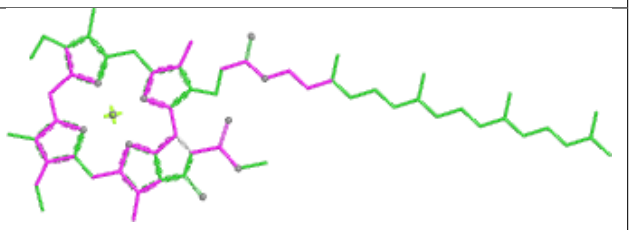

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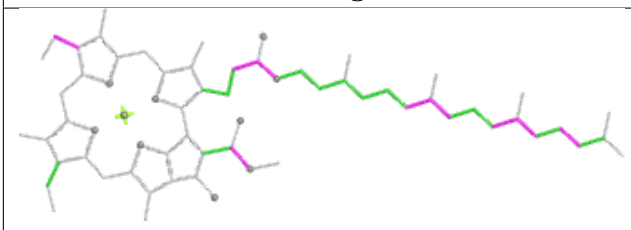

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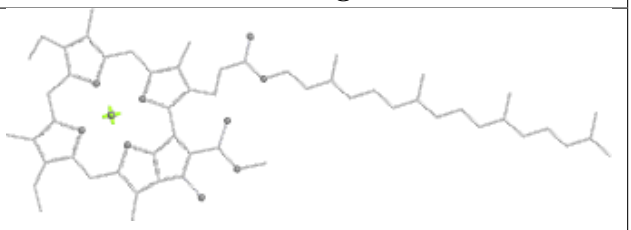
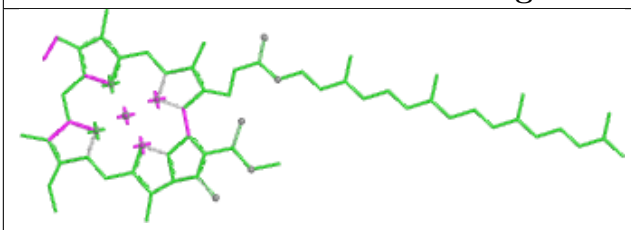


Rings

Ligand CLA B1 610



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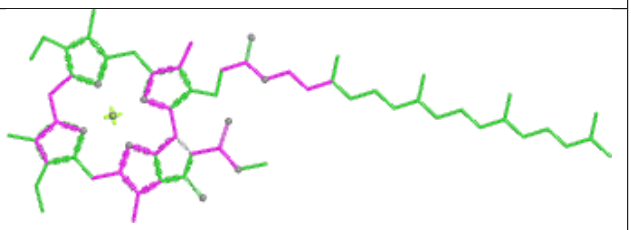
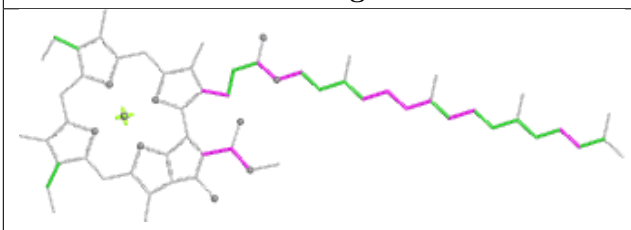


Bond angles



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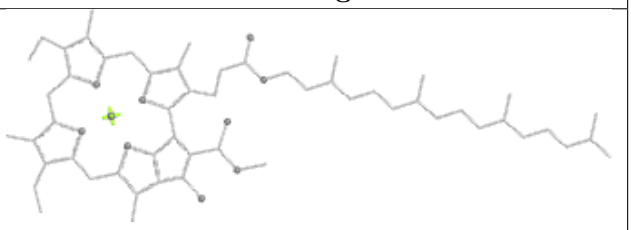
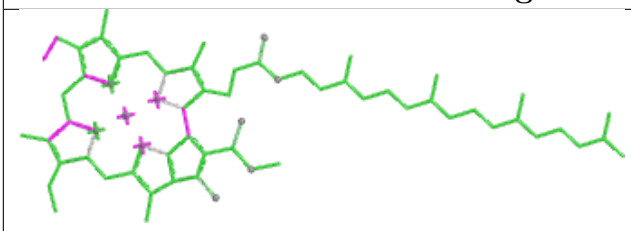


Rings

Ligand CLA C1 512



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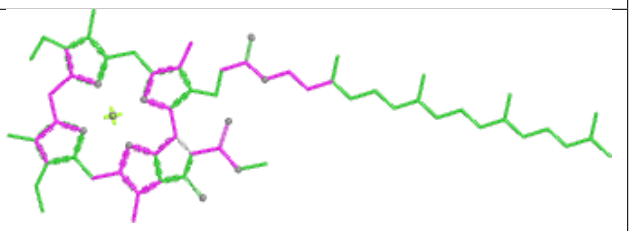
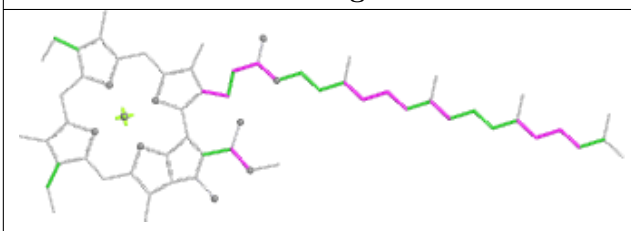
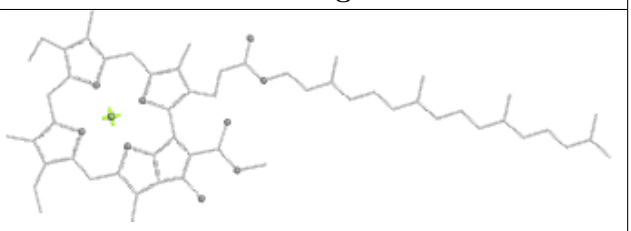


Bond angles

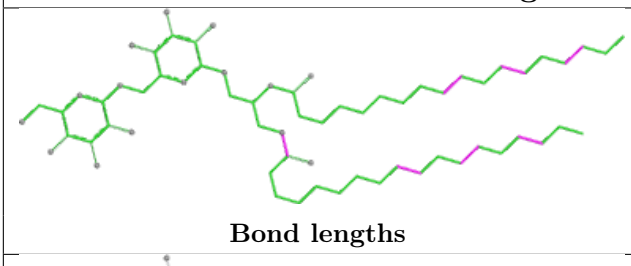


Torsions

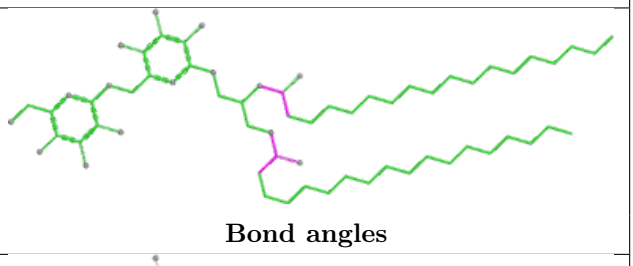


Rings

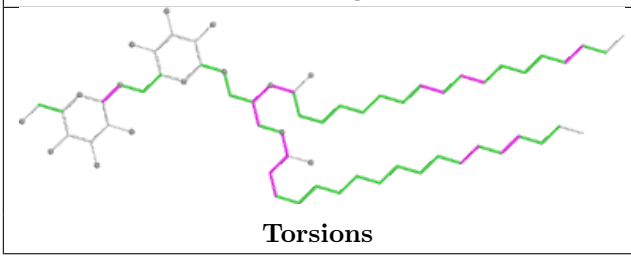
Ligand DGD C 523



Bond lengths



Bond angles



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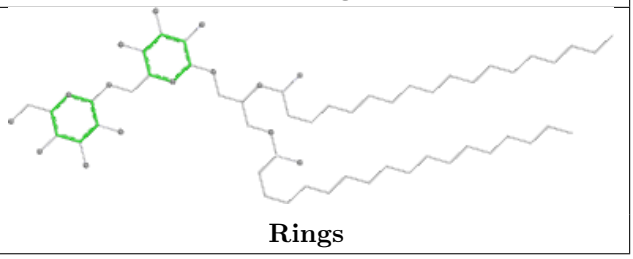
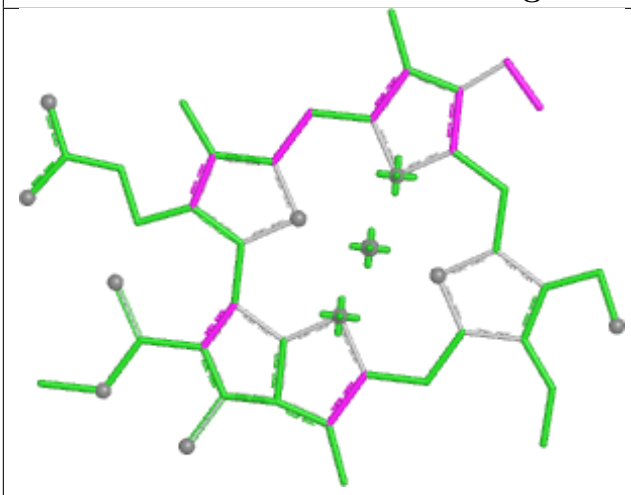
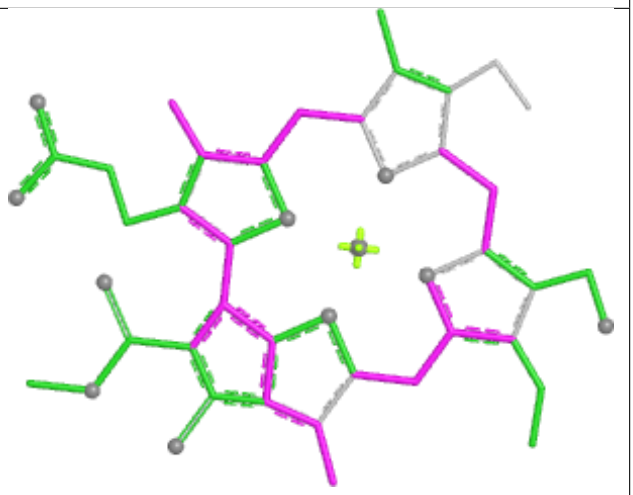


Rings

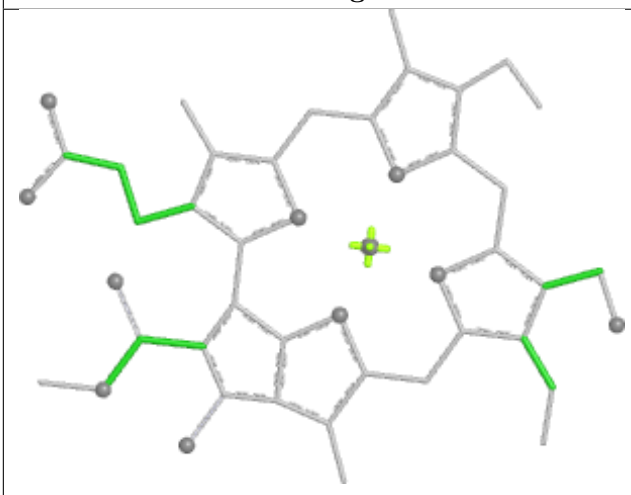
Ligand CHL Y 605



Bond lengths



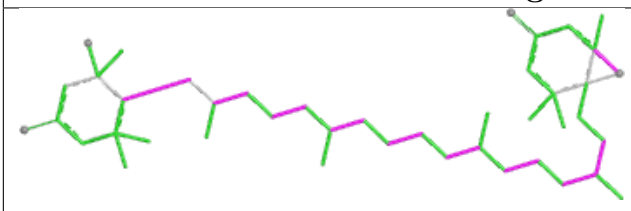
Bond angles



Torsions

Rings

Ligand NEX g 623



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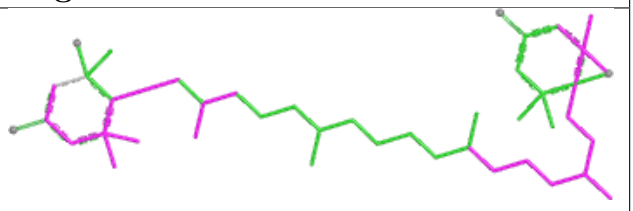
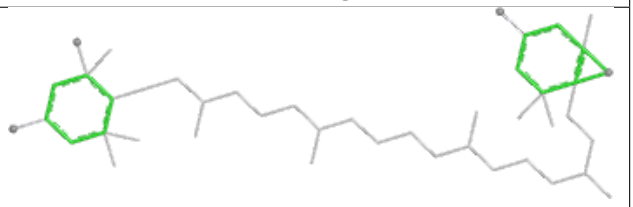


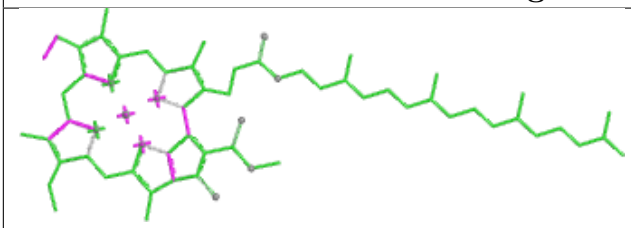
Bond angles

Torsions



Rings

Ligand CLA b 611



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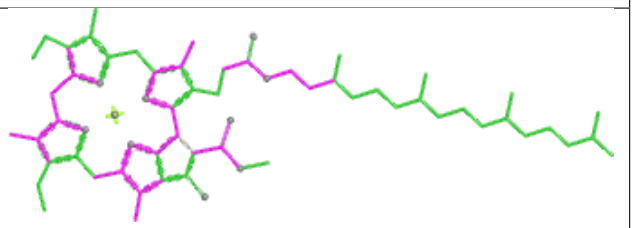

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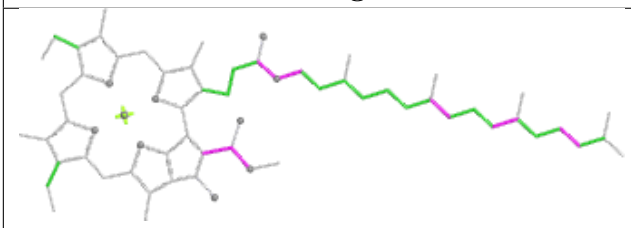
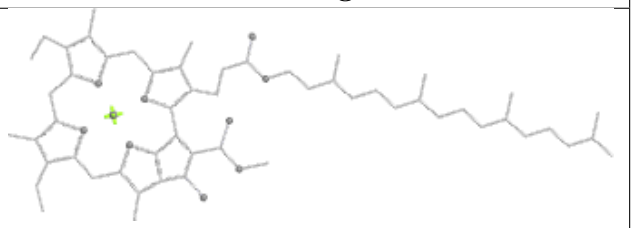
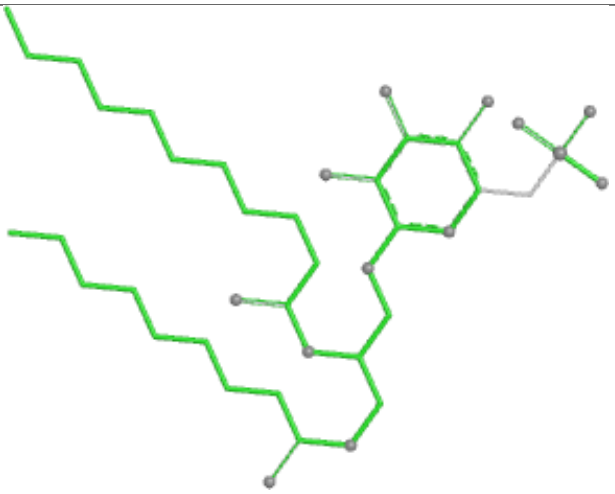


Torsions



Rings

Ligand SQD B1 621



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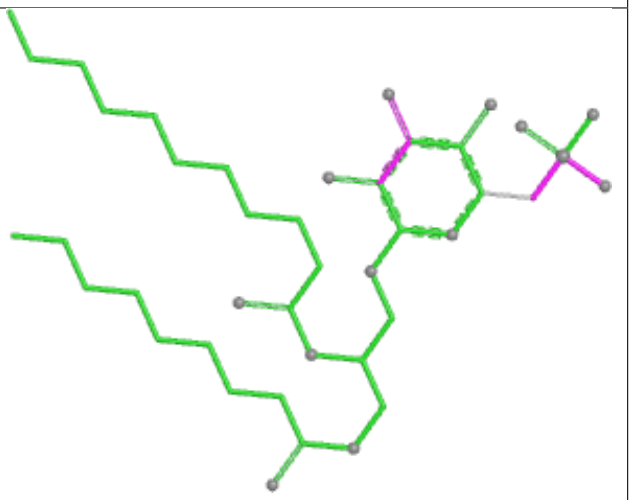
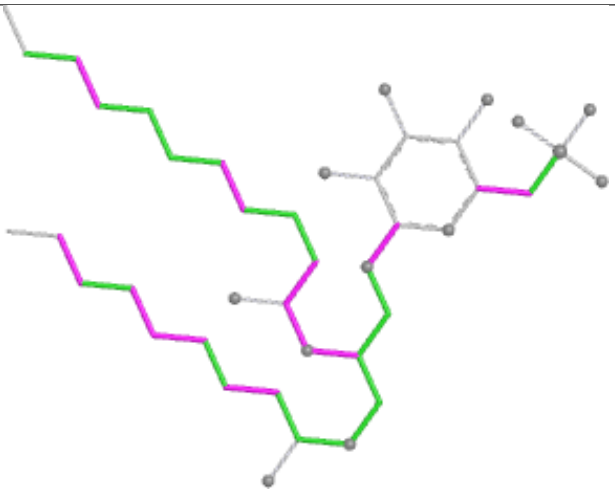


Bond angles



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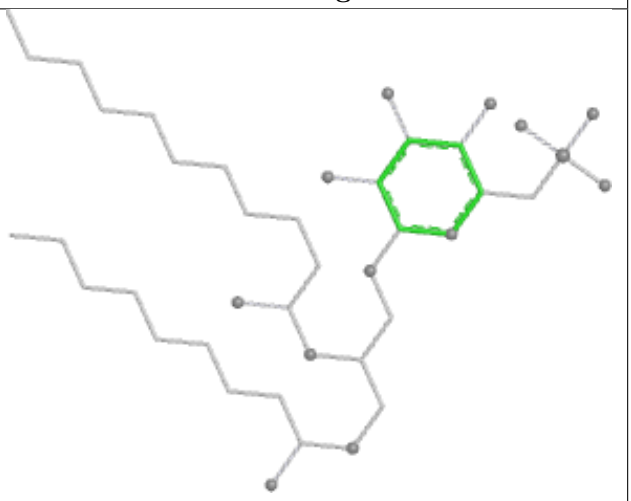
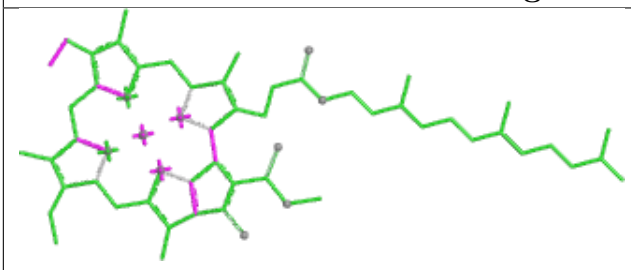


Rings

Ligand CLA A 410



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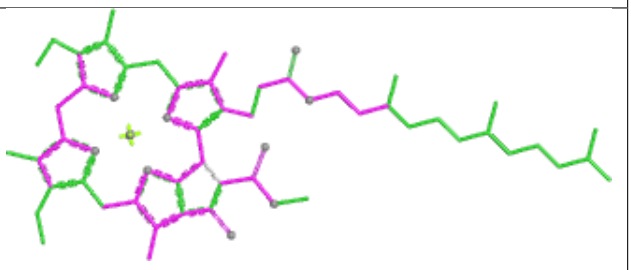

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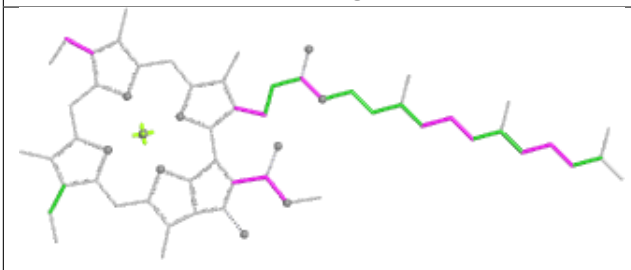

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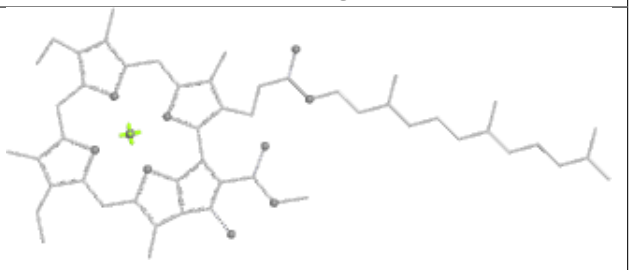
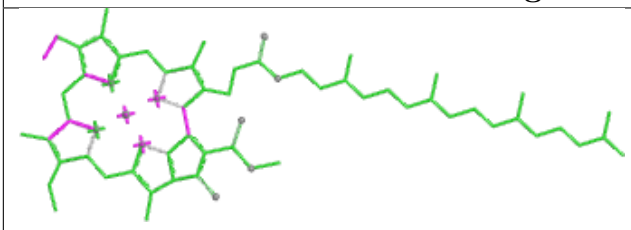


Rings

Ligand CLA C 512



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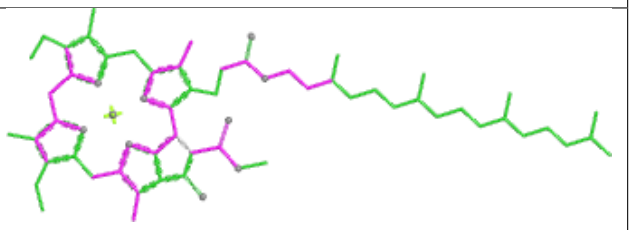

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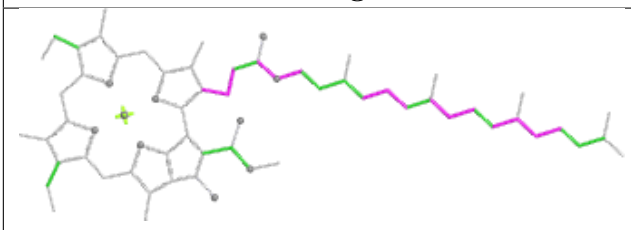

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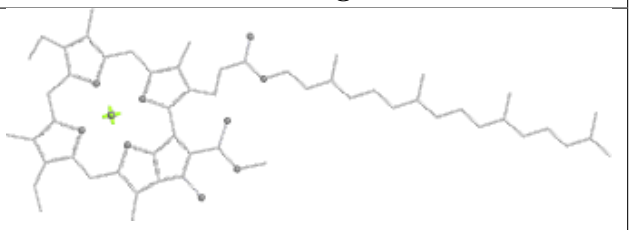
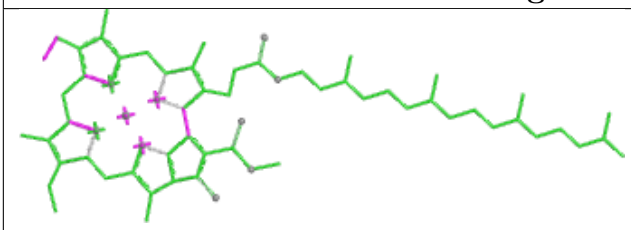


Rings

Ligand CLA n 603



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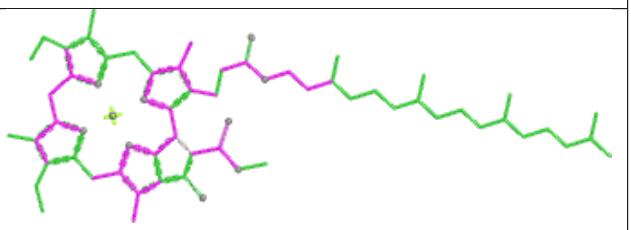

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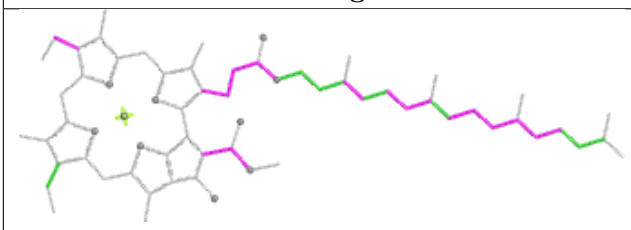

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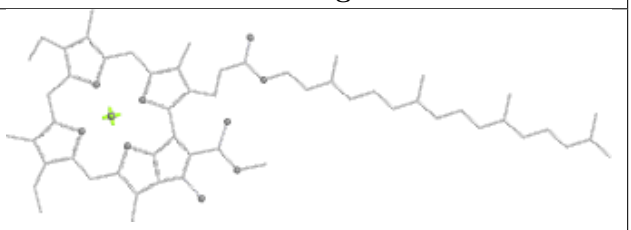
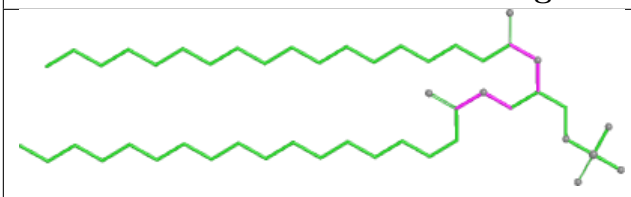


Rings

Ligand 3PH i 101



Bond lengths

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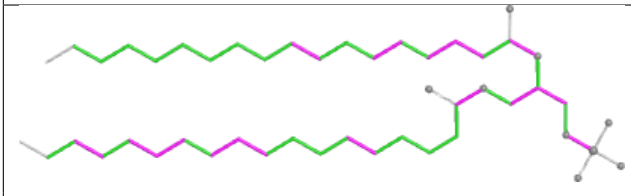

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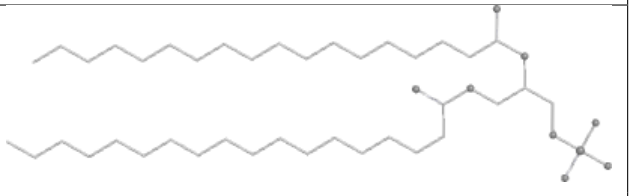
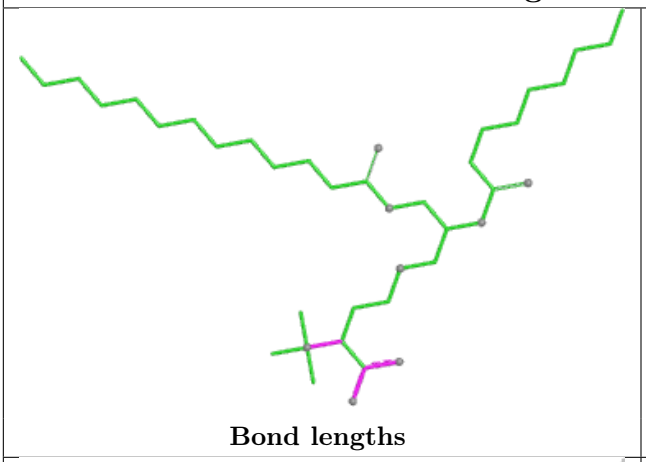


Rings

Ligand LMK c 627



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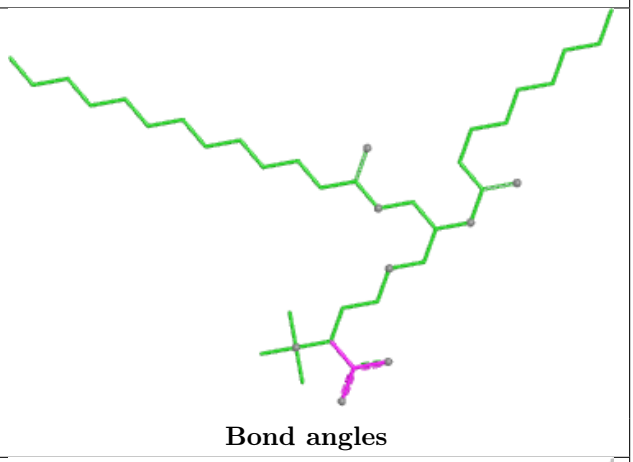

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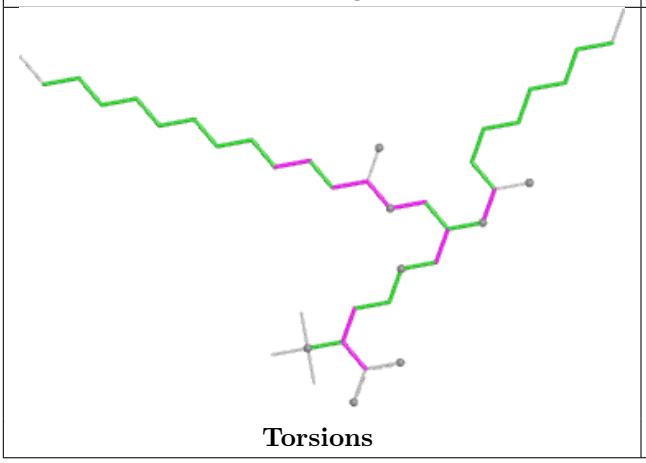

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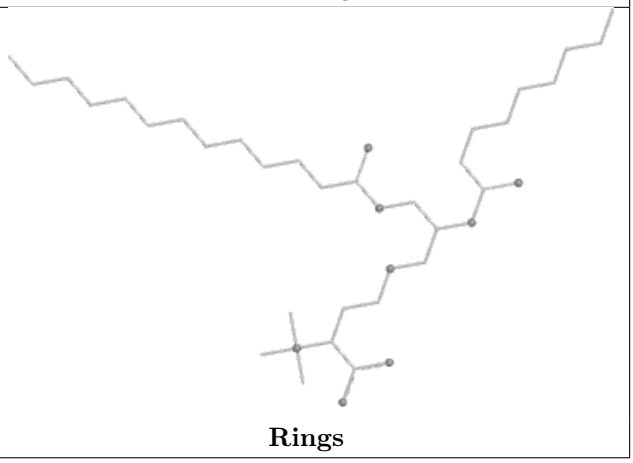
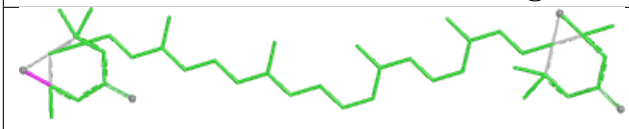


Rings

Ligand XAT n 622



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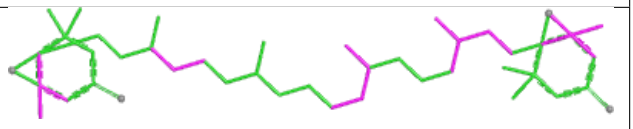
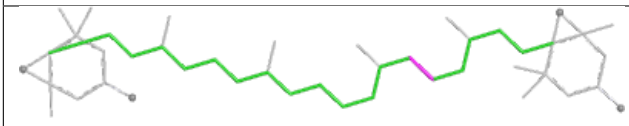


Bond angles



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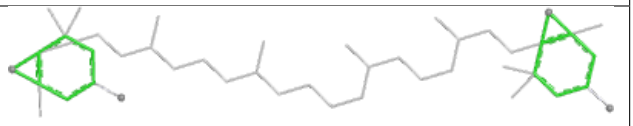
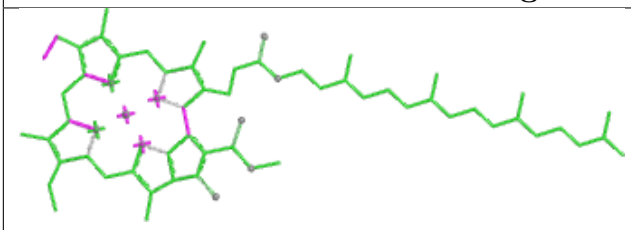


Rings

Ligand CLA c1 510



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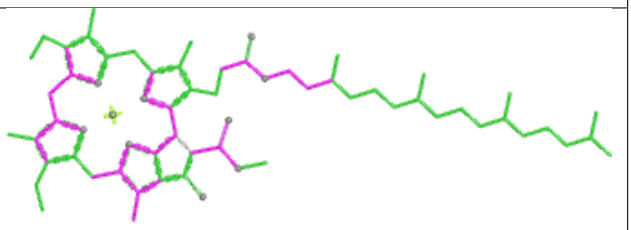

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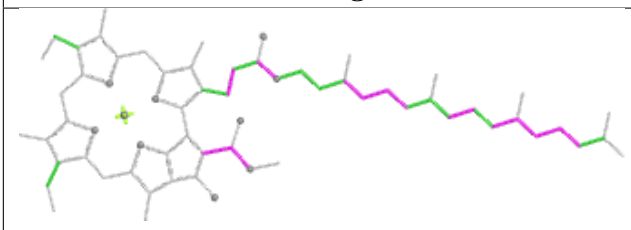

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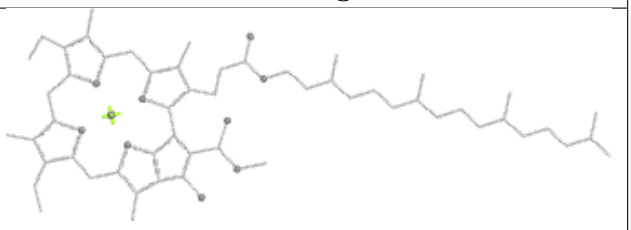
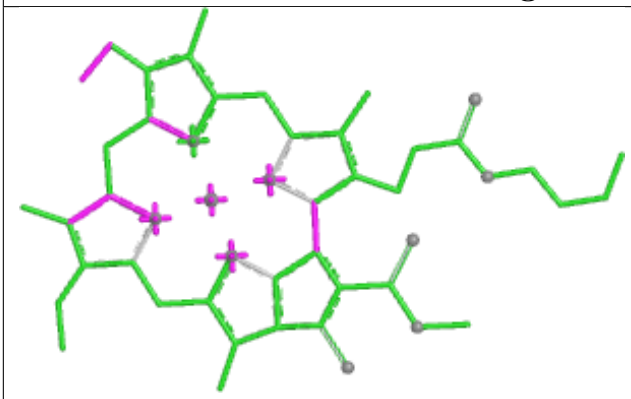


Rings

Ligand CLA g1 614



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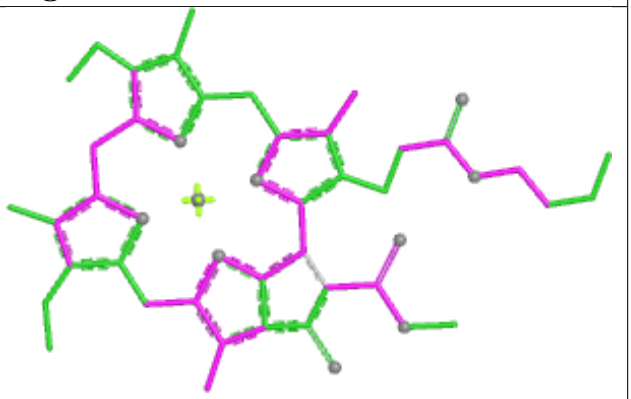
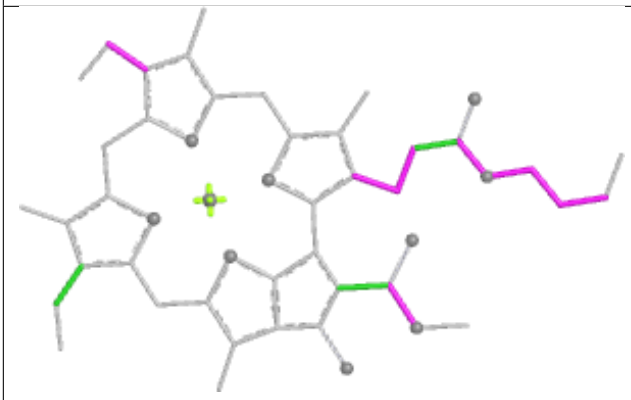


Bond angles



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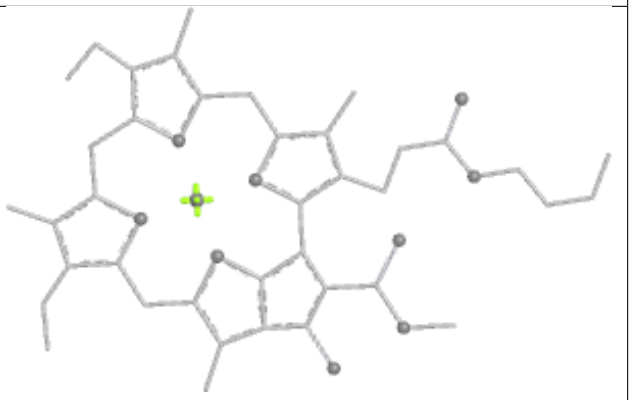
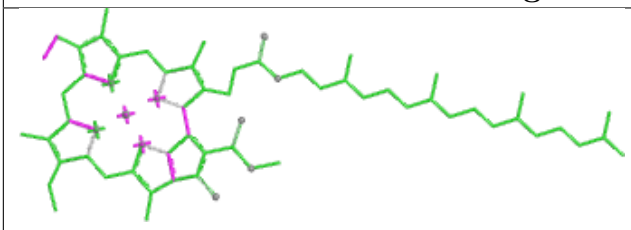
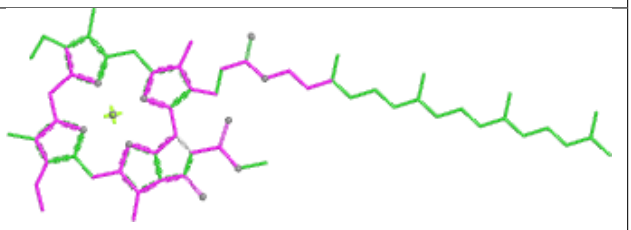
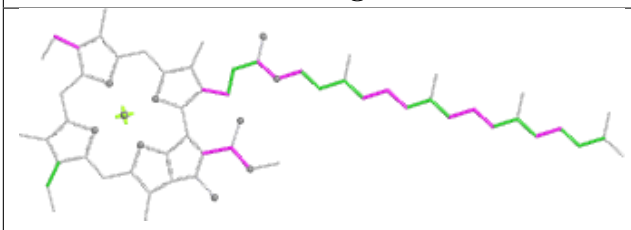
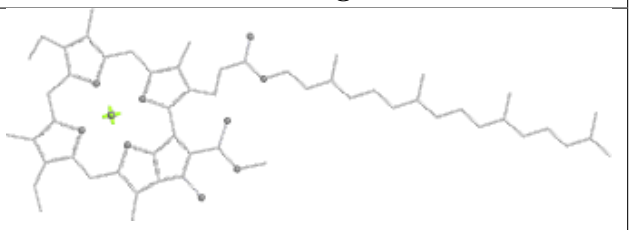
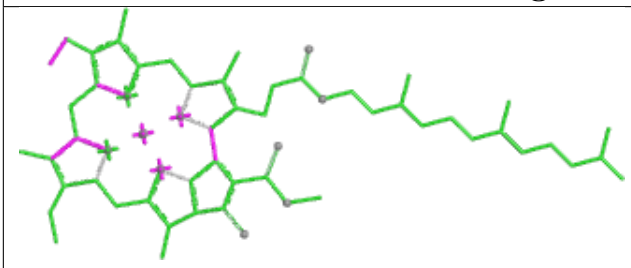
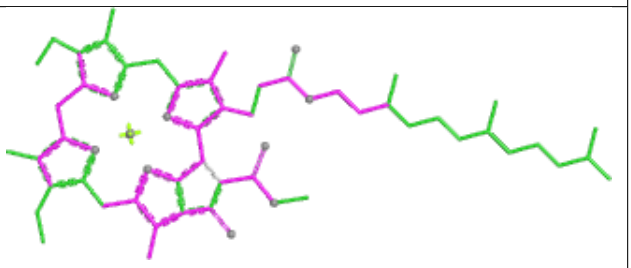
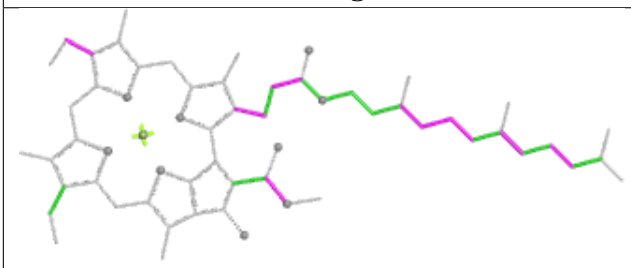
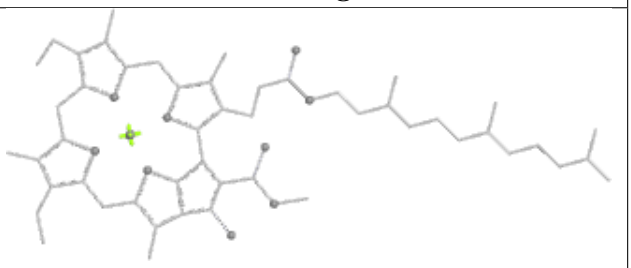
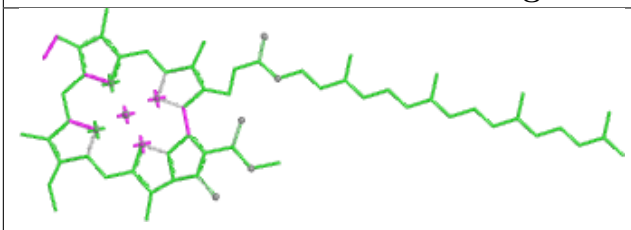


Rings

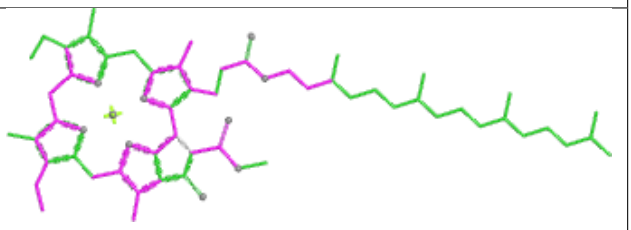
Ligand CLA N 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA r 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

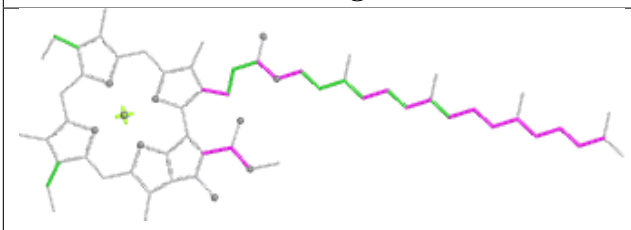
Ligand CLA G 603



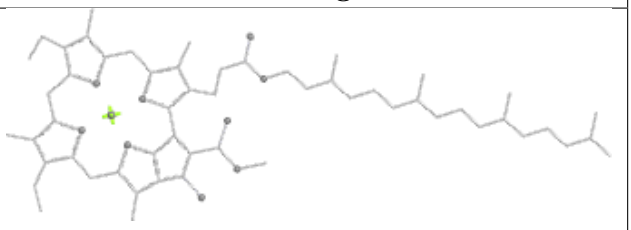
Bond lengths



Bond angles

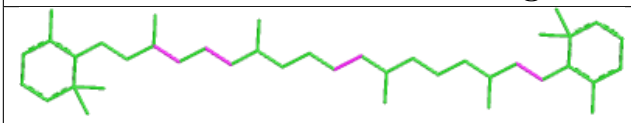


Torsions

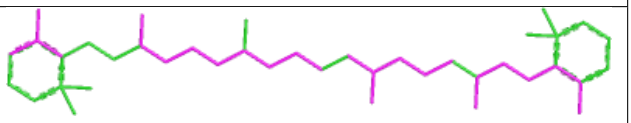


Rings

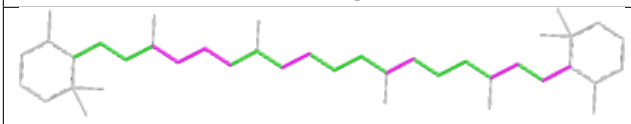
Ligand BCR B 618



Bond lengths



Bond angles



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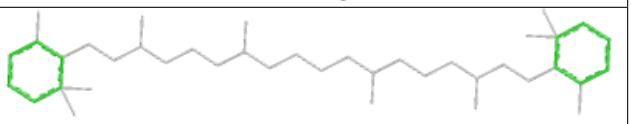
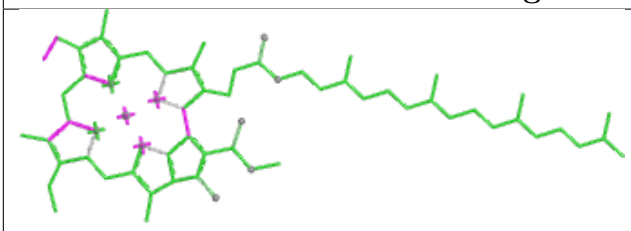


Rings

Ligand CLA N 604



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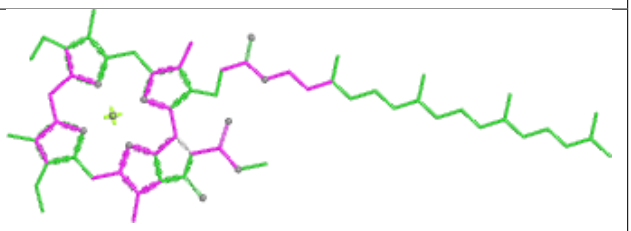
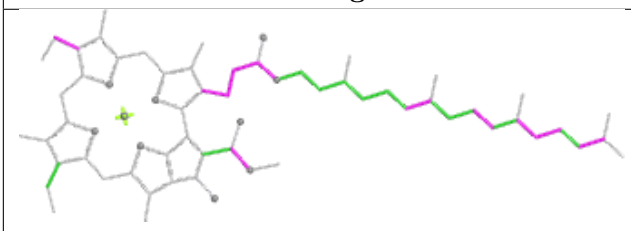


Bond angles



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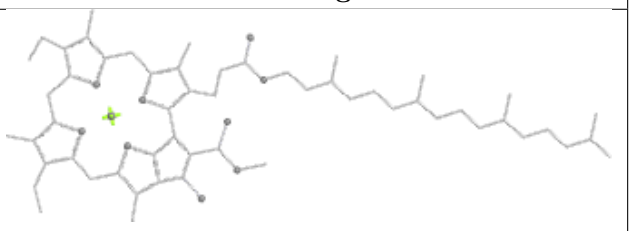
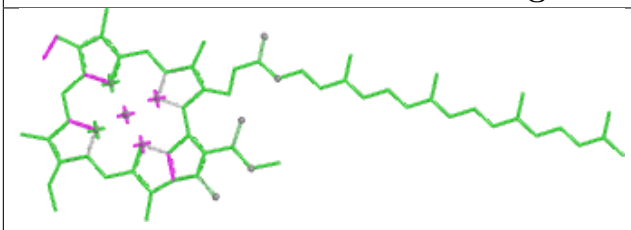


Rings

Ligand CLA a 405



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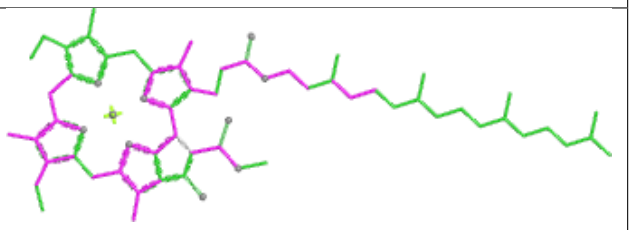
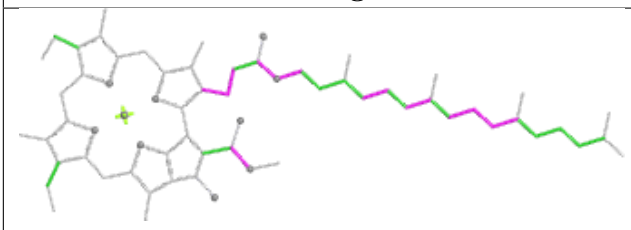


Bond angles



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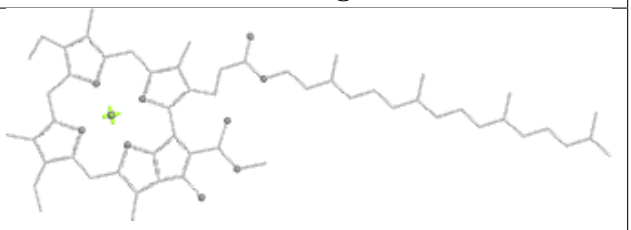
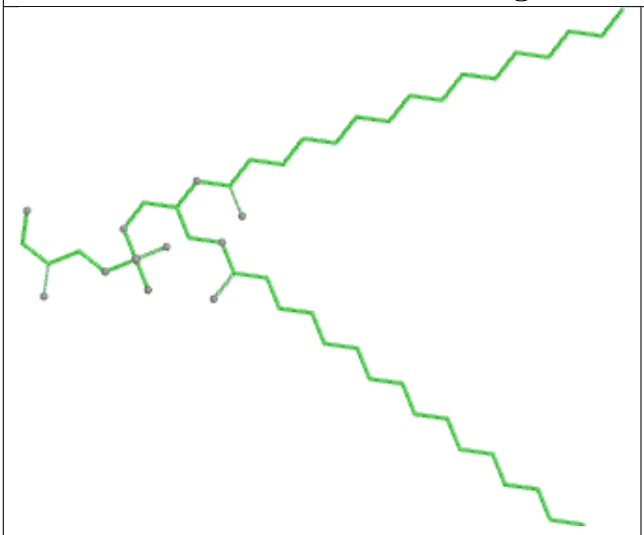


Rings

Ligand LHG N1 624



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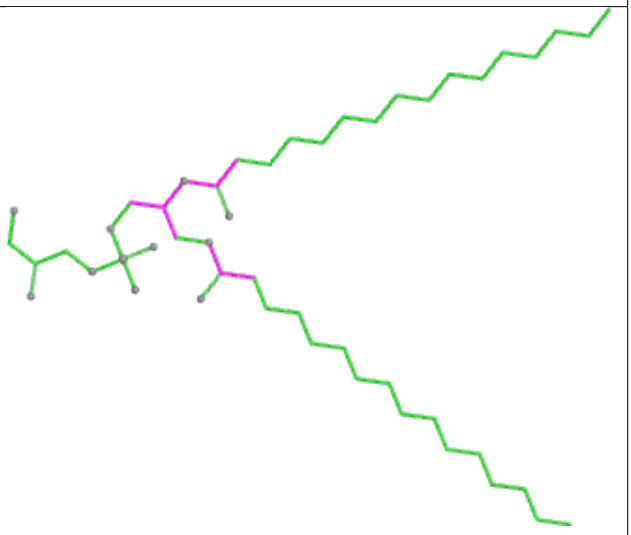
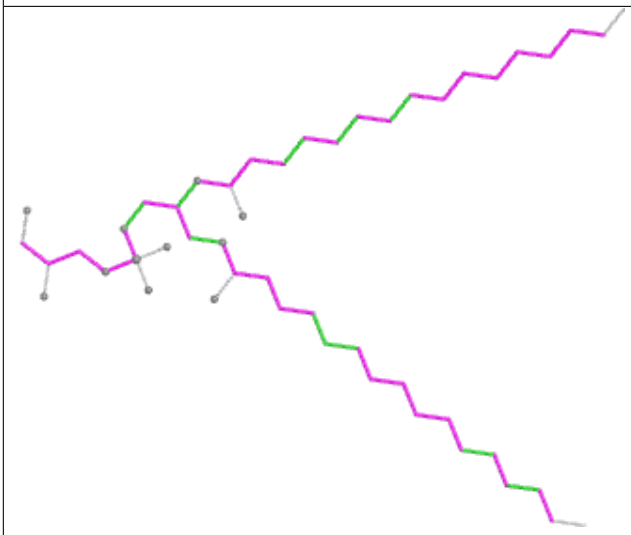


Bond angles



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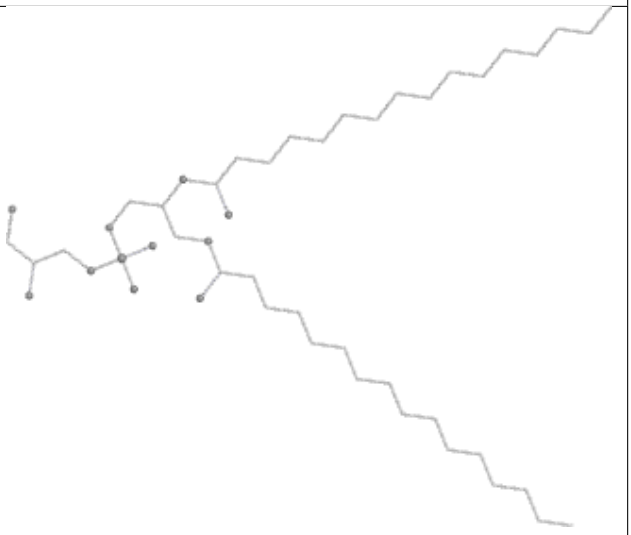
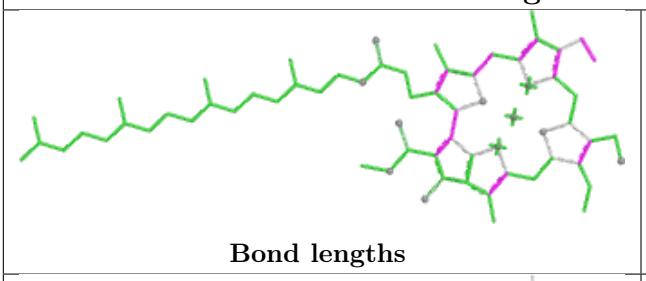


Rings

Ligand CHL Y 601



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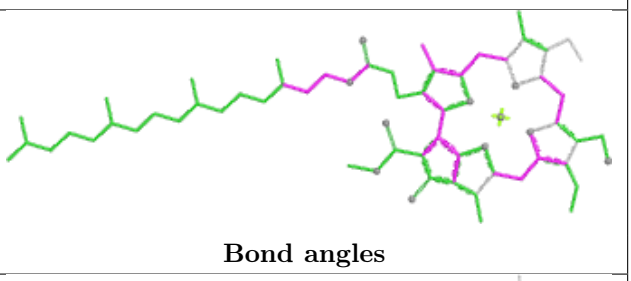
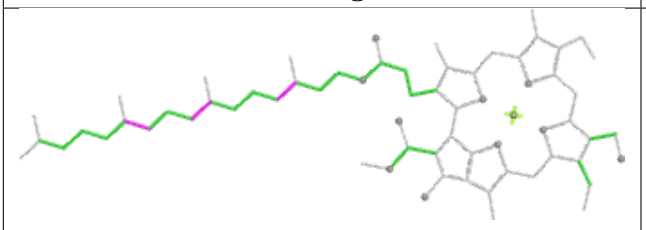


Bond angles



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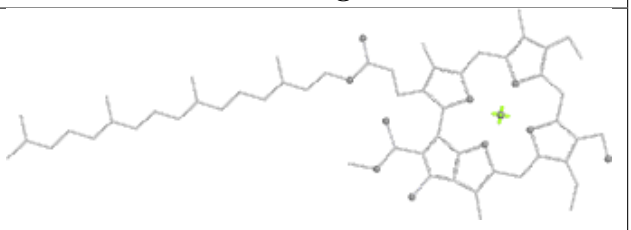
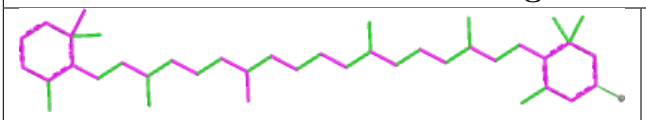


Rings

Ligand RRX h 101



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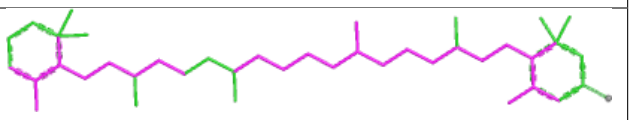
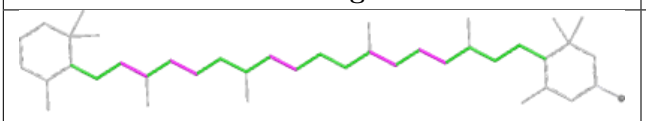


Bond angles



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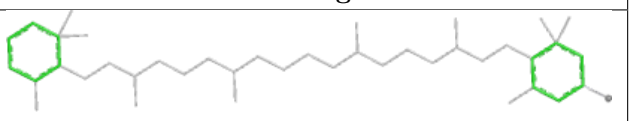
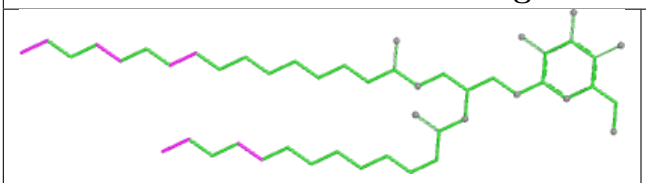
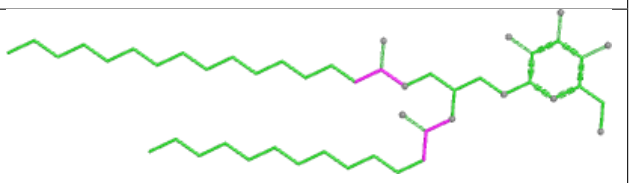


Rings

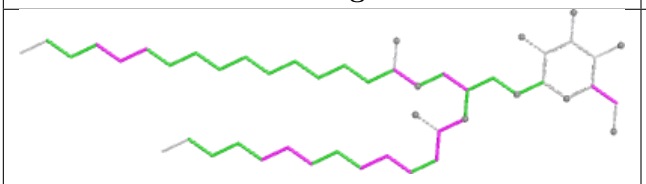
Ligand LMG h1 102



Bond lengths



Bond angles



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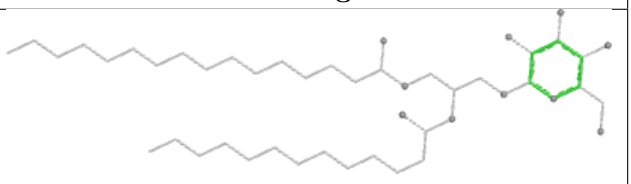
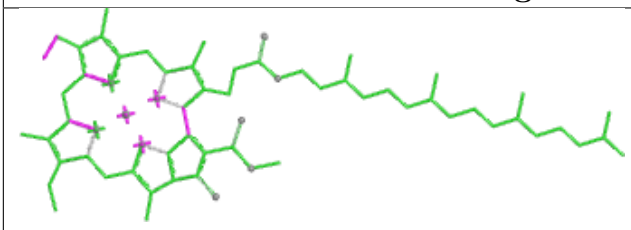
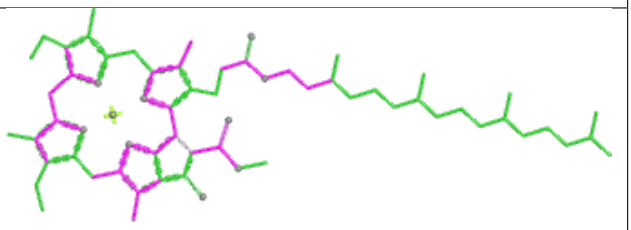
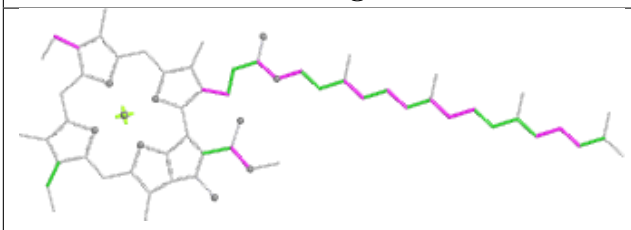
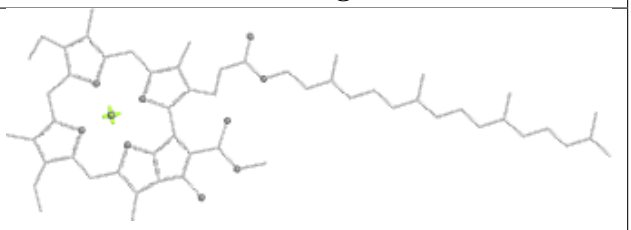
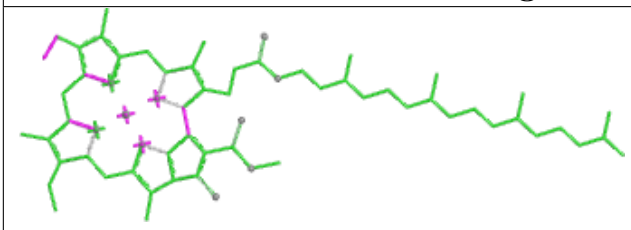
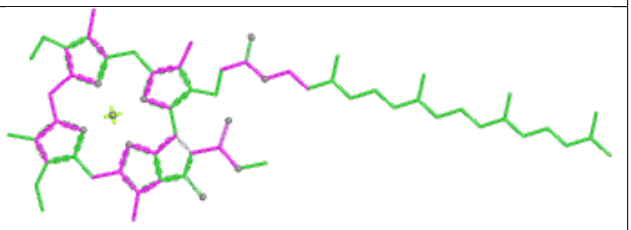
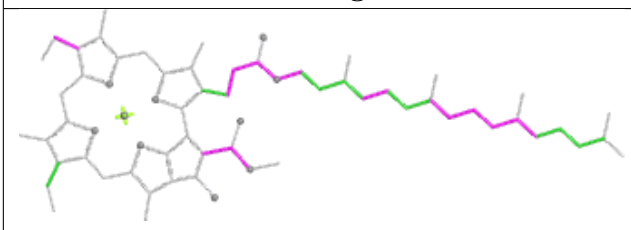
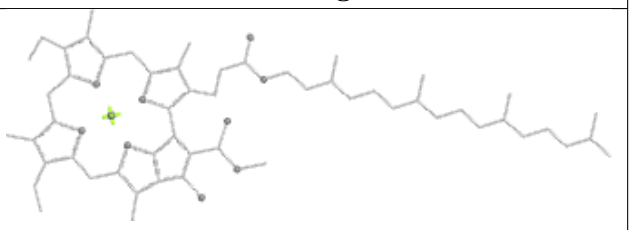
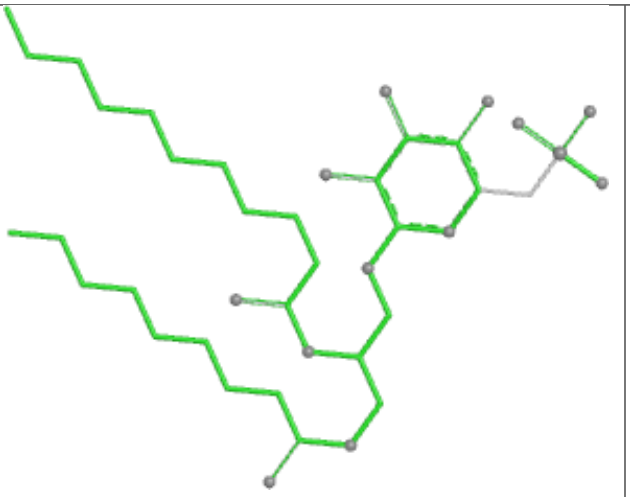


Rings

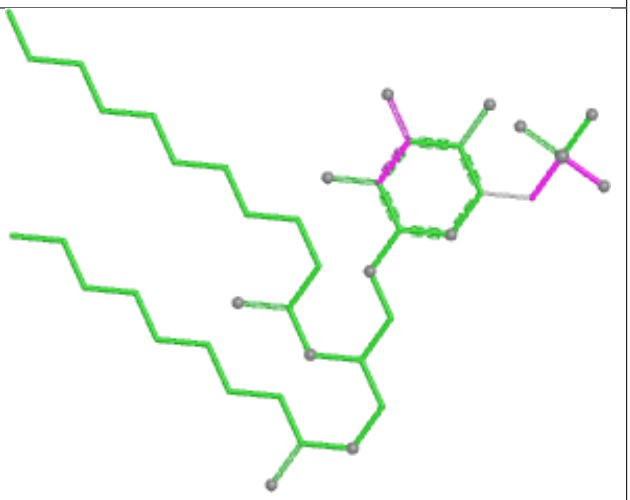
Ligand CLA N1 603	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA b1 613	
 Bond lengths	 Bond angles
 Torsions	 Rings

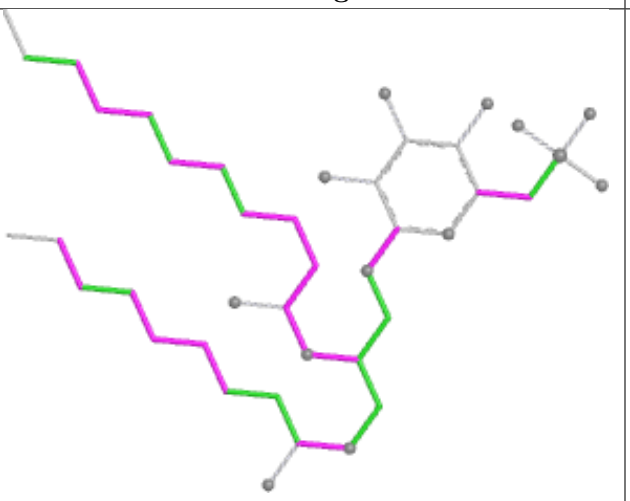
Ligand SQD M1 101



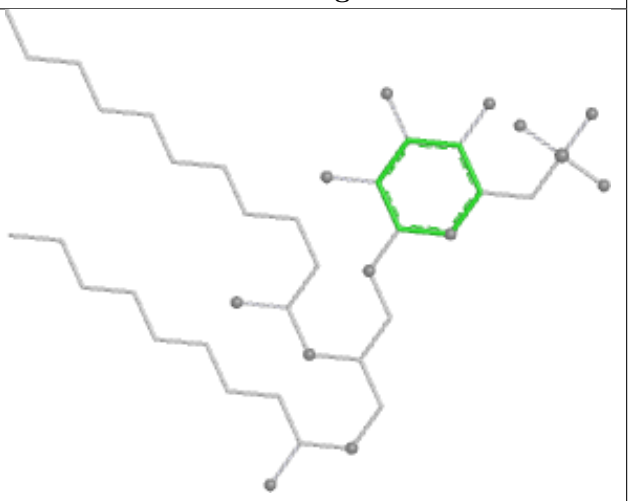
Bond lengths



Bond angles

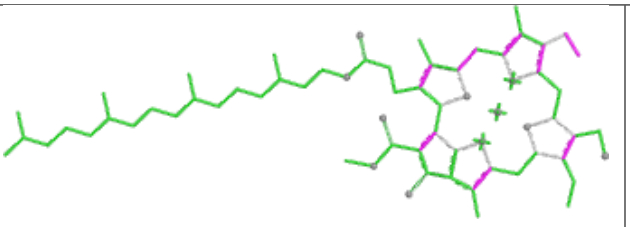


Torsions



Rings

Ligand CHL G1 607



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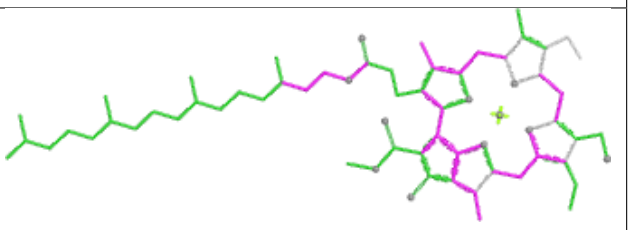
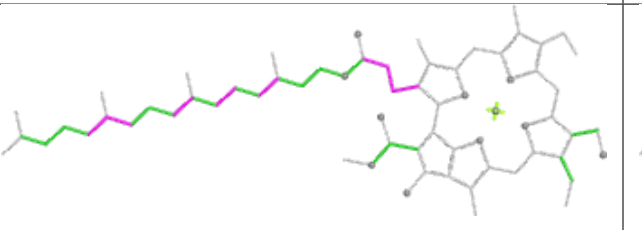


Bond angles



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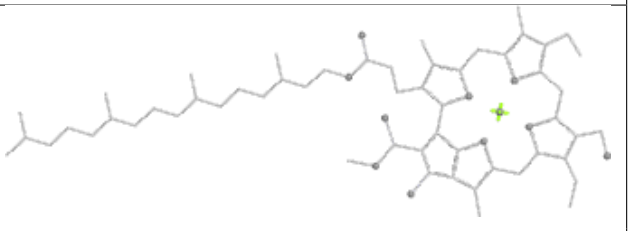
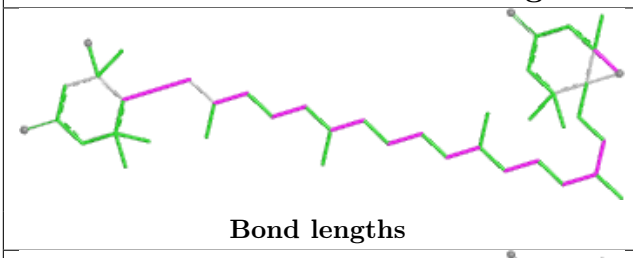
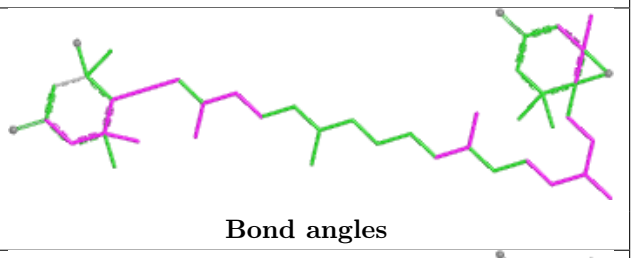


Rings

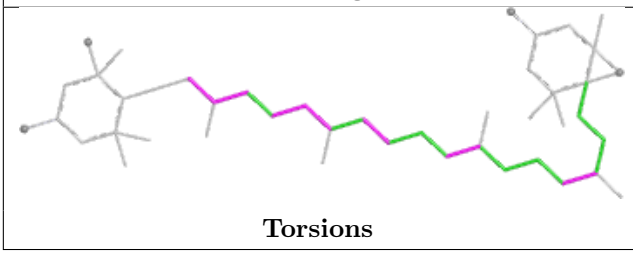
Ligand NEX S 622



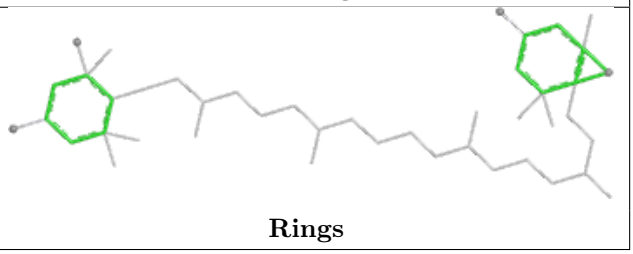
Bond lengths



Bond angles

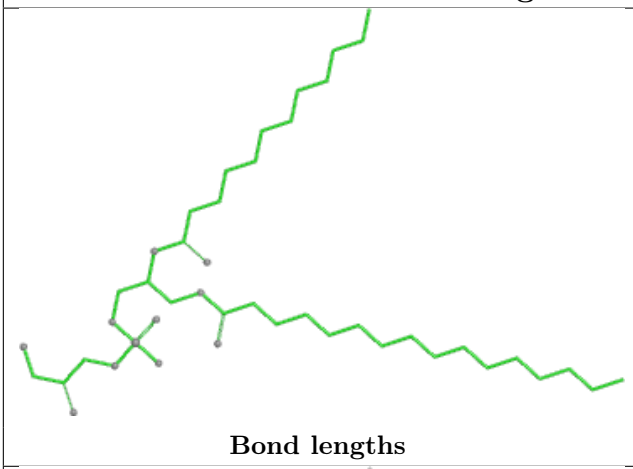


Torsions



Rings

Ligand LHG S1 624



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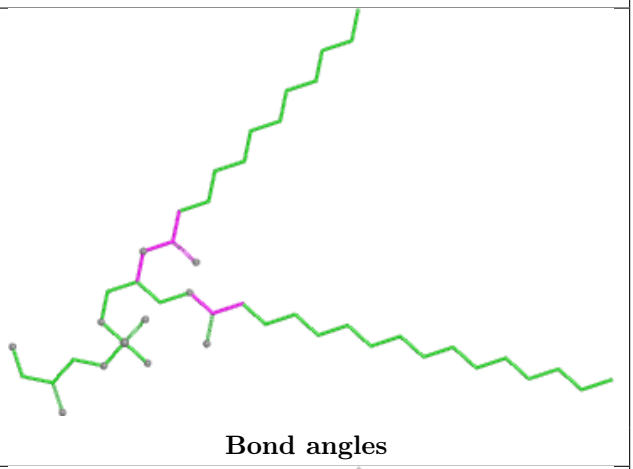
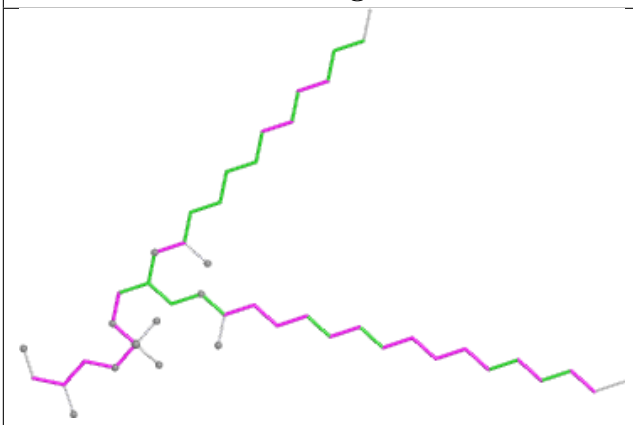
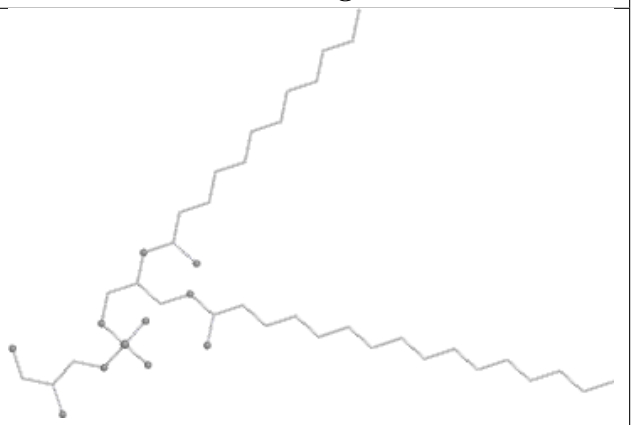


Bond angles

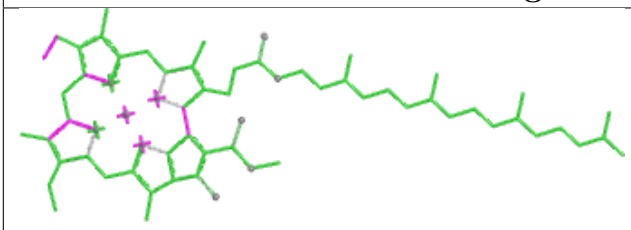


Torsions

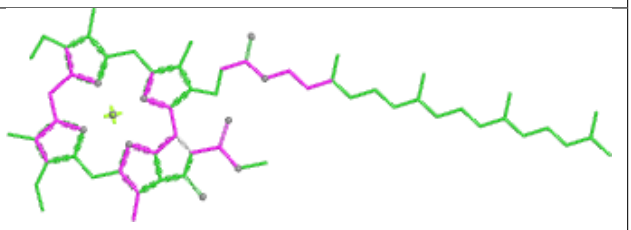


Rings

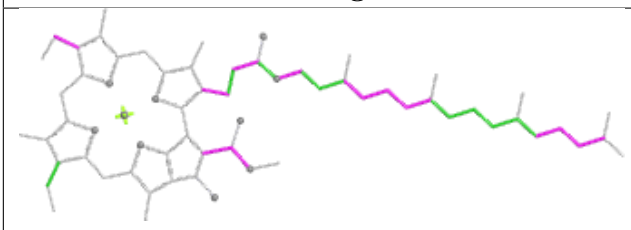
Ligand CLA B 610



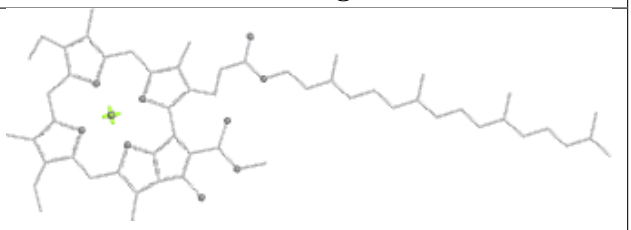
Bond lengths



Bond angles

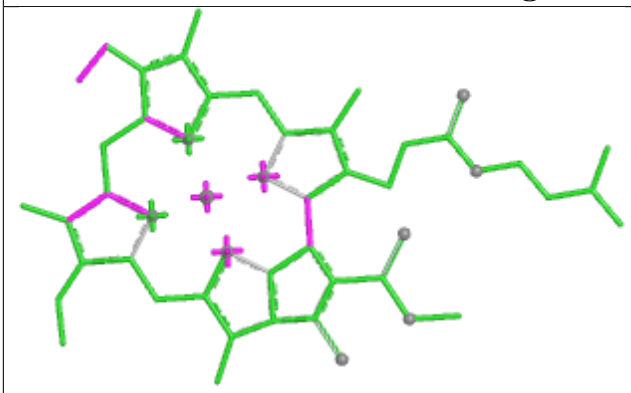


Torsions

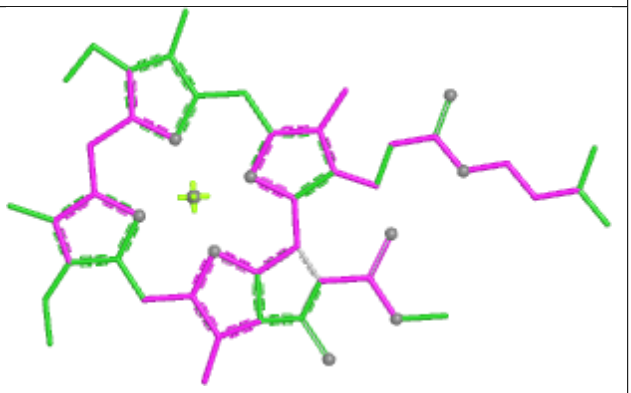


Rings

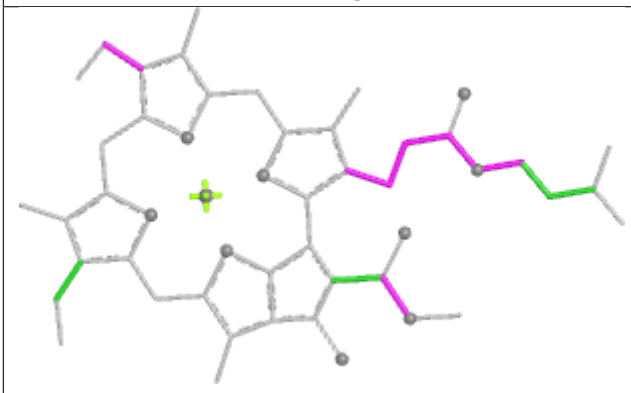
Ligand CLA s1 617



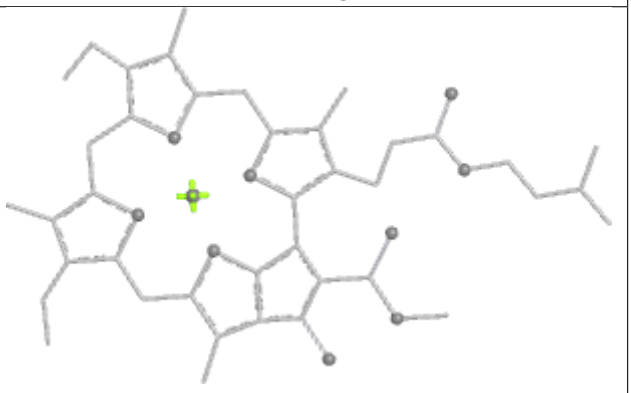
Bond lengths



Bond angles

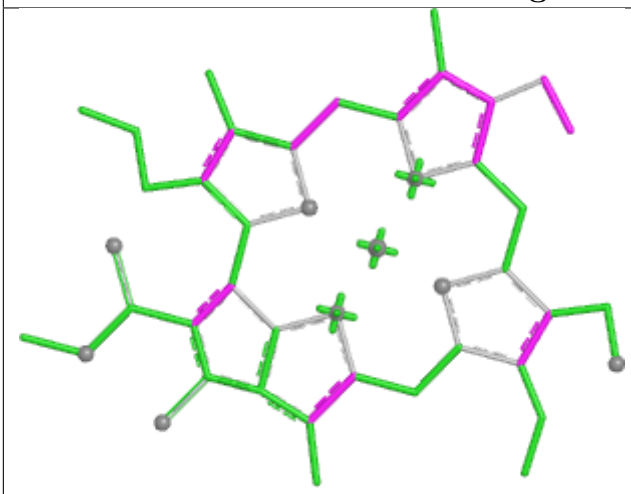


Torsions



Rings

Ligand CHL r 606



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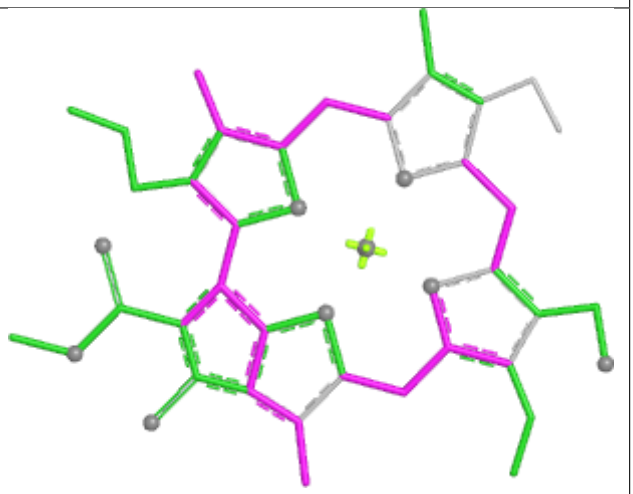
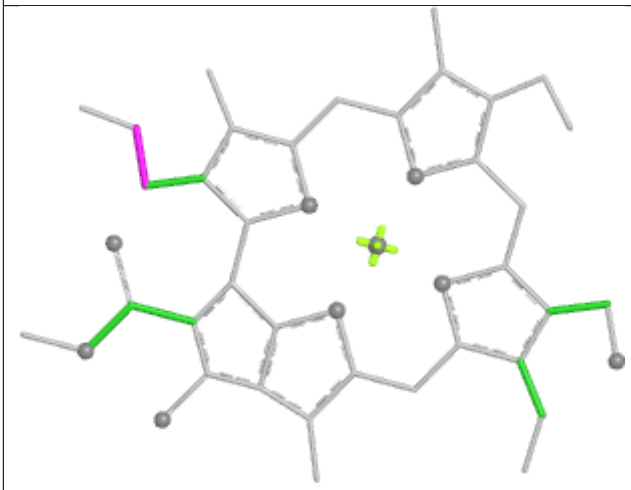
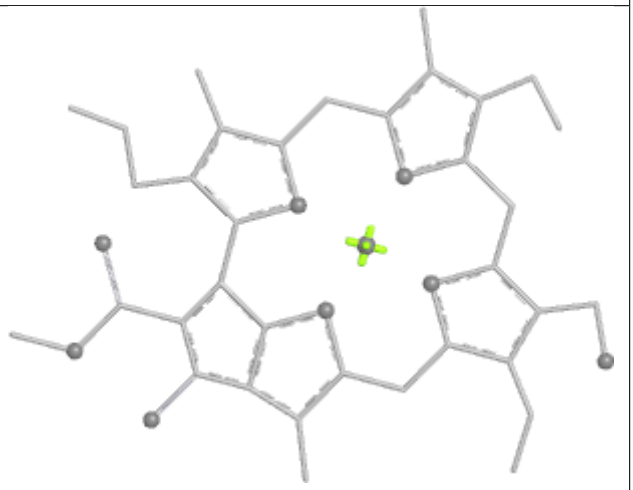


Bond angles

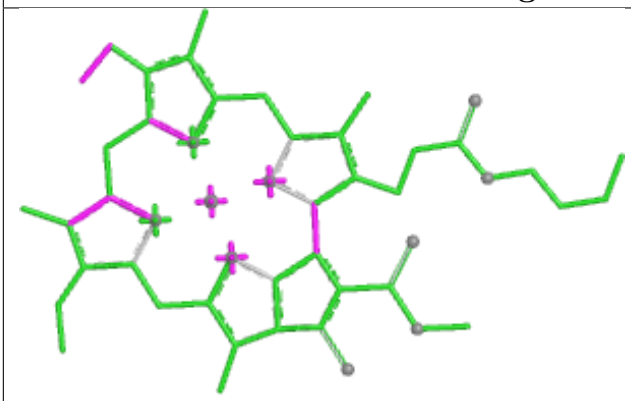


Torsions



Rings

Ligand CLA n1 611



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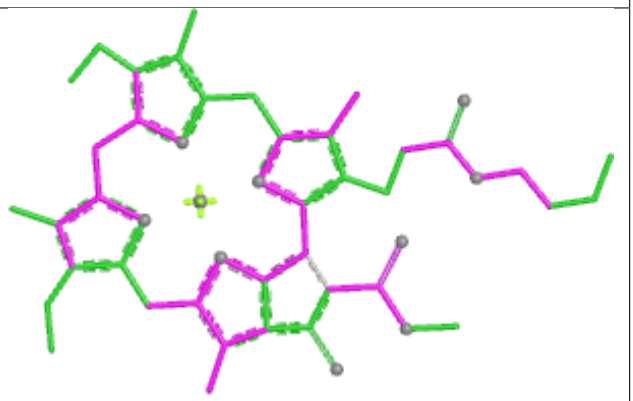
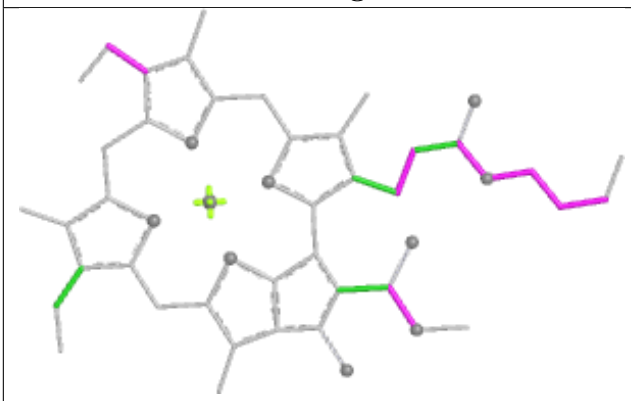


Bond angles



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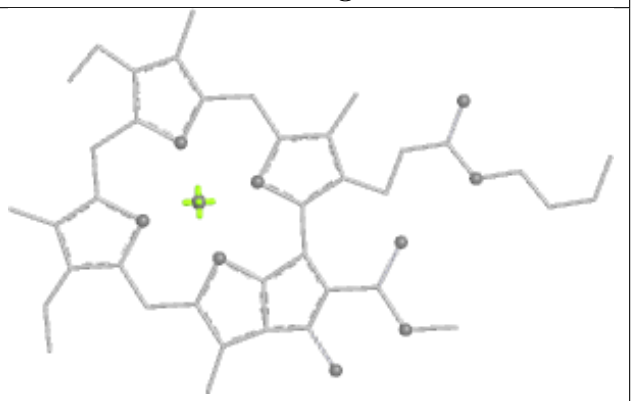
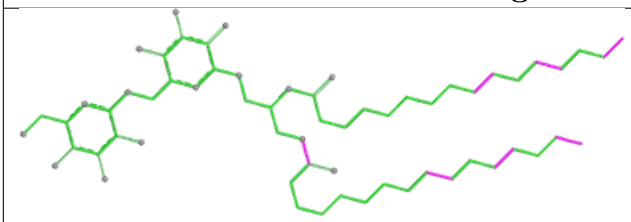
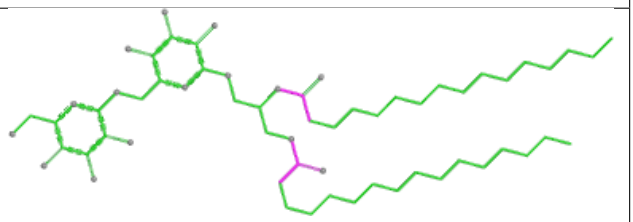


Rings

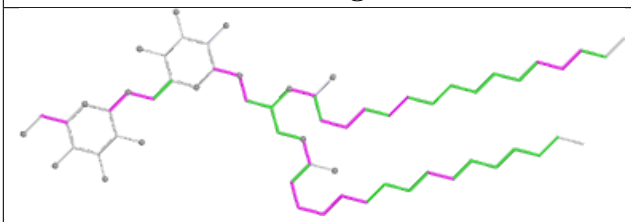
Ligand DGD C1 519



Bond lengths



Bond angles



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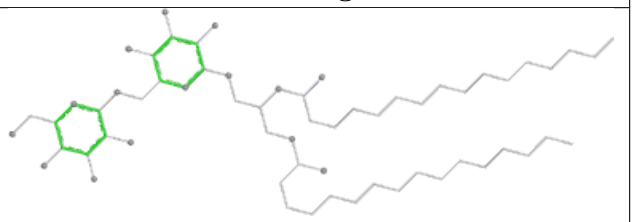
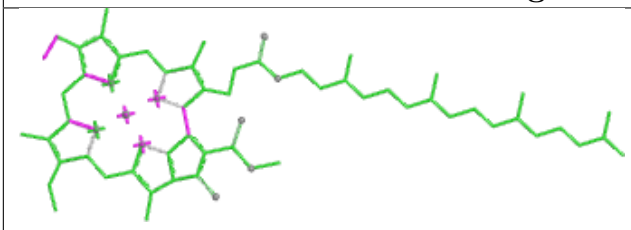
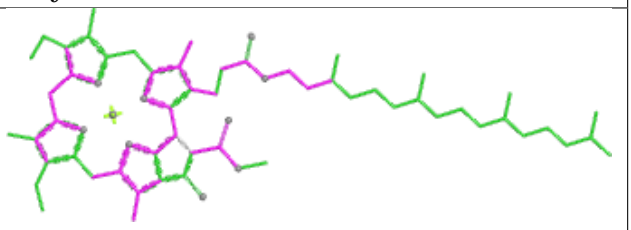
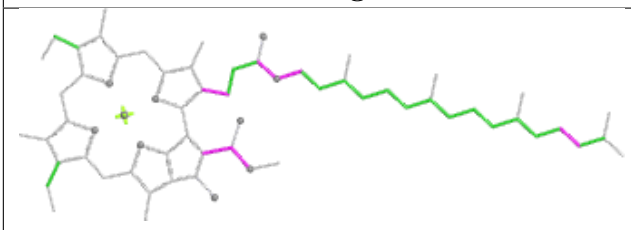
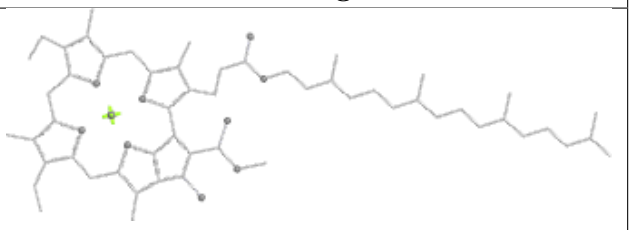
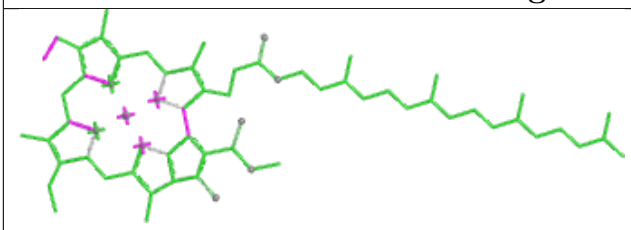
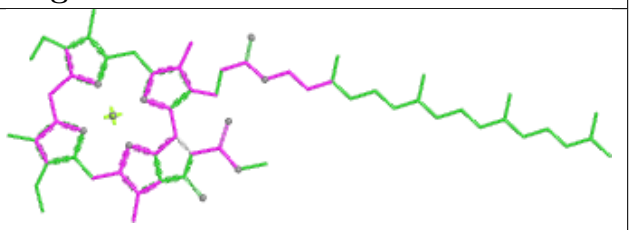
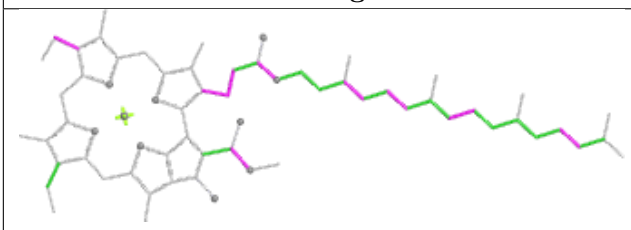
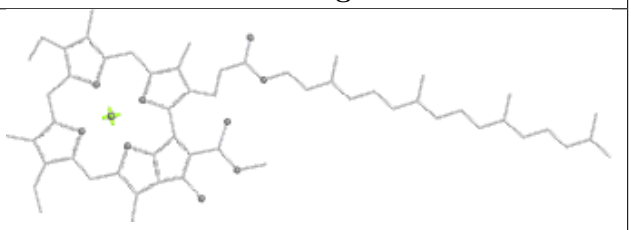
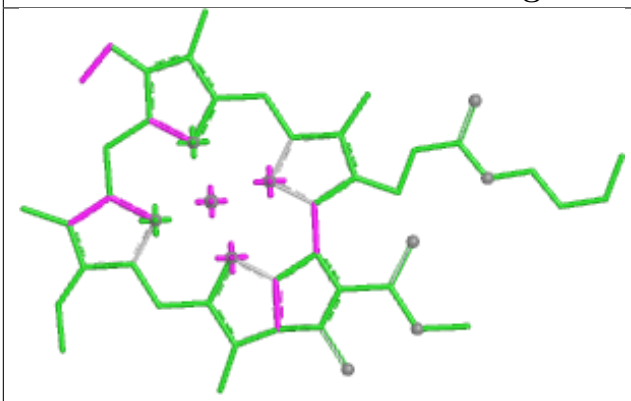


Rings

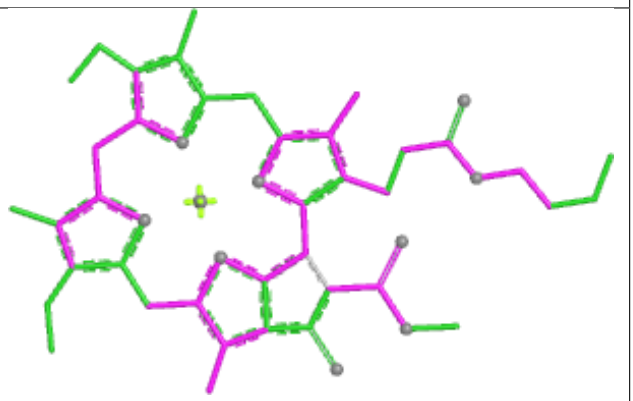
Ligand CLA y 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA g 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

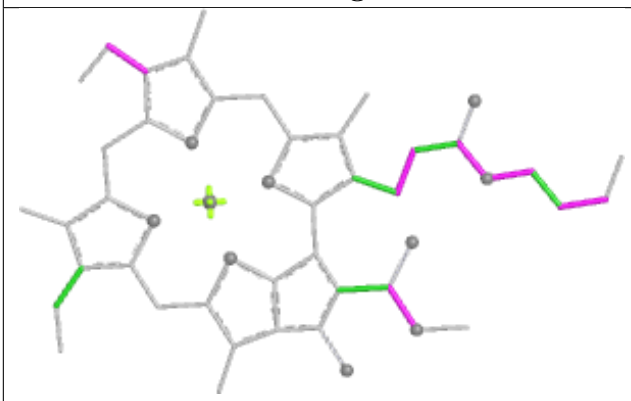
Ligand CLA G 604



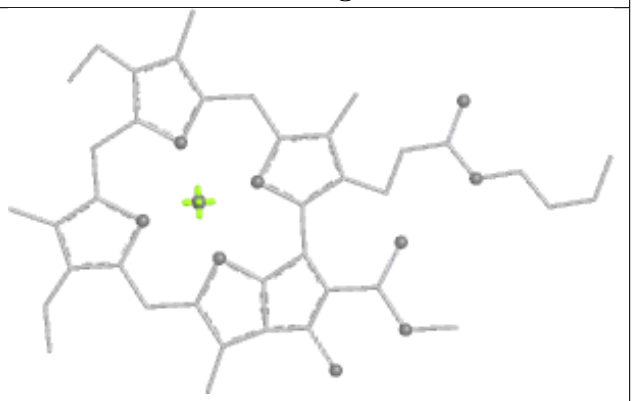
Bond lengths



Bond angles

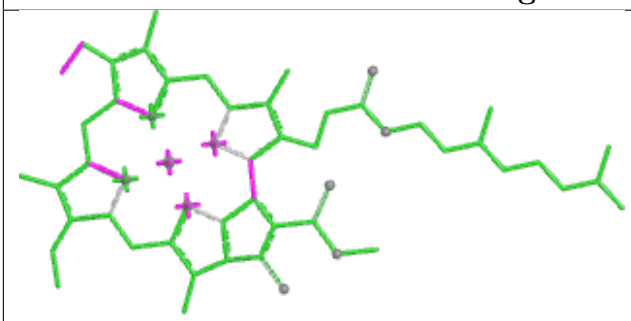


Torsions

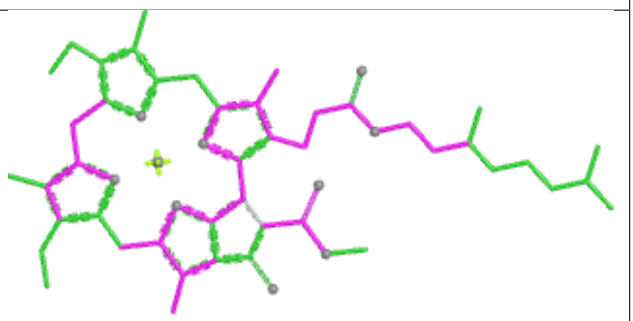


Rings

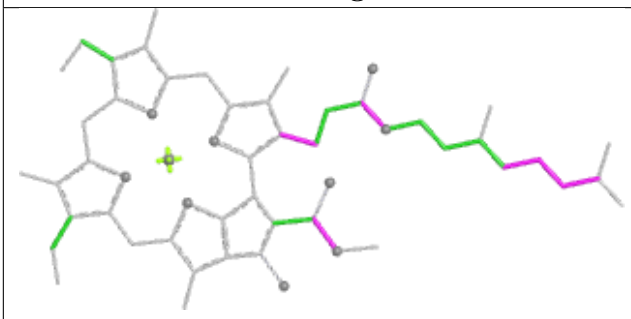
Ligand CLA S1 604



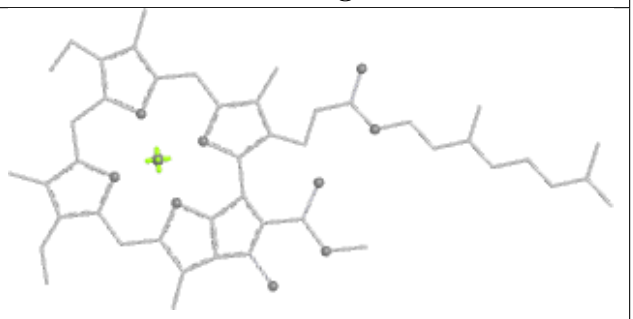
Bond lengths



Bond angles

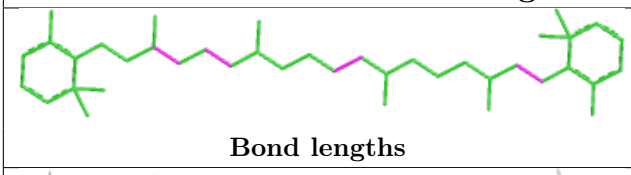


Torsions



Rings

Ligand BCR c1 516



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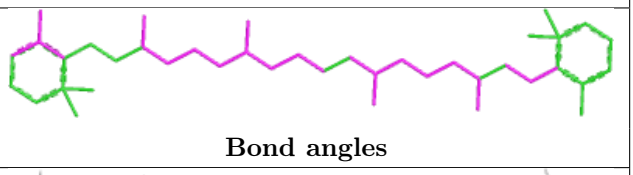
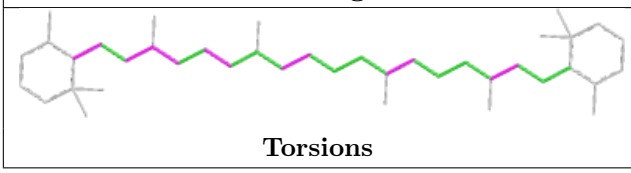
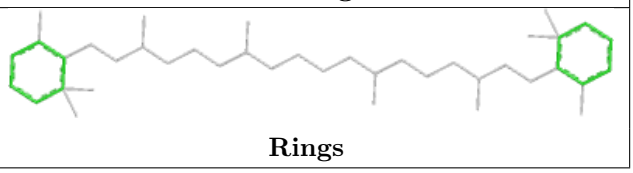


Bond angles

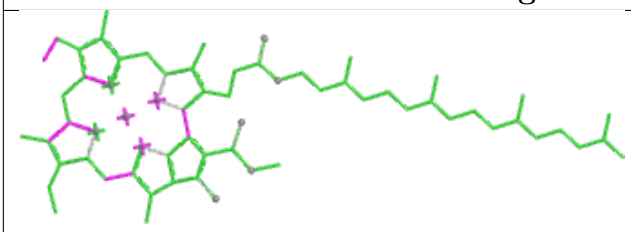


Torsions

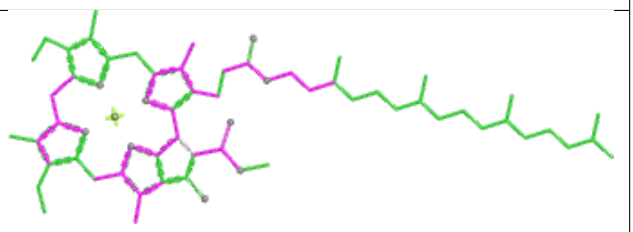


Rings

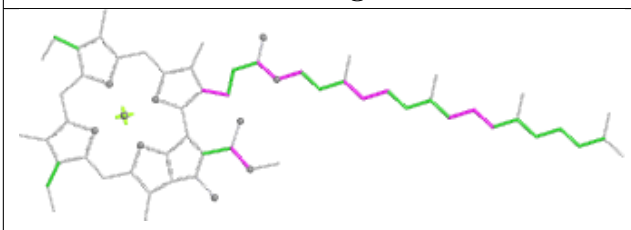
Ligand CLA d1 403



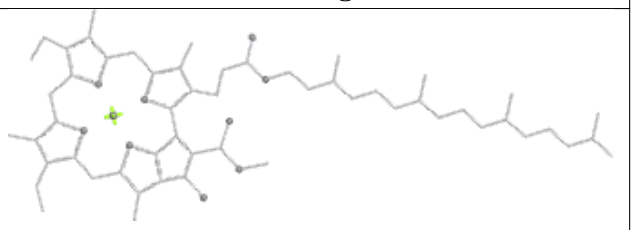
Bond lengths



Bond angles

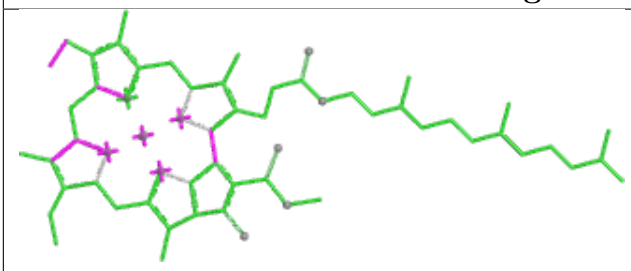


Torsions



Rings

Ligand CLA R 603



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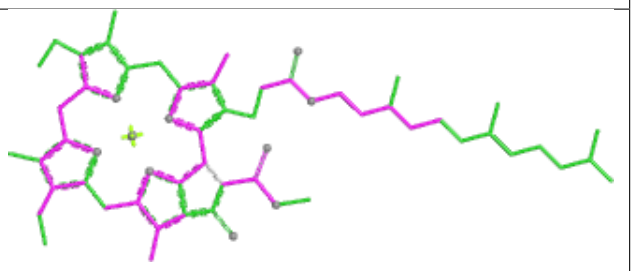
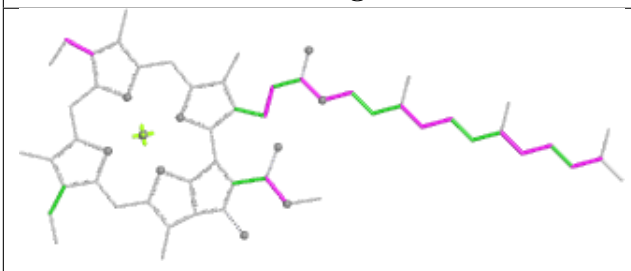
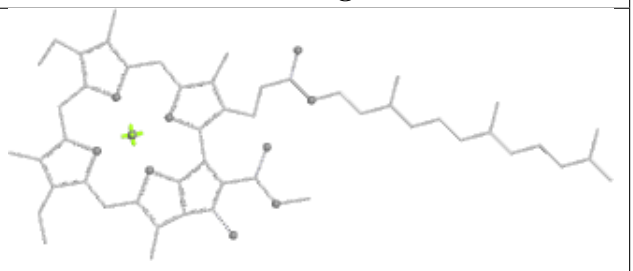


Bond angles

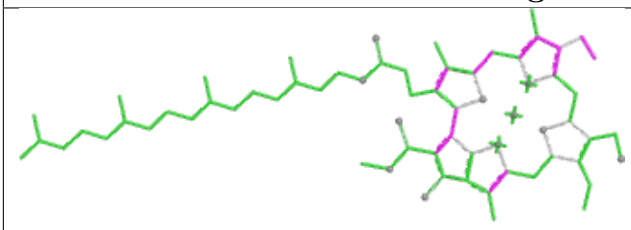


Torsions

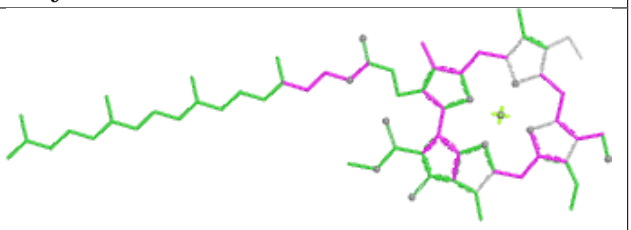


Rings

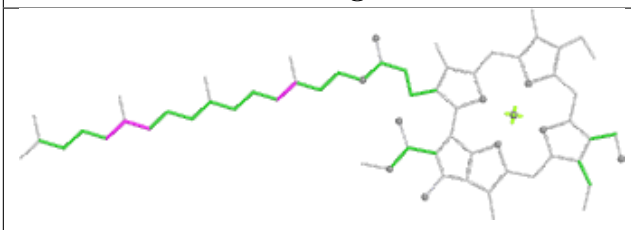
Ligand CHL y 609



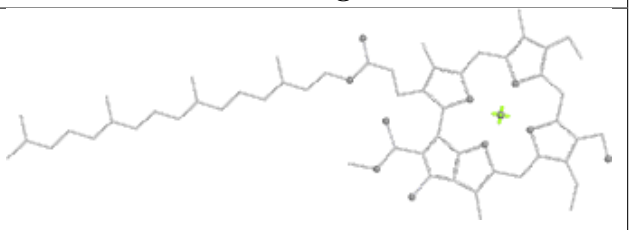
Bond lengths



Bond angles

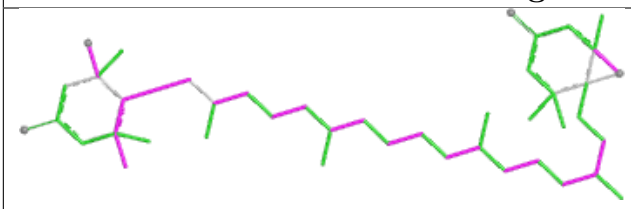


Torsions

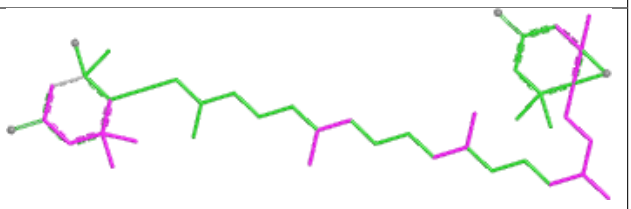


Rings

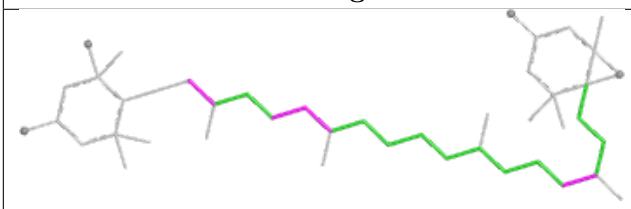
Ligand NEX s 623



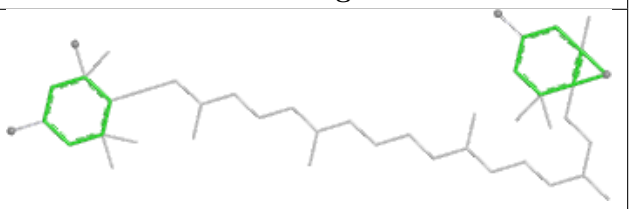
Bond lengths



Bond angles

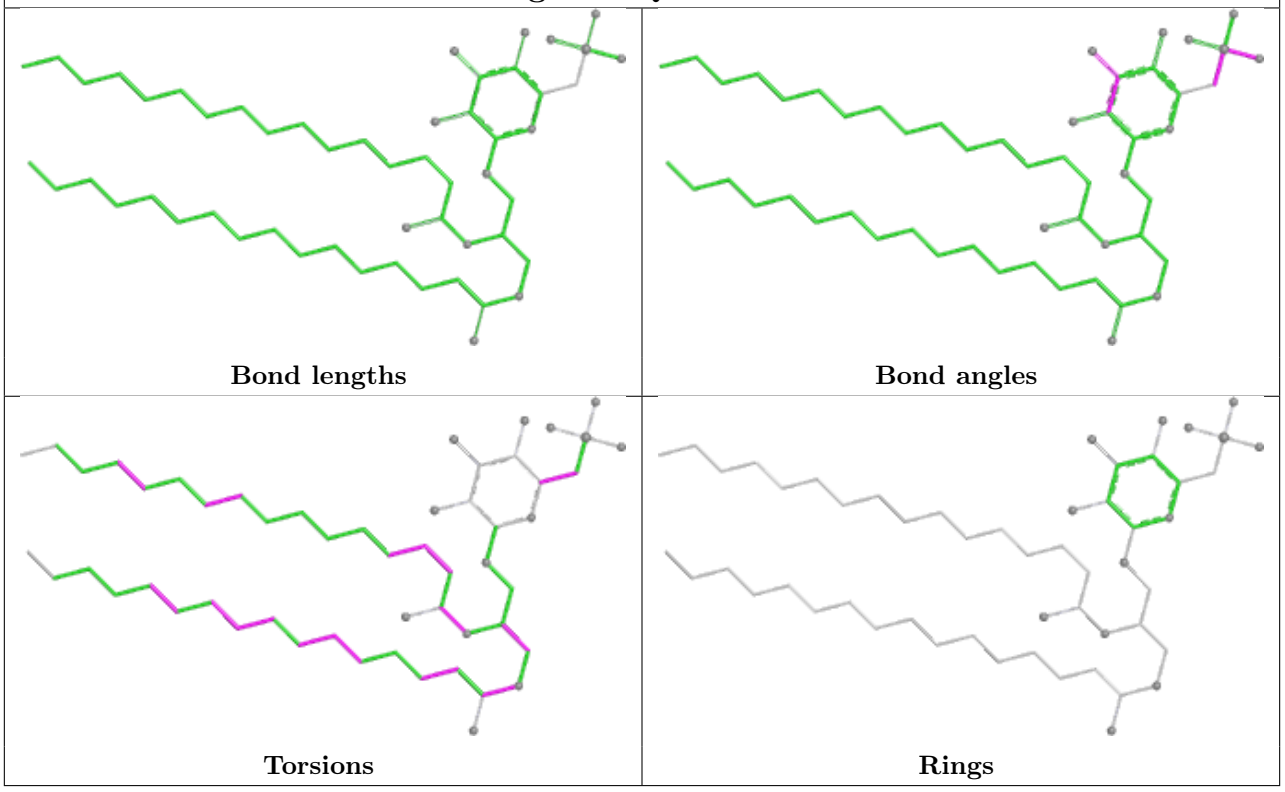


Torsions

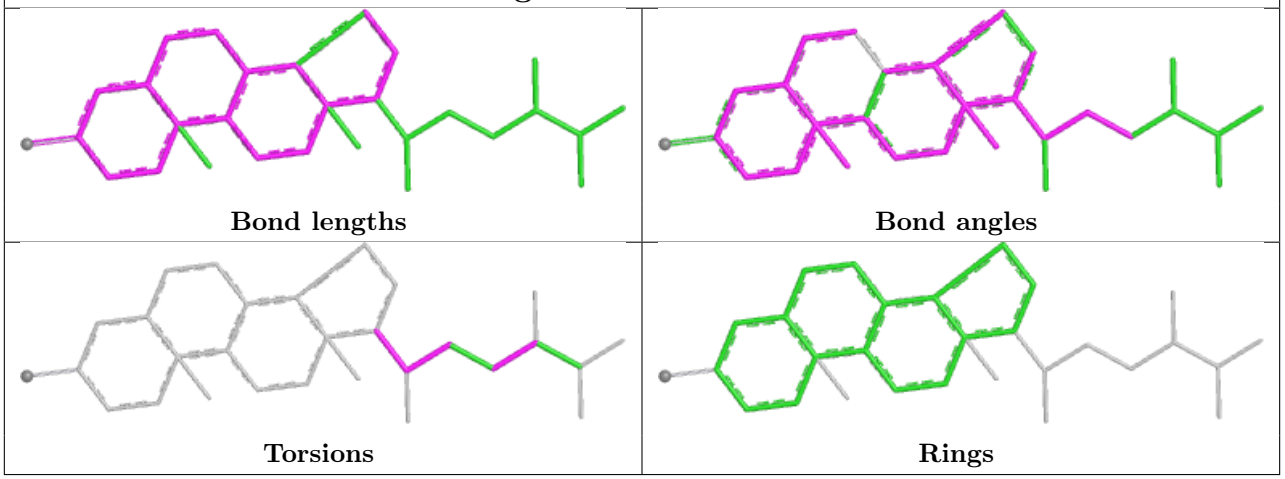


Rings

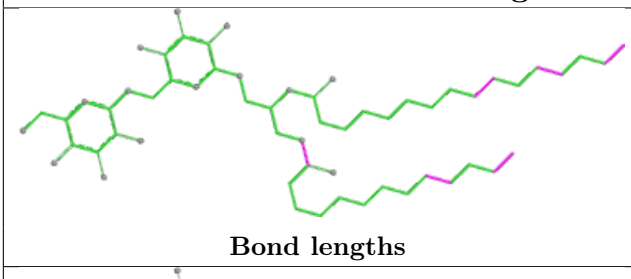
Ligand SQD b 621



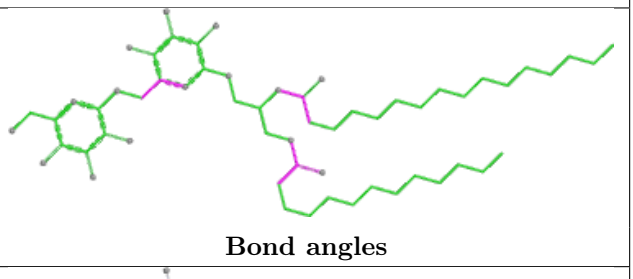
Ligand ERG R1 626



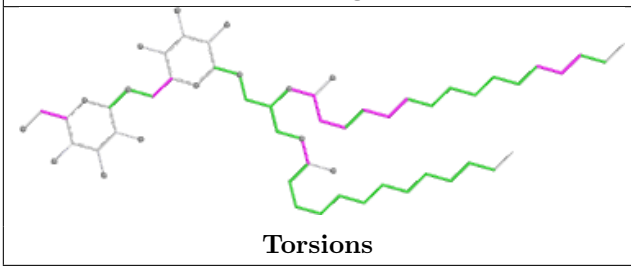
Ligand DGD C1 520



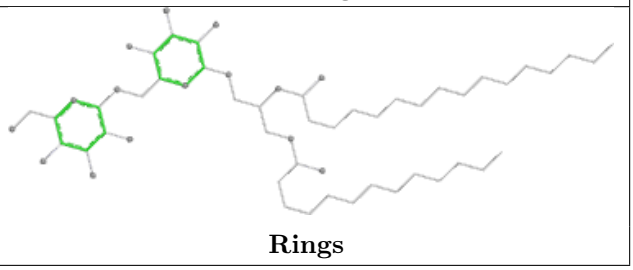
Bond lengths



Bond angles

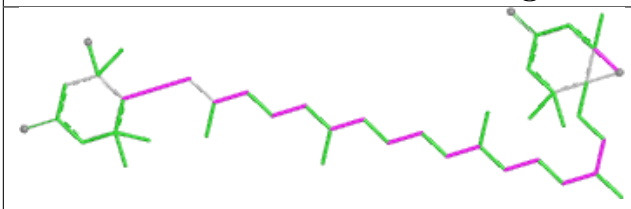


Torsions

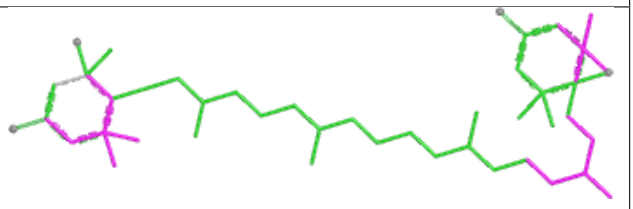


Rings

Ligand NEX G 623



Bond lengths

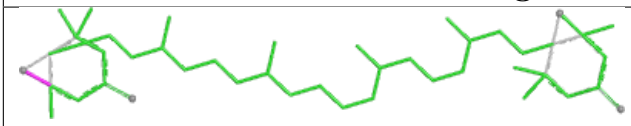


Bond angles

Torsions

Rings

Ligand XAT R1 621



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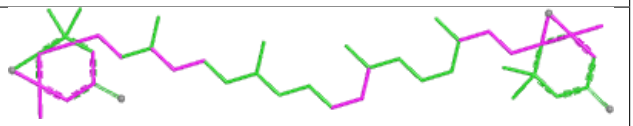
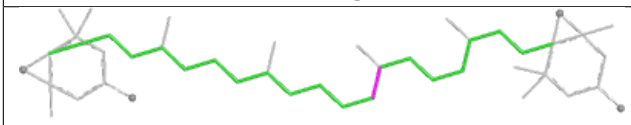
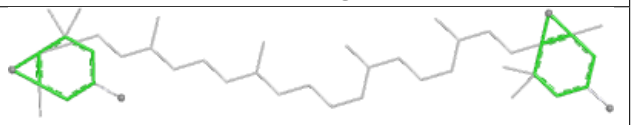


Bond angles

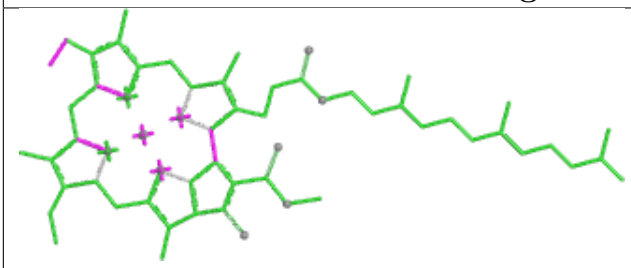


Torsions

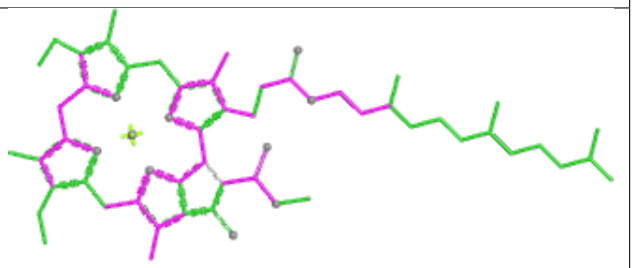


Rings

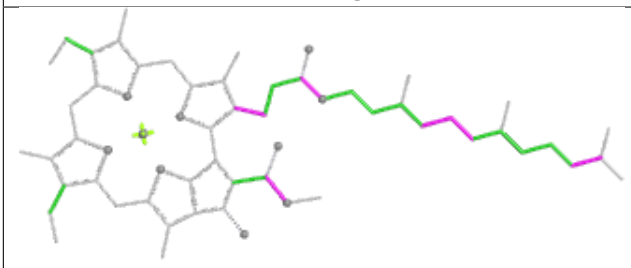
Ligand CLA a1 410



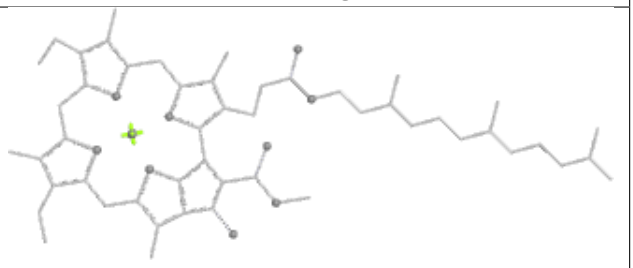
Bond lengths



Bond angles

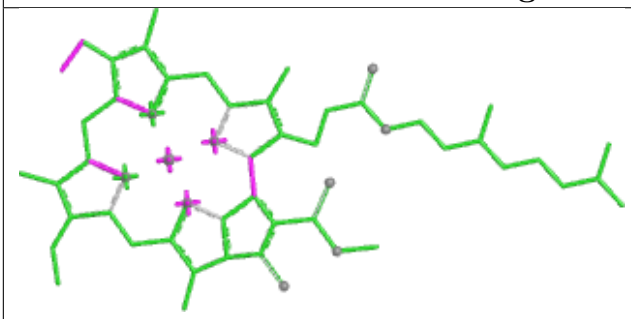


Torsions



Rings

Ligand CLA S1 614



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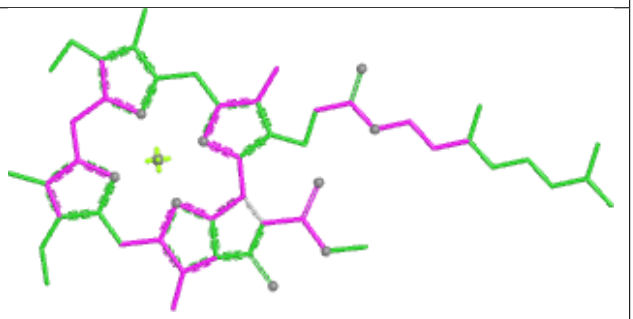
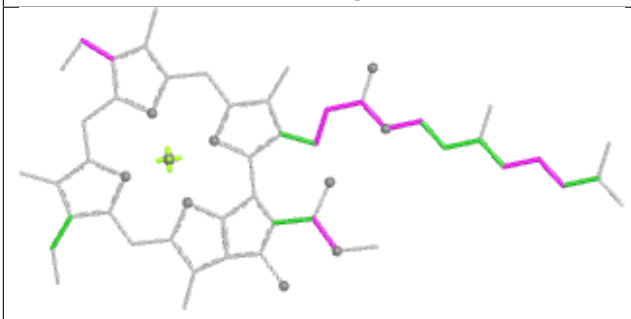


Bond angles



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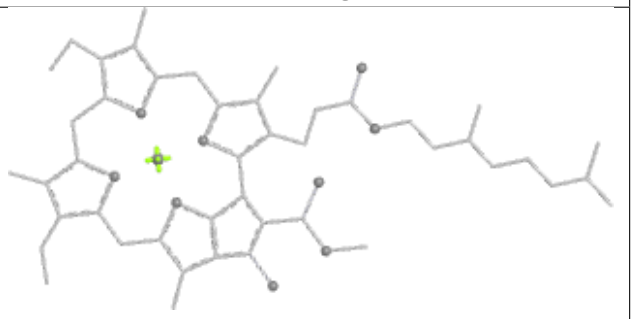
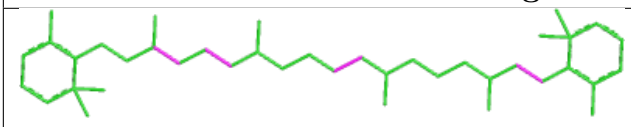


Rings

Ligand BCR C 516



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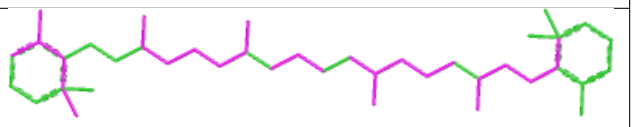
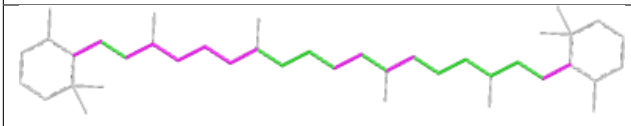
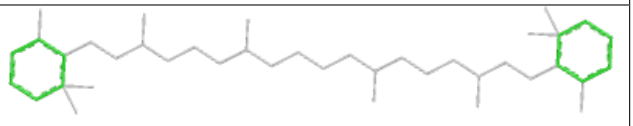


Bond angles

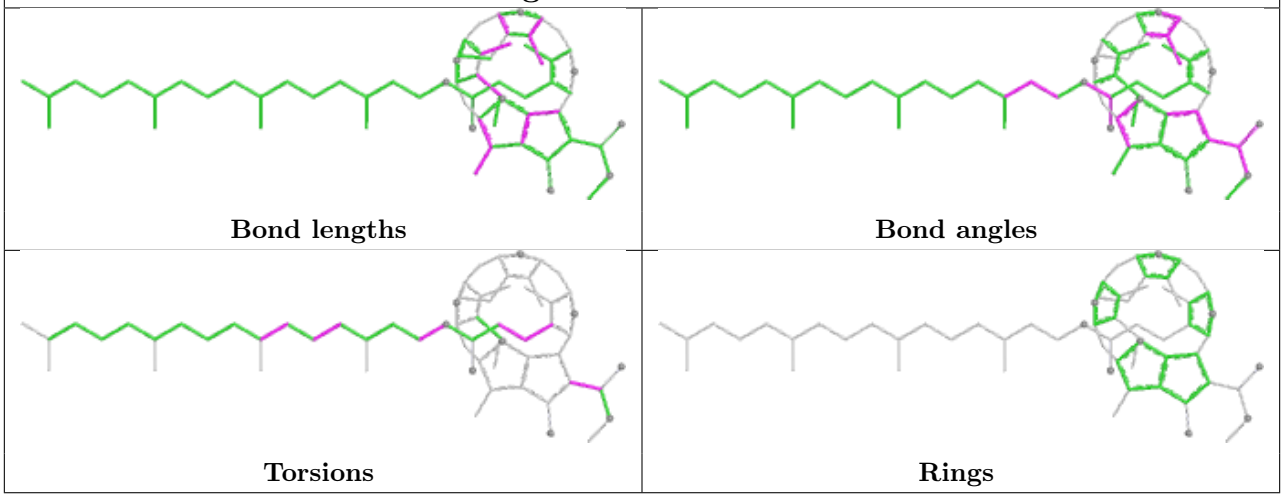


Torsions

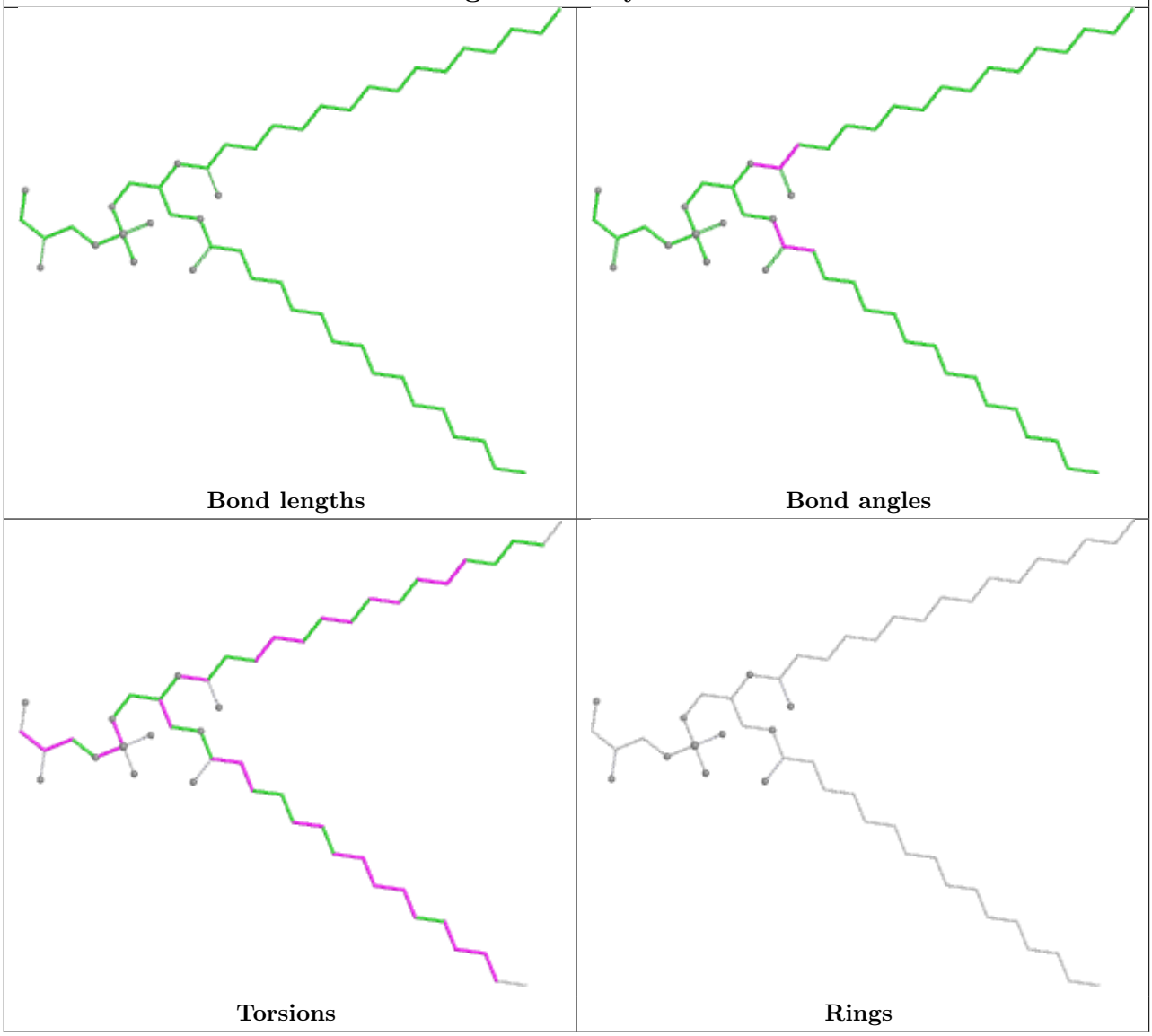


Rings

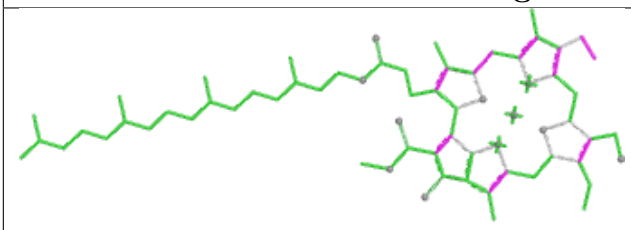
Ligand PHO A 409



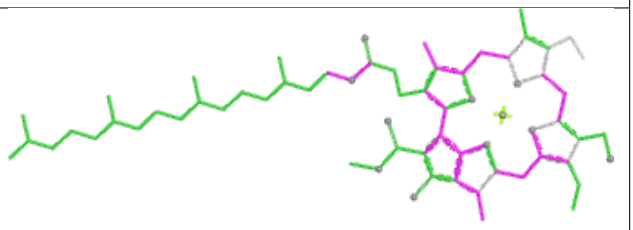
Ligand LHG y1 624



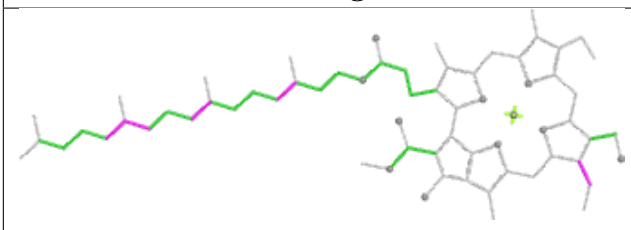
Ligand CHL G1 609



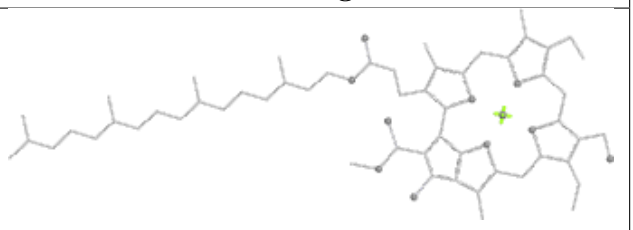
Bond lengths



Bond angles

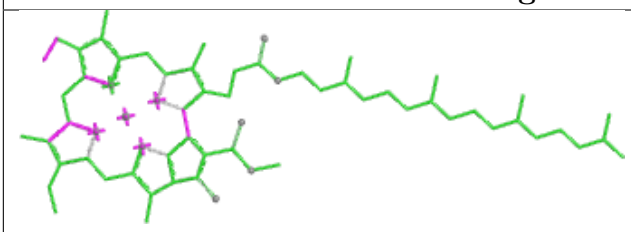


Torsions



Rings

Ligand CLA b1 614



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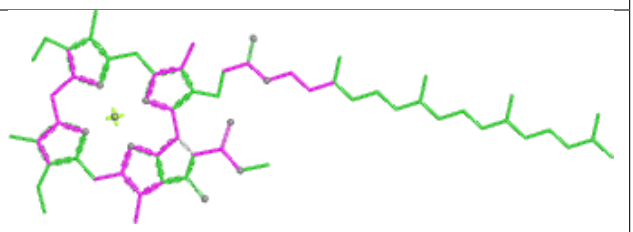
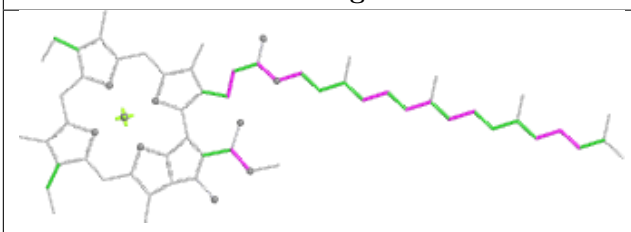
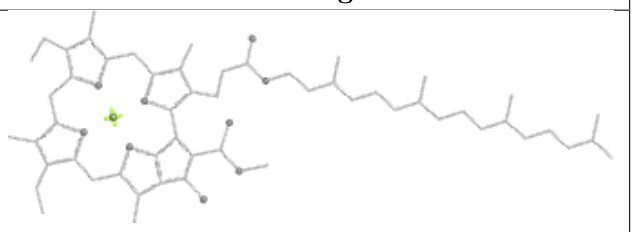


Bond angles

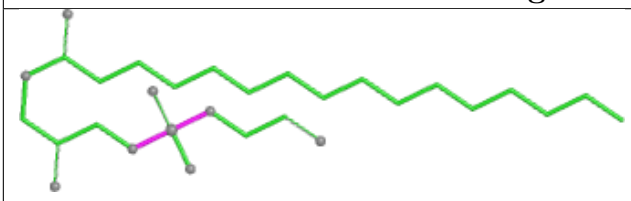


Torsions

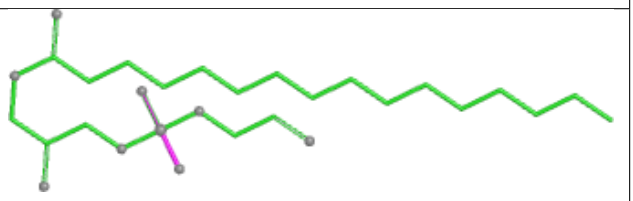


Rings

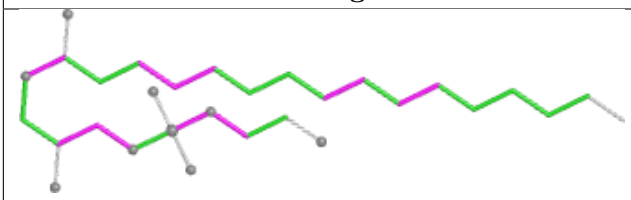
Ligand LPX S 625



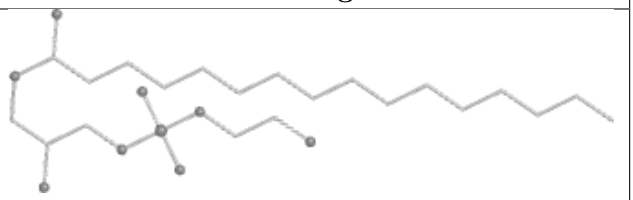
Bond lengths



Bond angles

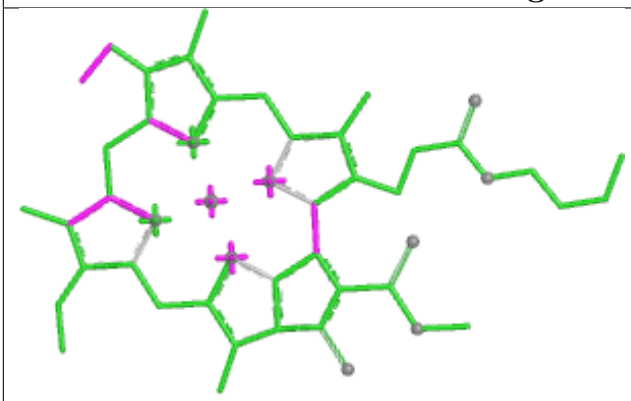


Torsions



Rings

Ligand CLA n 611



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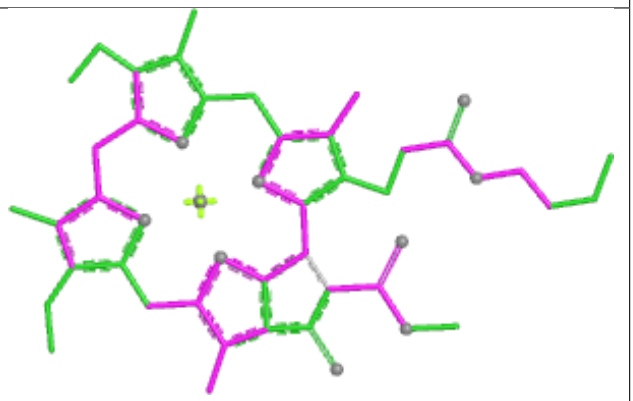
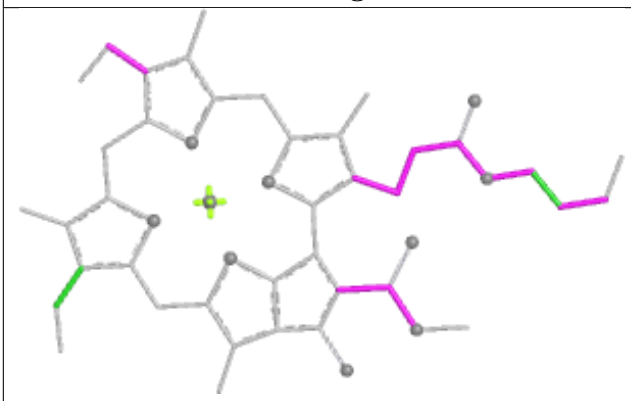
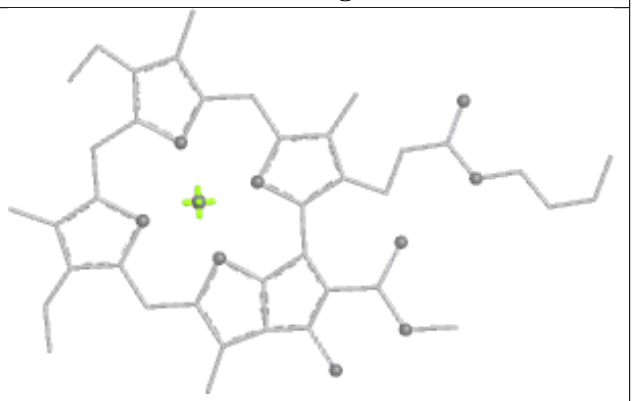


Bond angles

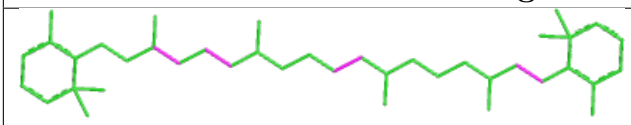


Torsions



Rings

Ligand BCR a1 411



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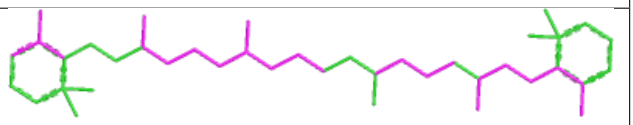
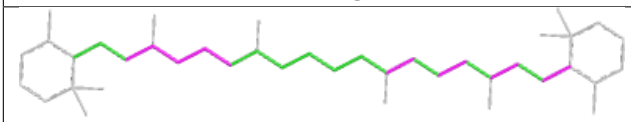
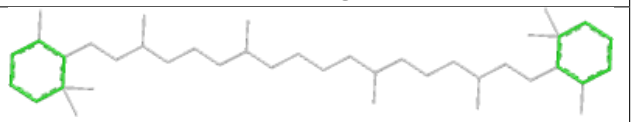


Bond angles

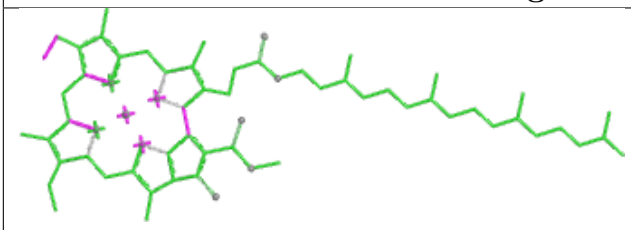


Torsions



Rings

Ligand CLA n 610



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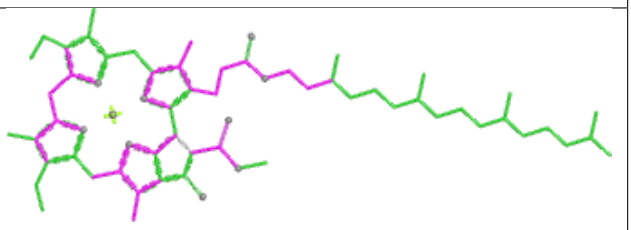
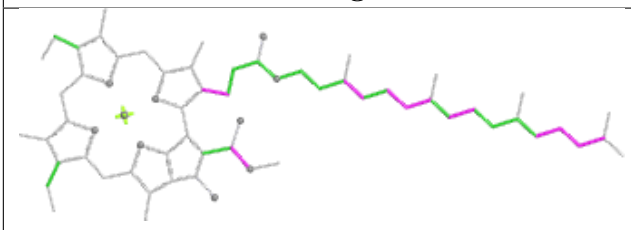
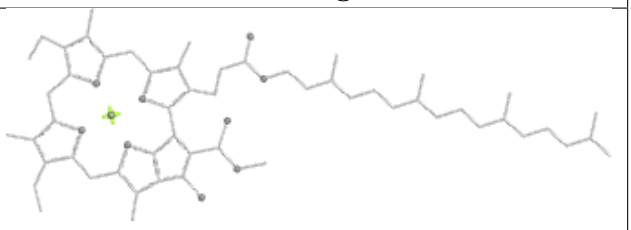


Bond angles

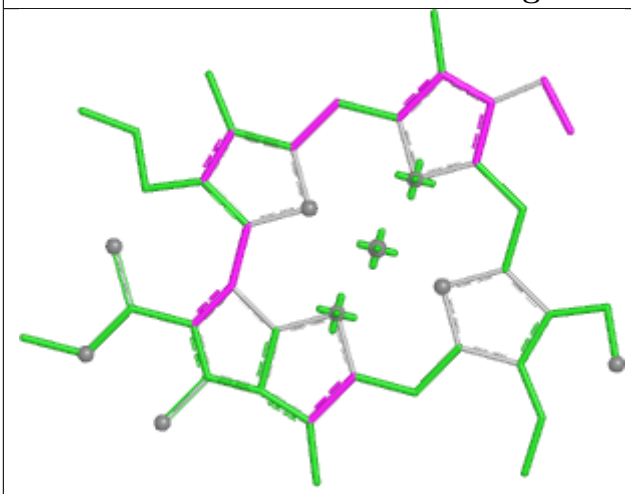


Torsions

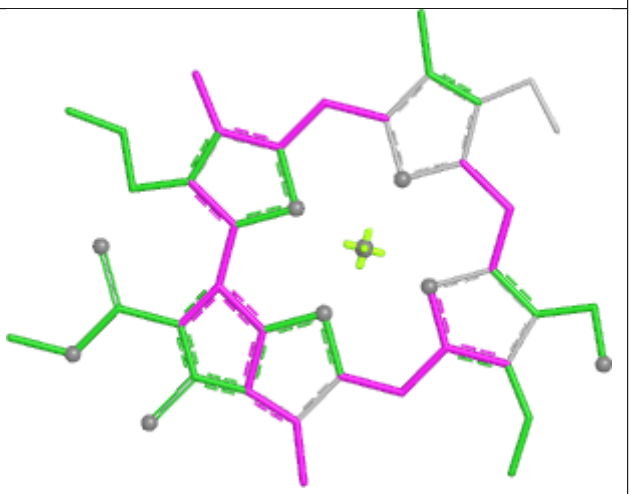


Rings

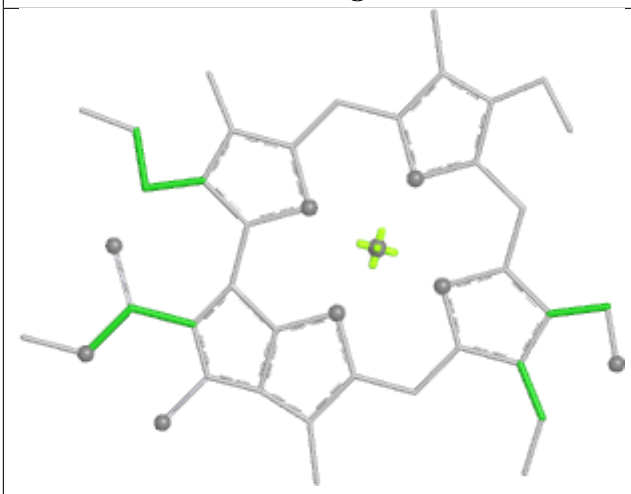
Ligand CHL G 608



Bond lengths



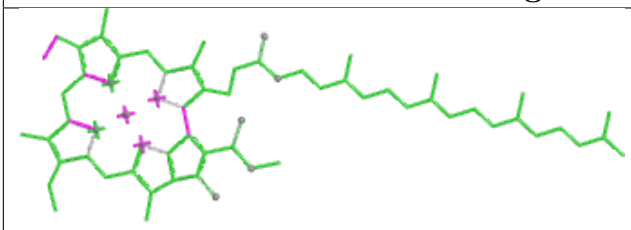
Bond angles



Torsions

Rings

Ligand CLA B 614



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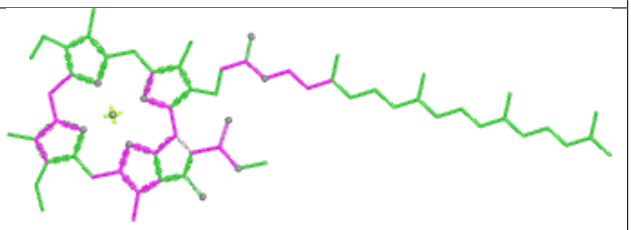
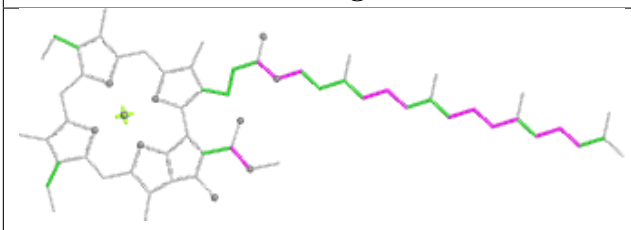
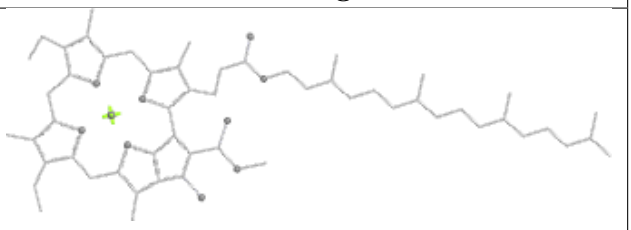


Bond angles

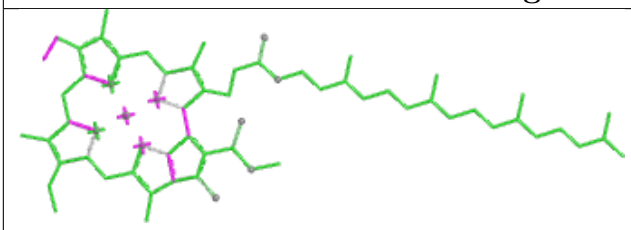


Torsions

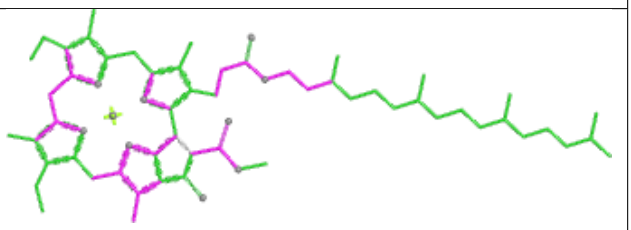


Rings

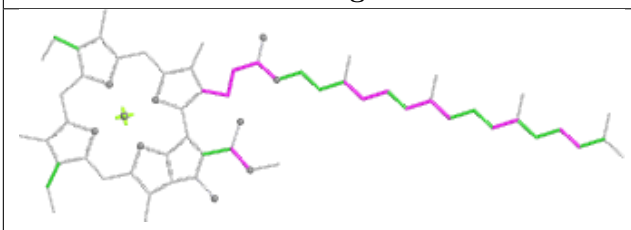
Ligand CLA D 402



Bond lengths



Bond angles



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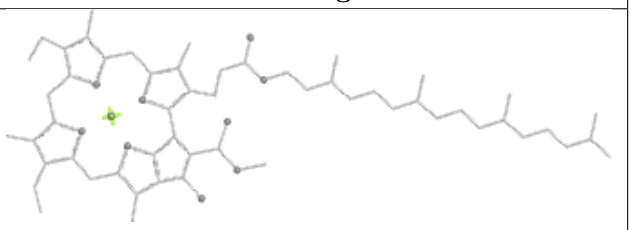
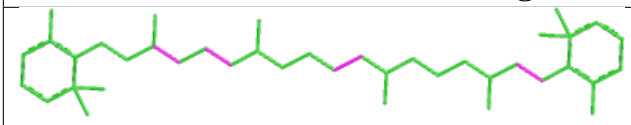


Rings

Ligand BCR b1 618



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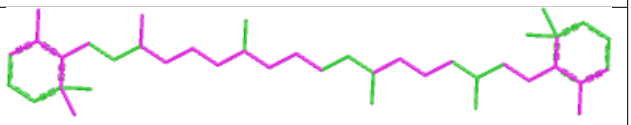
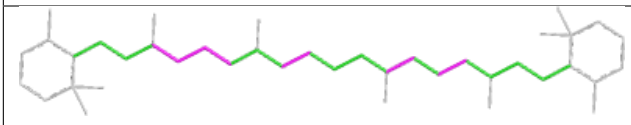


Bond angles



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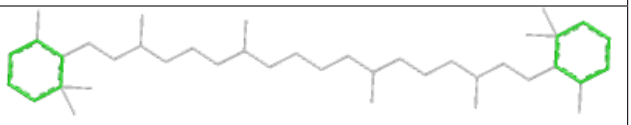
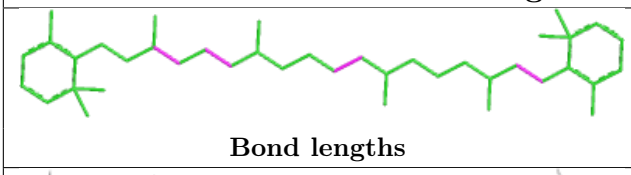


Rings

Ligand BCR d 404



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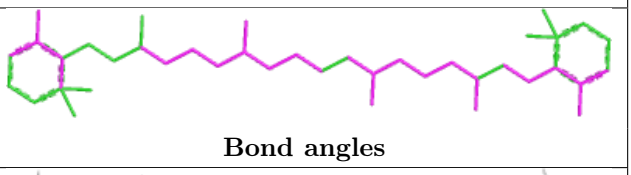
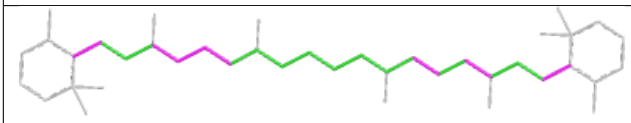


Bond angles



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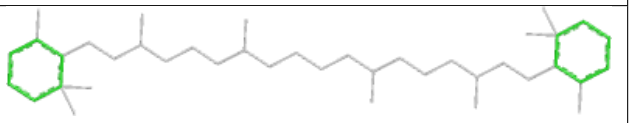
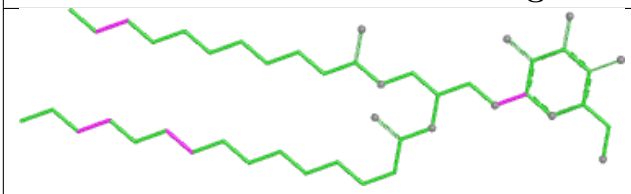


Rings

Ligand LMG j 101



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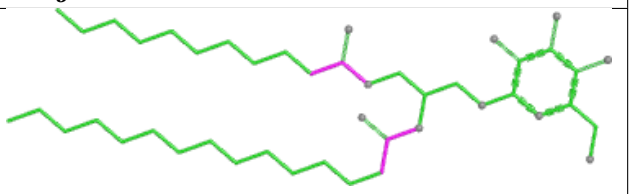
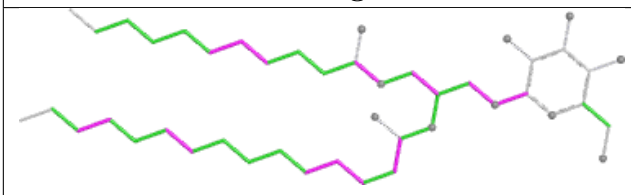


Bond angles



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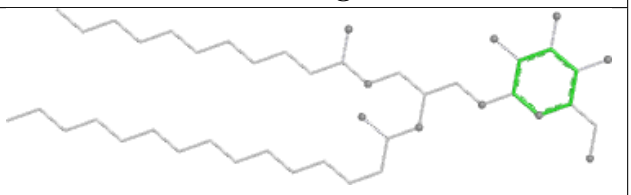
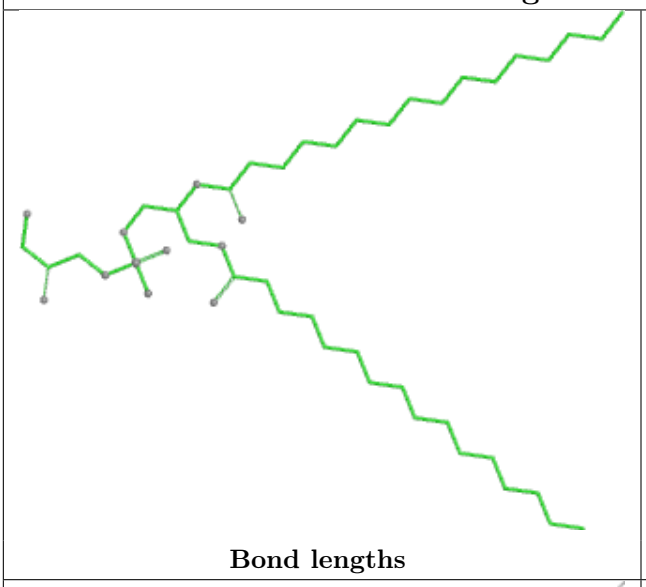


Rings

Ligand LHG D 409



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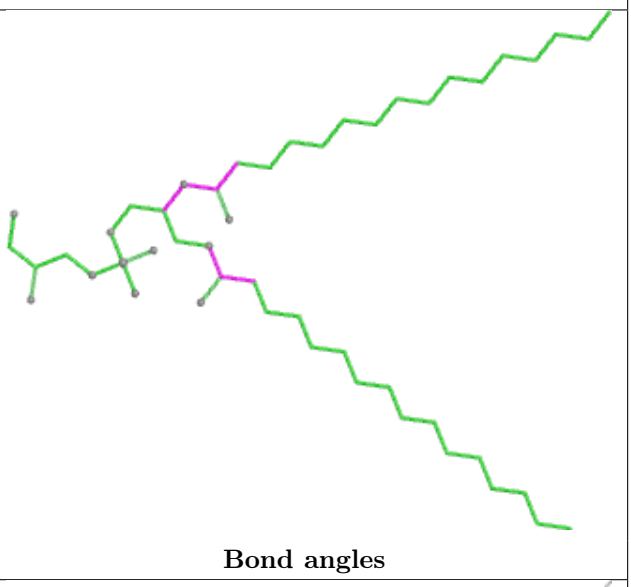
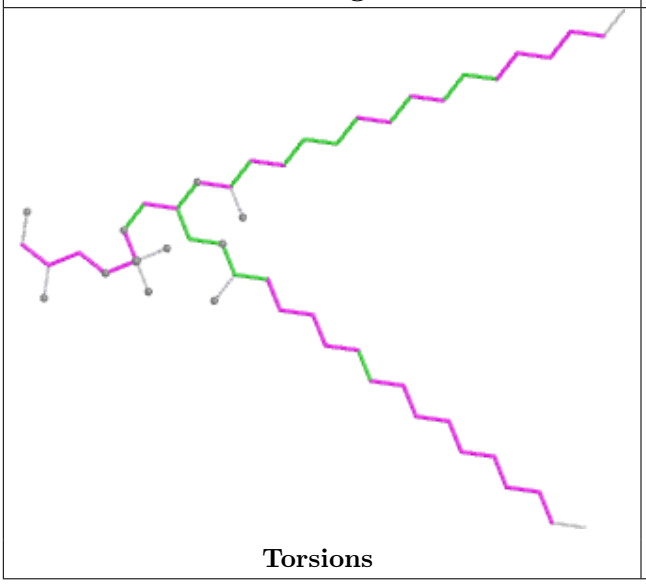


Bond angles



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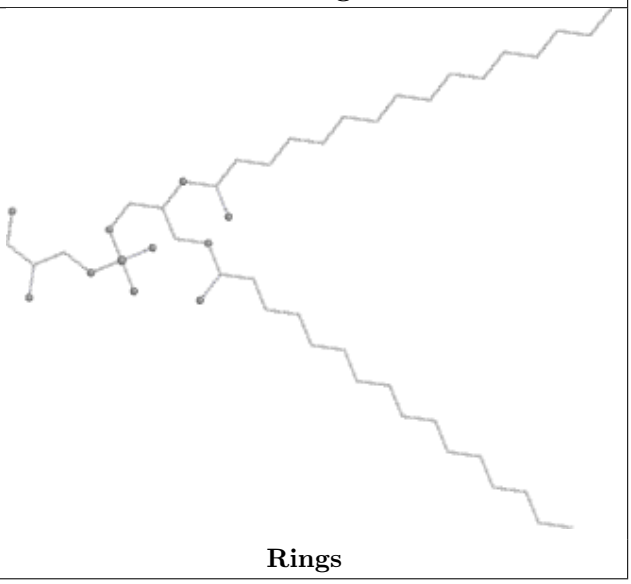
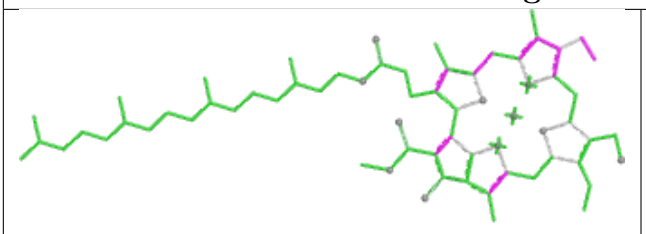


Rings

Ligand CHL Y 606



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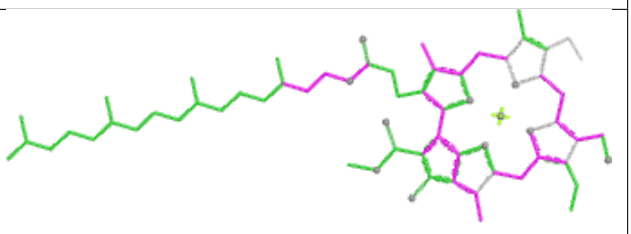
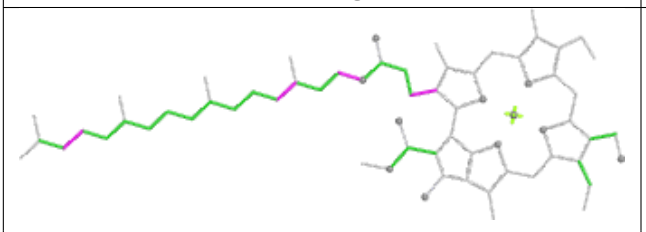


Bond angles



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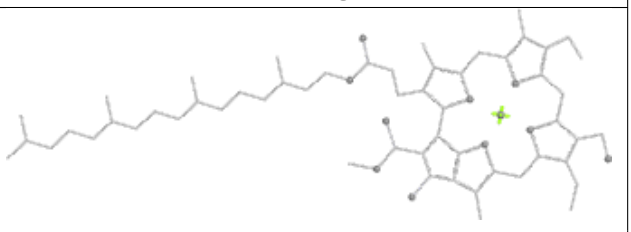
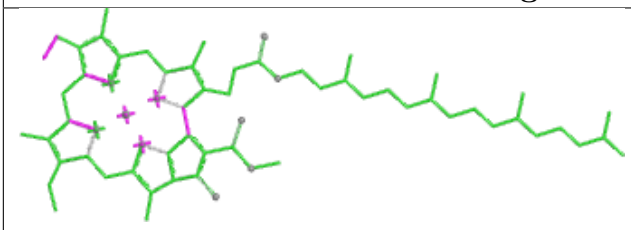


Rings

Ligand CLA c1 504



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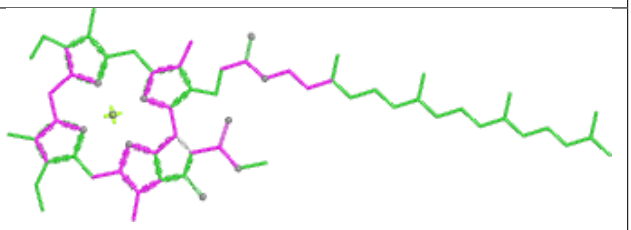
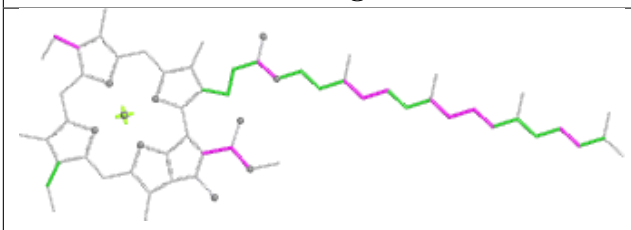


Bond angles



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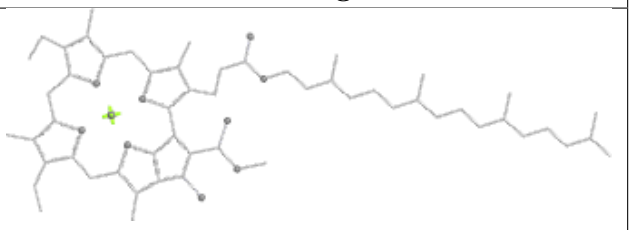
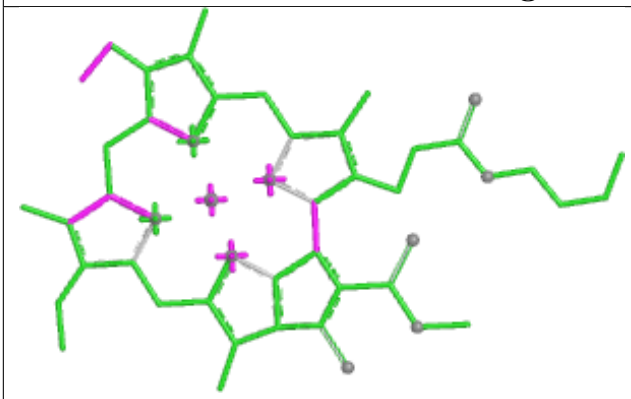


Rings

Ligand CLA g1 604



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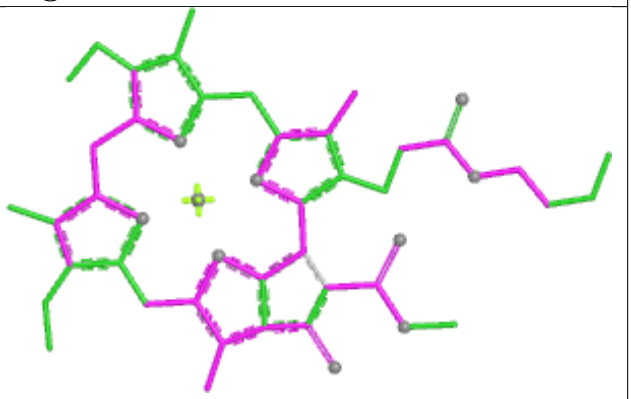
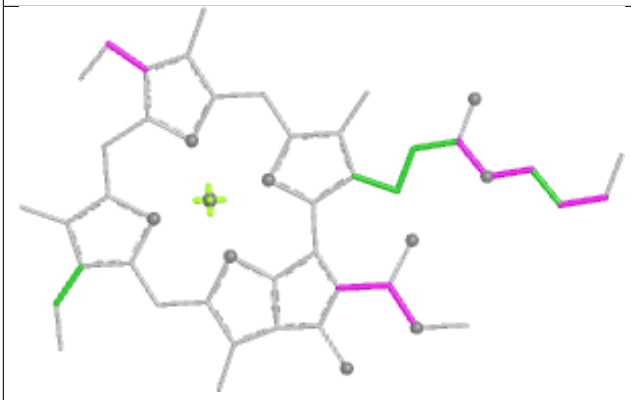


Bond angles



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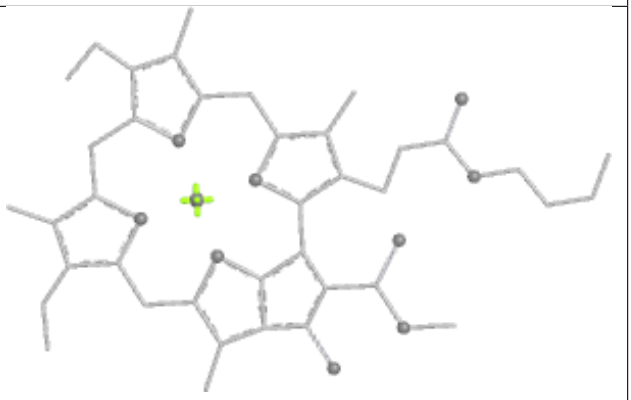
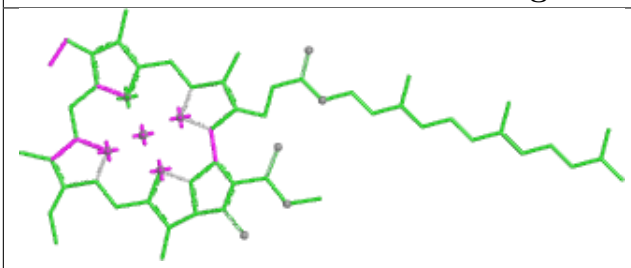


Rings

Ligand CLA r 602



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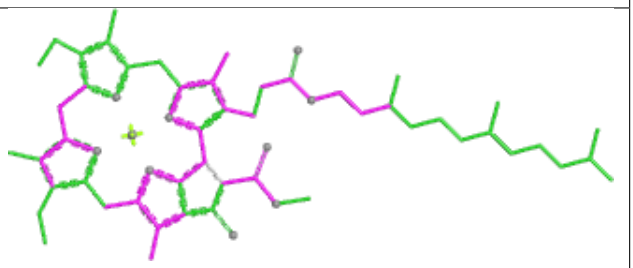
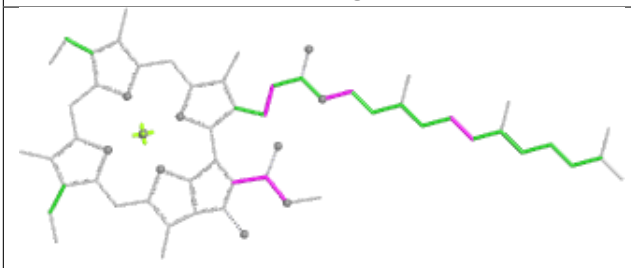


Bond angles



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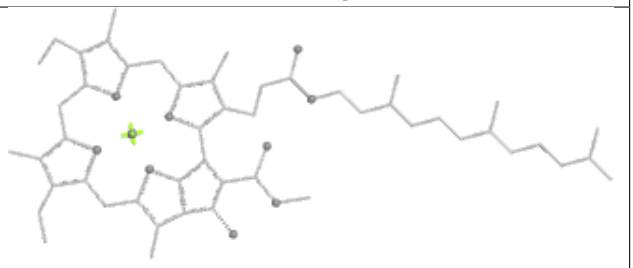
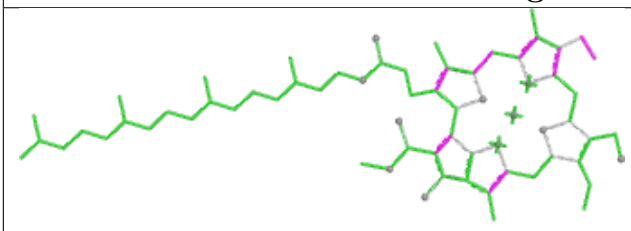


Rings

Ligand CHL n 607



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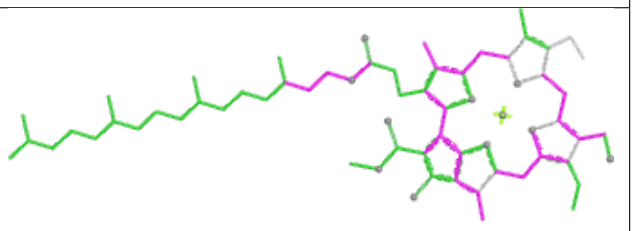

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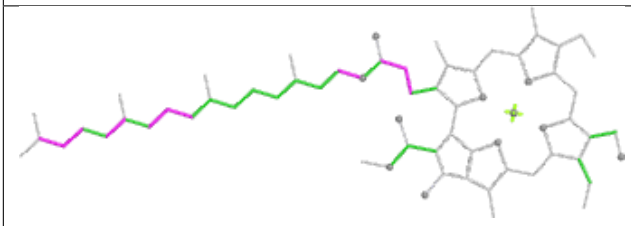

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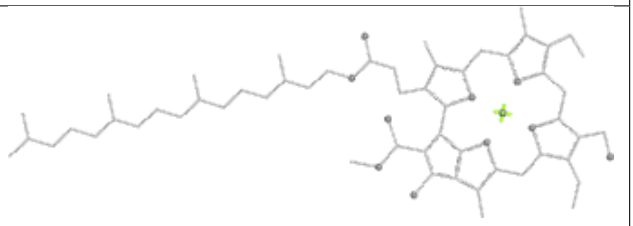
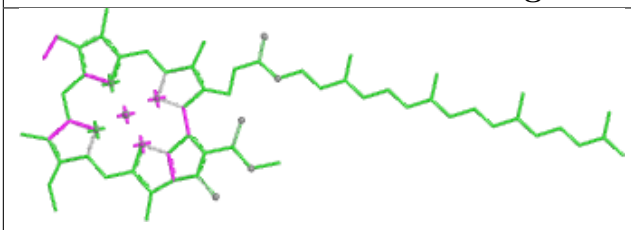


Rings

Ligand CLA C 503



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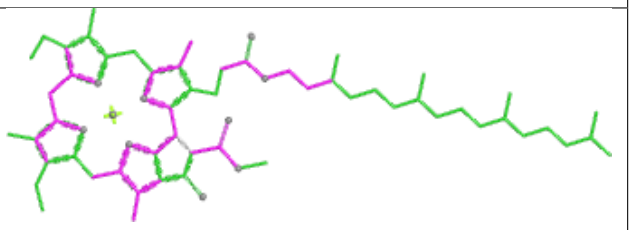
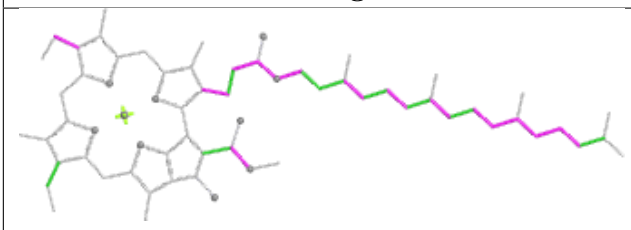


Bond angles



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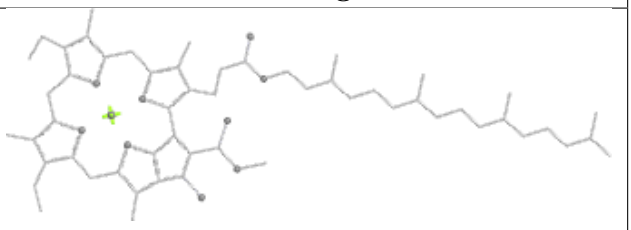
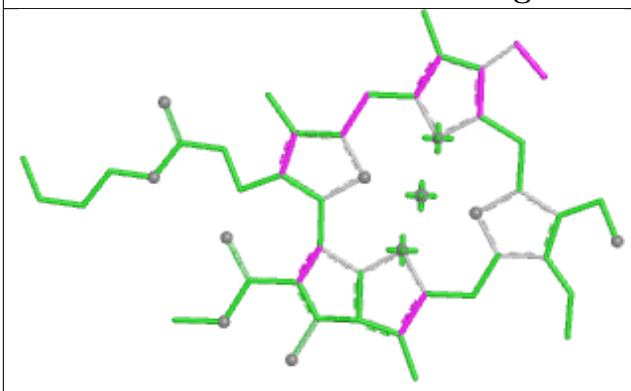


Rings

Ligand CHL N1 608



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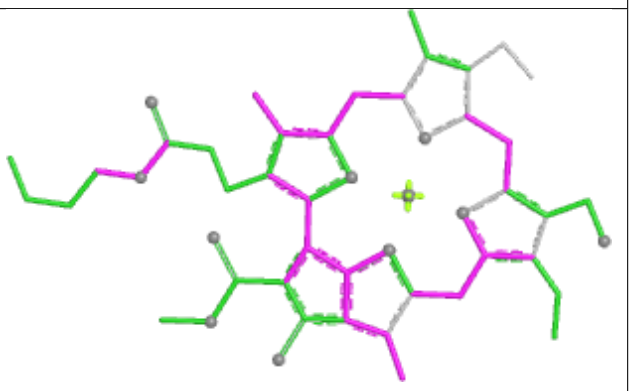
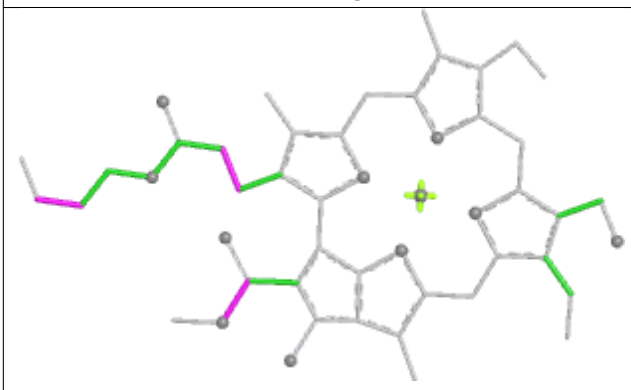


Bond angles



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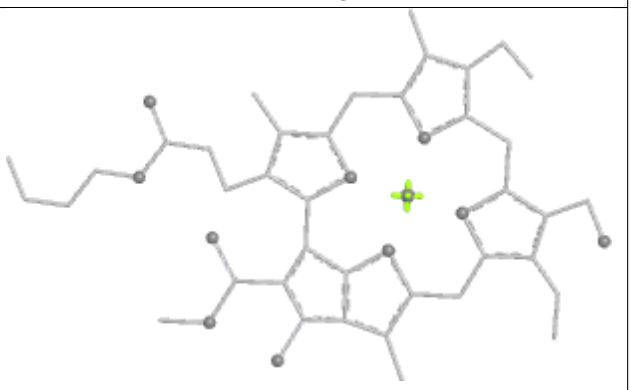
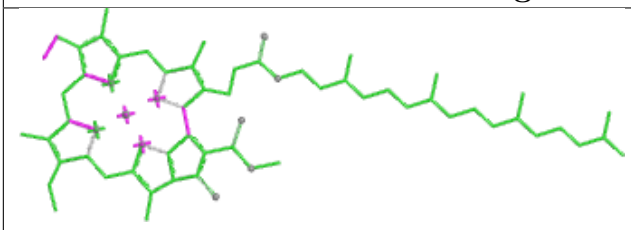


Rings

Ligand CLA G1 611



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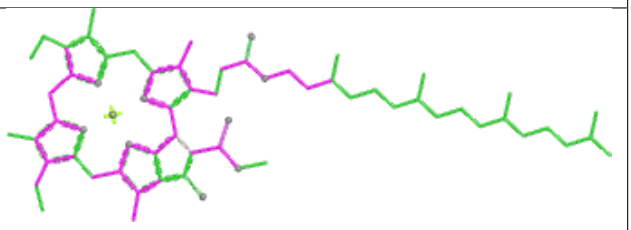
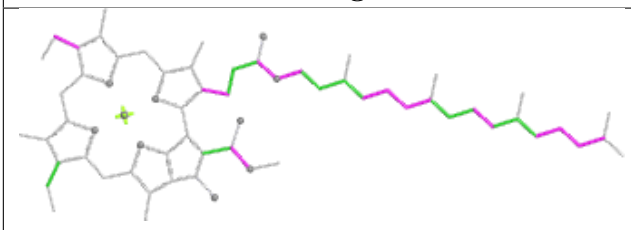
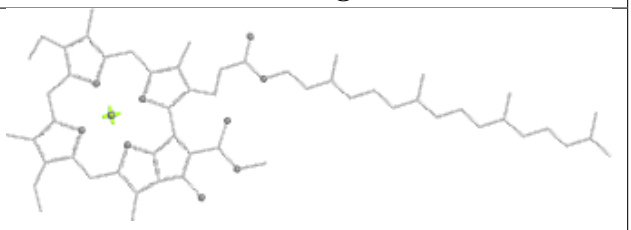


Bond angles

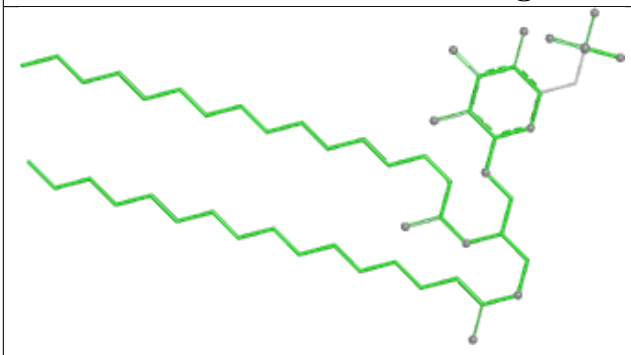


Torsions

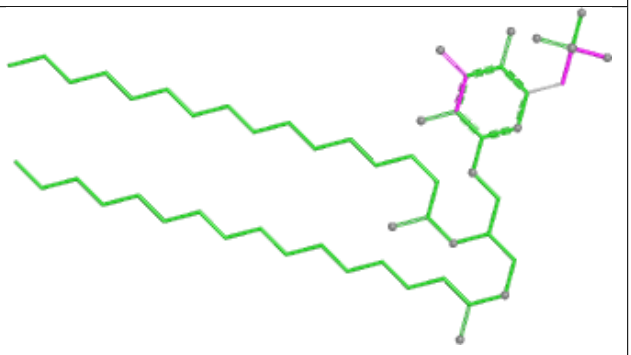


Rings

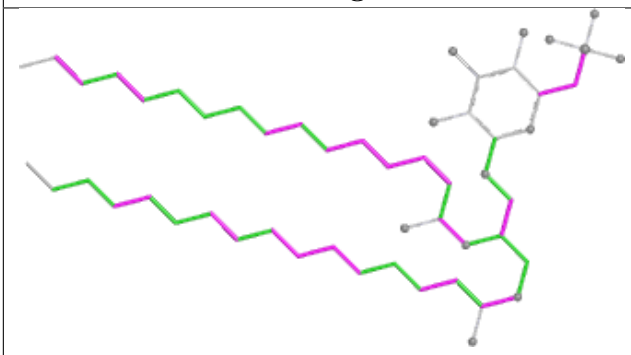
Ligand SQD C1 526



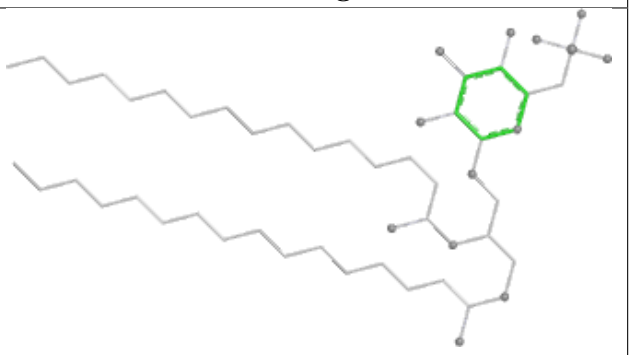
Bond lengths



Bond angles

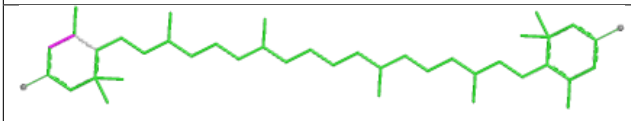


Torsions

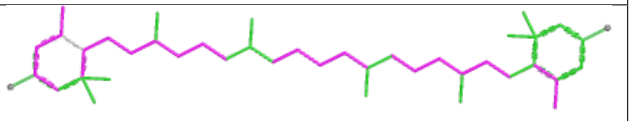


Rings

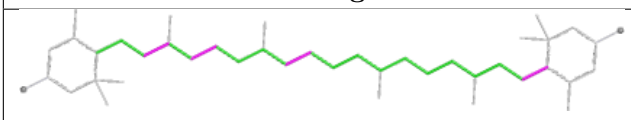
Ligand LUT Y 620



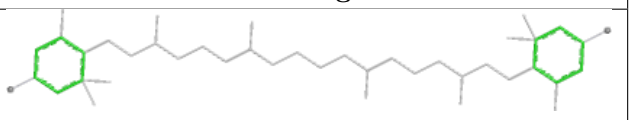
Bond lengths



Bond angles

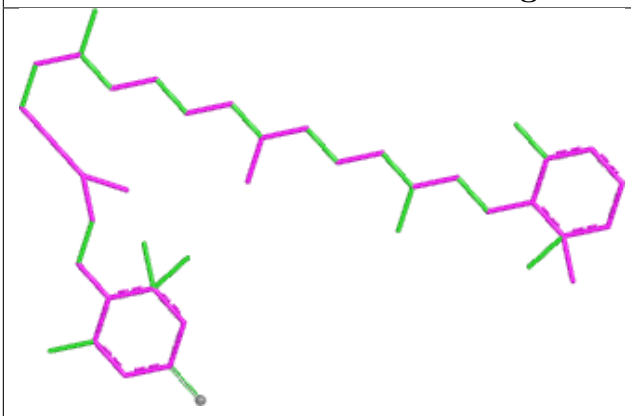


Torsions



Rings

Ligand RRX H 101



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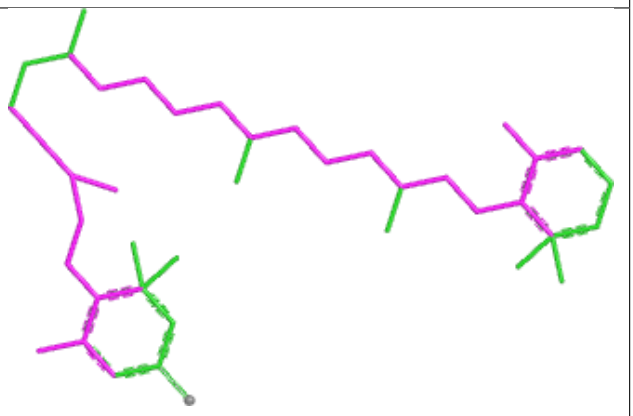
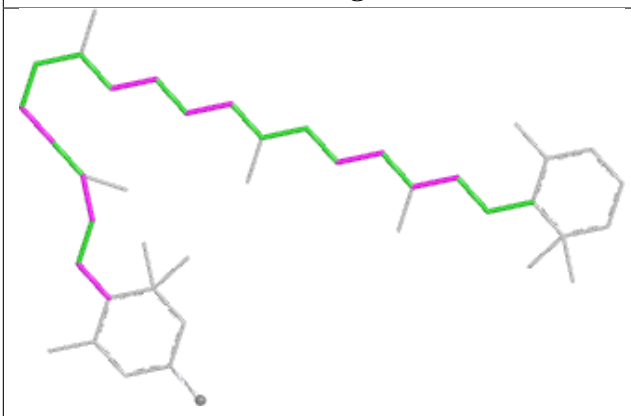
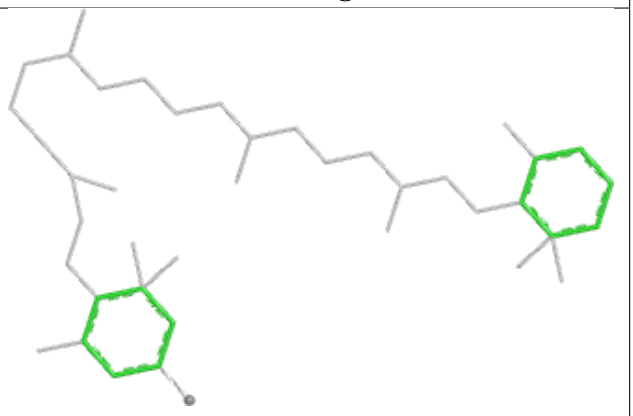


Bond angles

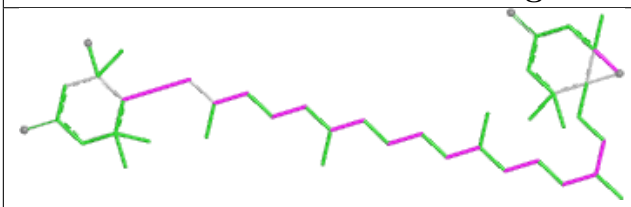


Torsions



Rings

Ligand NEX n 623



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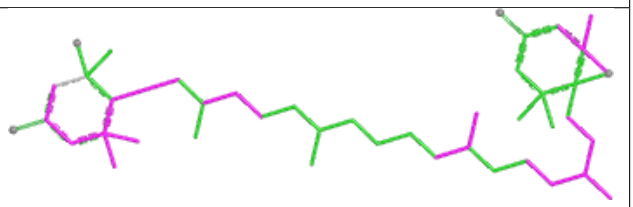
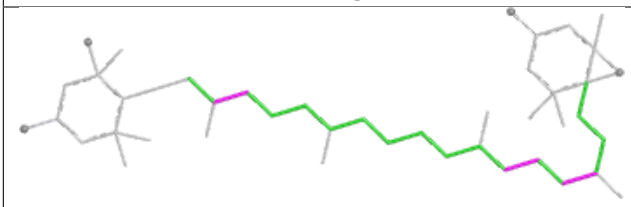
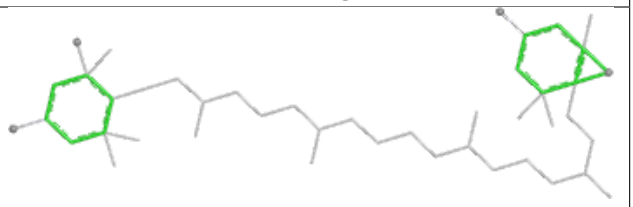


Bond angles

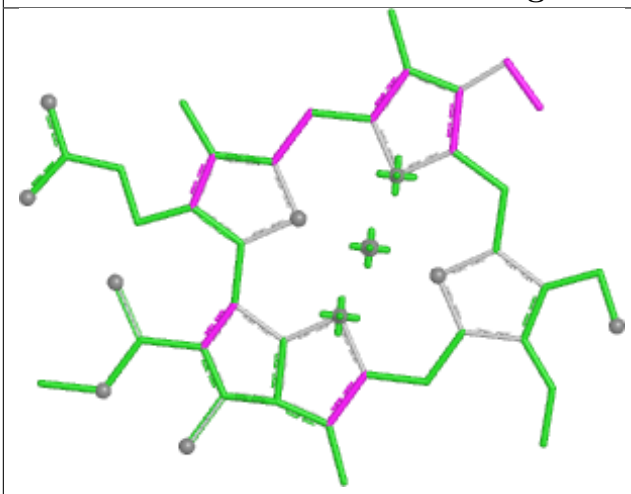


Torsions

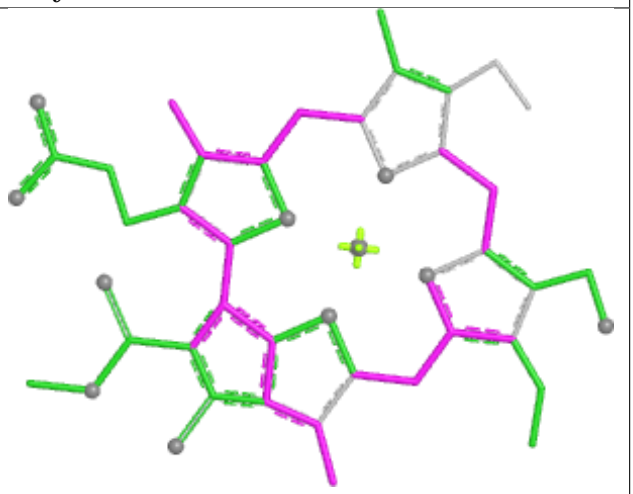


Rings

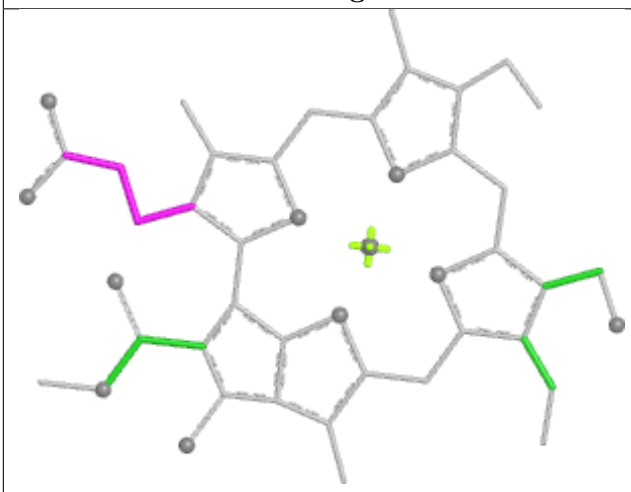
Ligand CHL y 605



Bond lengths



Bond angles



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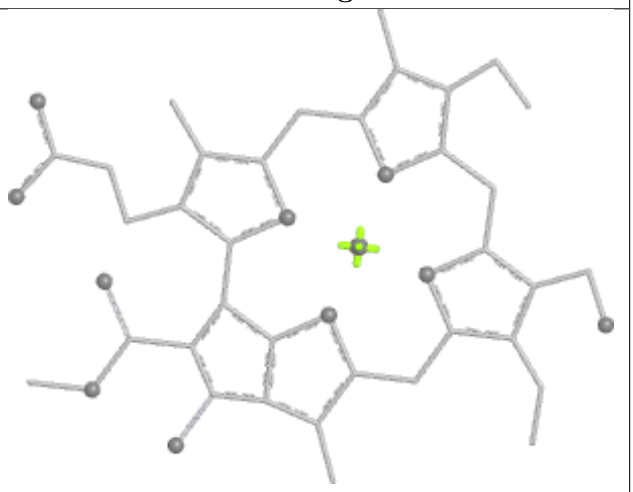
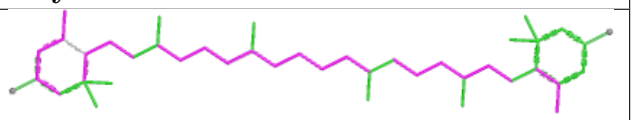


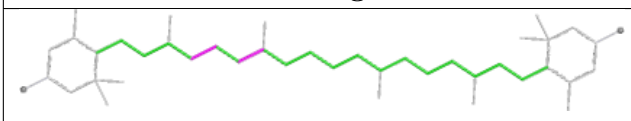
Rings

Ligand LUT y 621

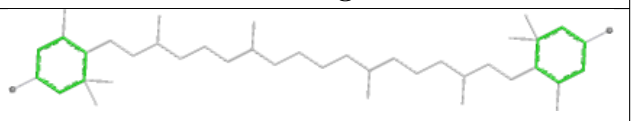
Bond lengths



Bond angles

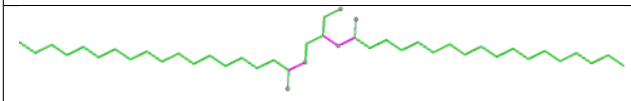


Torsions



Rings

Ligand DGA c1 524



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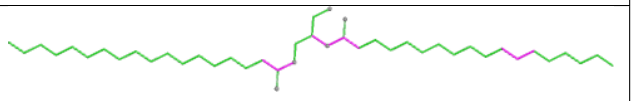
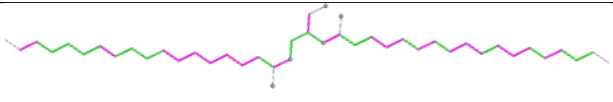
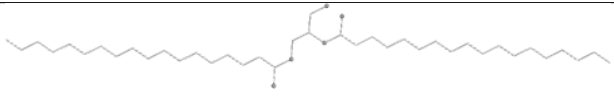


Bond angles

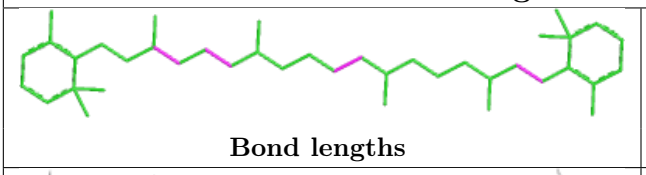


Torsions



Rings

Ligand BCR A1 411



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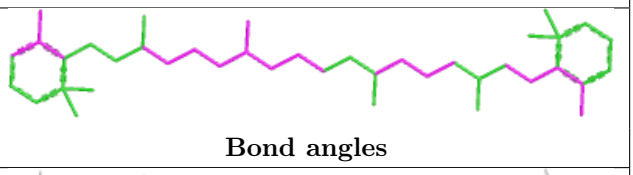
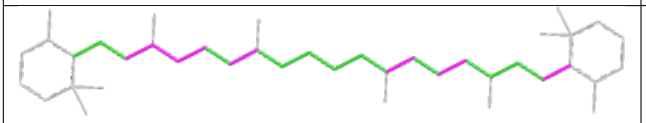


Bond angles



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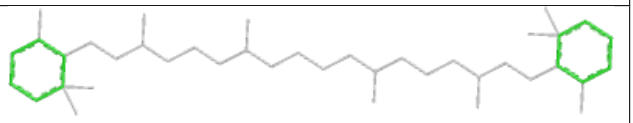
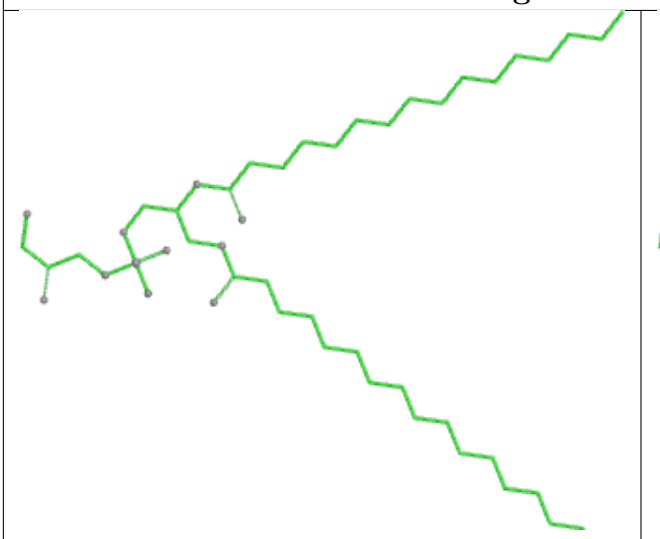


Rings

Ligand LHG Y1 624



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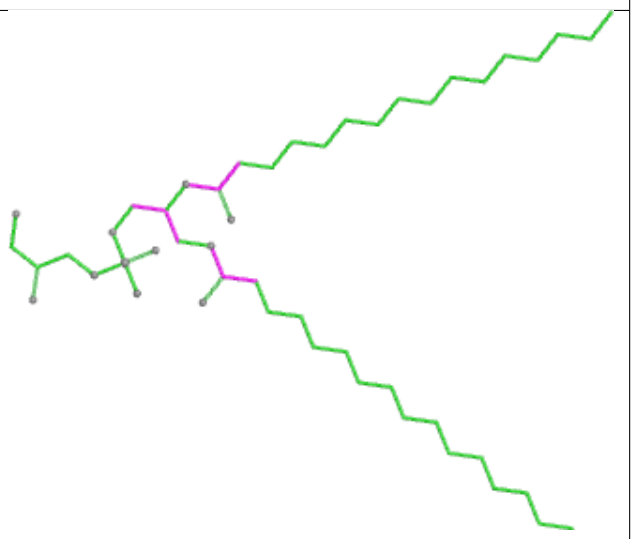
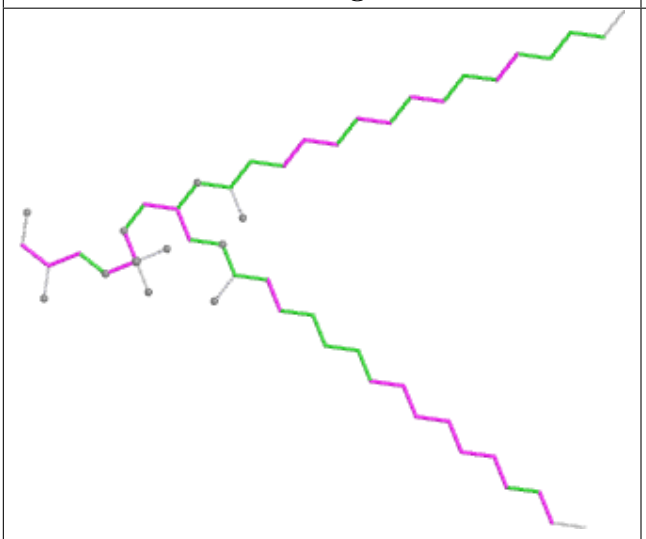


Bond angles



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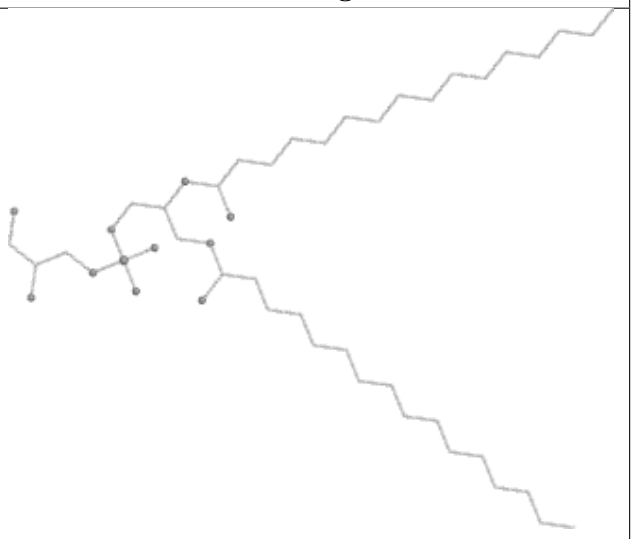
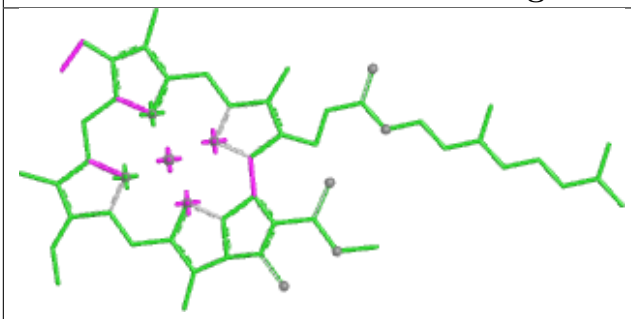
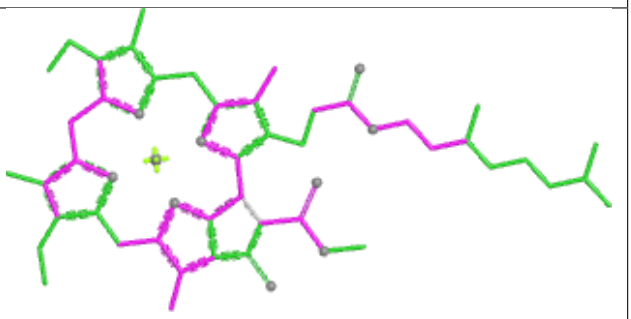
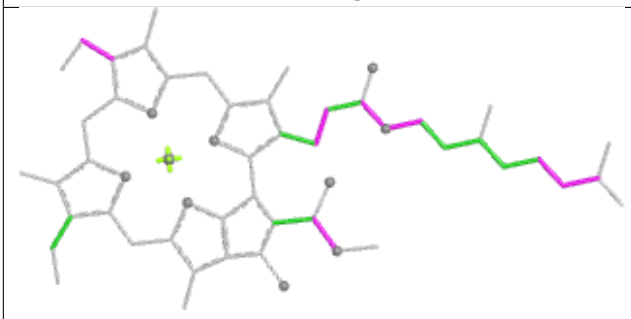
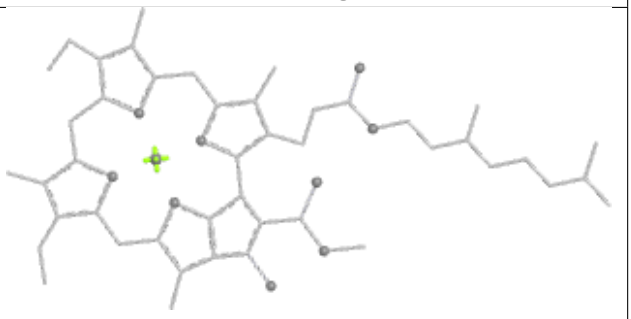
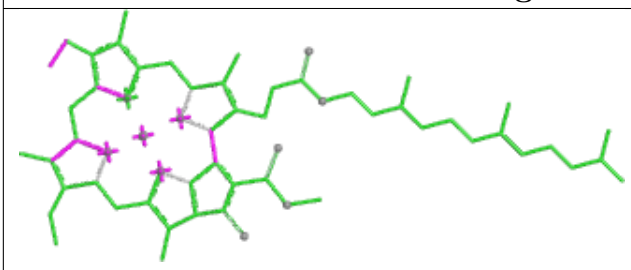
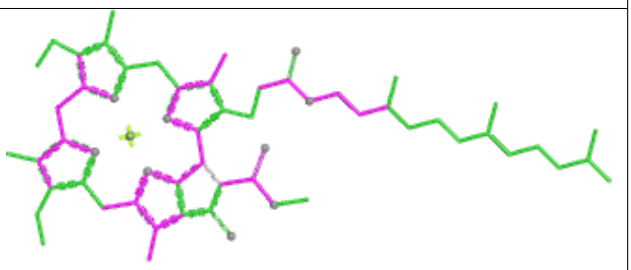
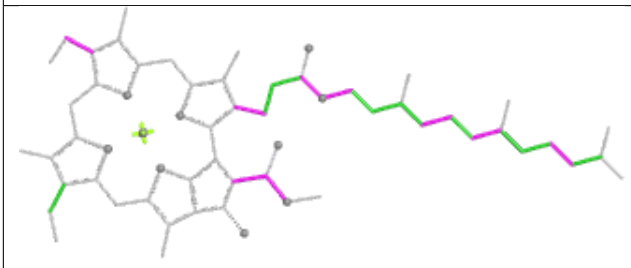
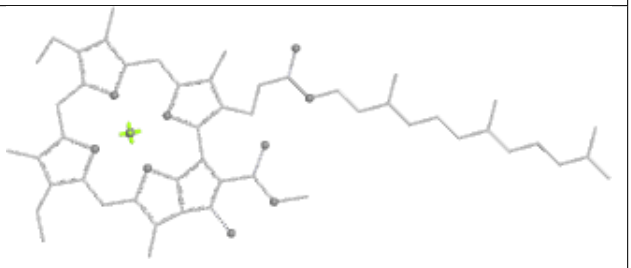
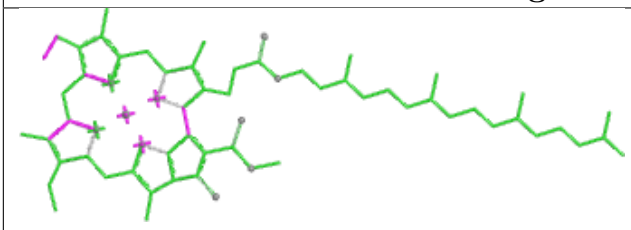


Rings

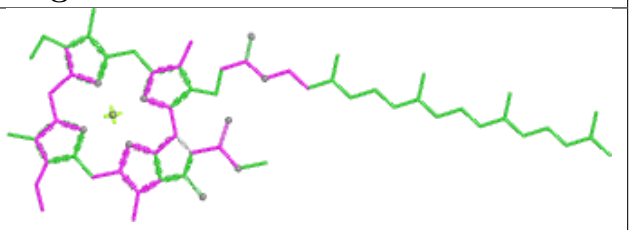
Ligand CLA S 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA R1 612	
	
Bond lengths	Bond angles
	
Torsions	Rings

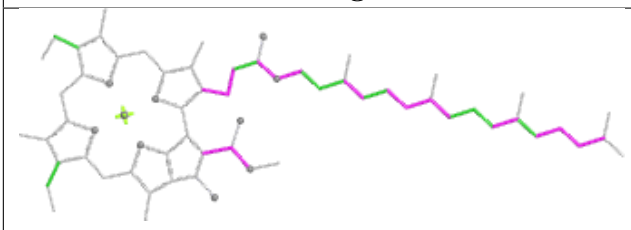
Ligand CLA g 602



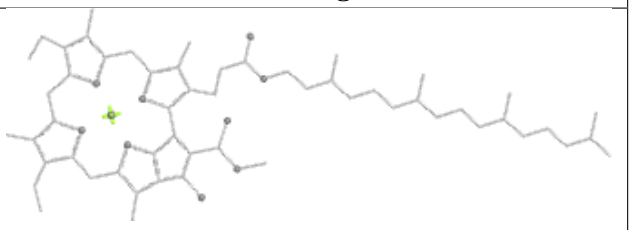
Bond lengths



Bond angles

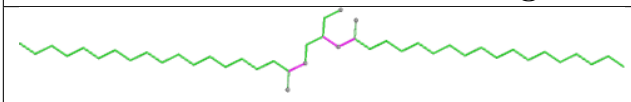


Torsions

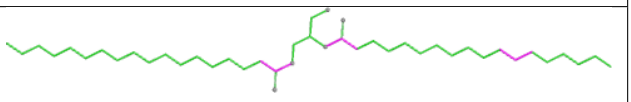


Rings

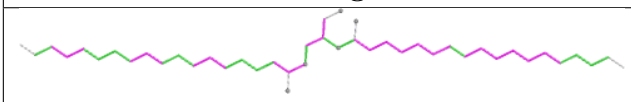
Ligand DGA C 524



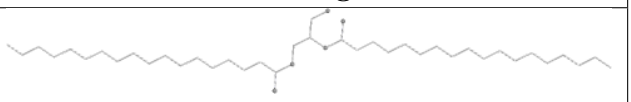
Bond lengths



Bond angles

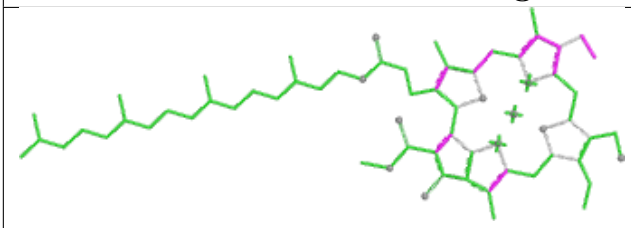


Torsions

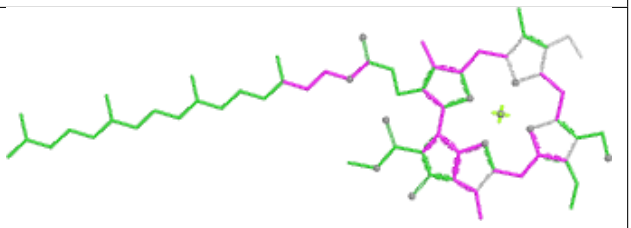


Rings

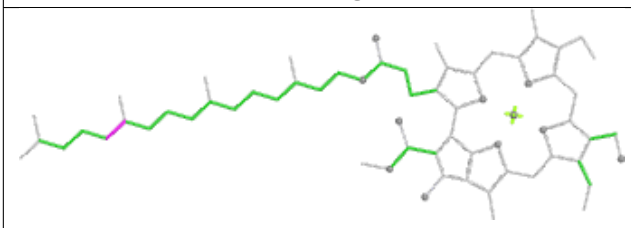
Ligand CHL N1 601



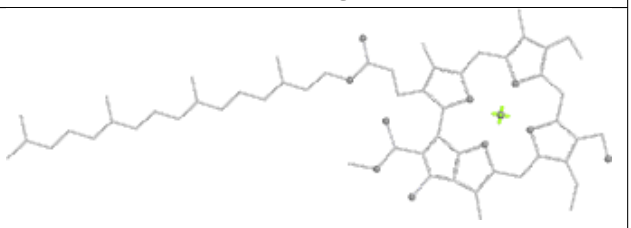
Bond lengths



Bond angles

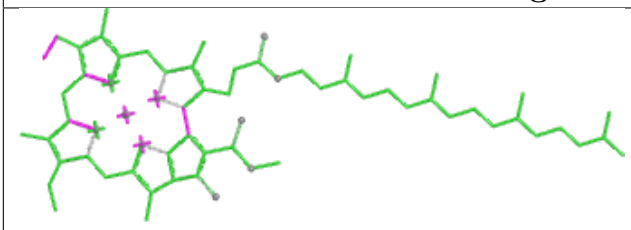


Torsions

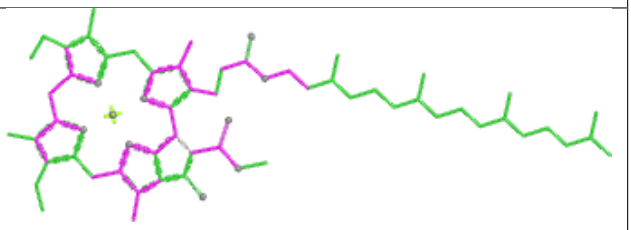


Rings

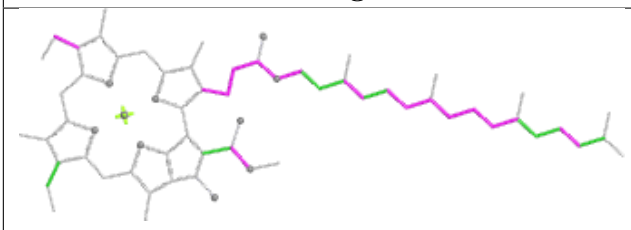
Ligand CLA s 610



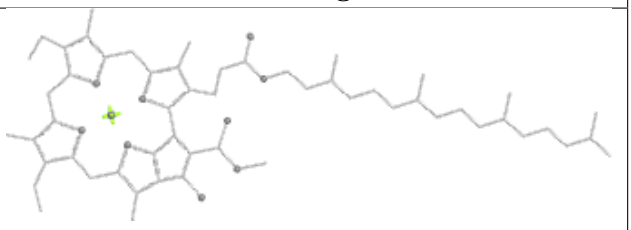
Bond lengths



Bond angles

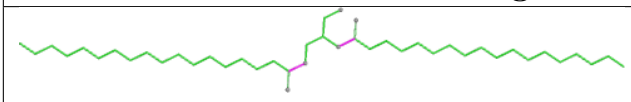


Torsions

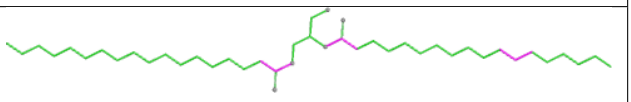


Rings

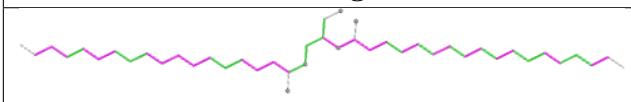
Ligand DGA B1 625



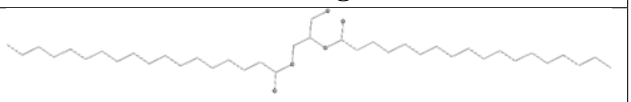
Bond lengths



Bond angles

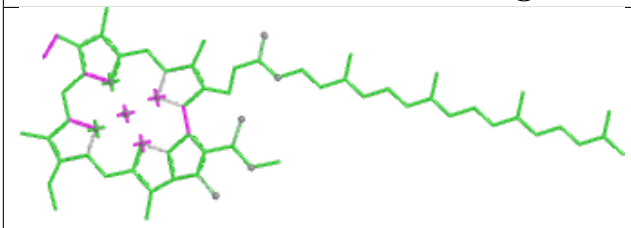


Torsions



Rings

Ligand CLA C1 508



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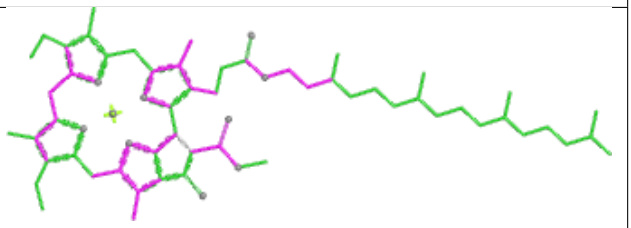
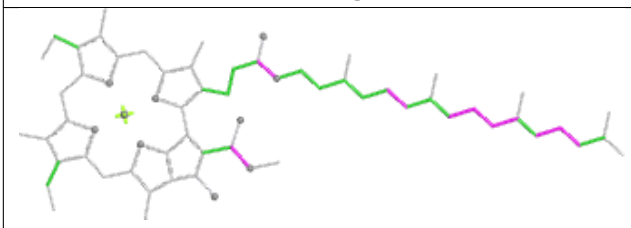
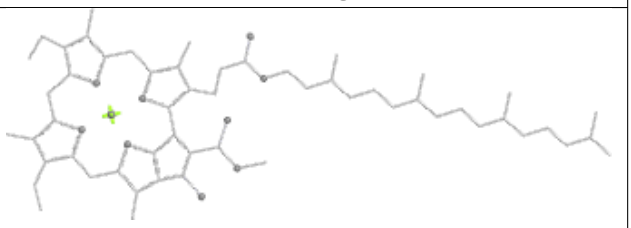


Bond angles

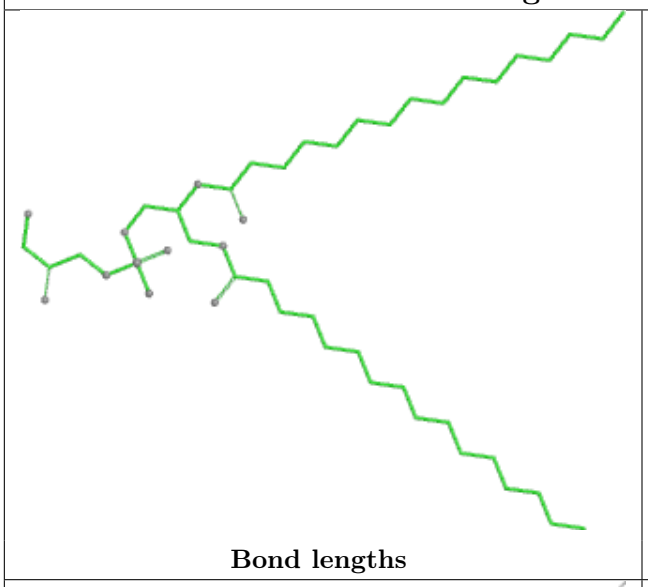


Torsions



Rings

Ligand LHG N 624



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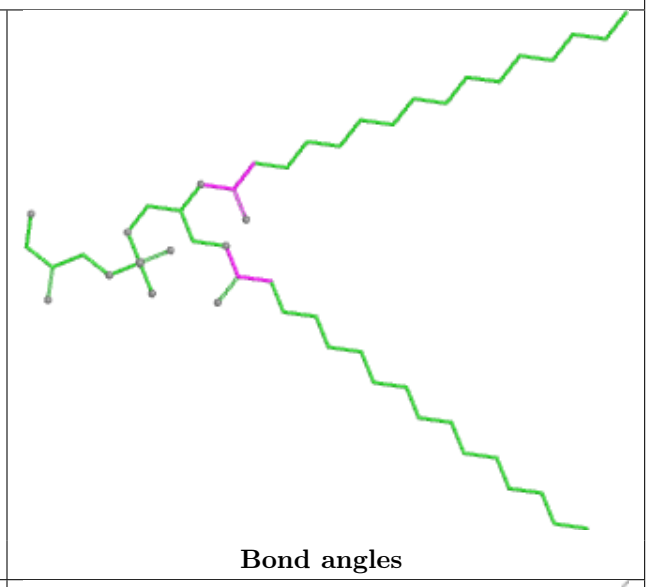
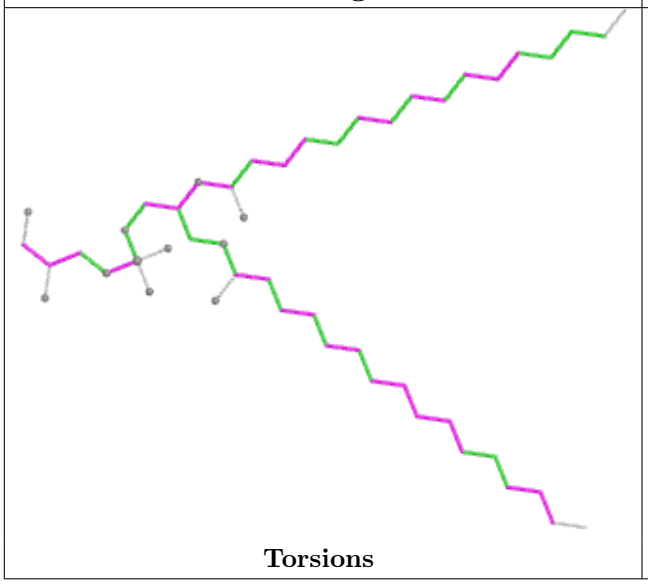


Bond angles



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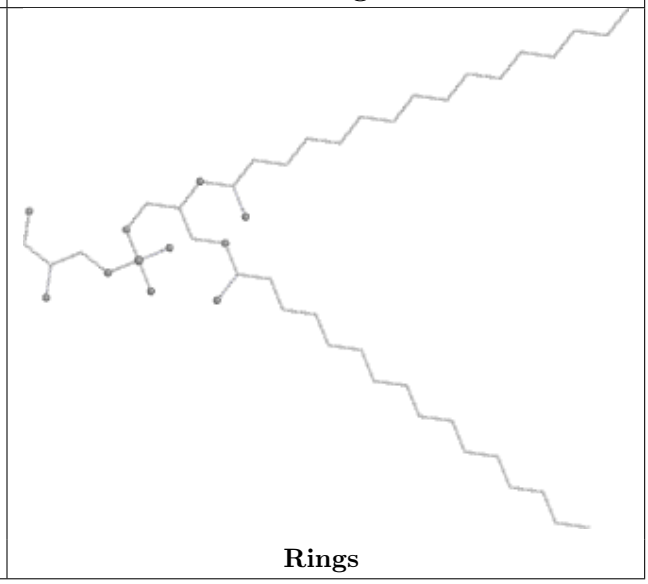
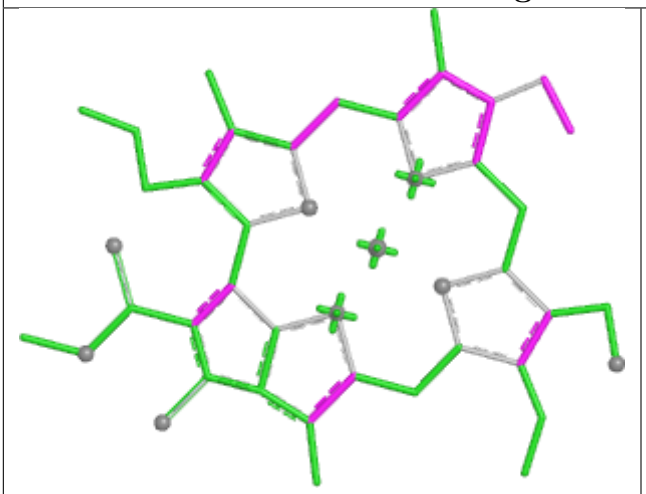


Rings

Ligand CHL R1 606



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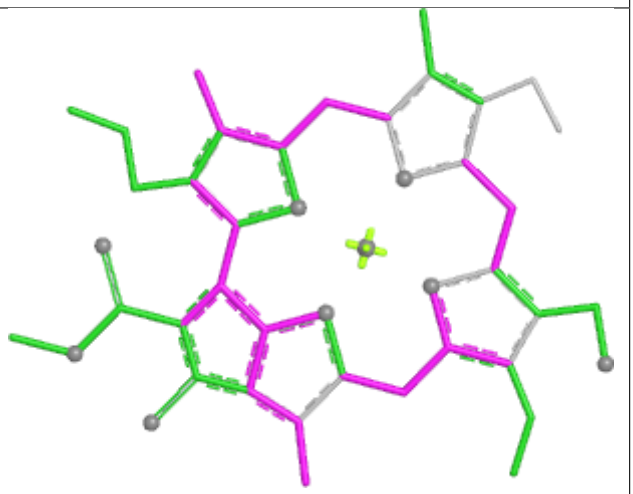
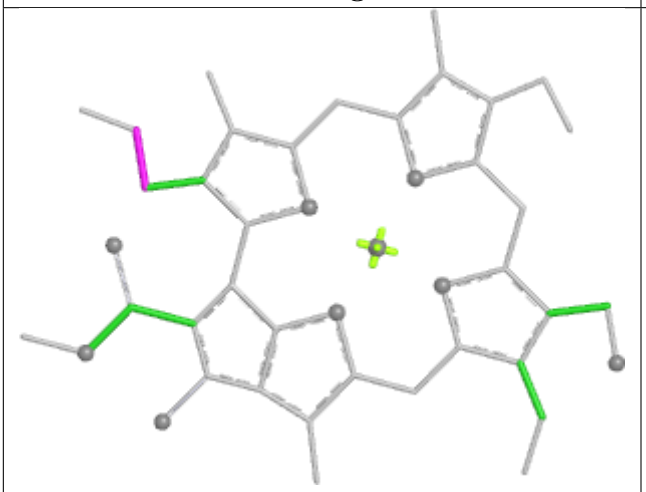


Bond angles



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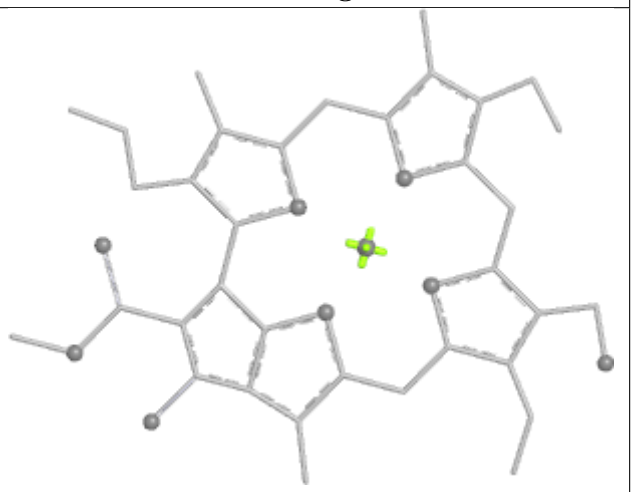
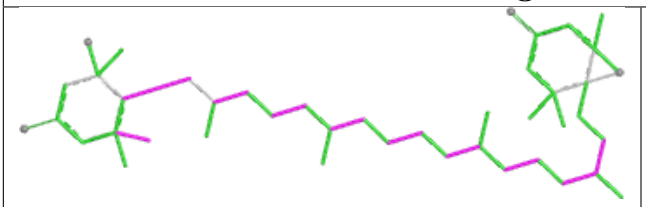


Rings

Ligand NEX n1 623



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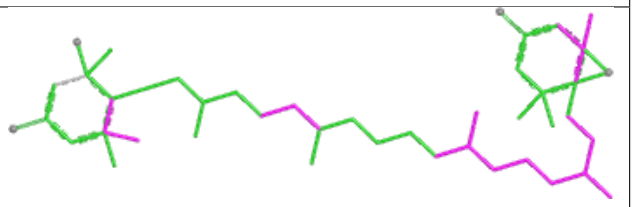
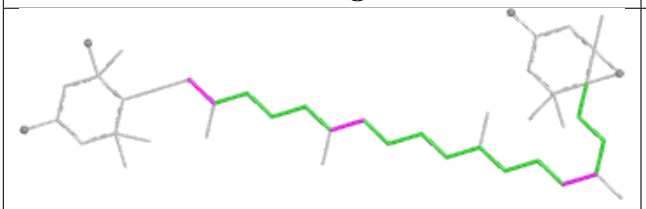


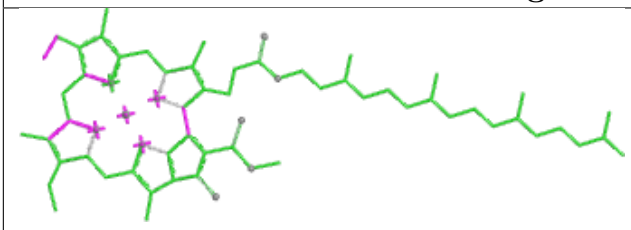
Bond angles



Torsions

Rings

Ligand CLA n 613



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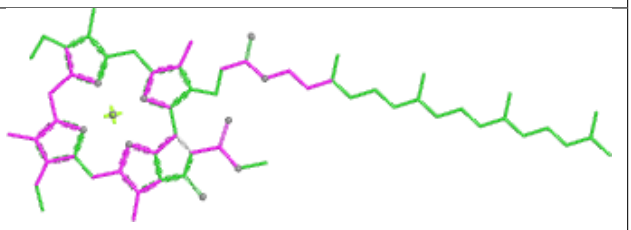
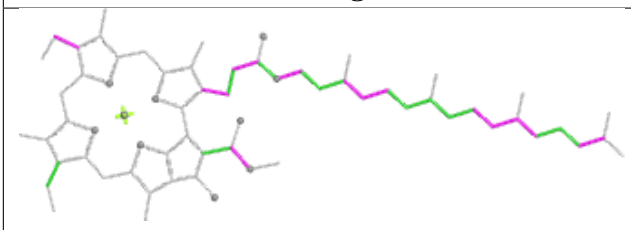


Bond angles



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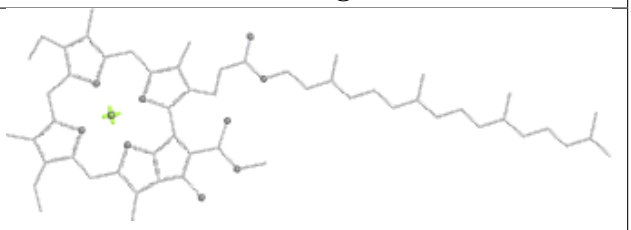
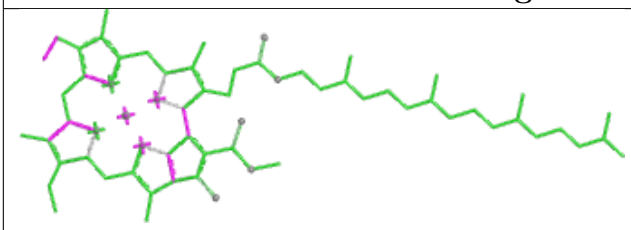


Rings

Ligand CLA Y1 614



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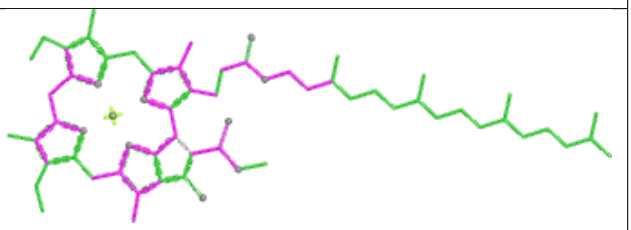
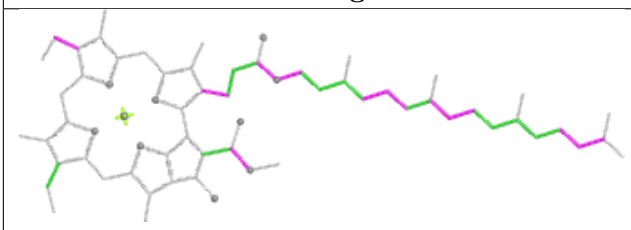


Bond angles



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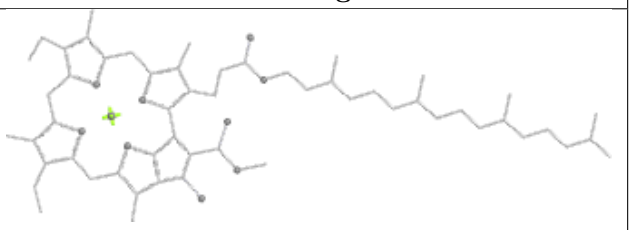
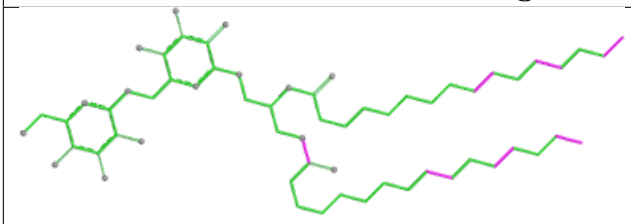
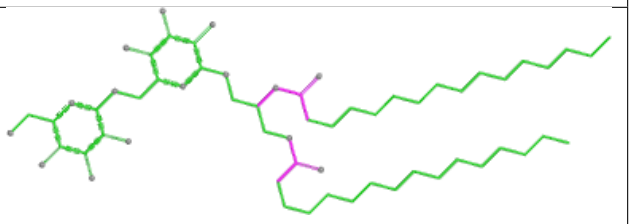


Rings

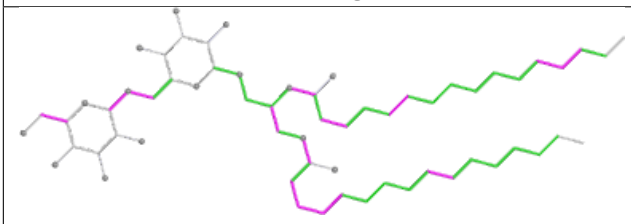
Ligand DGD c1 519



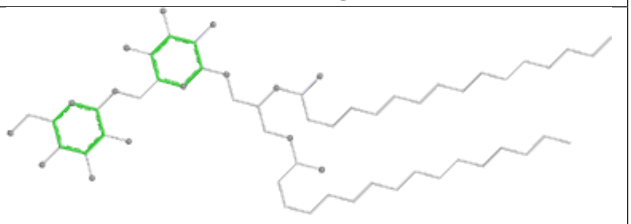
Bond lengths



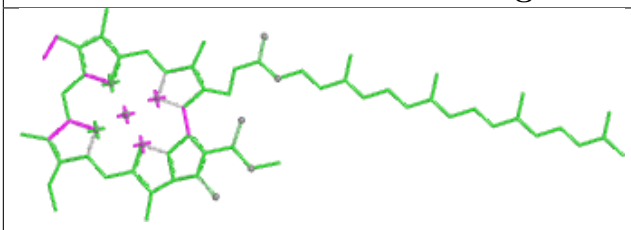
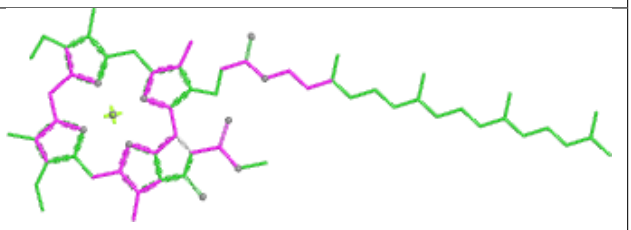
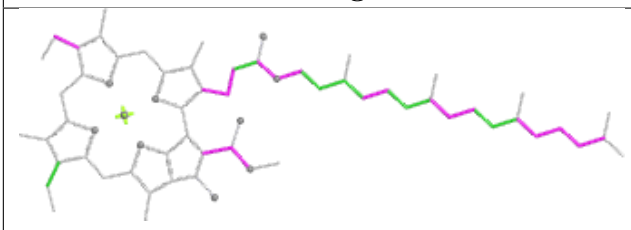
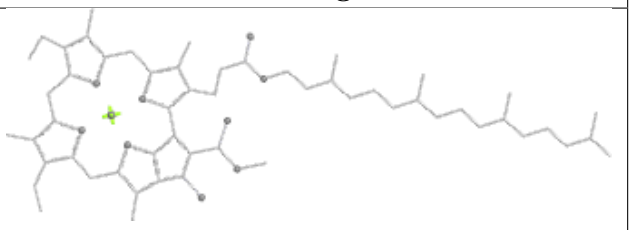
Bond angles

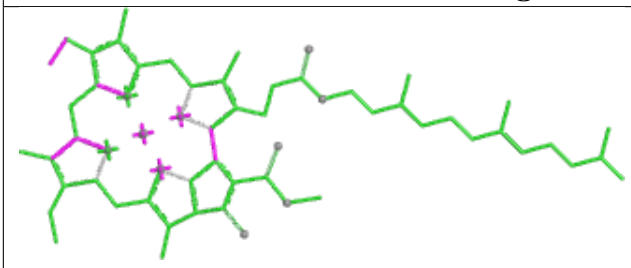
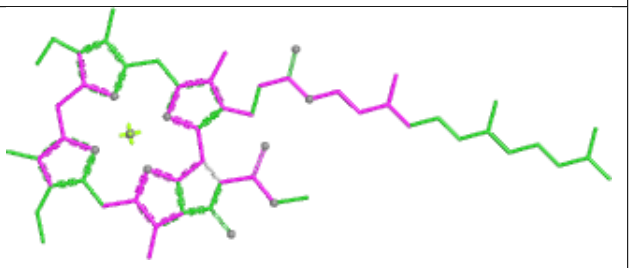
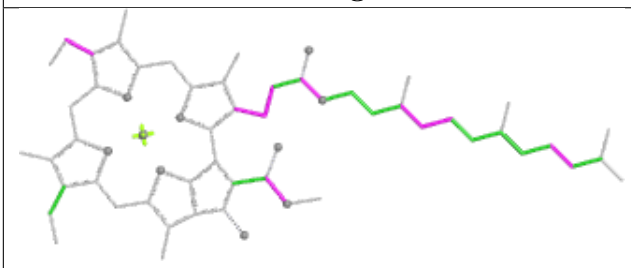
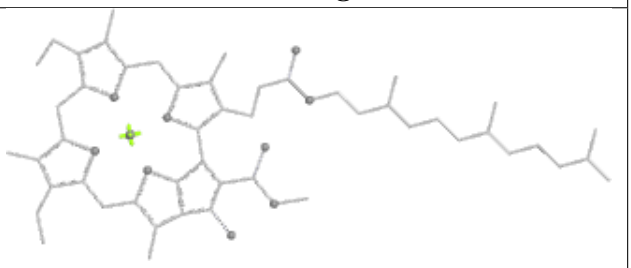


Torsions

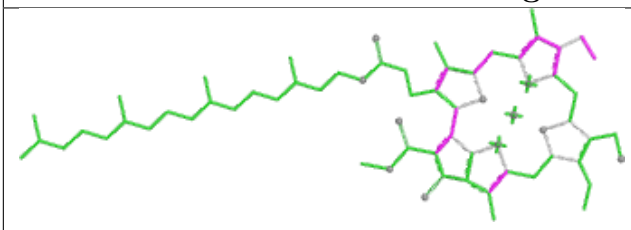


Rings

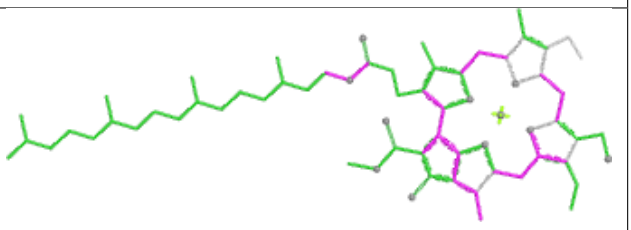
Ligand CLA B1 602	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA R1 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

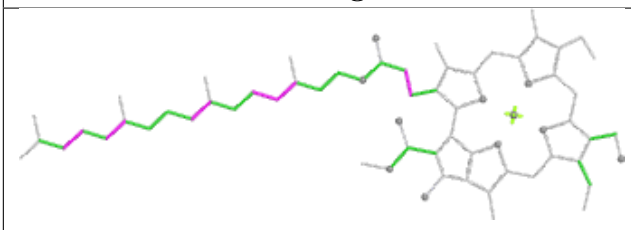
Ligand CHL N 605



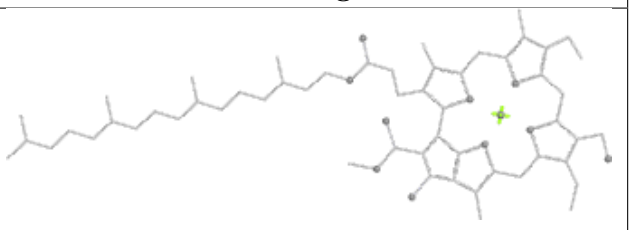
Bond lengths



Bond angles

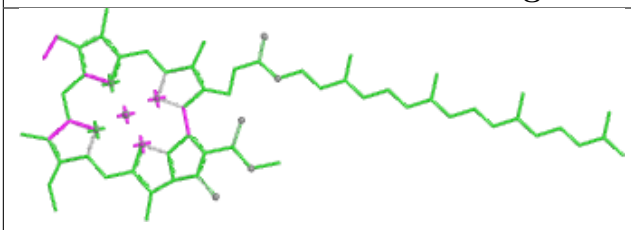


Torsions

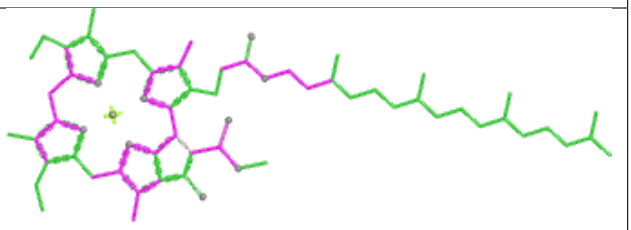


Rings

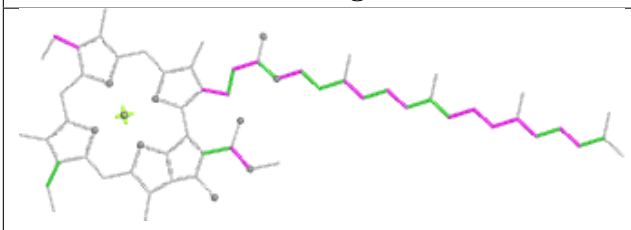
Ligand CLA N 613



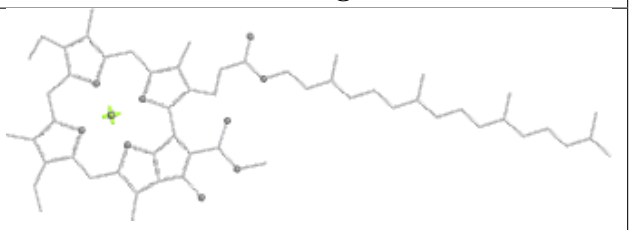
Bond lengths



Bond angles

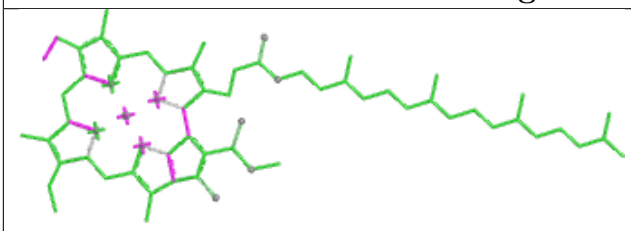


Torsions



Rings

Ligand CLA b1 617



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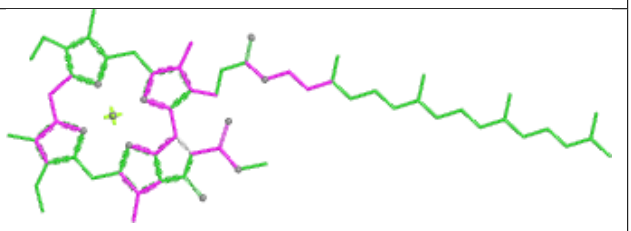
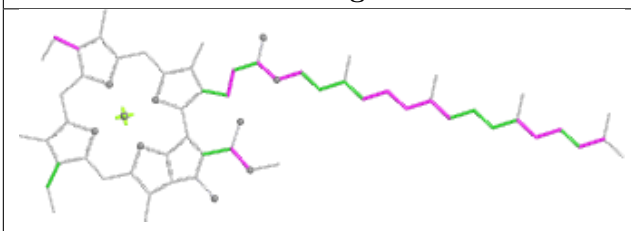
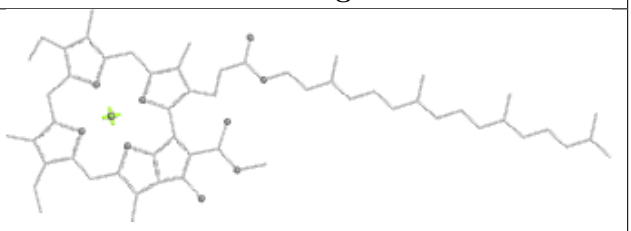


Bond angles

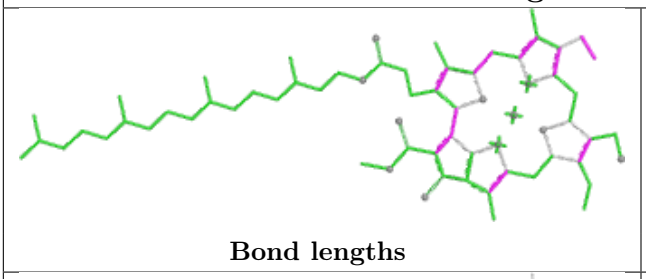


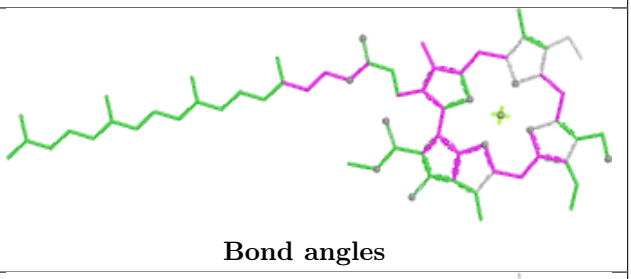
Torsions

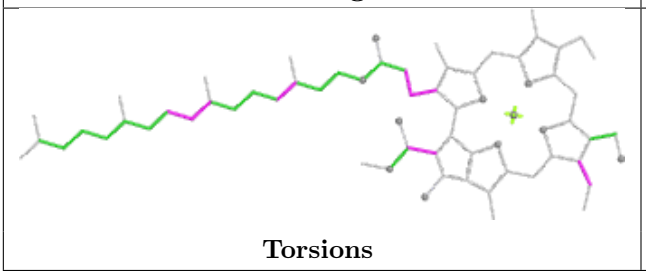


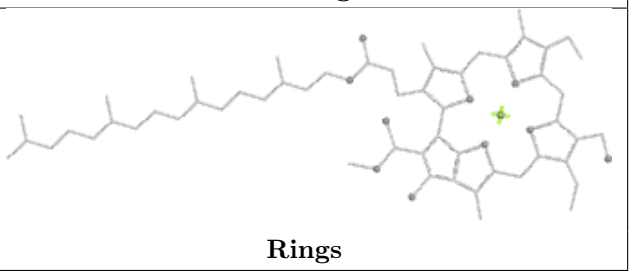
Rings

Ligand CHL n 609

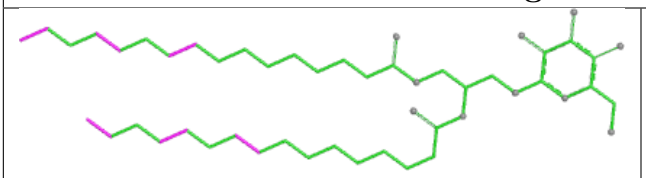

Bond lengths


Bond angles


Torsions


Rings

Ligand LMG c 521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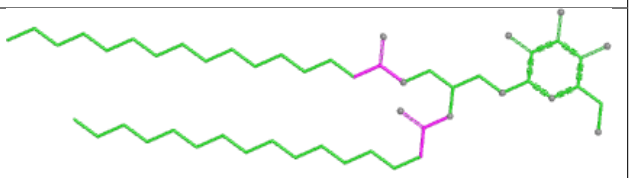
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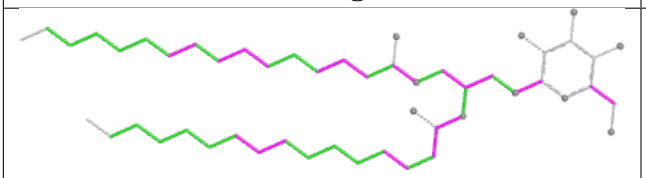
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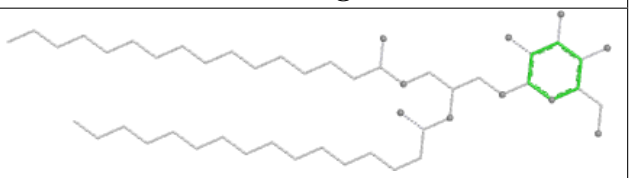
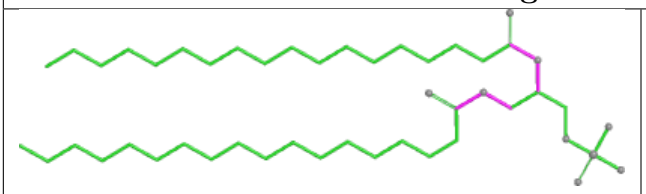

Rings

Ligand 3PH b1 624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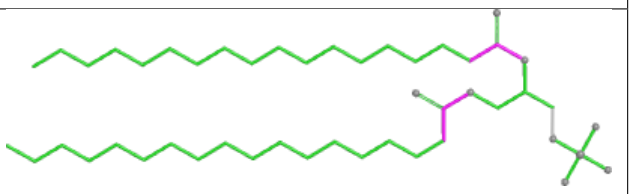
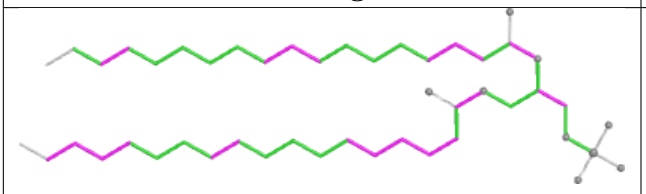

Bond angles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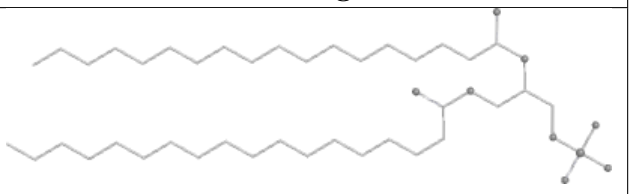
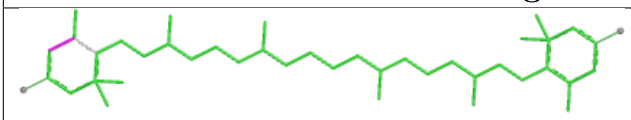

Rings

Ligand LUT G 621



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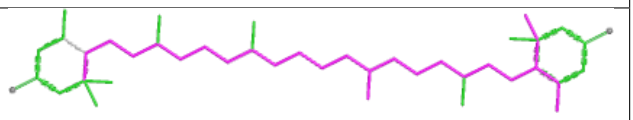
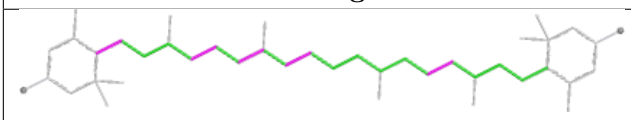


Bond angles



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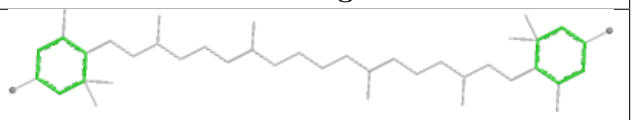
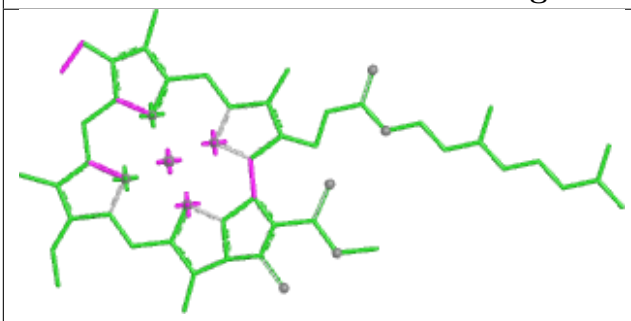


Rings

Ligand CLA s 613



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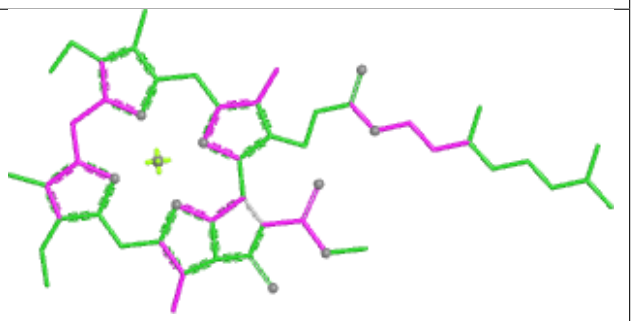

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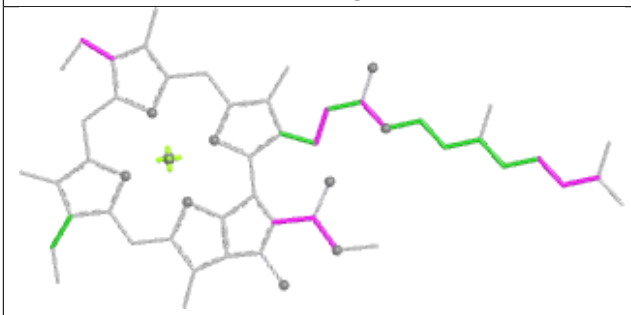

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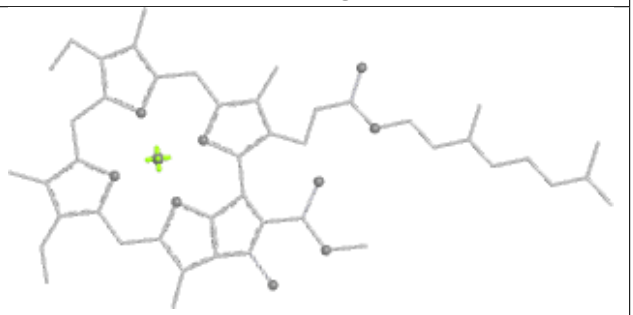
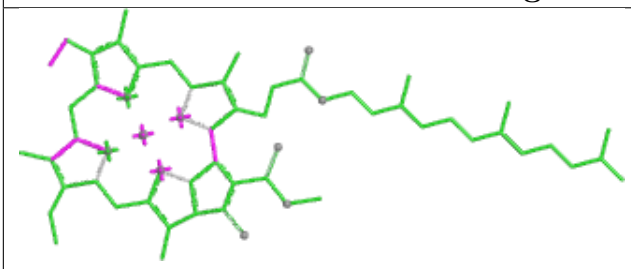


Rings

Ligand CLA R 610



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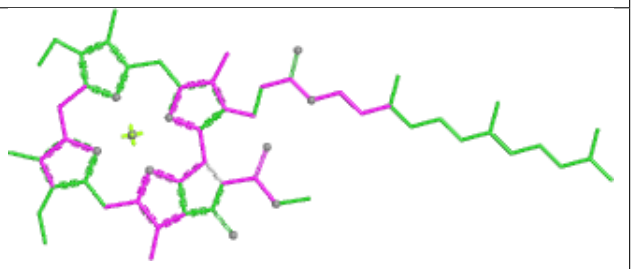
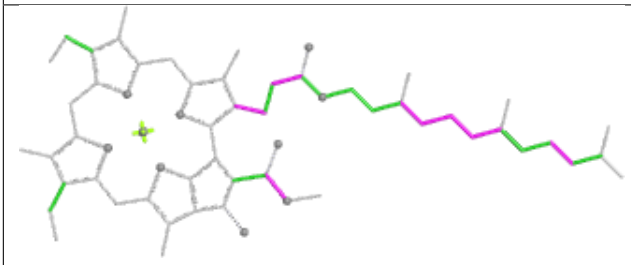


Bond angles



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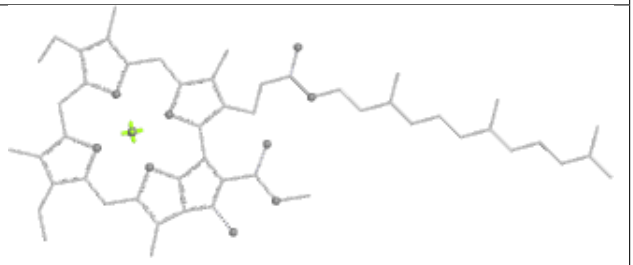
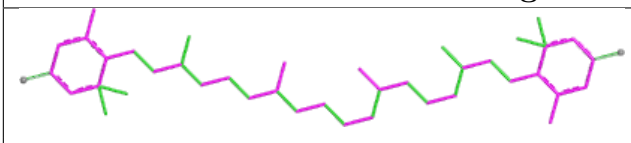


Rings

Ligand C7Z B1 620



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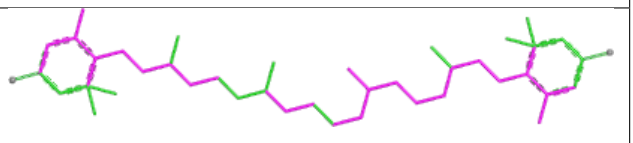

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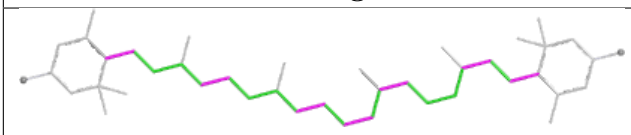

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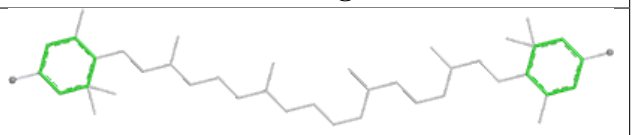
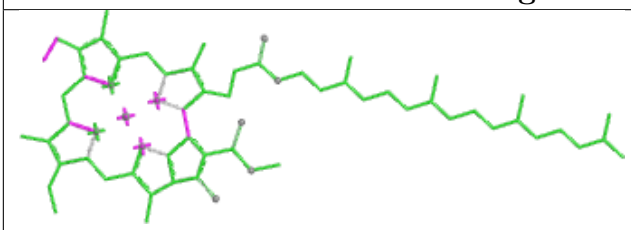


Rings

Ligand CLA b1 608



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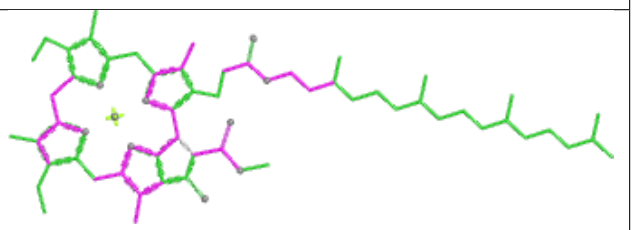

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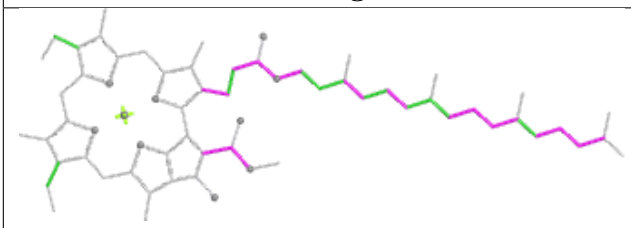

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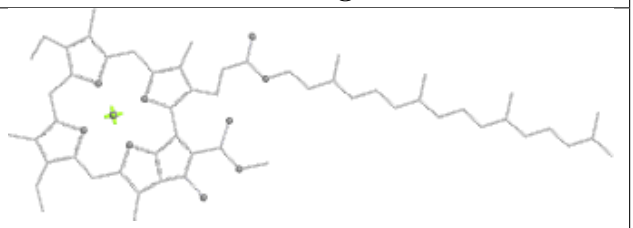
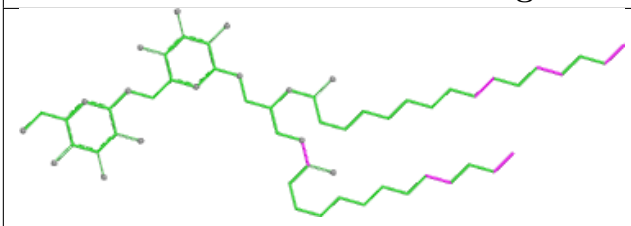


Rings

Ligand DGD c1 520



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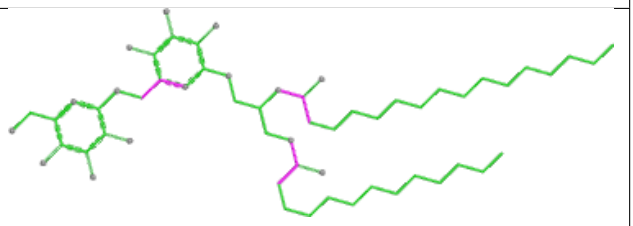
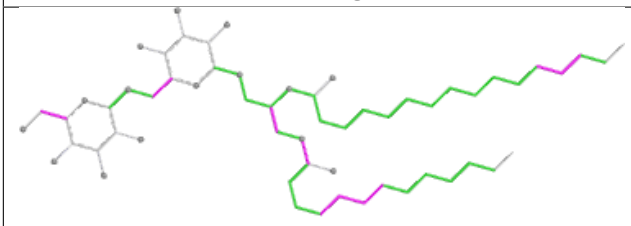


Bond angles



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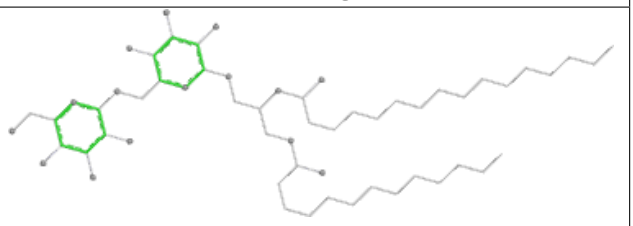
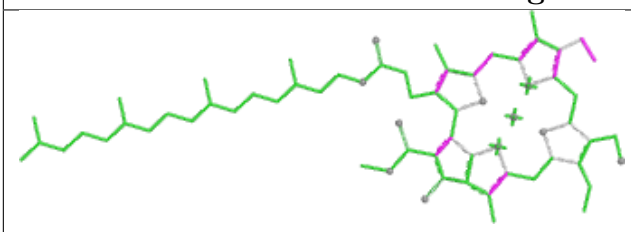


Rings

Ligand CHL y 607



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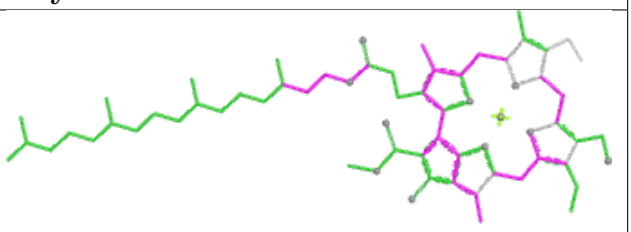
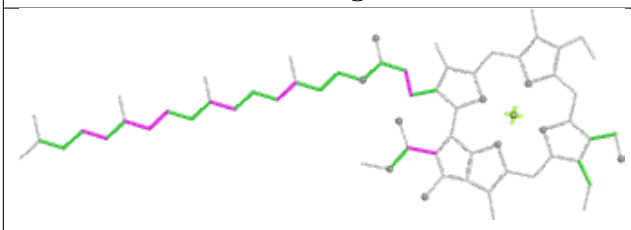


Bond angles



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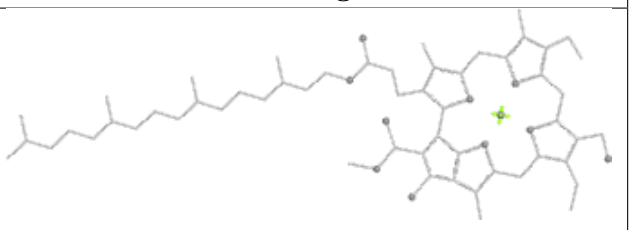
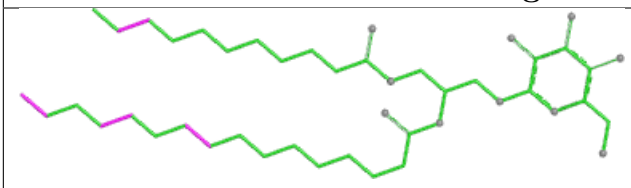


Rings

Ligand LMG d 411



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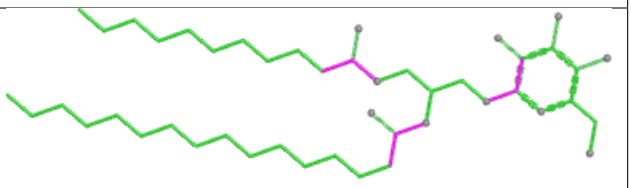

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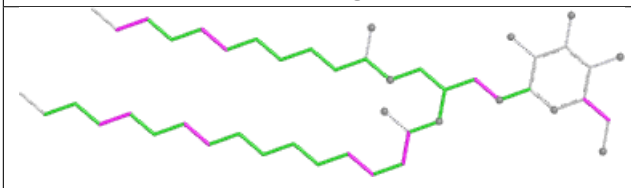

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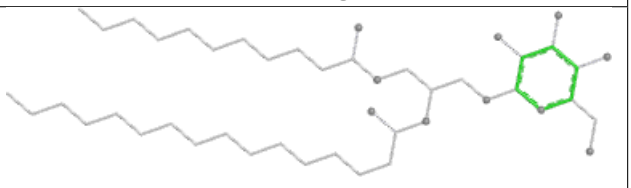
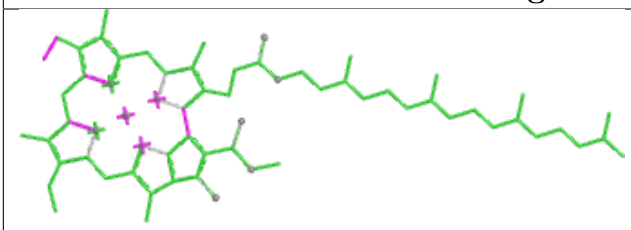


Rings

Ligand CLA y 604



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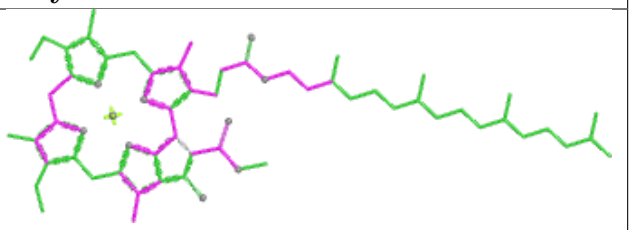
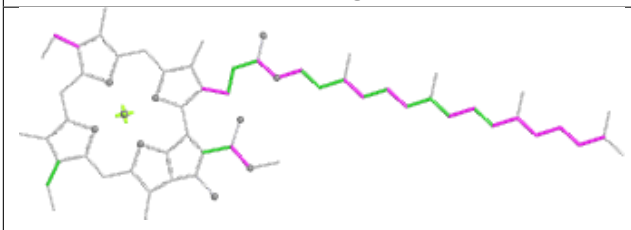


Bond angles



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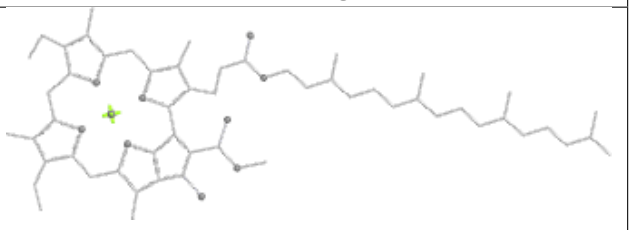
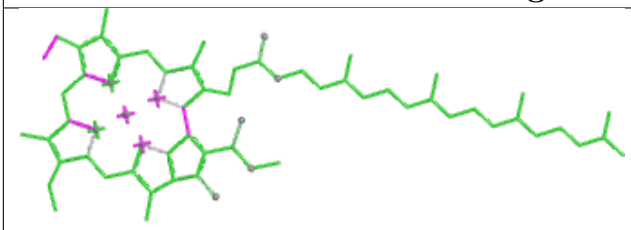


Rings

Ligand CLA d 403



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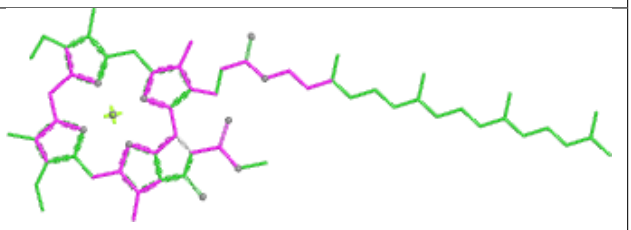
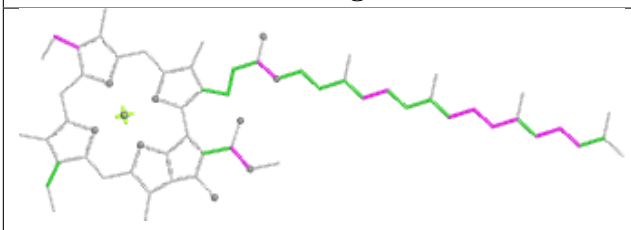


Bond angles



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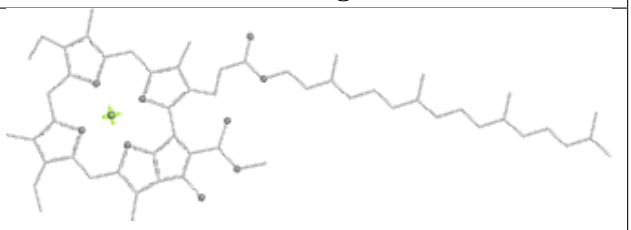
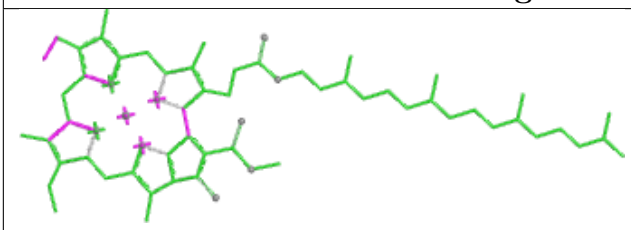


Rings

Ligand CLA Y1 604



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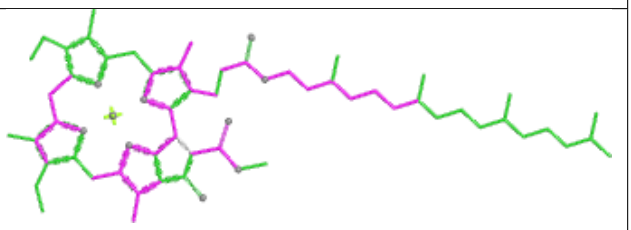
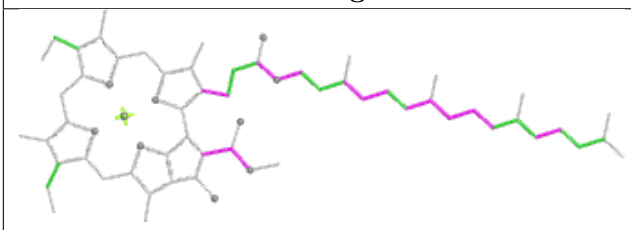
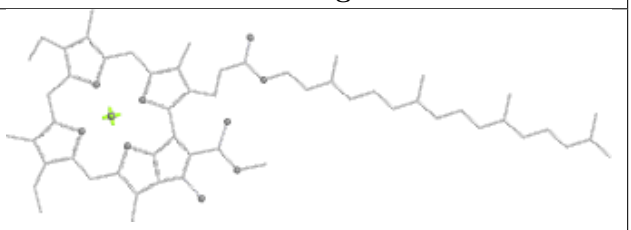


Bond angles

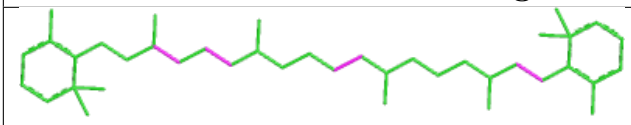


Torsions

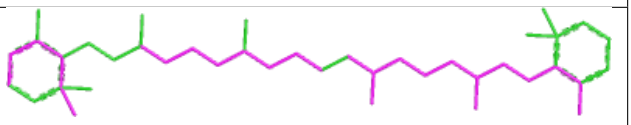


Rings

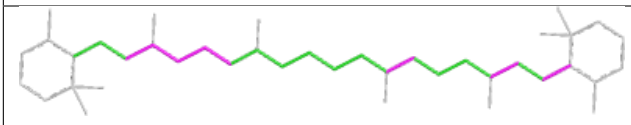
Ligand BCR C1 517



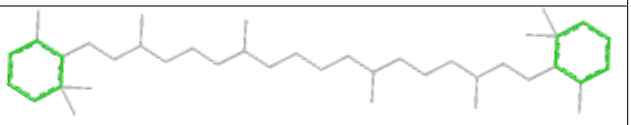
Bond lengths



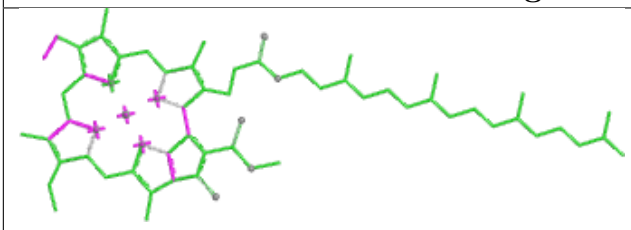
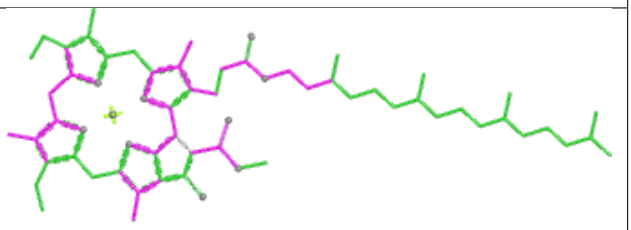
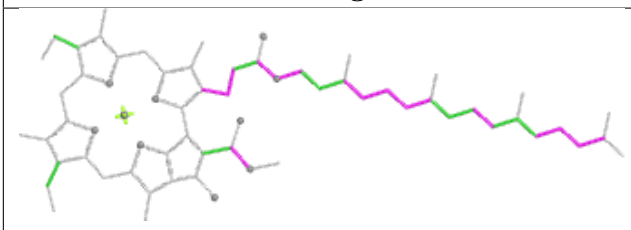
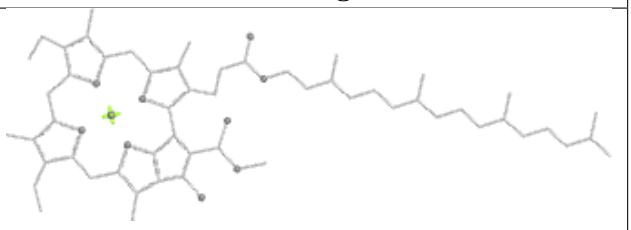
Bond angles

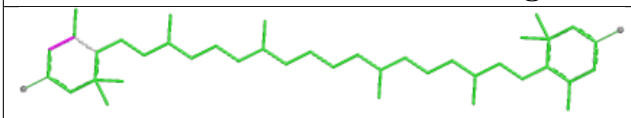
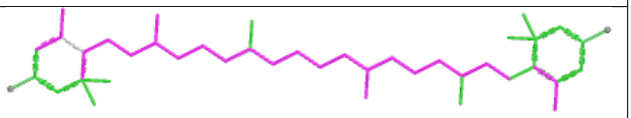
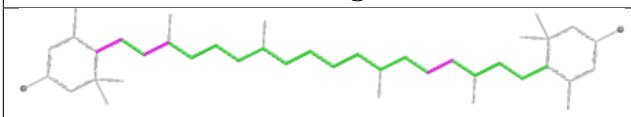
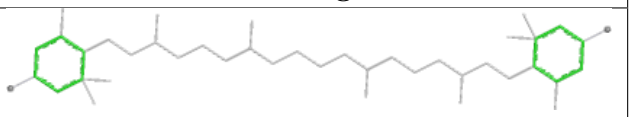


Torsions

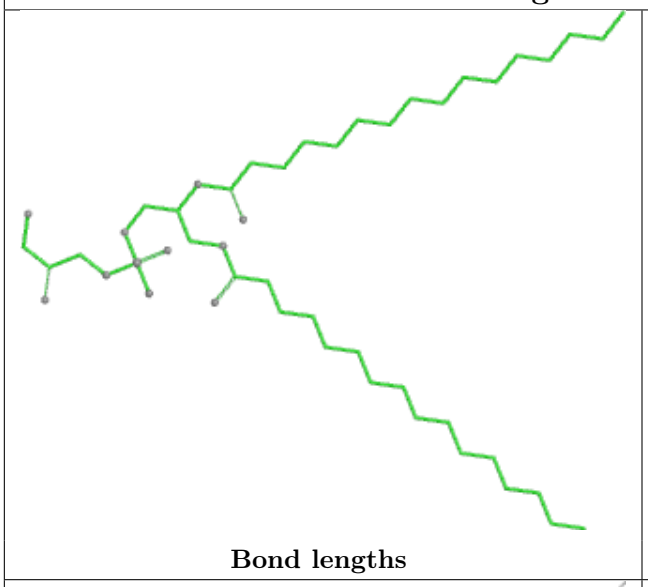


Rings

Ligand CLA B 604	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LUT N 620	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand LHG l 101



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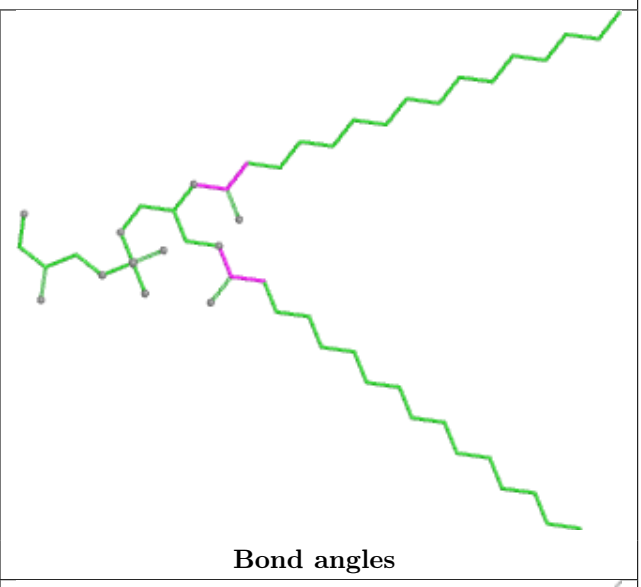
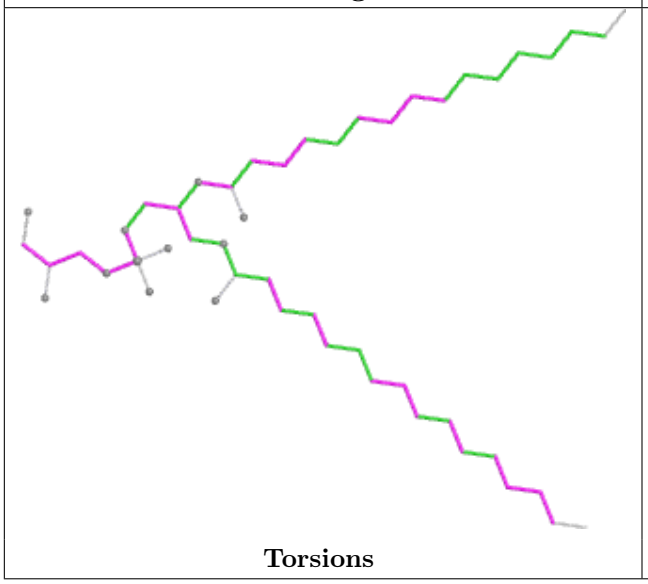
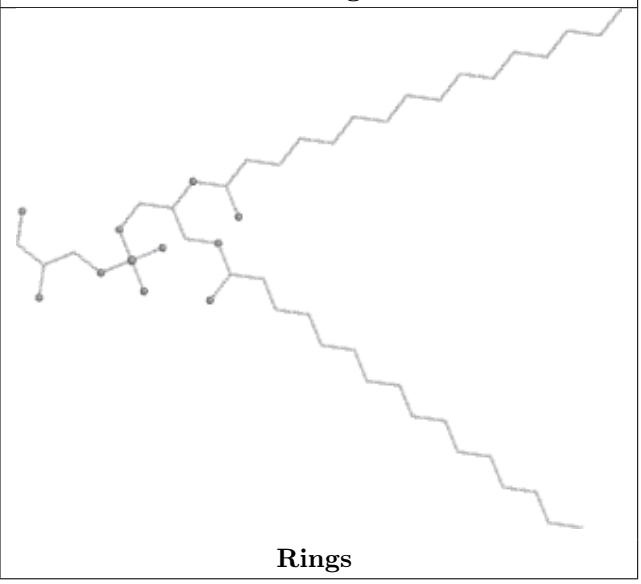


Bond angles

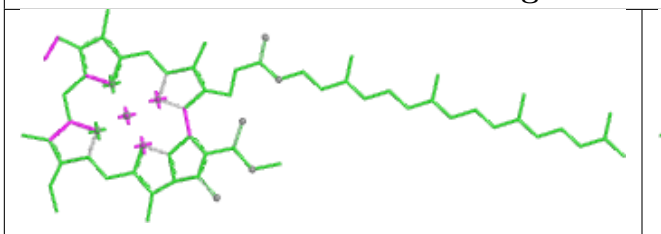


Torsions

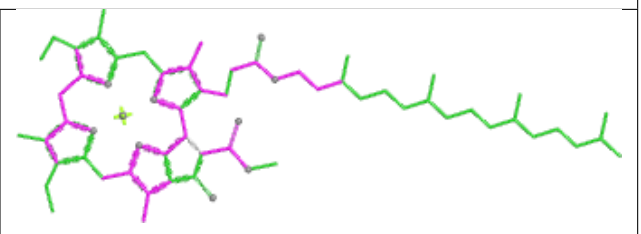


Rings

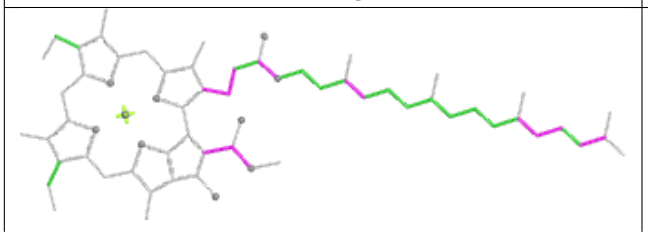
Ligand CLA c1 501



Bond lengths



Bond angles



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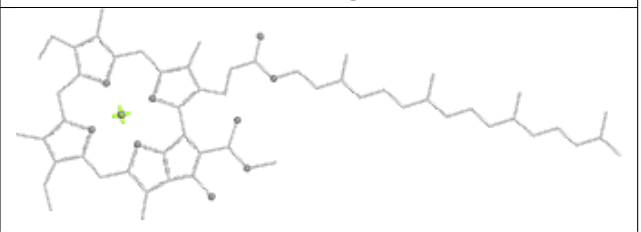
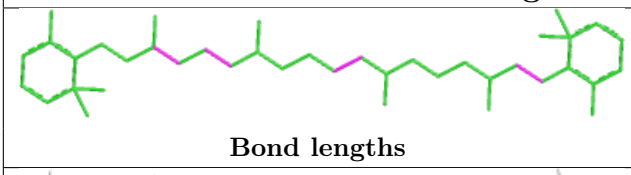


Rings

Ligand BCR B 619



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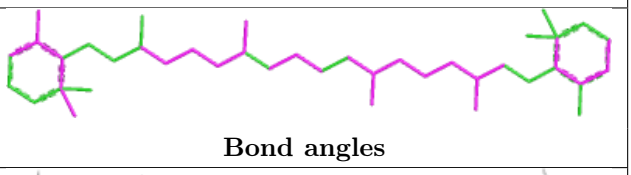
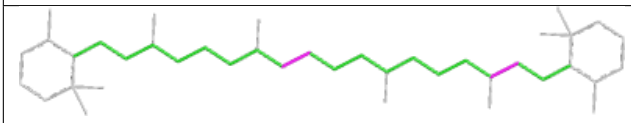


Bond angles



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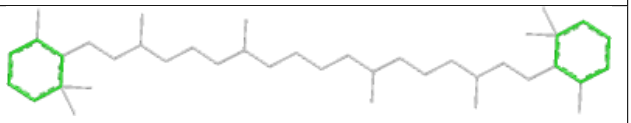
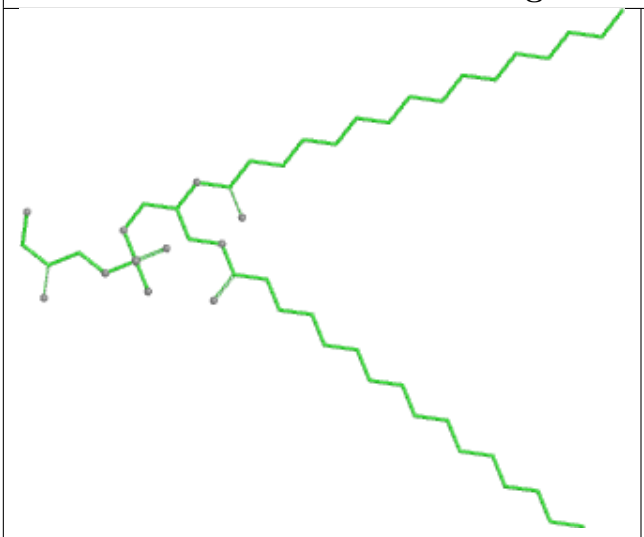


Rings

Ligand LHG d 409



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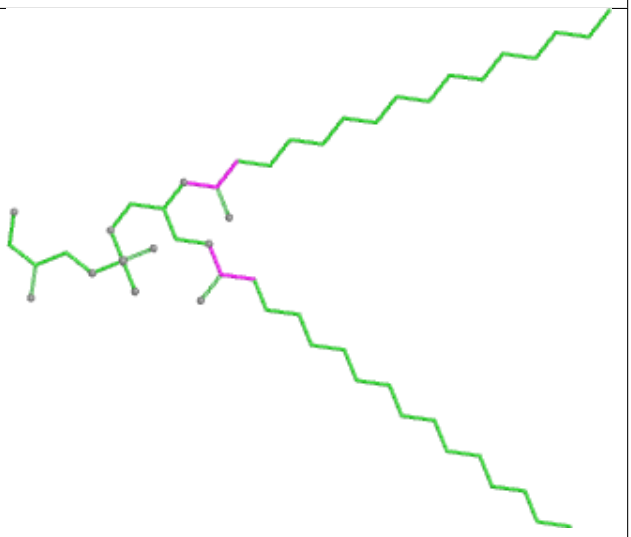
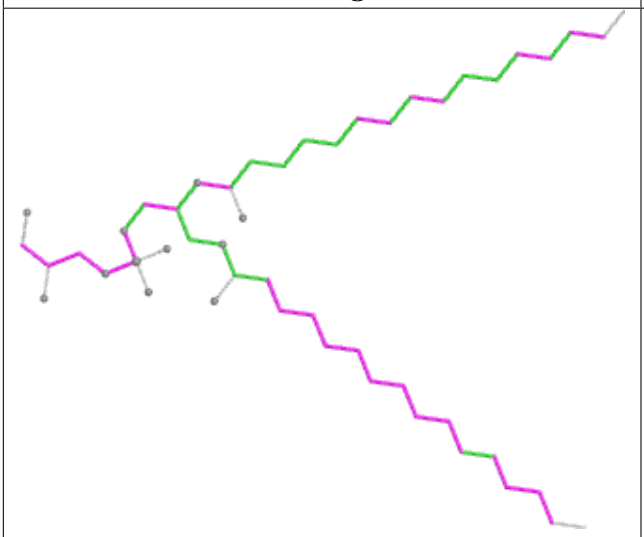
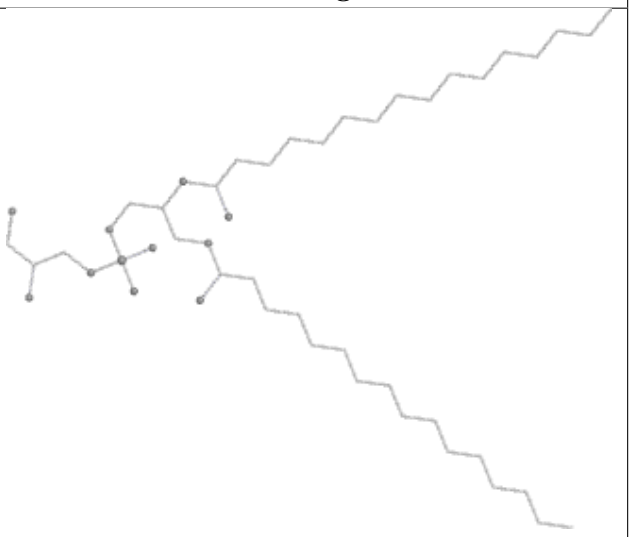


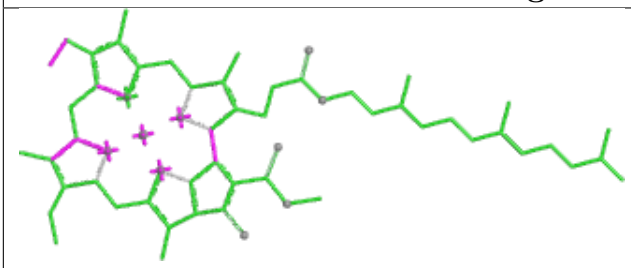
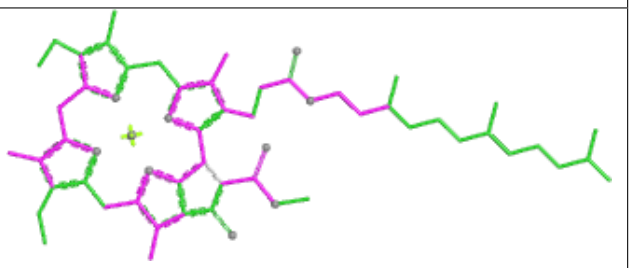
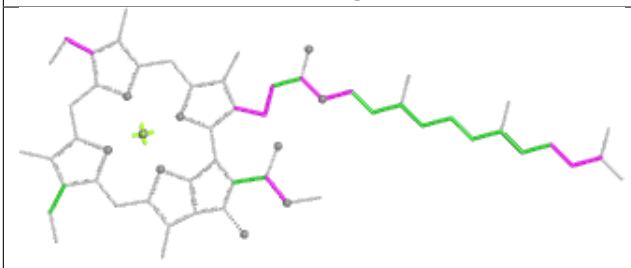
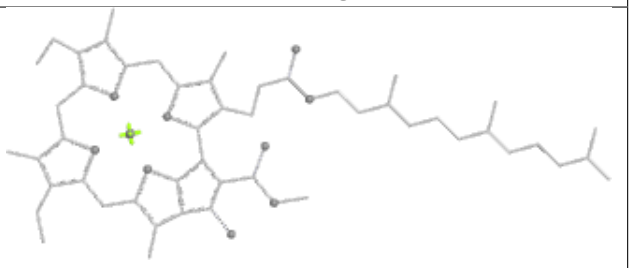
Bond angles

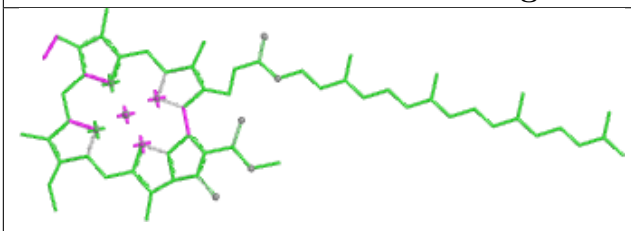
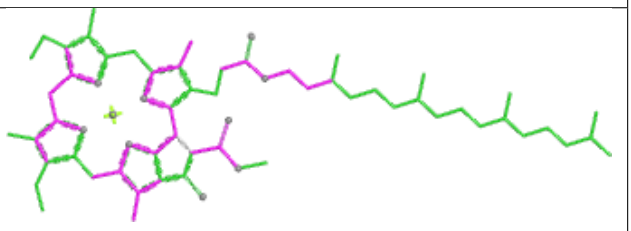
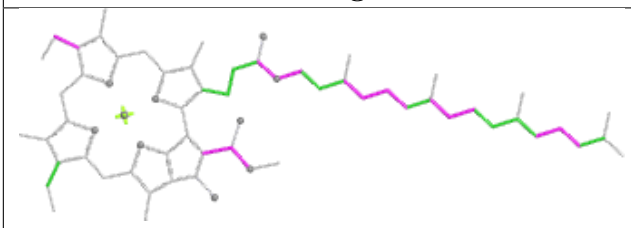
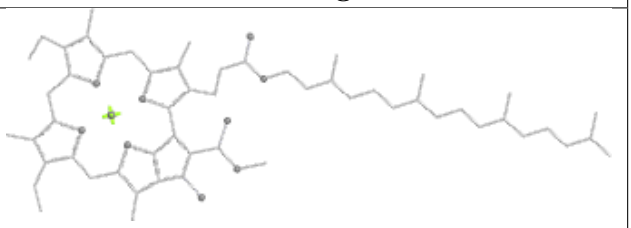


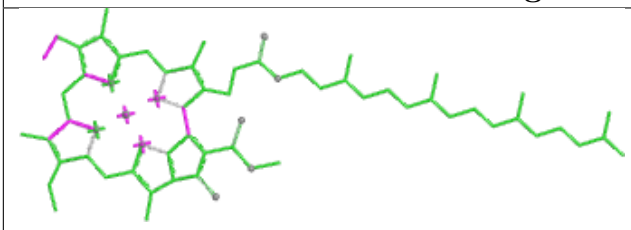
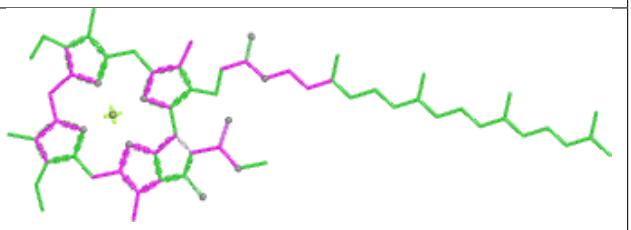
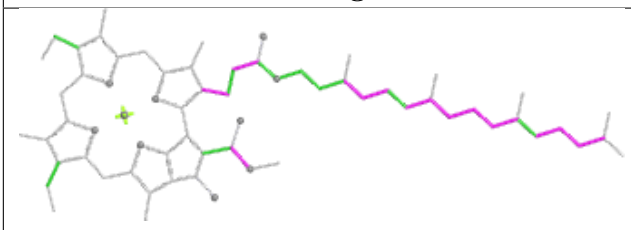
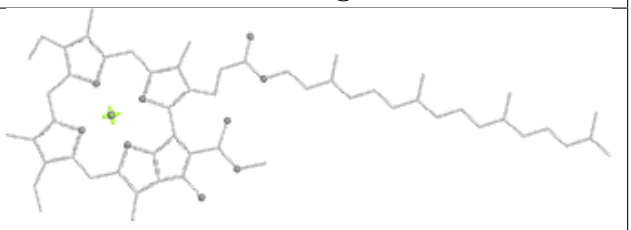
Torsions

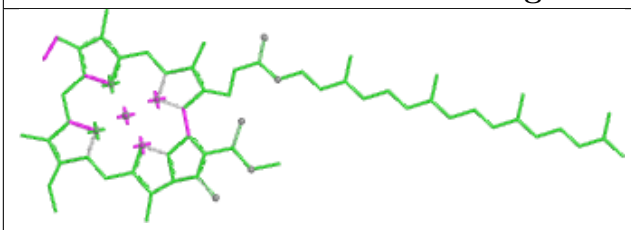
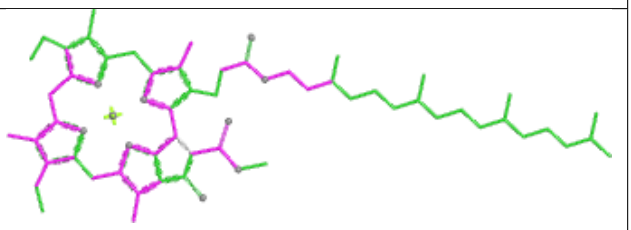


Rings

Ligand CLA S 609	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA c1 506	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA C 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA B 603	
	
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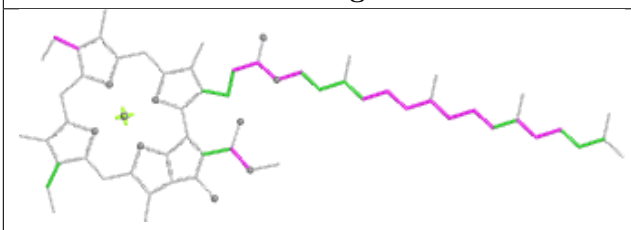
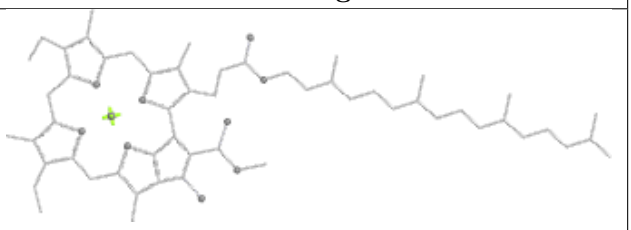
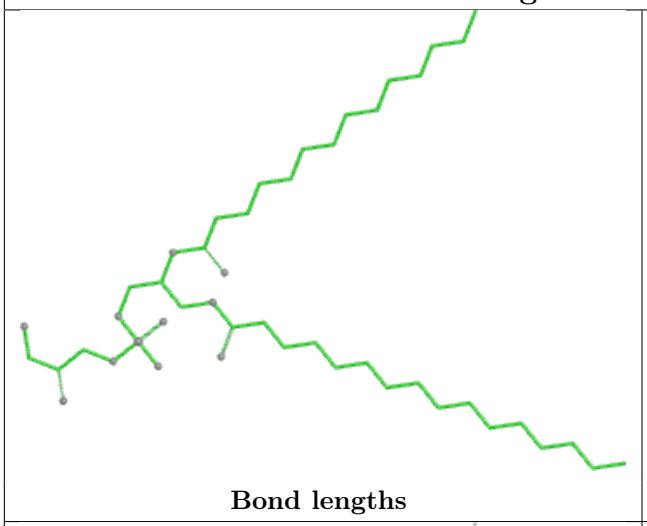
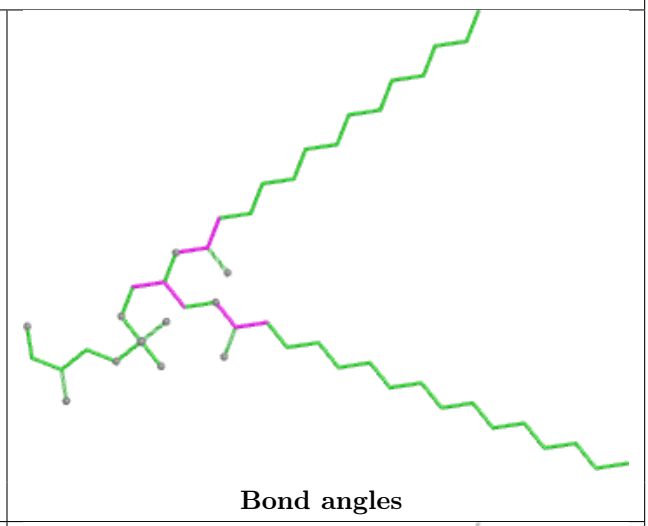
	
Torsions	Rings

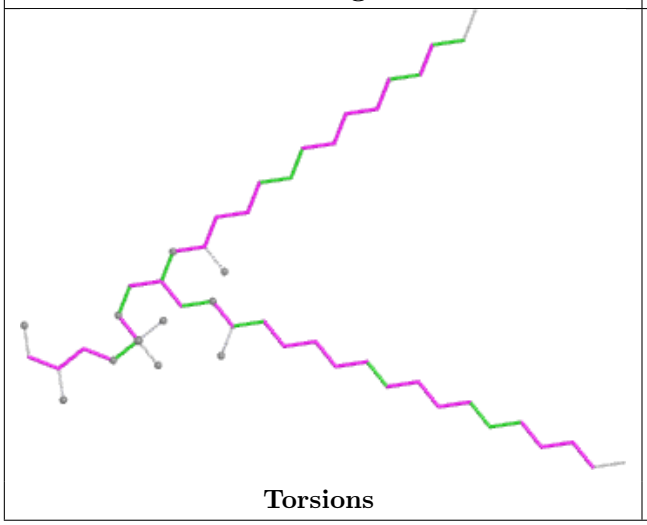
Ligand LHG c1 525



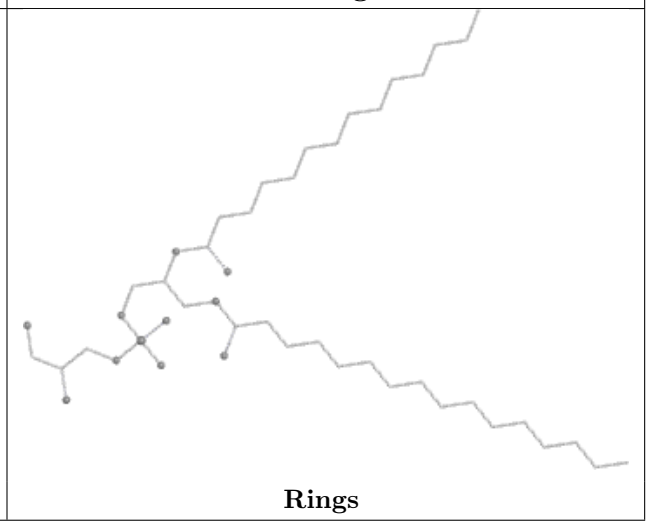
Bond lengths



Bond angles

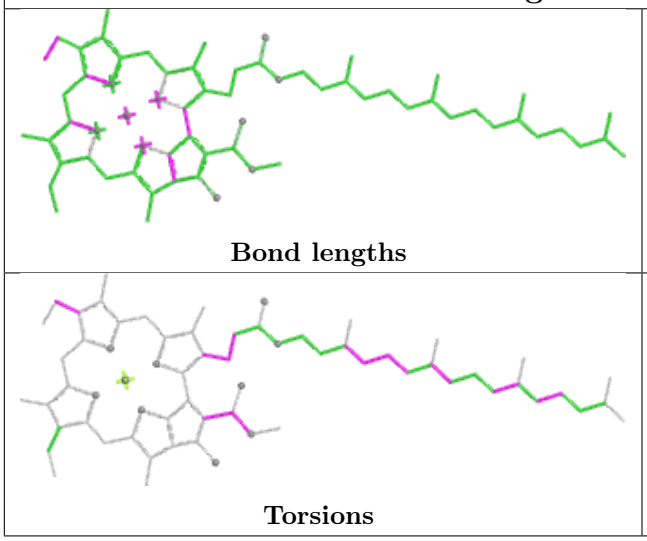


Torsions

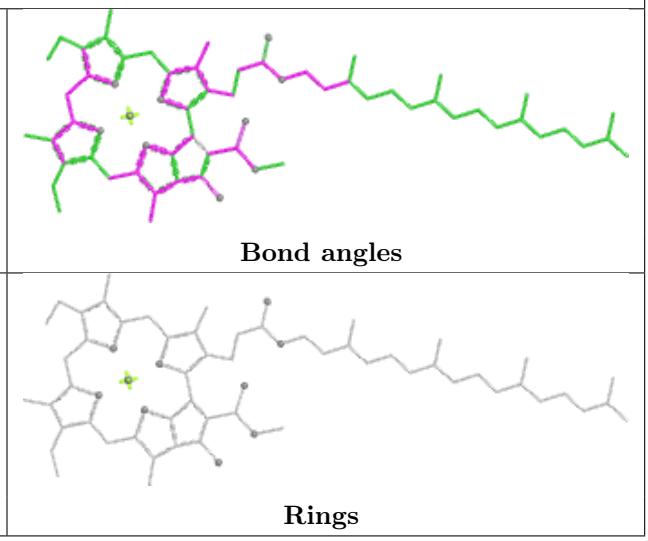


Rings

Ligand CLA C 501



Bond lengths

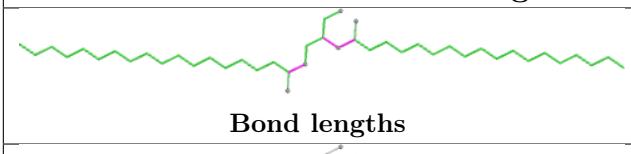


Bond angles

Torsions

Rings

Ligand DGA C1 524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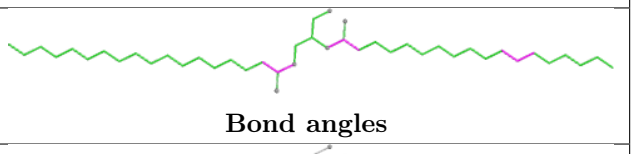
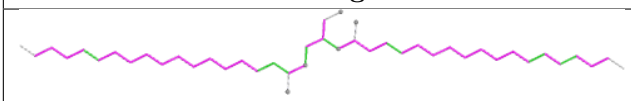

Bond angles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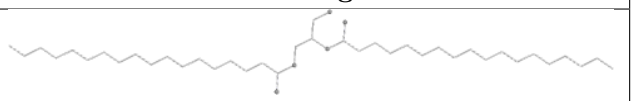
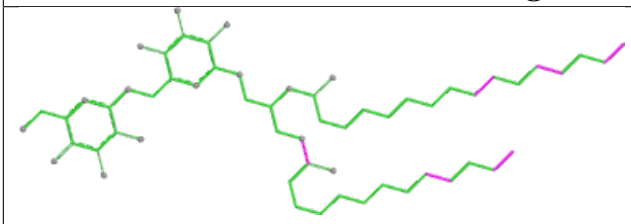
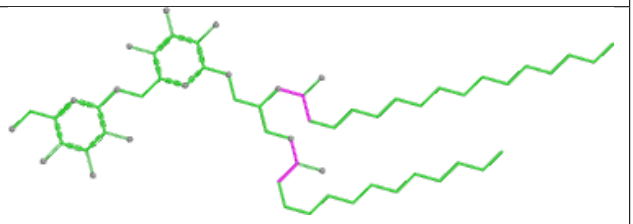
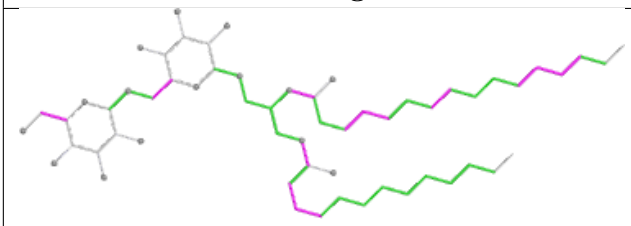
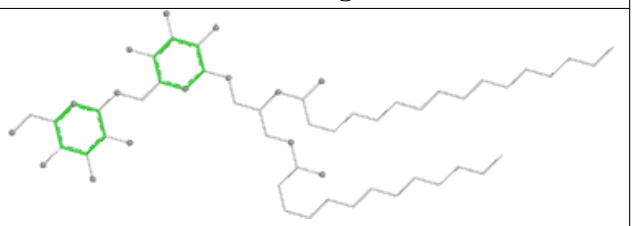

Rings

Ligand DGD c 520

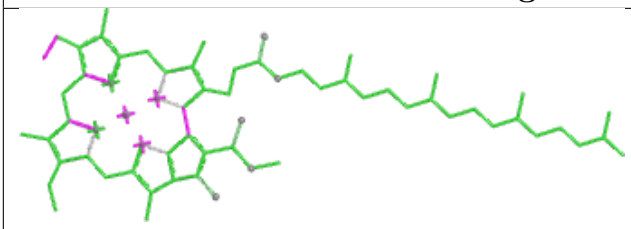

Bond lengths

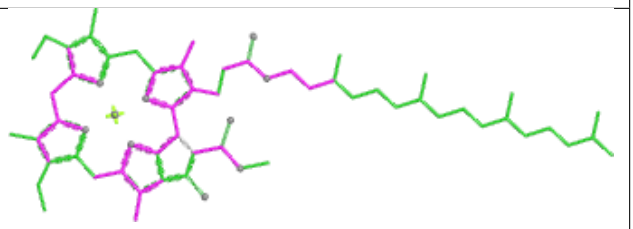

Bond angles


Torsions


Rings

Ligand CLA n1 610


Bond lengths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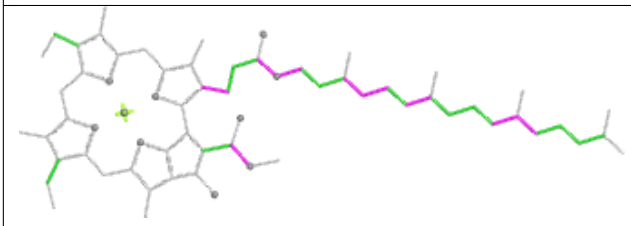
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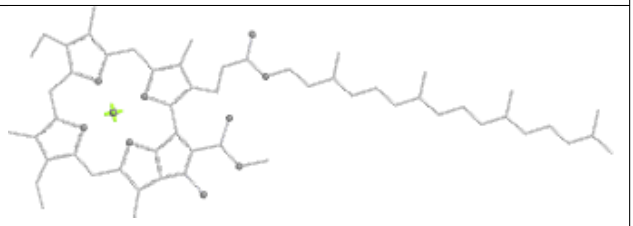
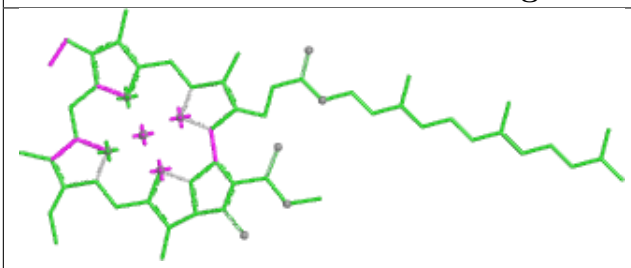
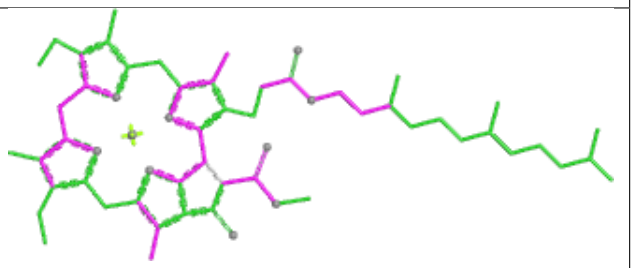

Rings

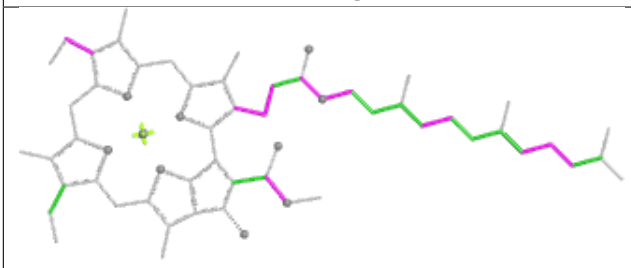
Ligand CLA r1 603



Bond lengths



Bond angles



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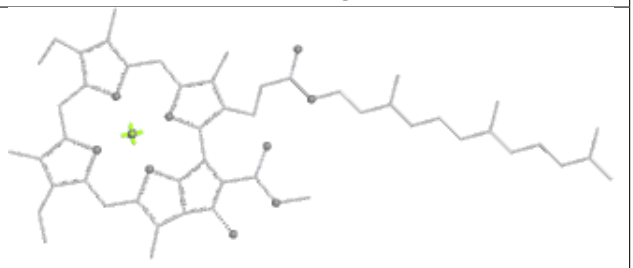
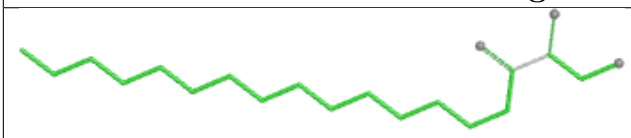


Rings

Ligand SPH y 625



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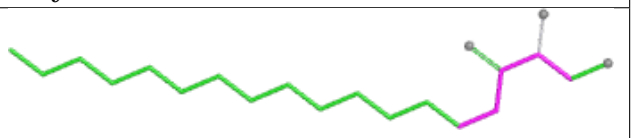
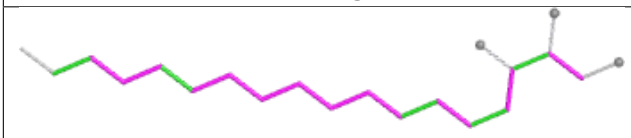


Bond angles



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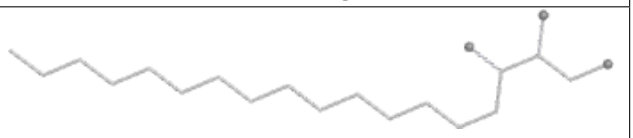
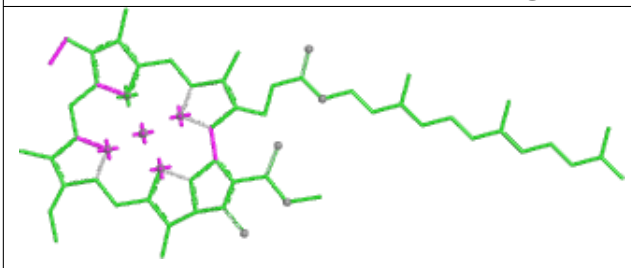


Rings

Ligand CLA R 608



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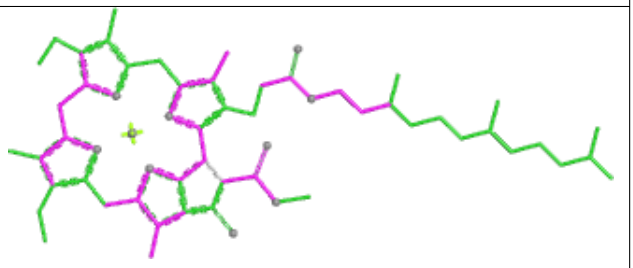

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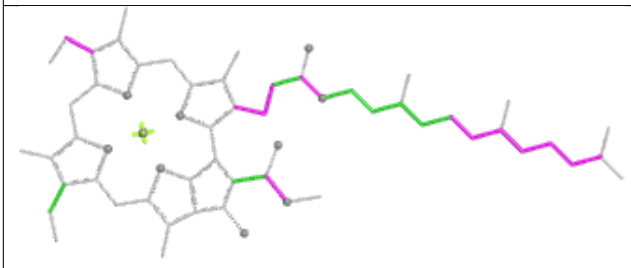

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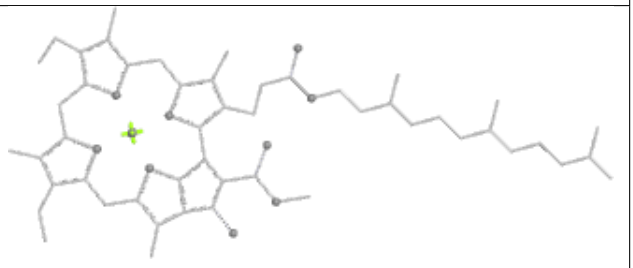
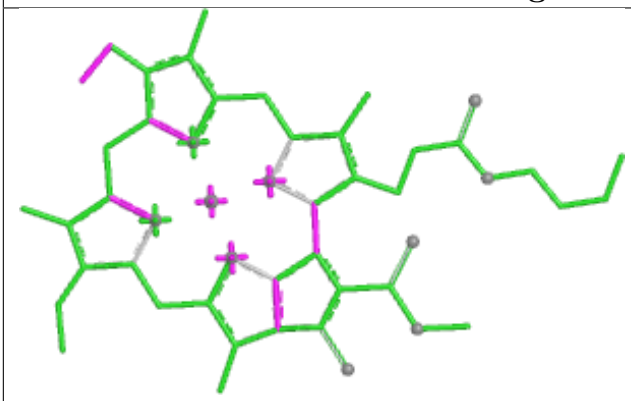


Rings

Ligand CLA a 407



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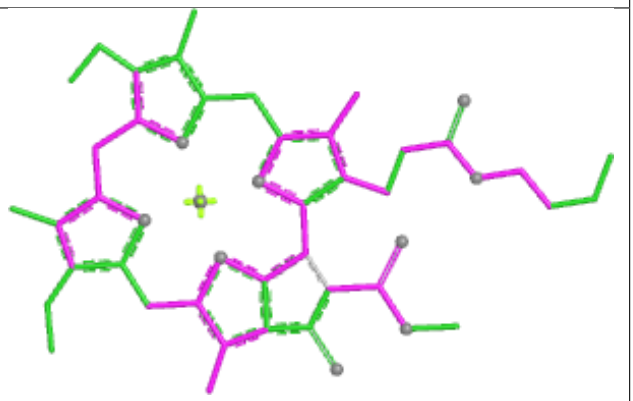
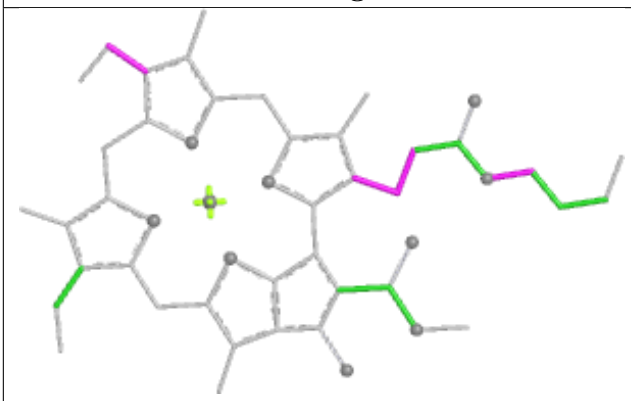


Bond angles



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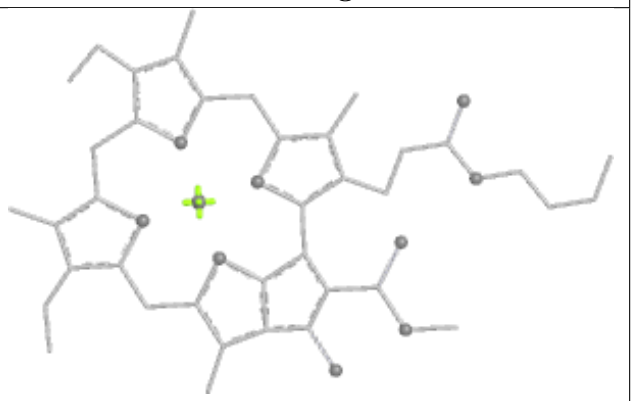
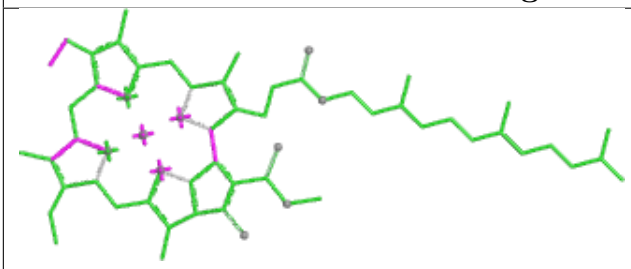


Rings

Ligand CLA r1 602



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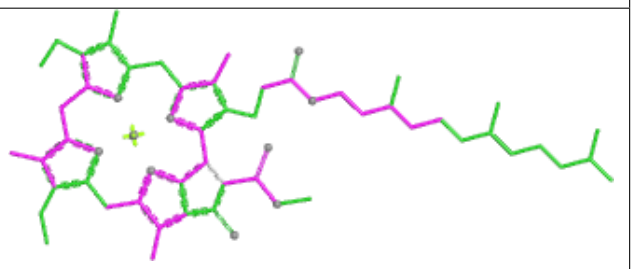

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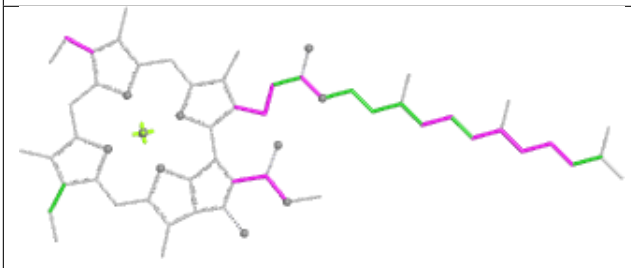

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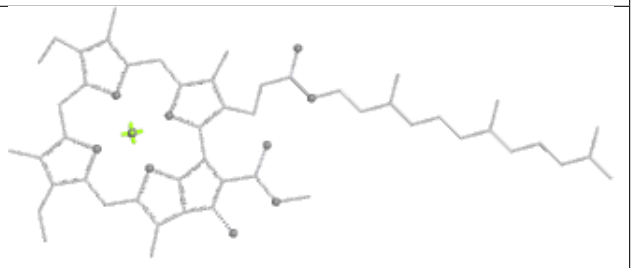
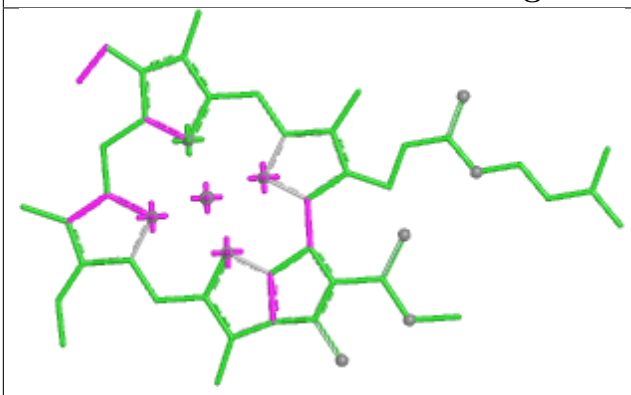


Rings

Ligand CLA Y 608



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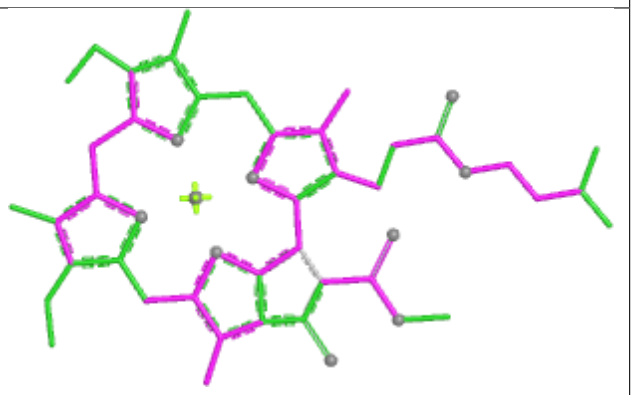

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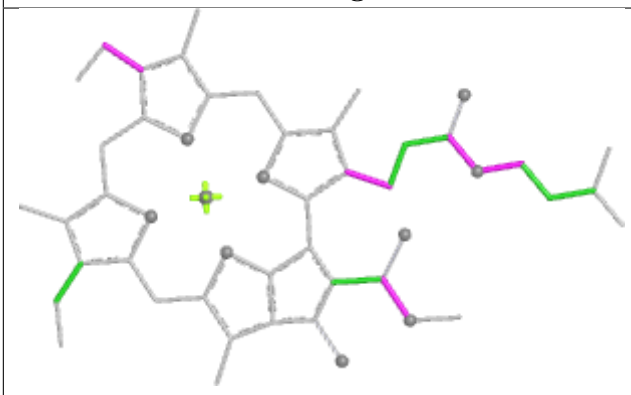

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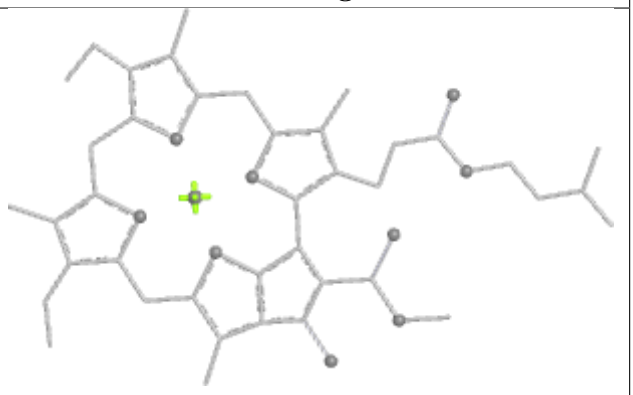
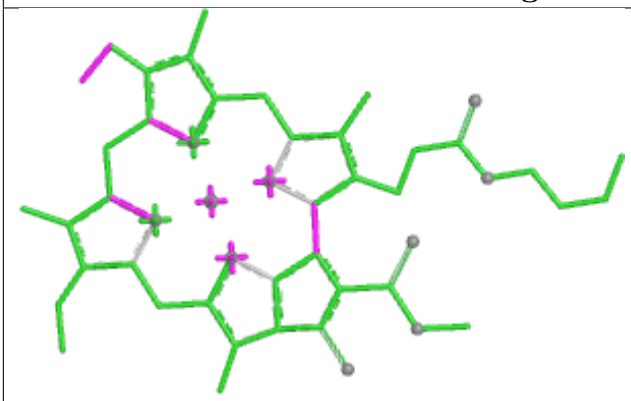


Rings

Ligand CLA r1 604



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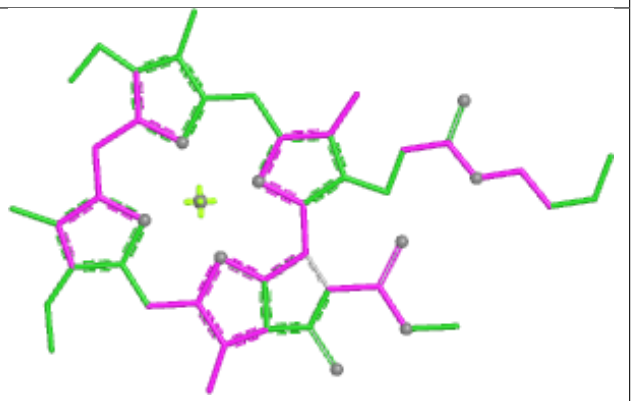

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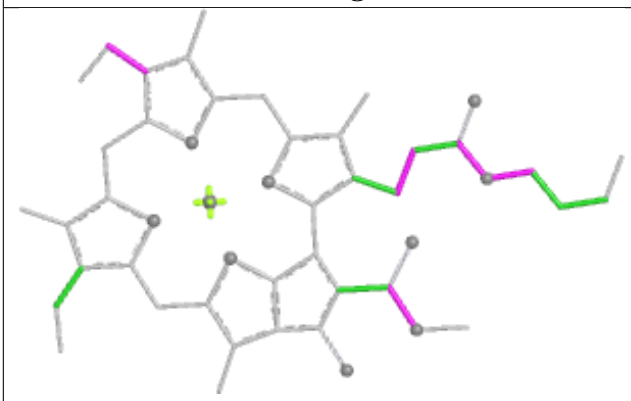

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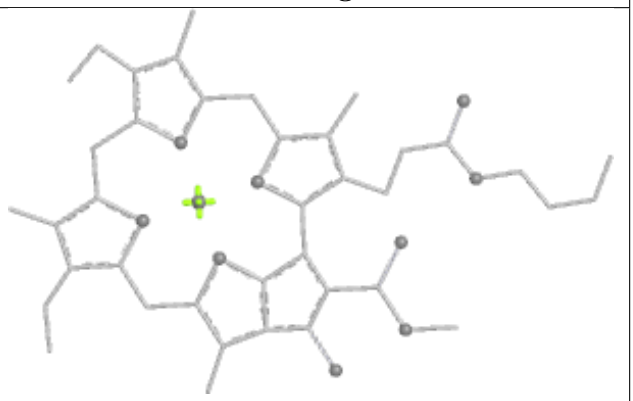
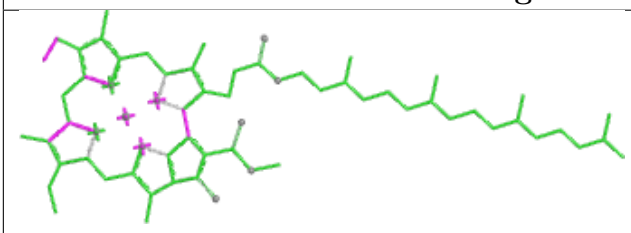


Rings

Ligand CLA A1 405



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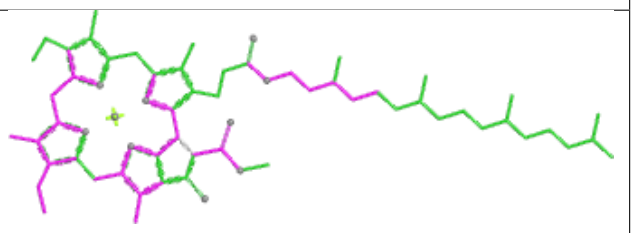

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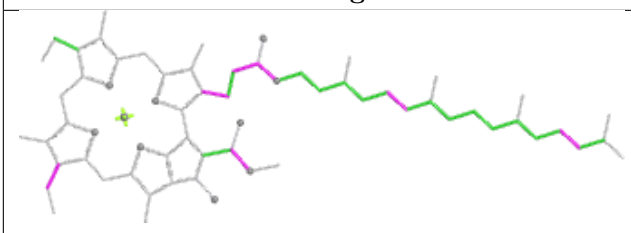

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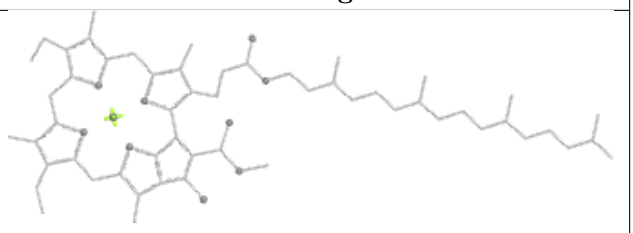
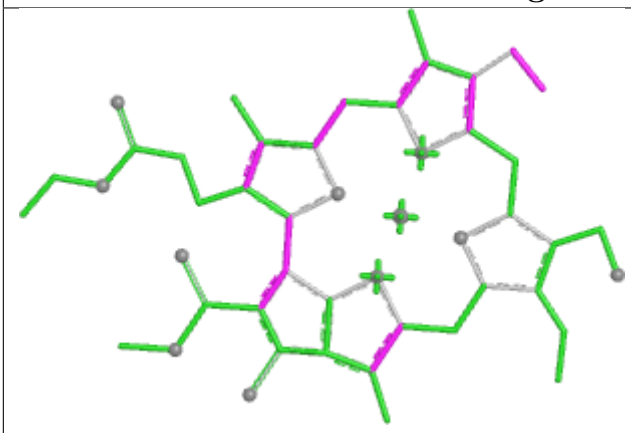


Rings

Ligand CHL g 605



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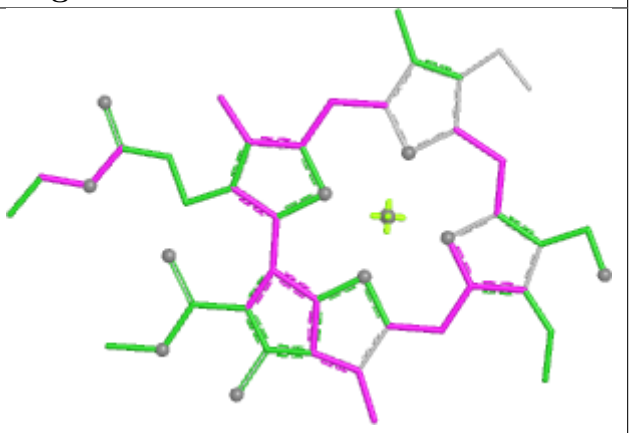

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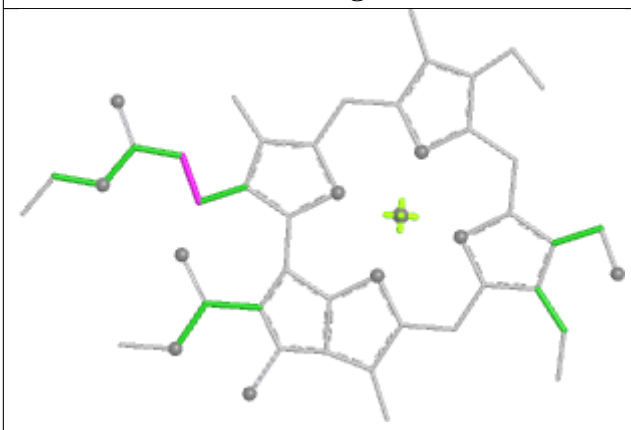
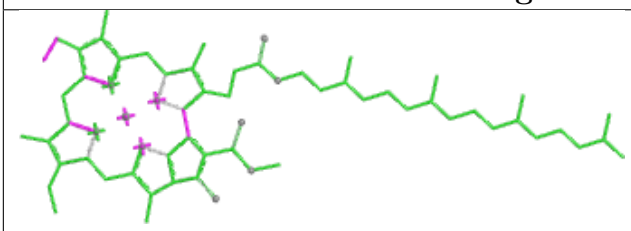


Torsions

Rings

Ligand CLA C1 511



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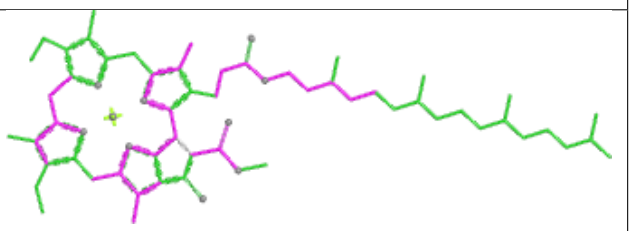

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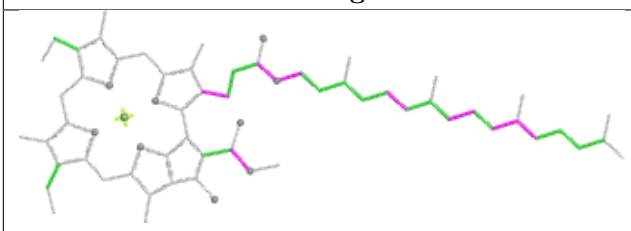

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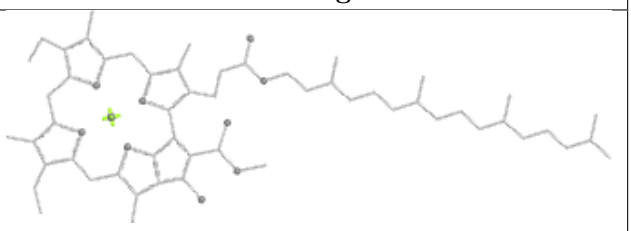
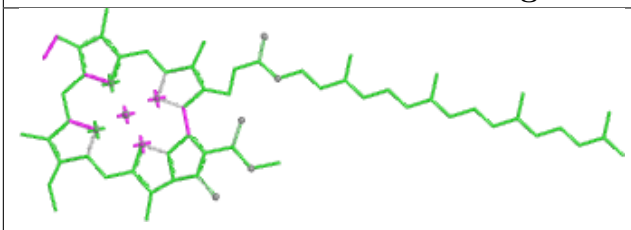


Rings

Ligand CLA c1 503



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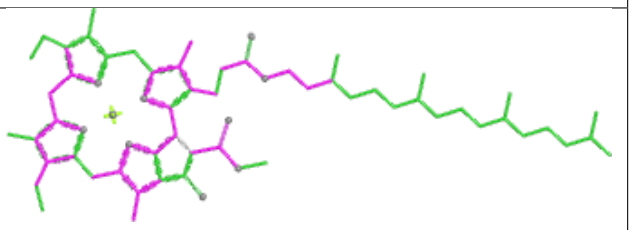
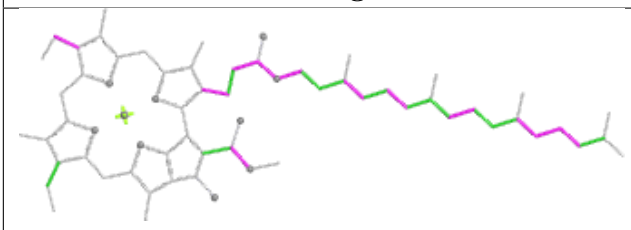


Bond angles



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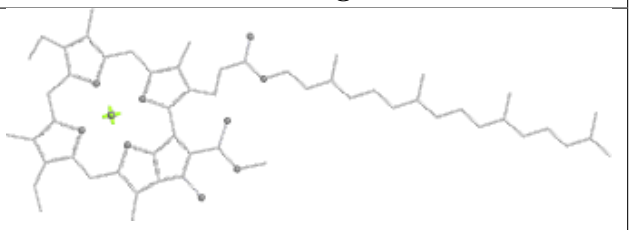
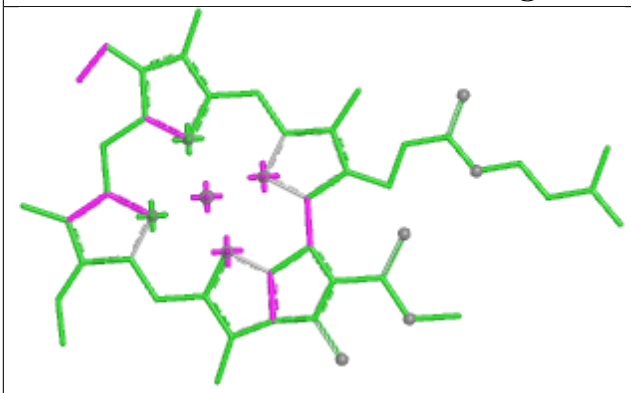


Rings

Ligand CLA y1 608



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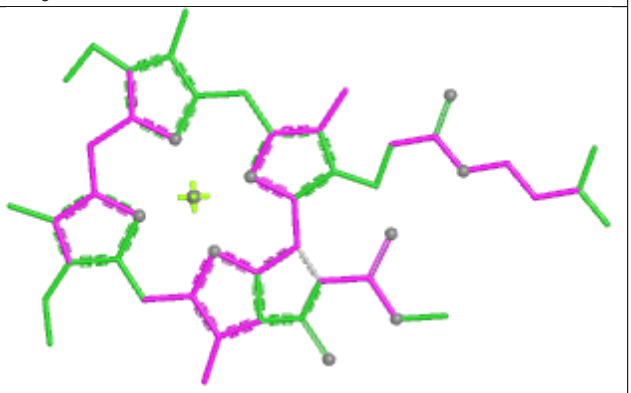

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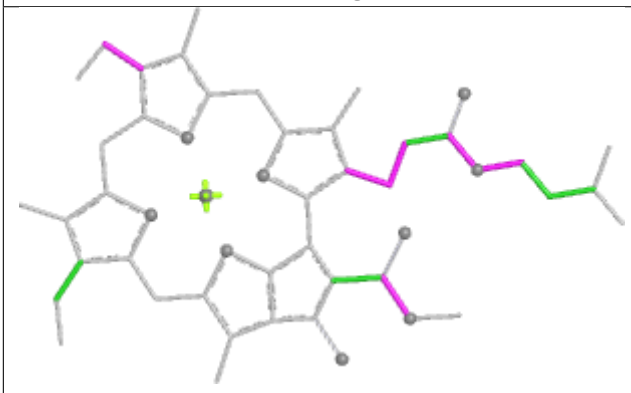

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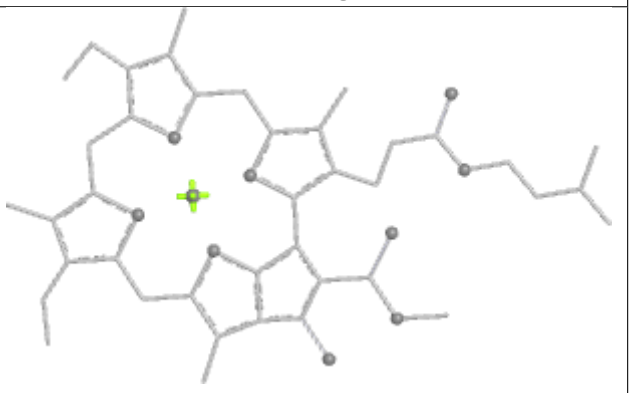
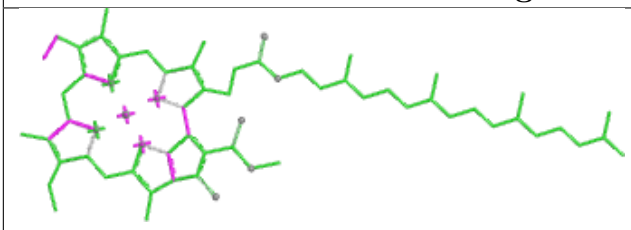
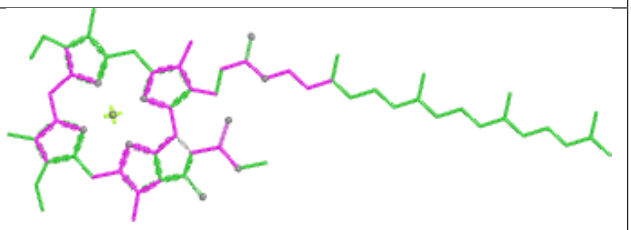
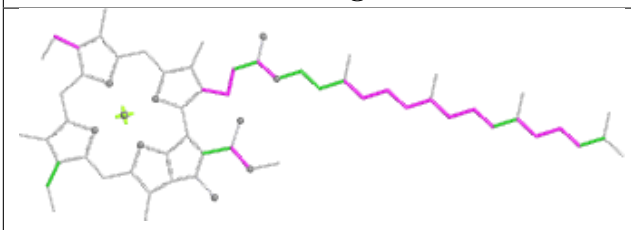
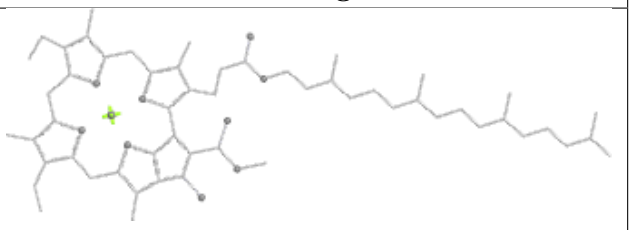
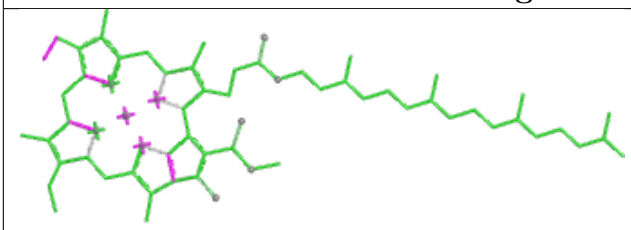
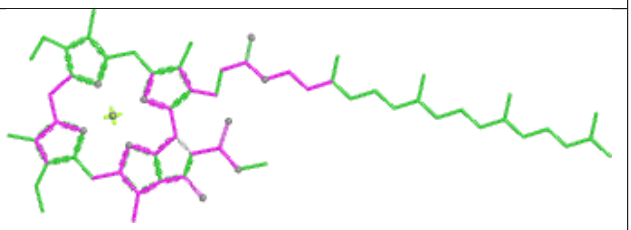


Rings

Ligand CLA B1 604	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA C1 510	
	
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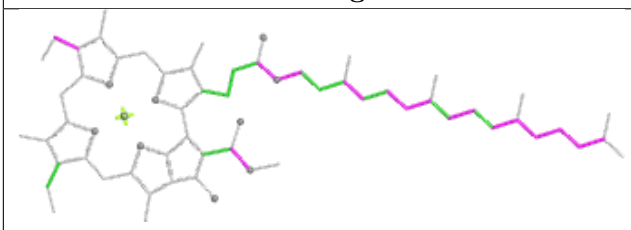	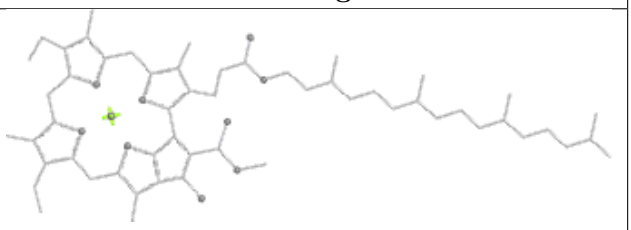
Torsions	Rings

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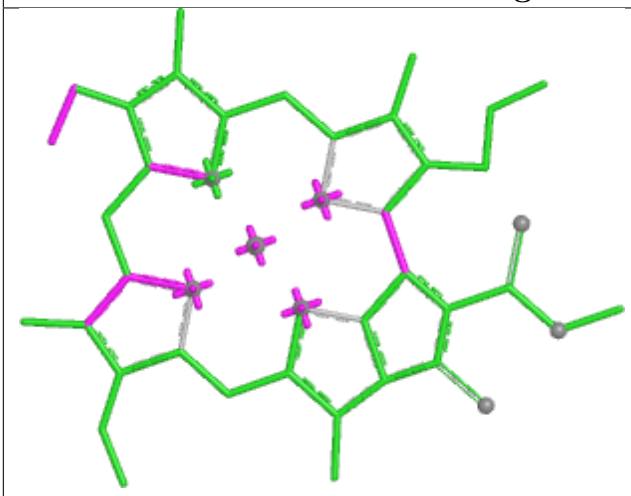
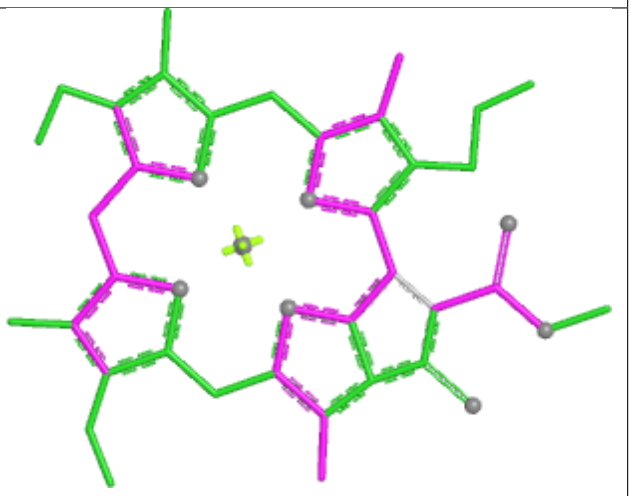
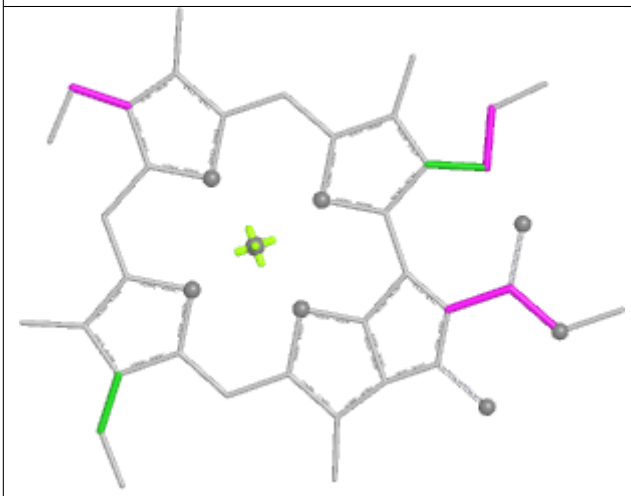
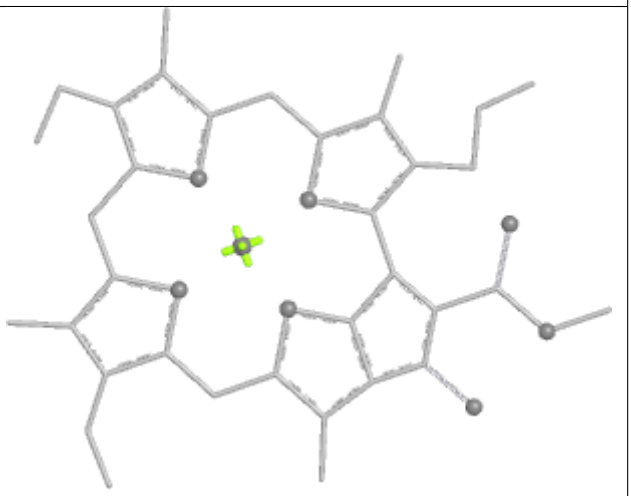
 Bond lengths	 Bond angles
 Torsions	 Rings

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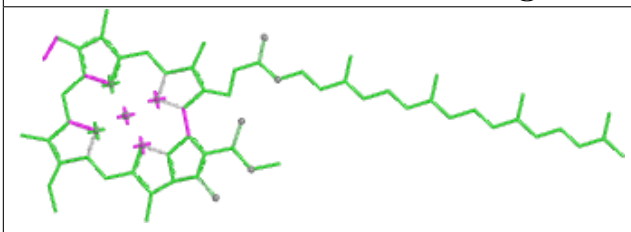
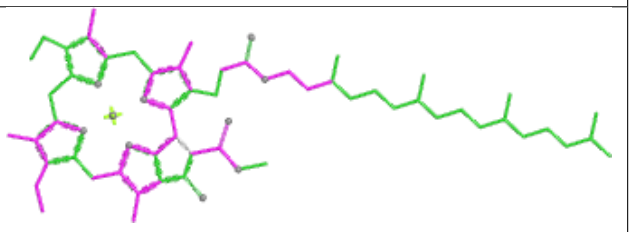
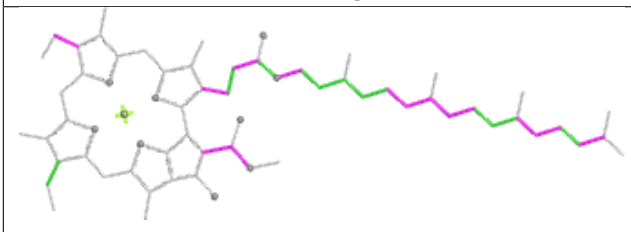
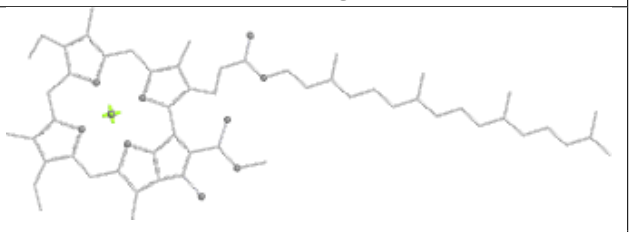
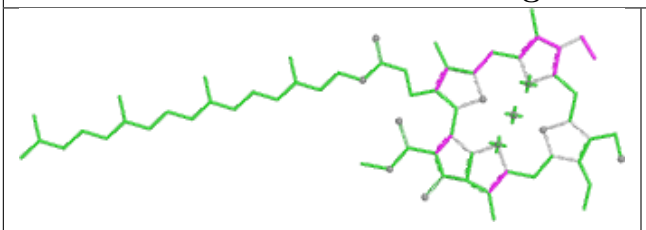
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CHL N 601



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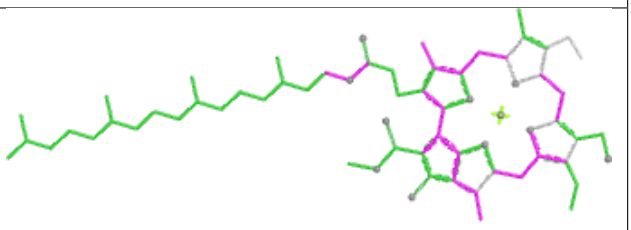

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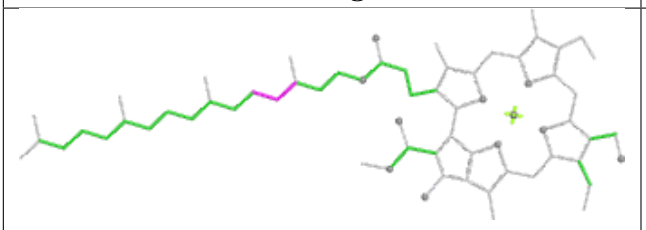

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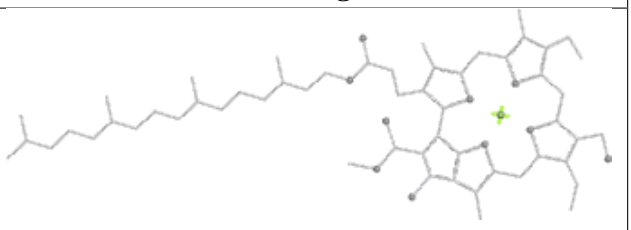
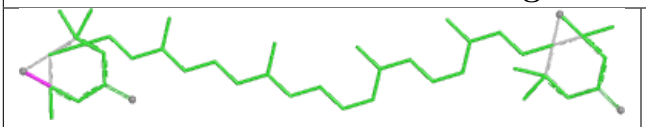


Rings

Ligand XAT Y 622



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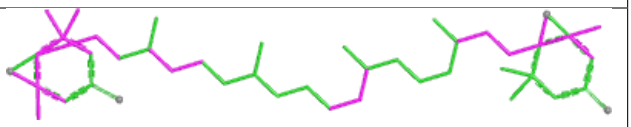

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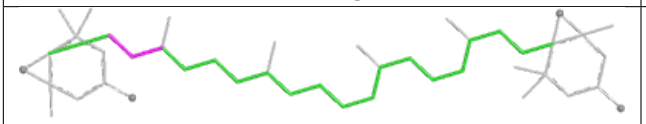

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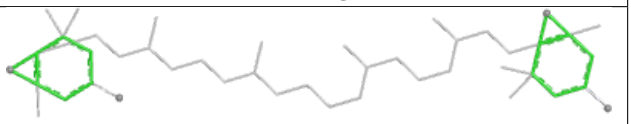
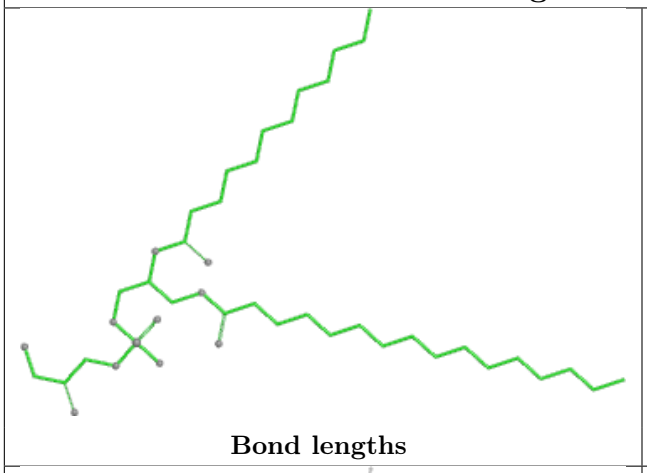


Rings

Ligand LHG s 624



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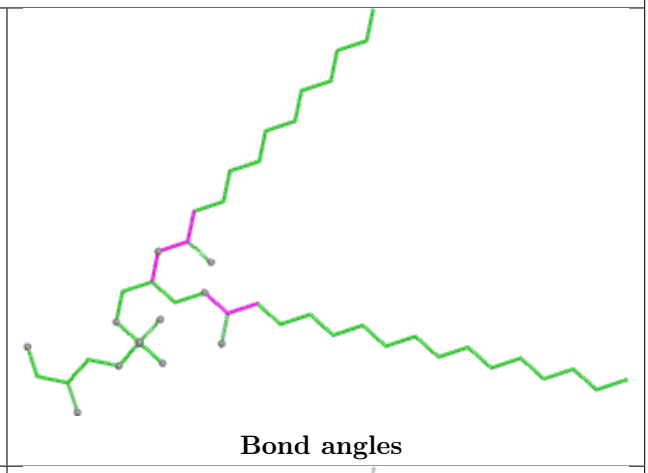

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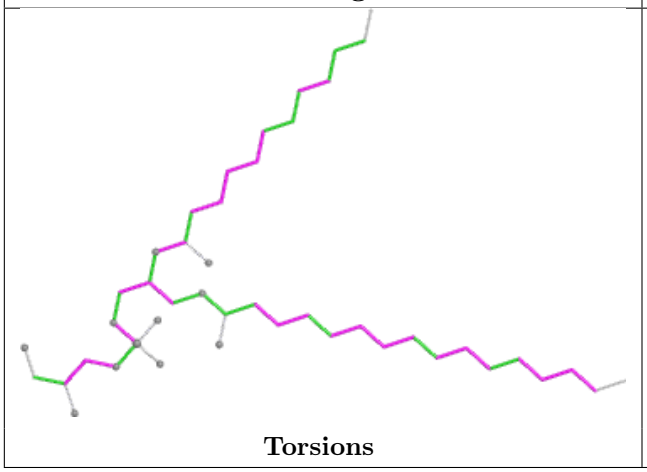

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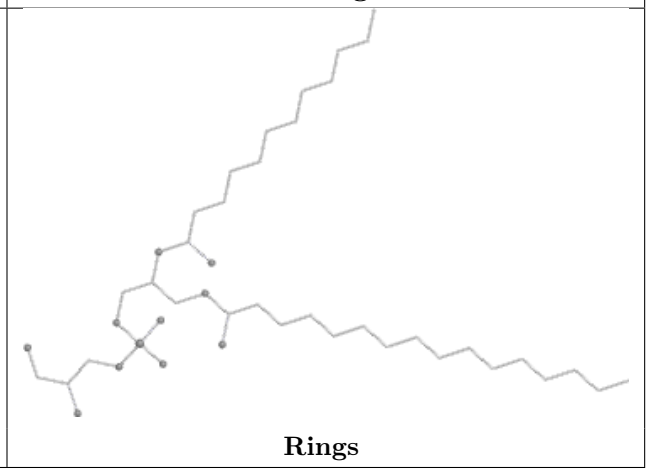
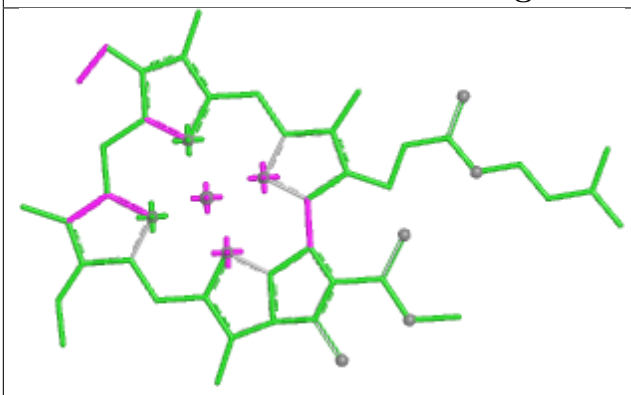


Rings

Ligand CLA A1 407



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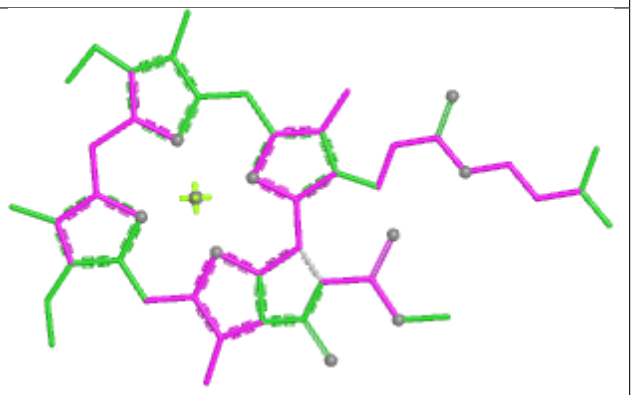

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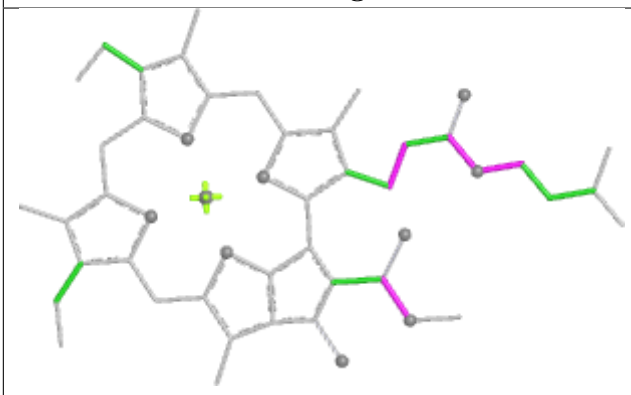

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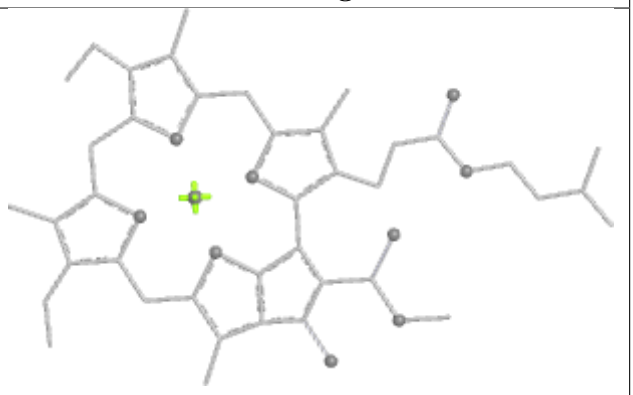
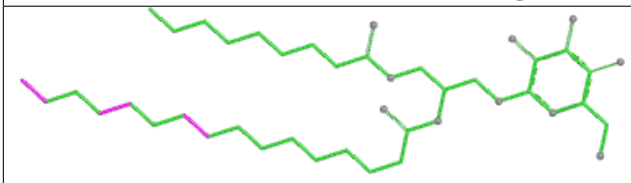


Rings

Ligand LMG B1 622



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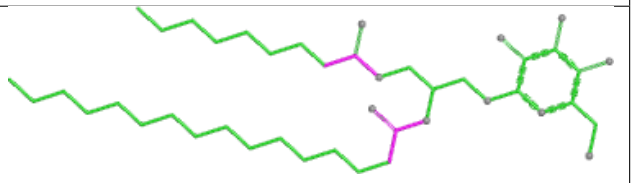

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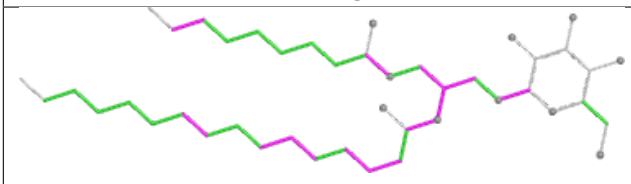

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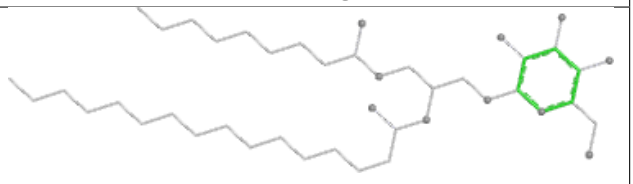
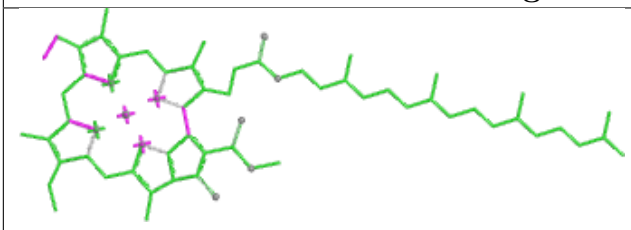
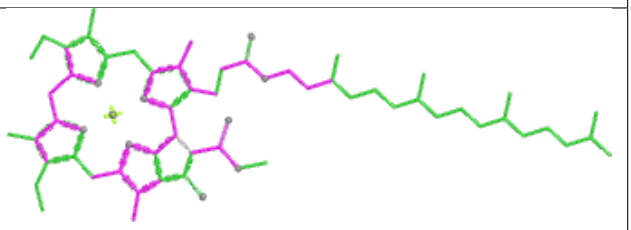
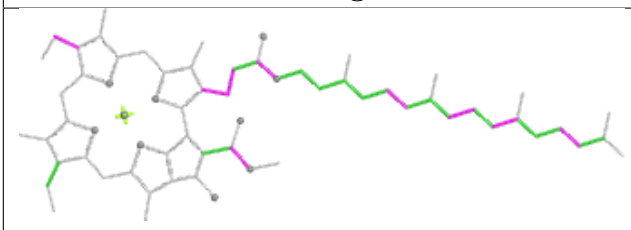
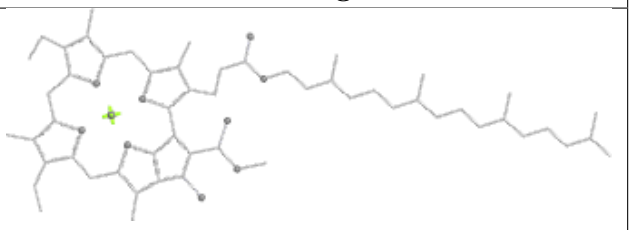


Rings

Ligand CLA G 610	
 Bond lengths	 Bond angles
 Torsions	 Rings

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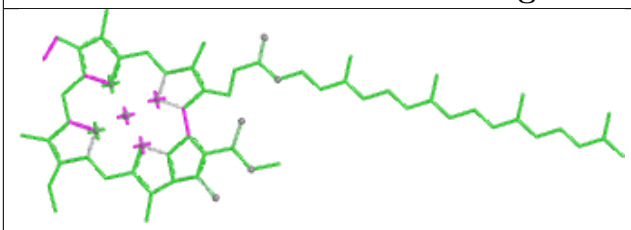
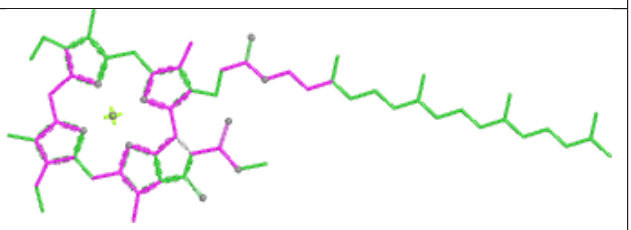
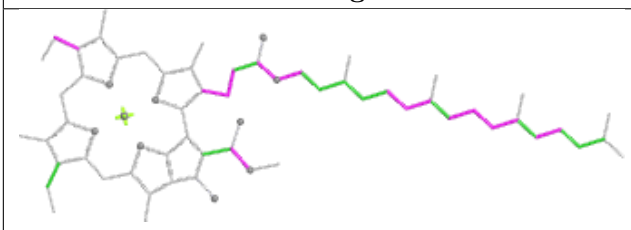
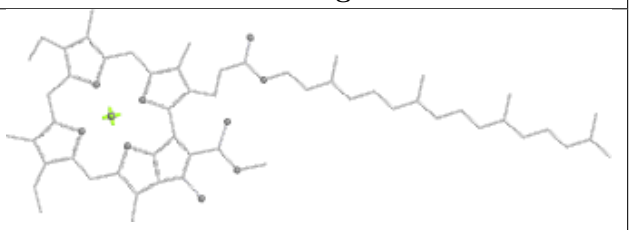
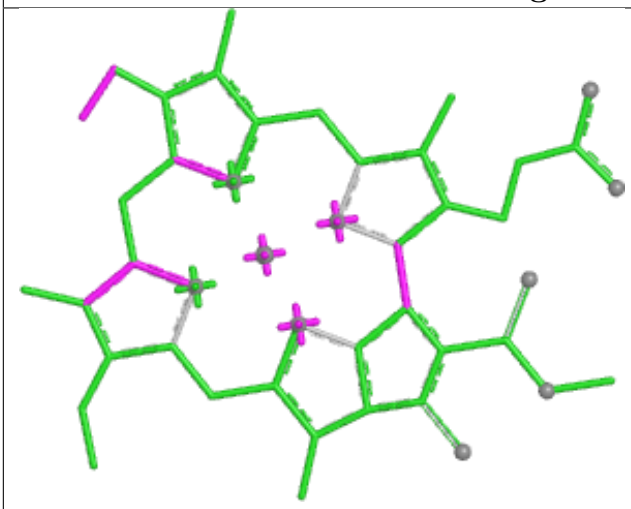
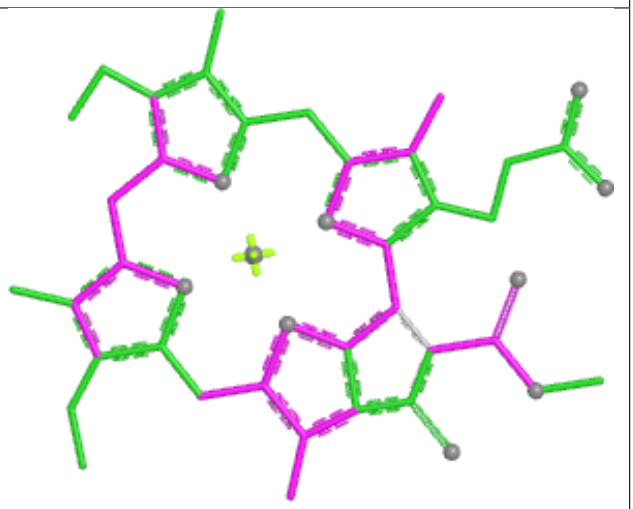
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand CLA s 612



Bond lengths



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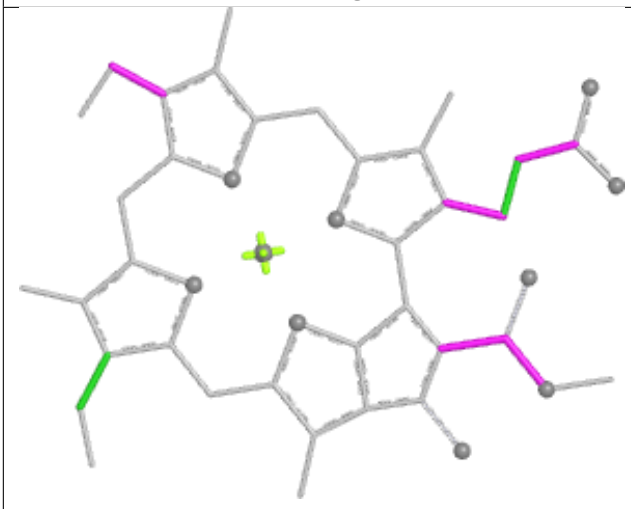
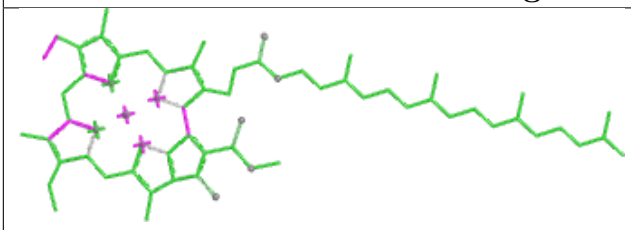


Torsions

Rings

Ligand CLA N 610



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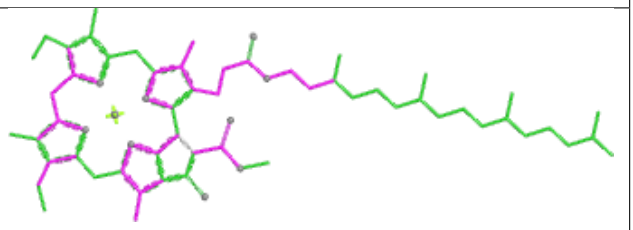

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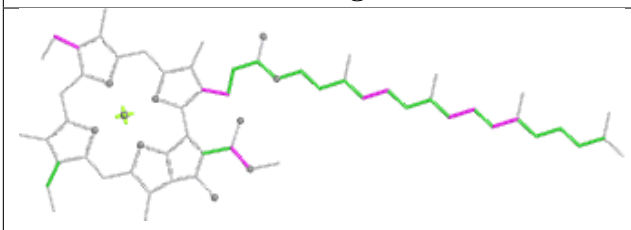
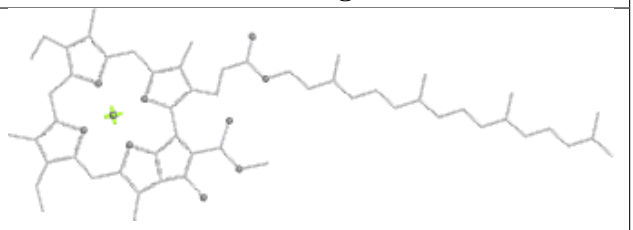
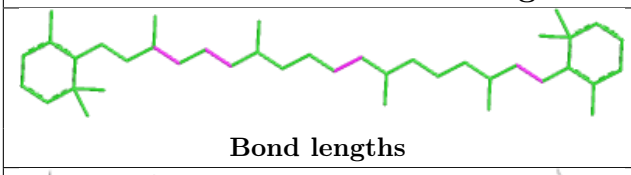


Torsions



Rings

Ligand BCR c1 514



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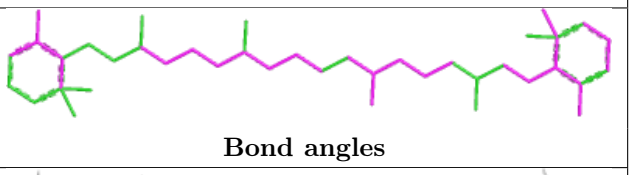
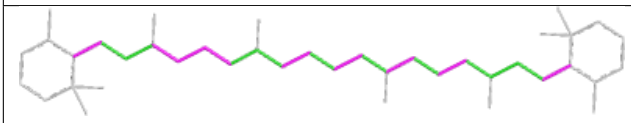


Bond angles



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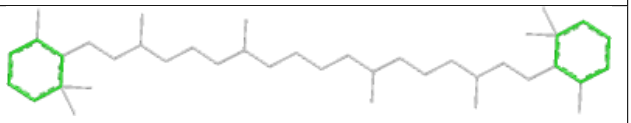
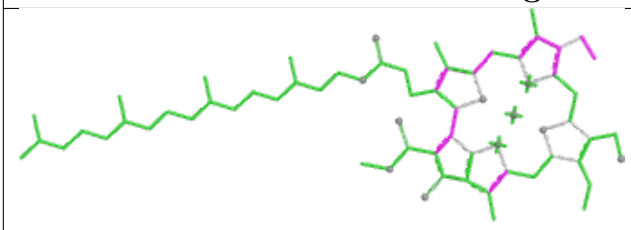
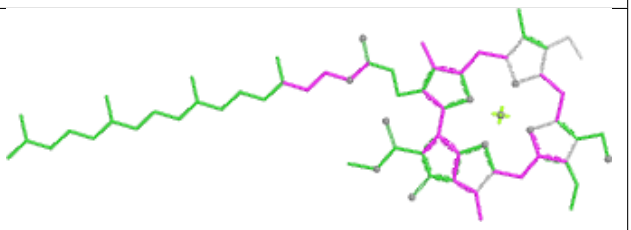


Rings

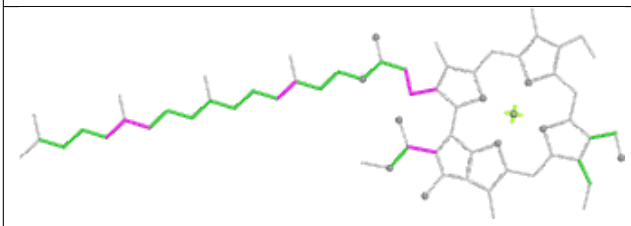
Ligand CHL Y 609



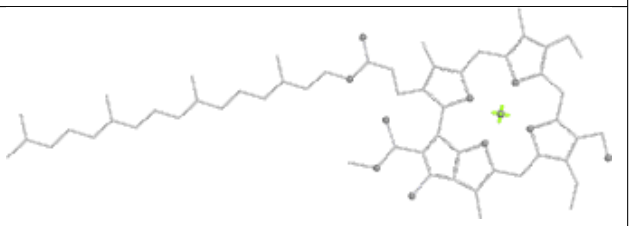
Bond lengths



Bond angles

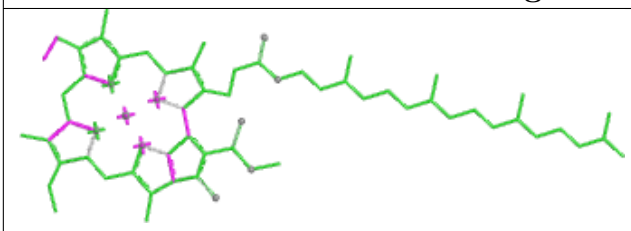


Torsions



Rings

Ligand CLA B 606



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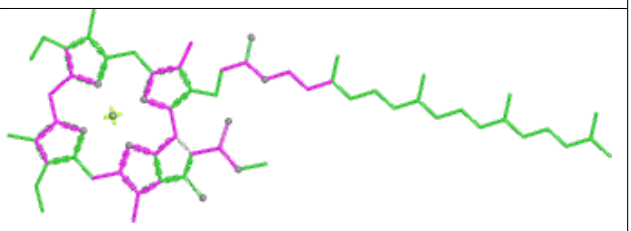
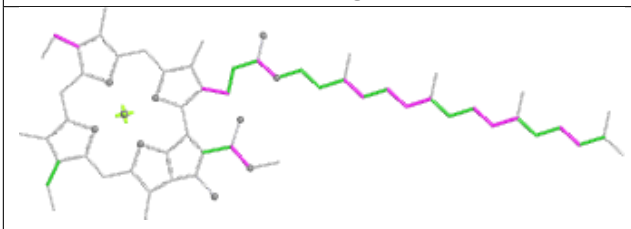


Bond angles



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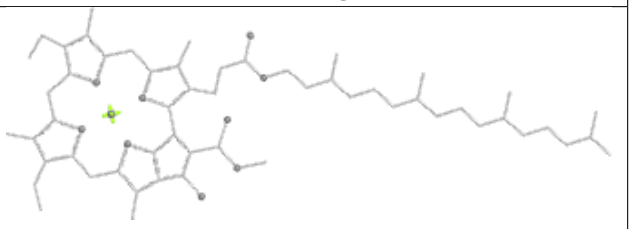
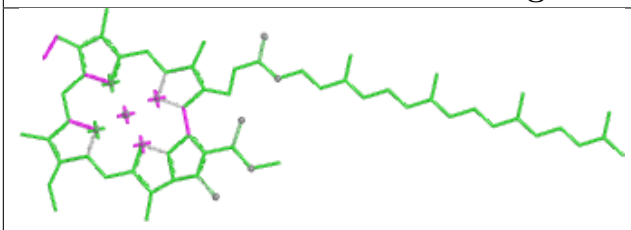


Rings

Ligand CLA b 616



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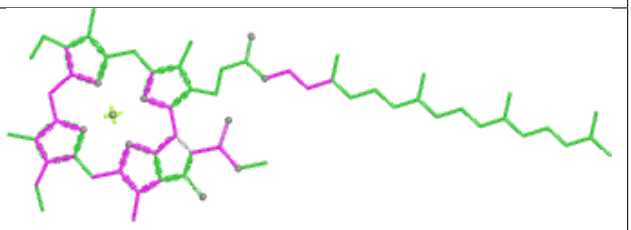
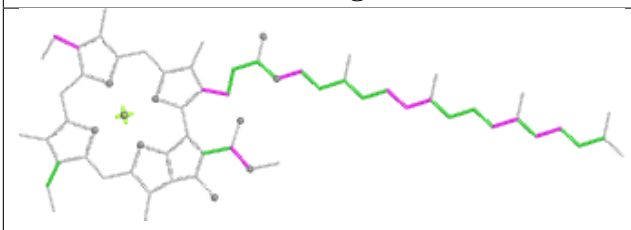


Bond angles



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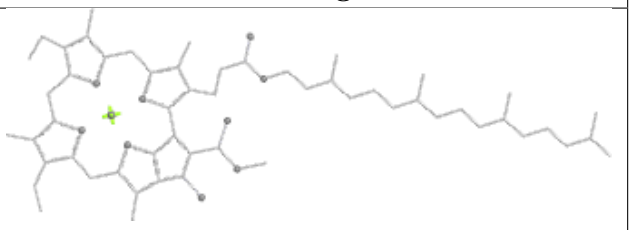
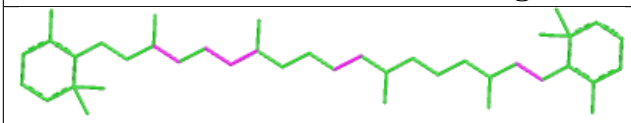


Rings

Ligand BCR C1 516



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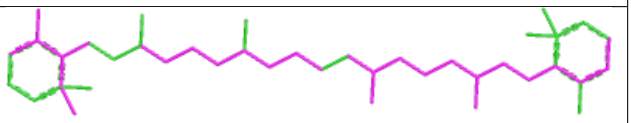
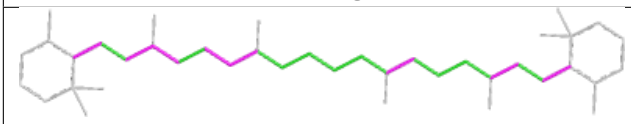


Bond angles



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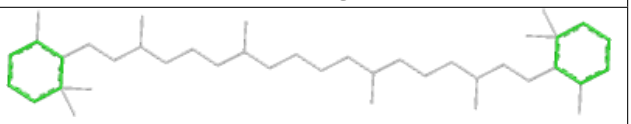
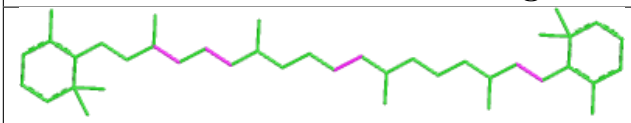


Rings

Ligand BCR C 514



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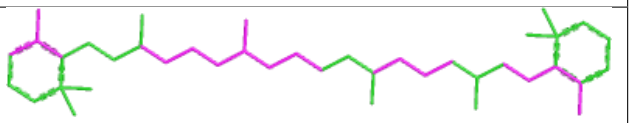
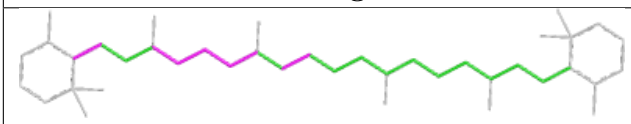


Bond angles



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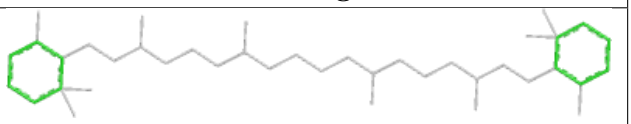
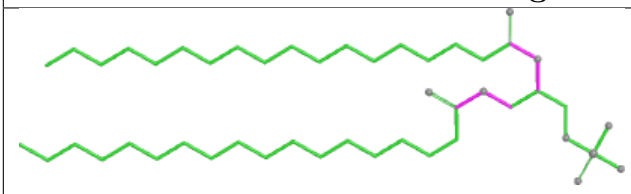


Rings

Ligand 3PH S 626



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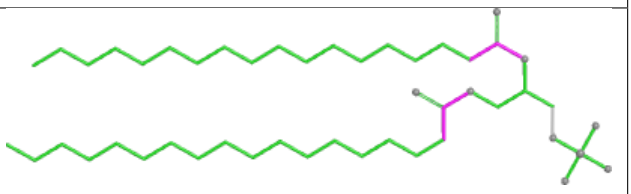
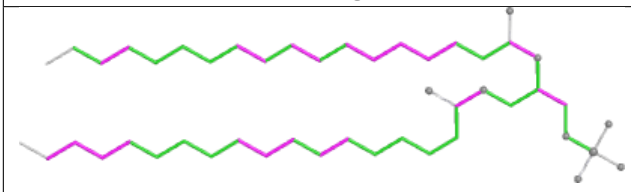


Bond angles



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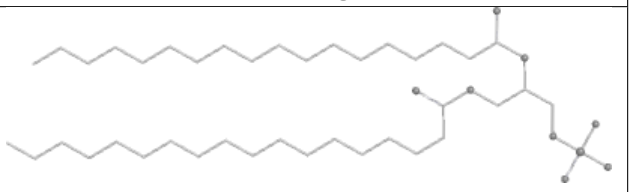
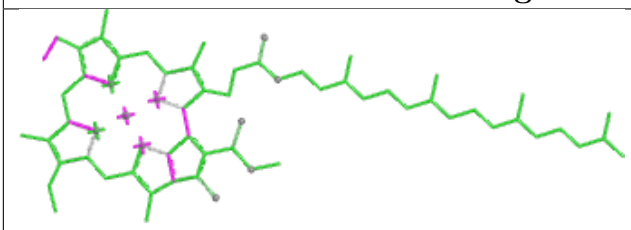


Rings

Ligand CLA N1 604



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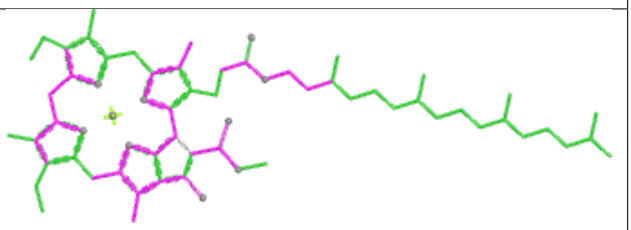
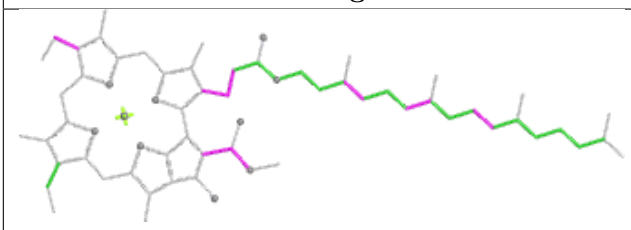


Bond angles



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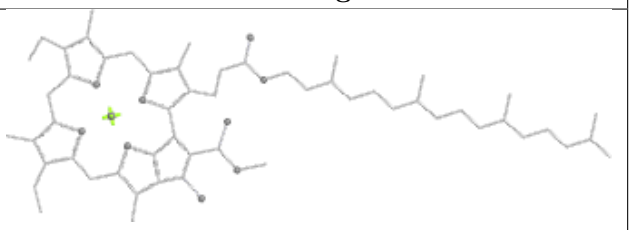
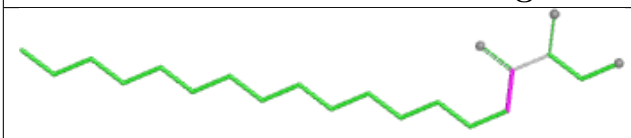


Rings

Ligand SPH A1 414



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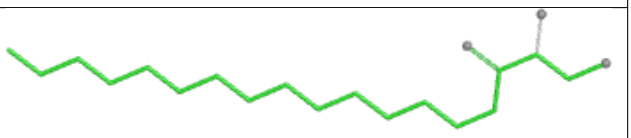

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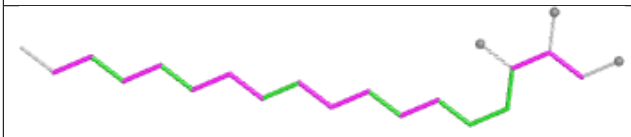

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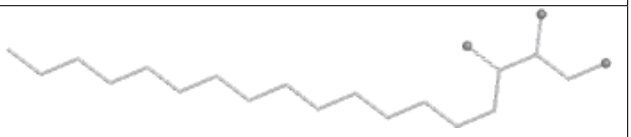
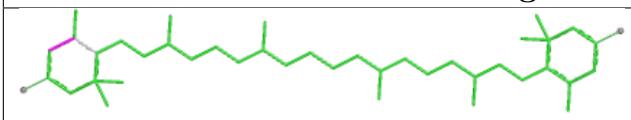


Rings

Ligand LUT y1 621



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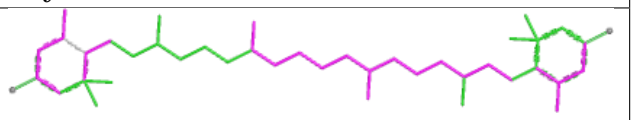
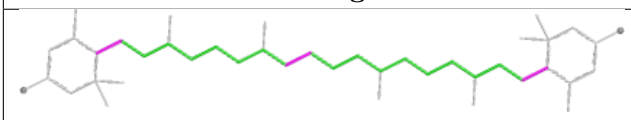
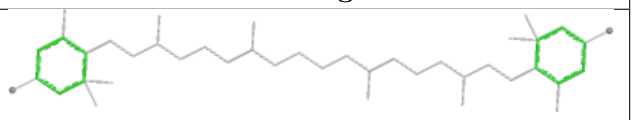


Bond angles

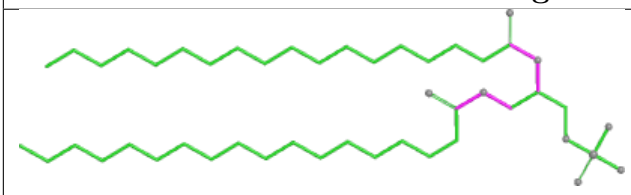


Torsions



Rings

Ligand 3PH s 626



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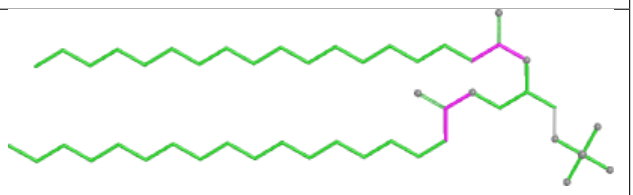
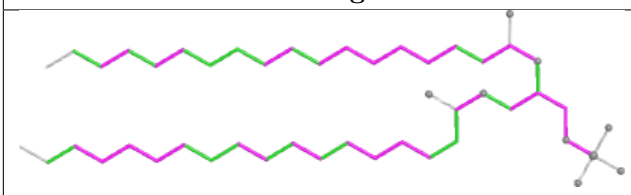


Bond angles



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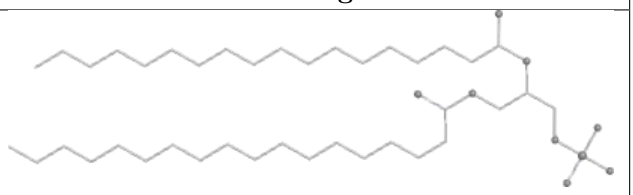
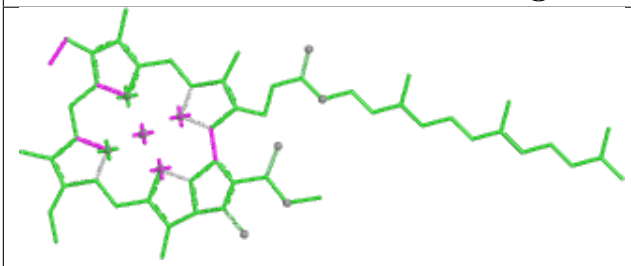


Rings

Ligand CLA s 602



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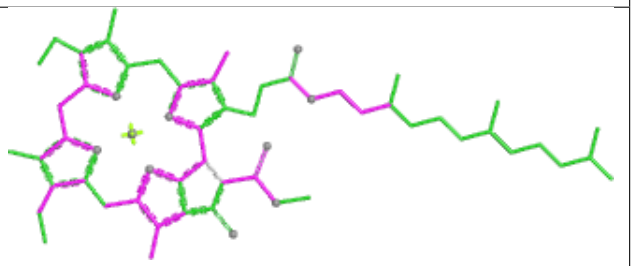
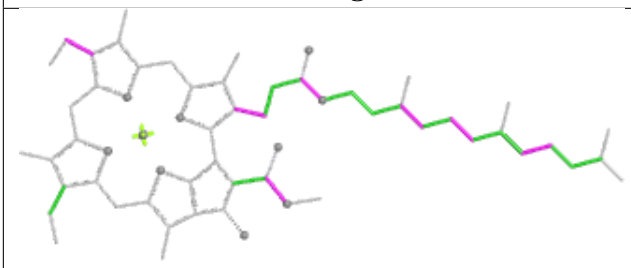


Bond angles



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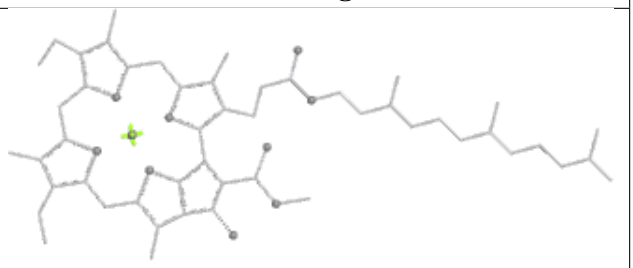
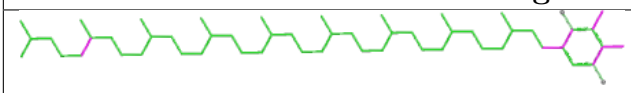


Rings

Ligand PL9 d 405



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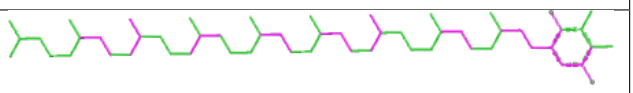
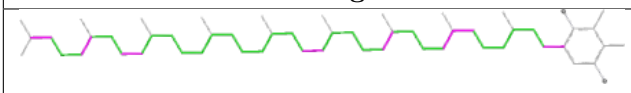


Bond angles



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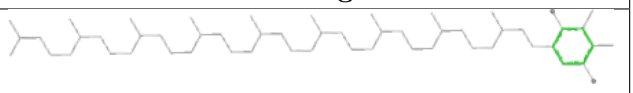
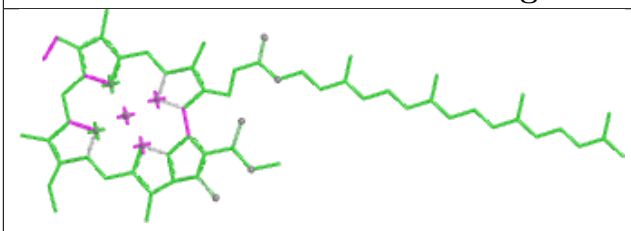


Rings

Ligand CLA c1 509



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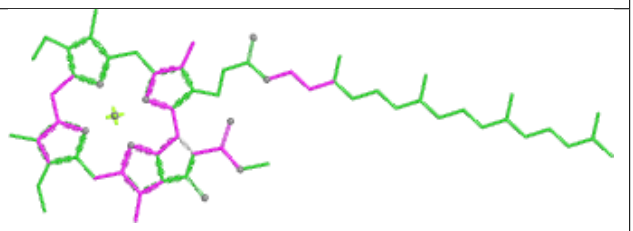
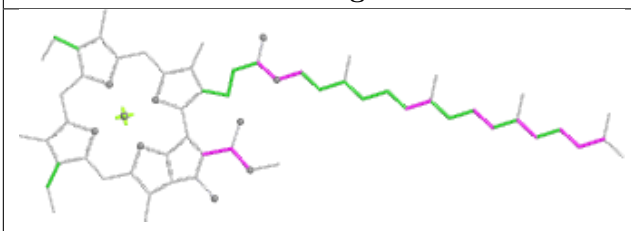


Bond angles



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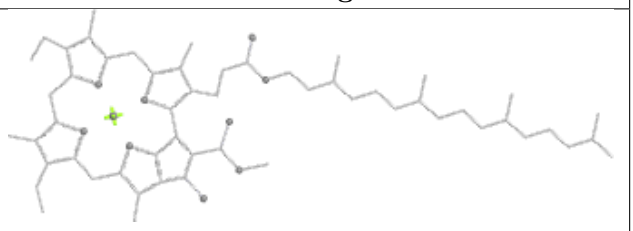
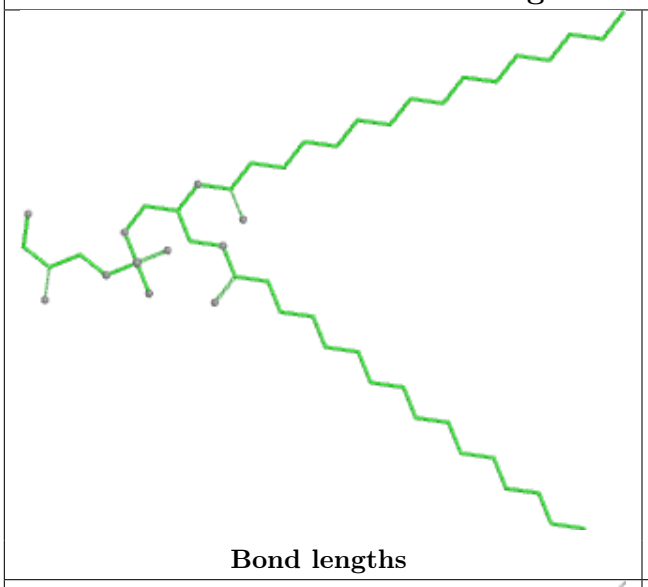


Rings

Ligand LHG y 624



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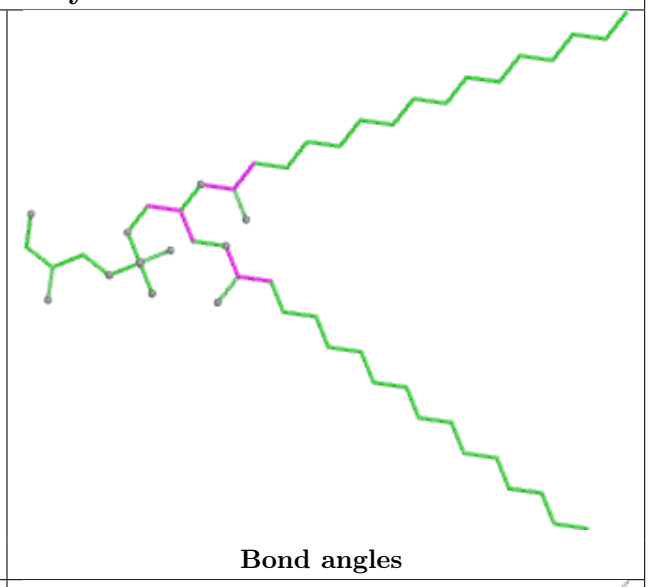
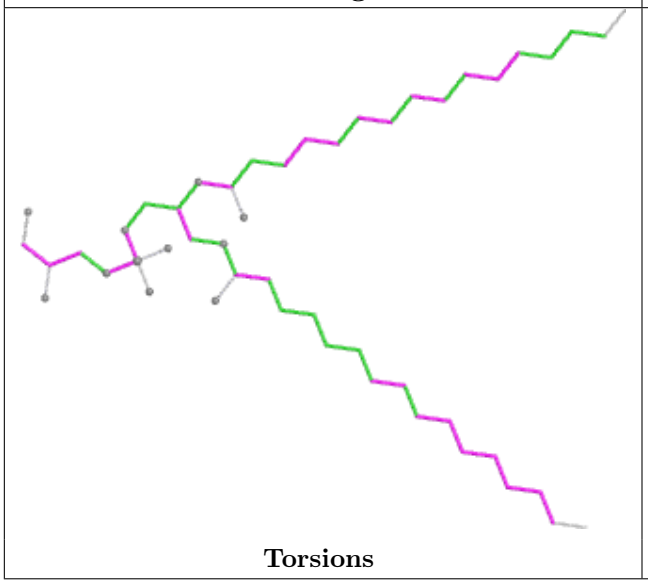
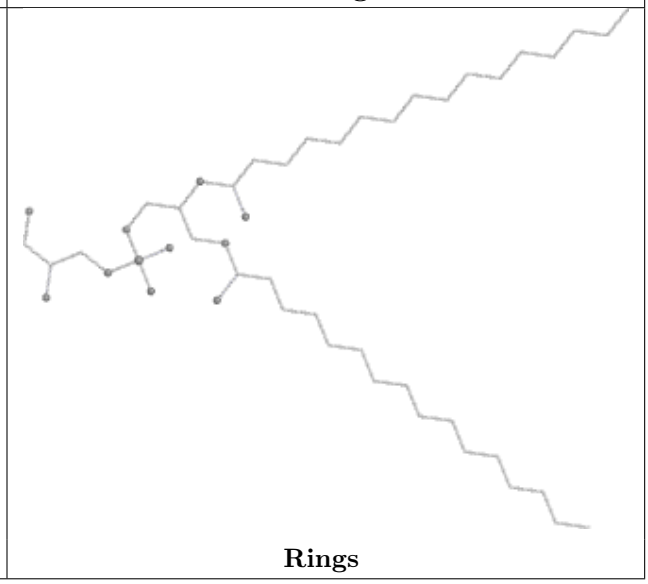


Bond angles

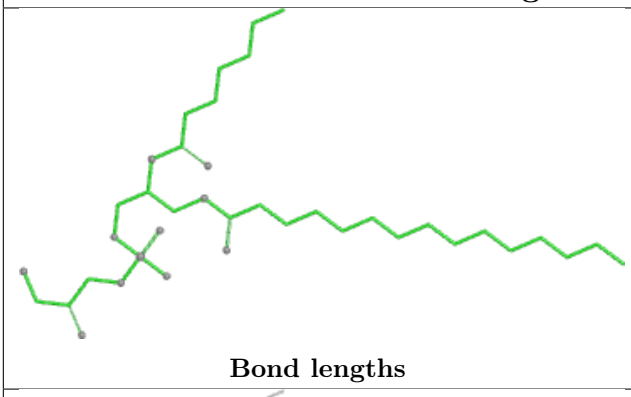


Torsions

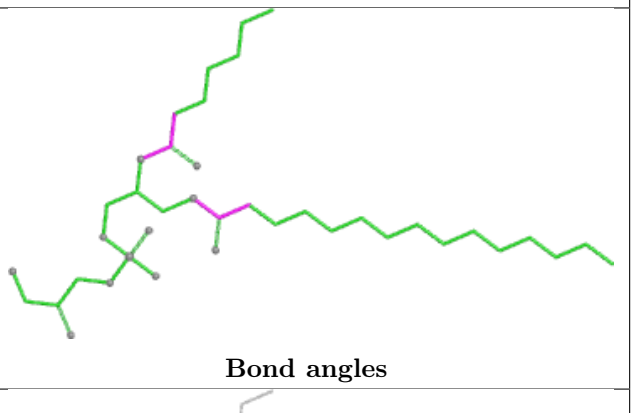


Rings

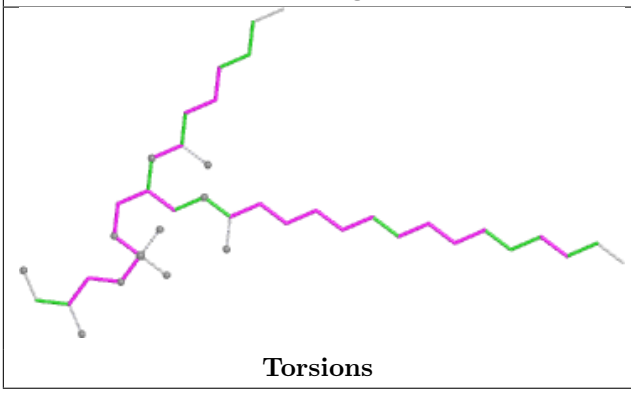
Ligand LHG D 410



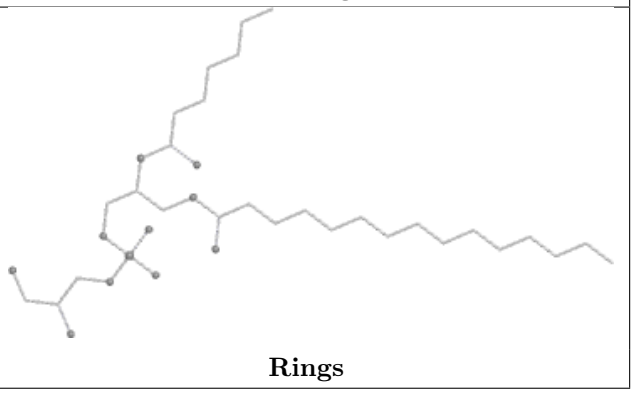
Bond lengths



Bond angles

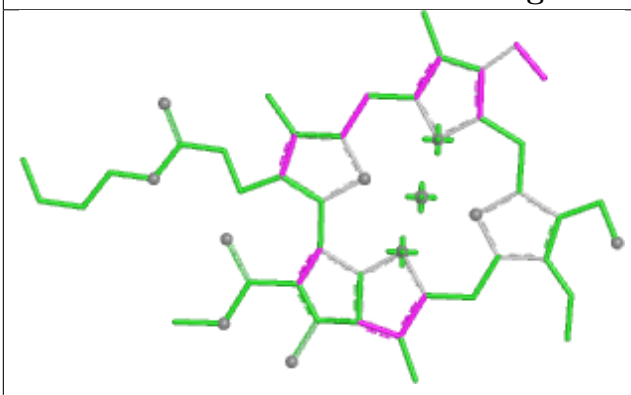


Torsions



Rings

Ligand CHL n 608



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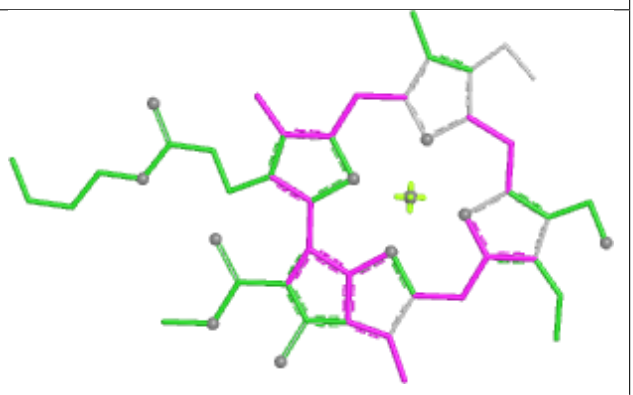

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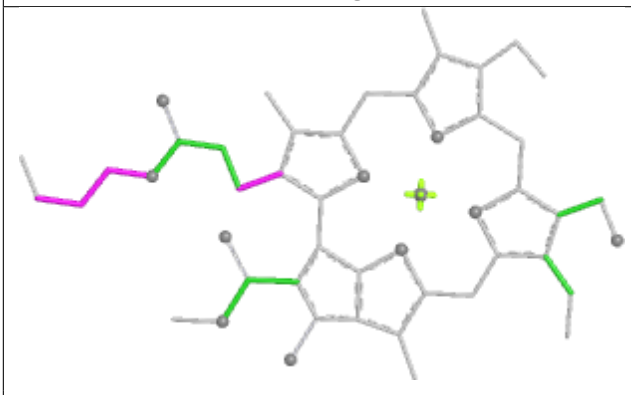

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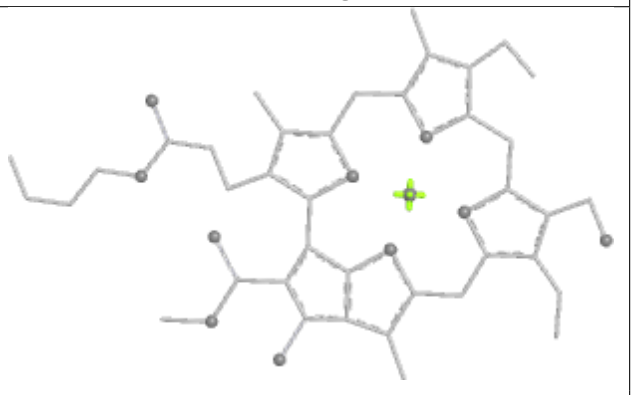
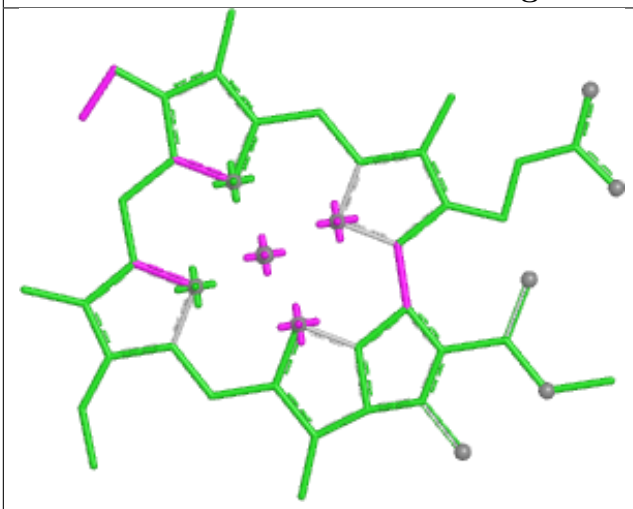


Rings

Ligand CLA s1 612



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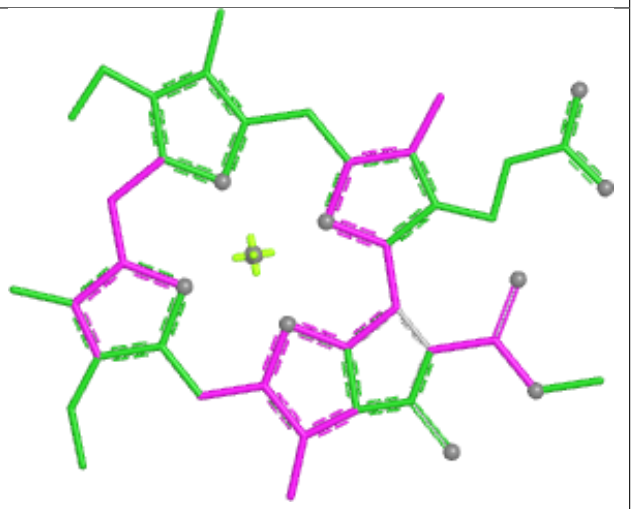

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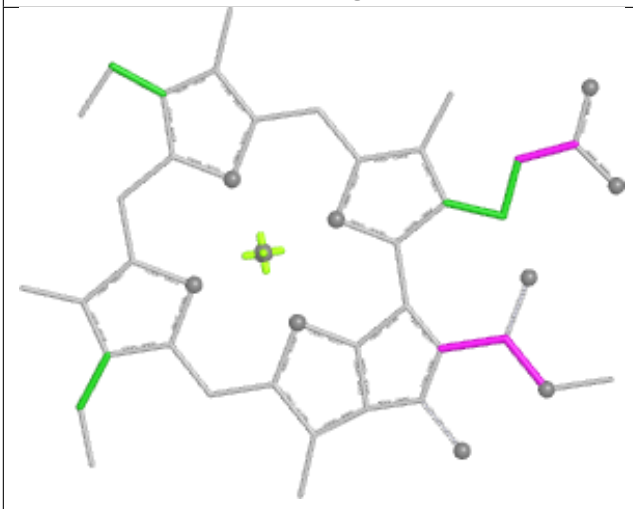
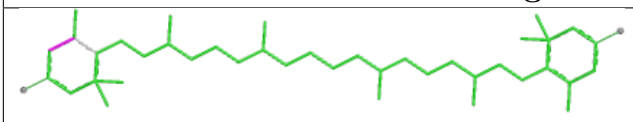


Torsions

Rings

Ligand LUT Y 621



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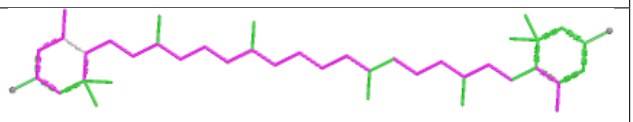

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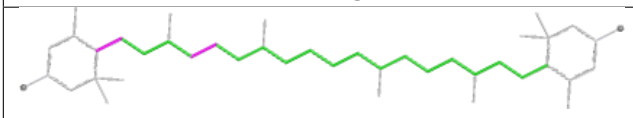
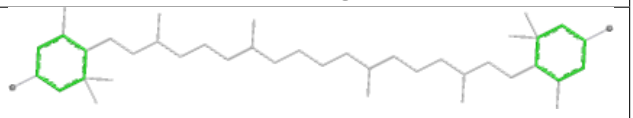
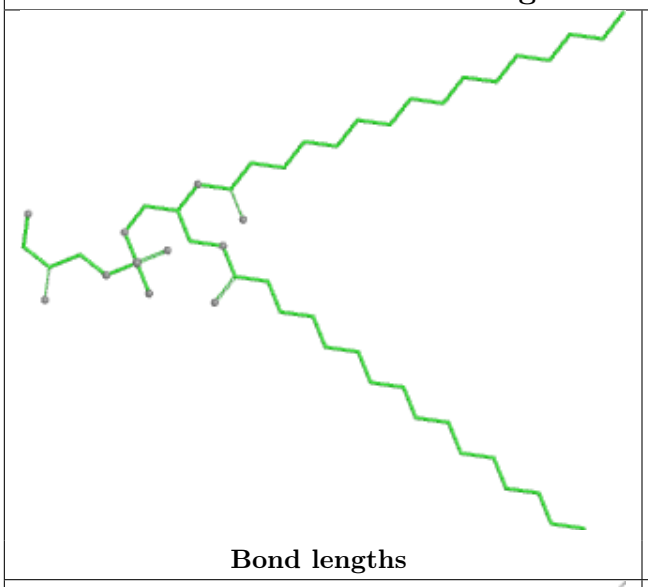


Torsions



Rings

Ligand LHG g1 624



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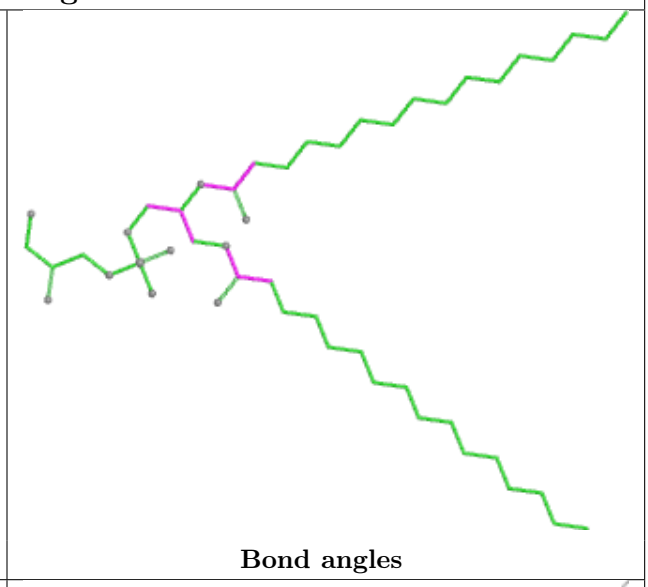
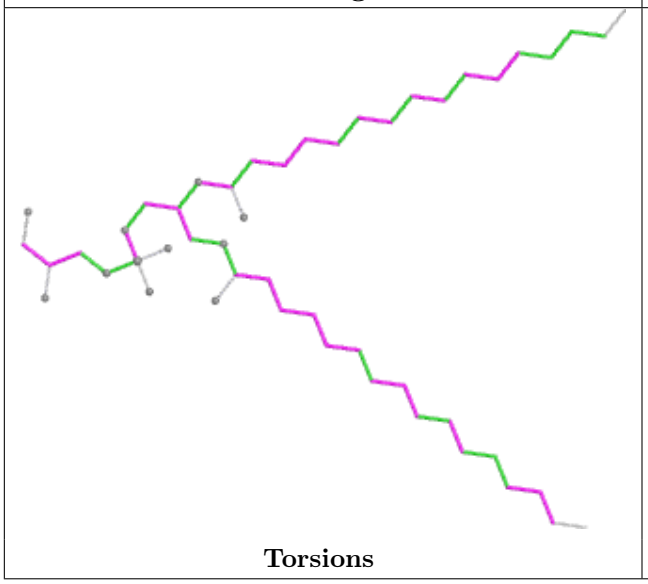


Bond angles



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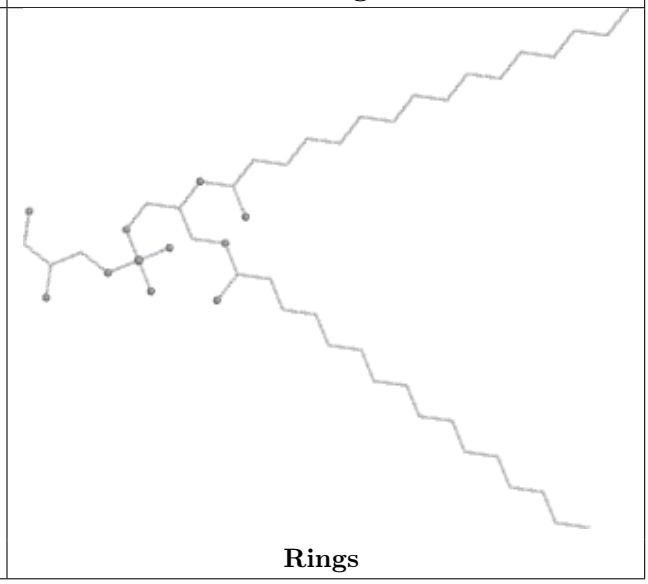
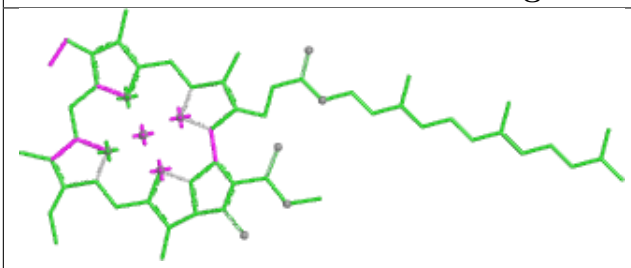


Rings

Ligand CLA R 602



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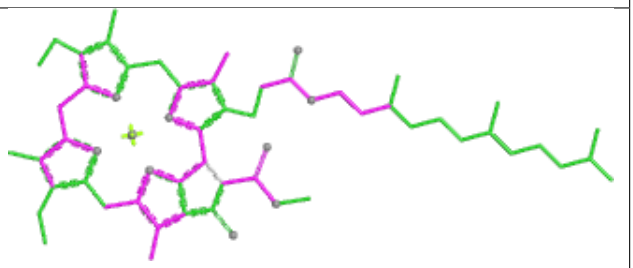
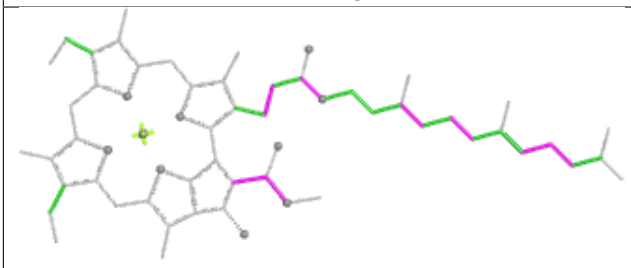


Bond angles



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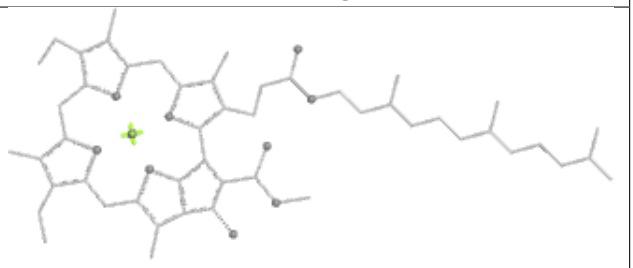
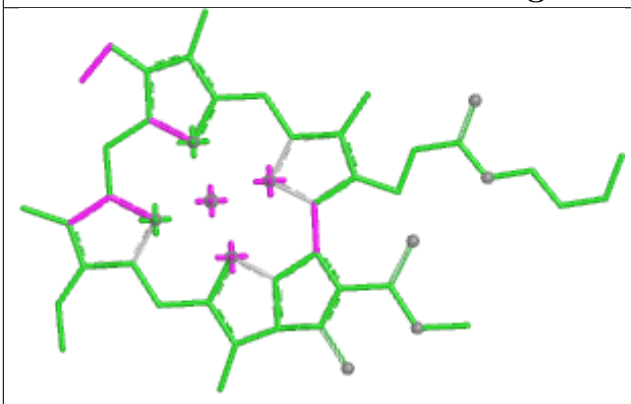


Rings

Ligand CLA n 614



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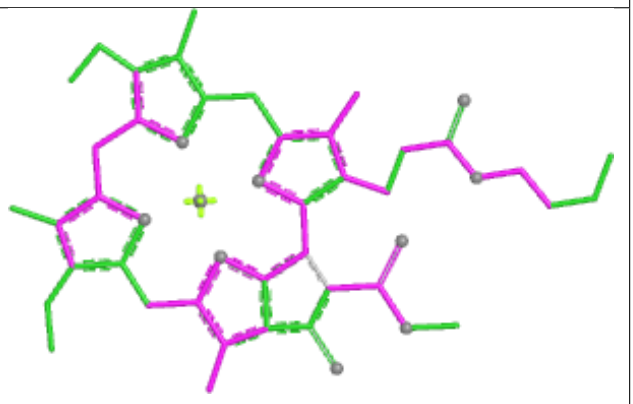
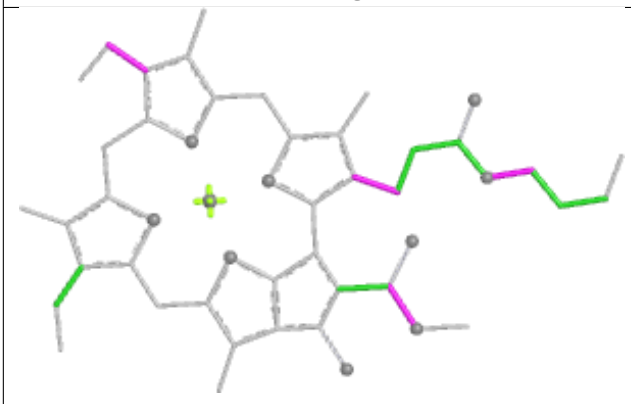


Bond angles



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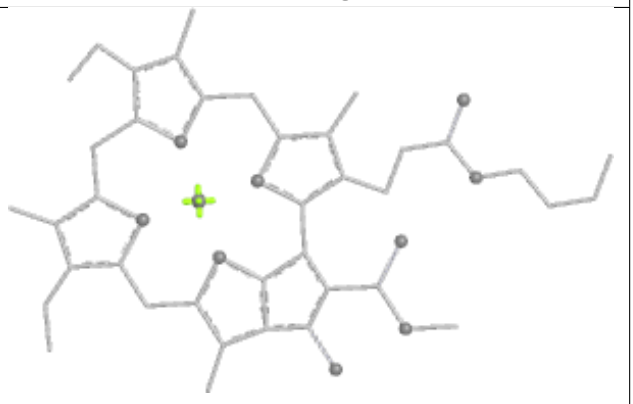
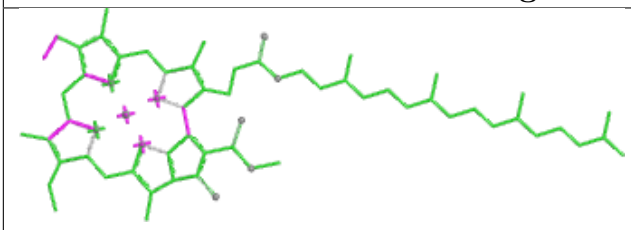


Rings

Ligand CLA g1 613



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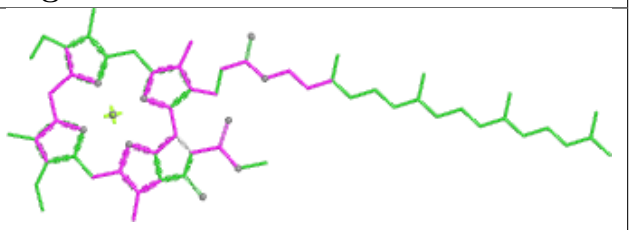
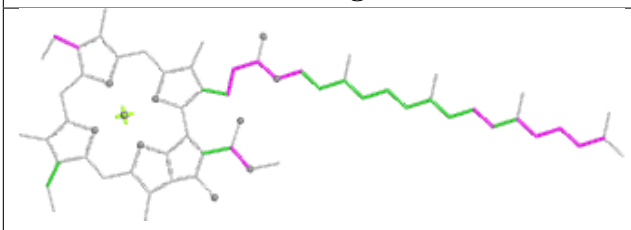


Bond angles



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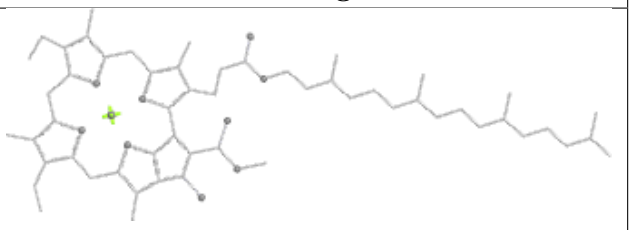
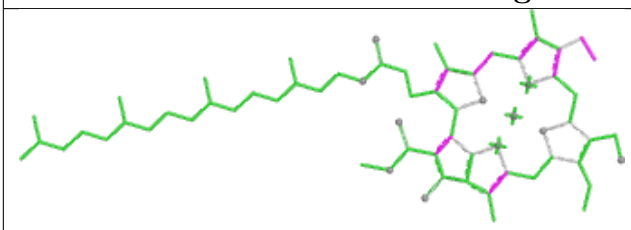


Rings

Ligand CHL N1 607



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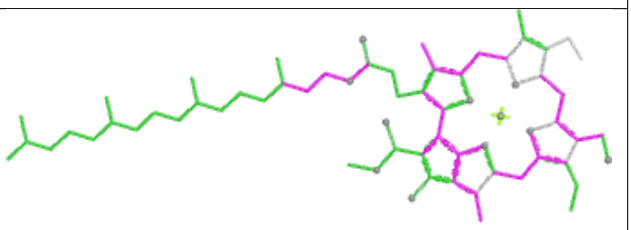
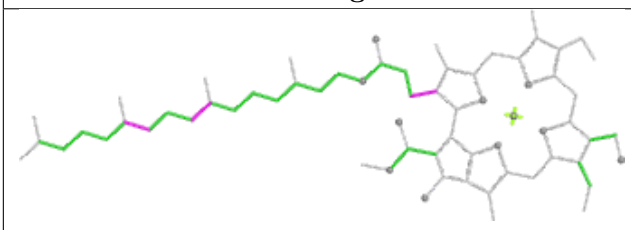
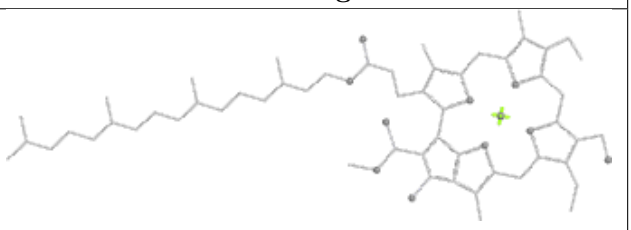


Bond angles

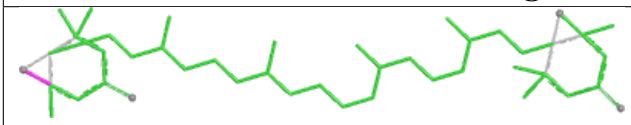


Torsions



Rings

Ligand XAT R 621



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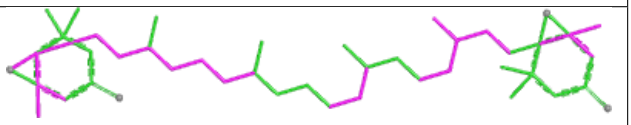
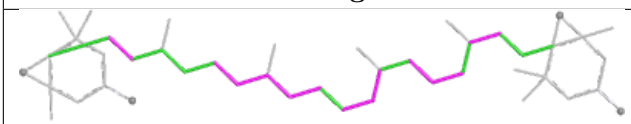


Bond angles



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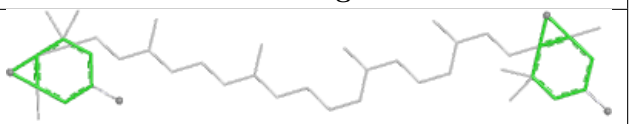
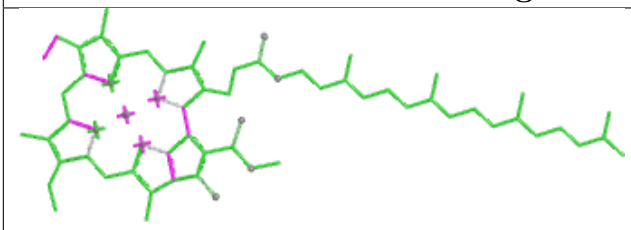


Rings

Ligand CLA C1 503



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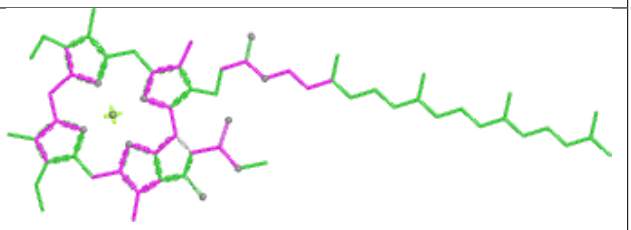
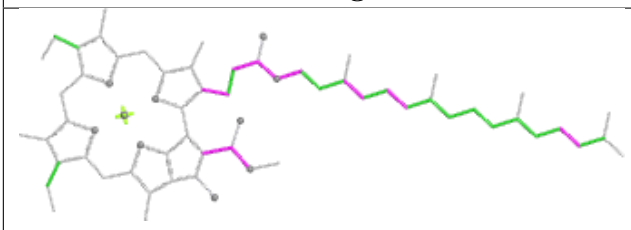


Bond angles



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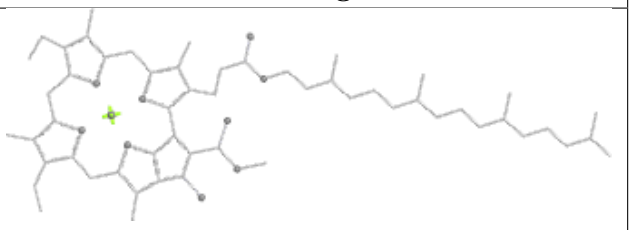
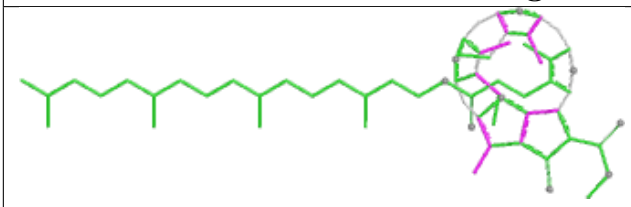


Rings

Ligand PHO a 409



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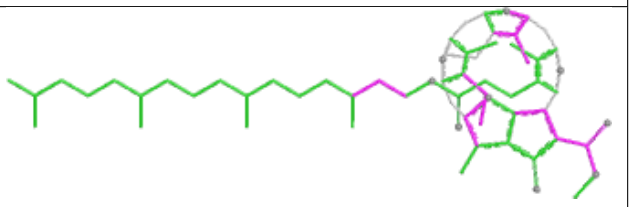
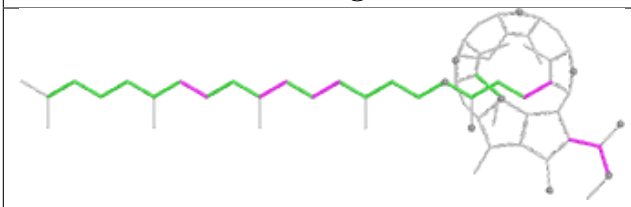
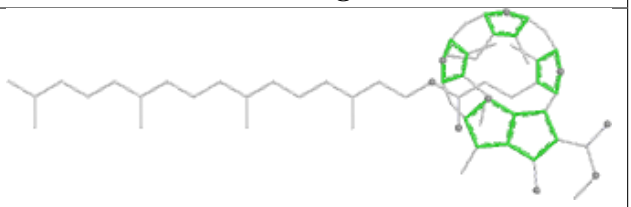


Bond angles

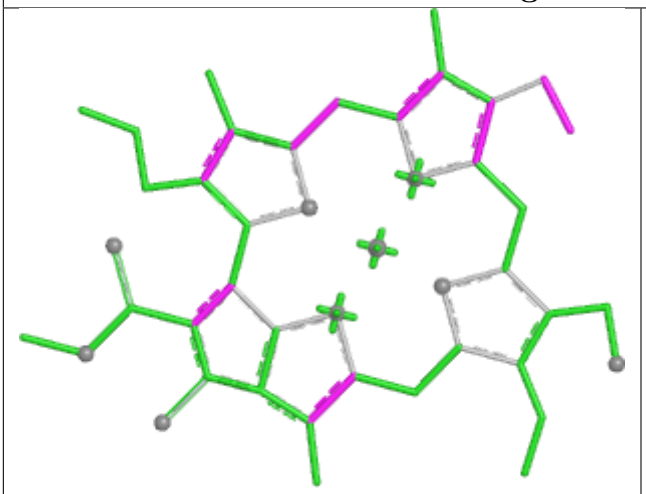


Torsions



Rings

Ligand CHL s1 606



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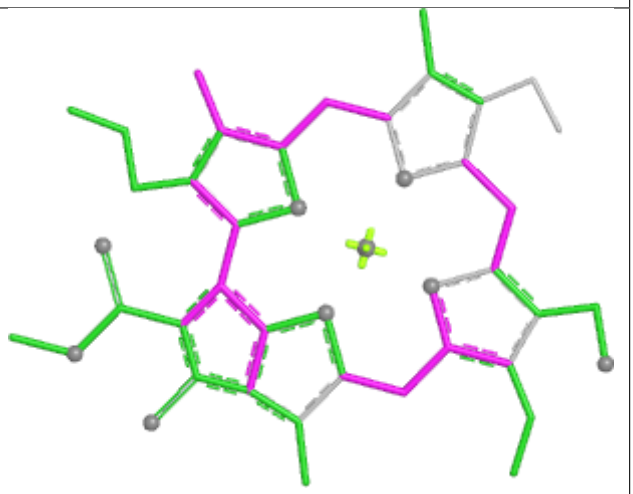
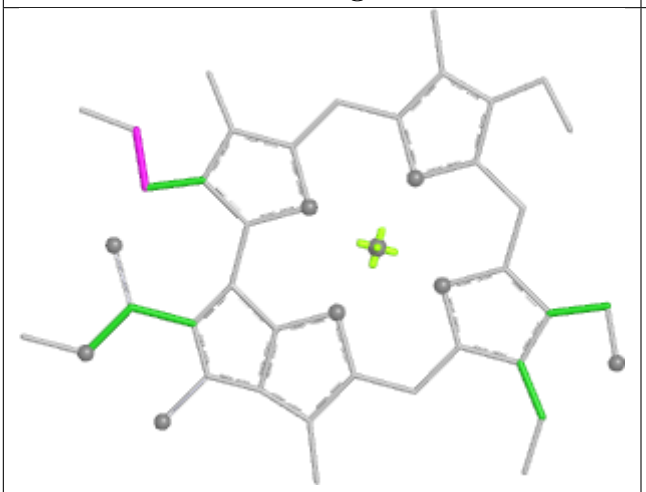


Bond angles



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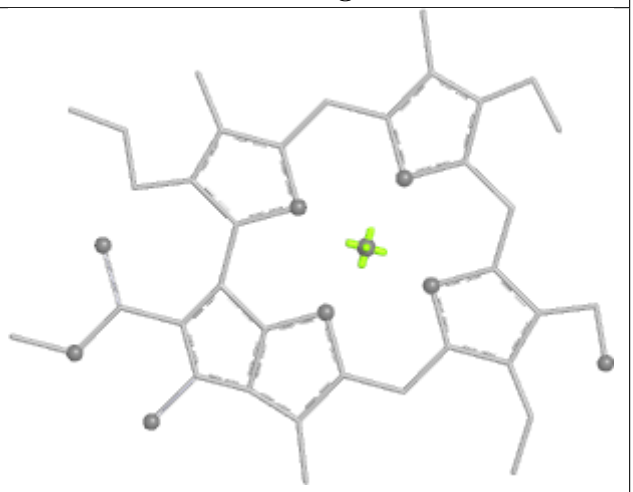
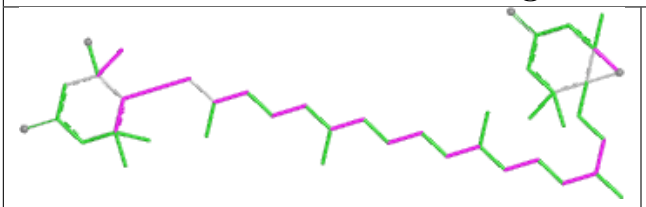


Rings

Ligand NEX R 622



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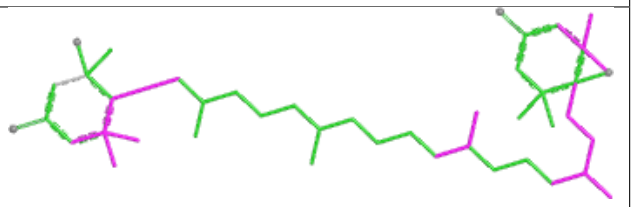
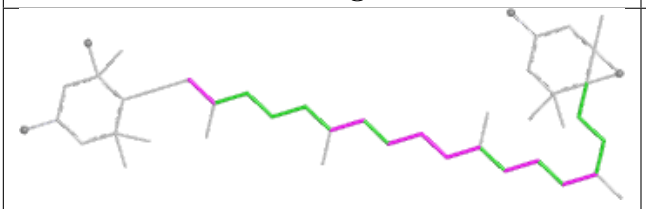


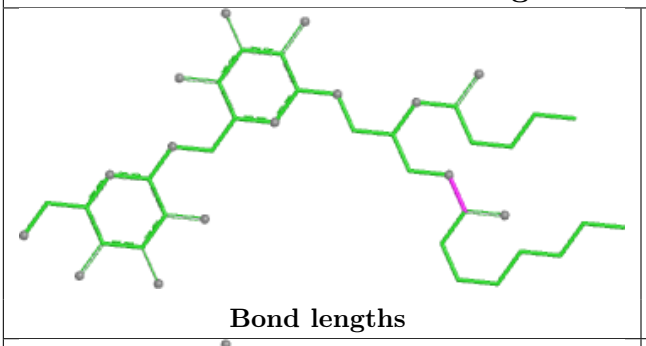
Bond angles



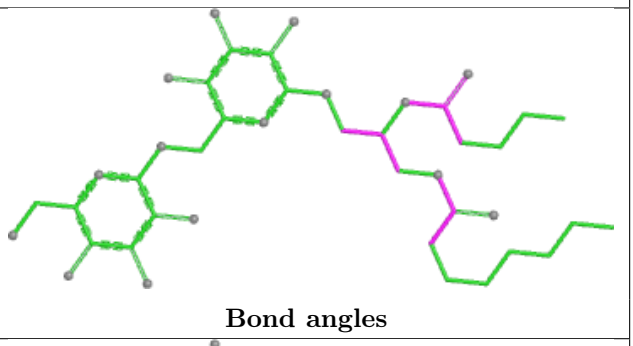
Torsions

Rings

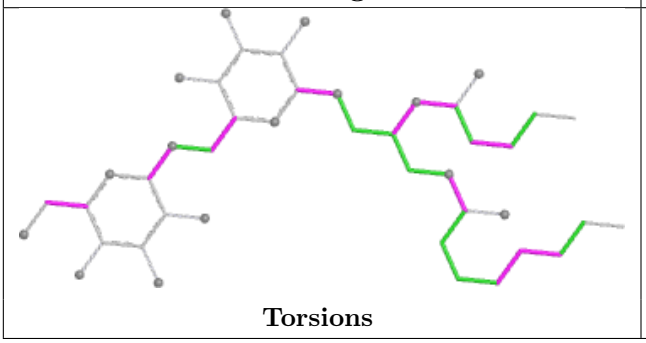
Ligand DGD B1 623



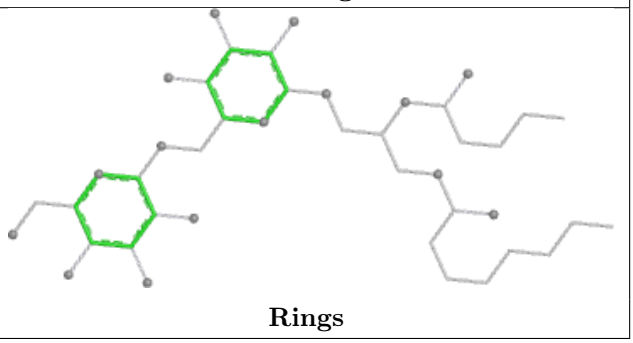
Bond lengths



Bond angles

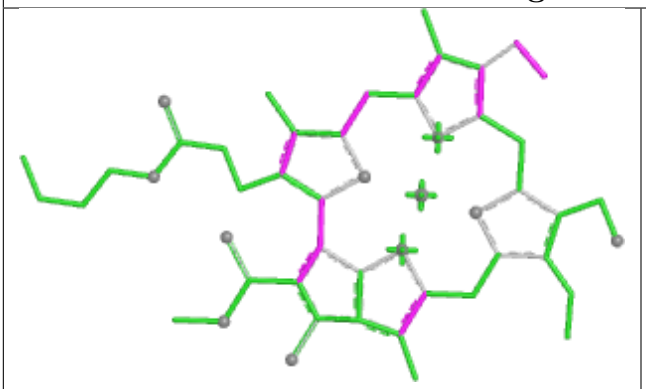


Torsions

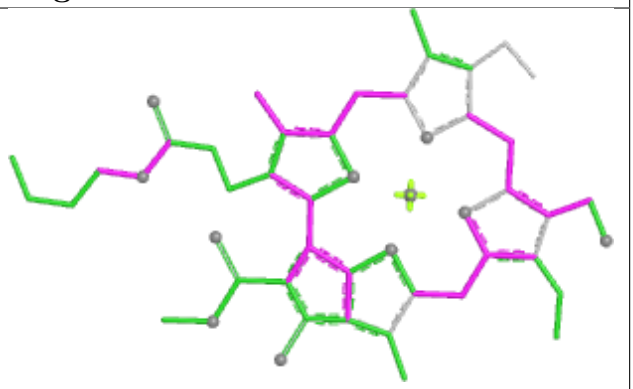


Rings

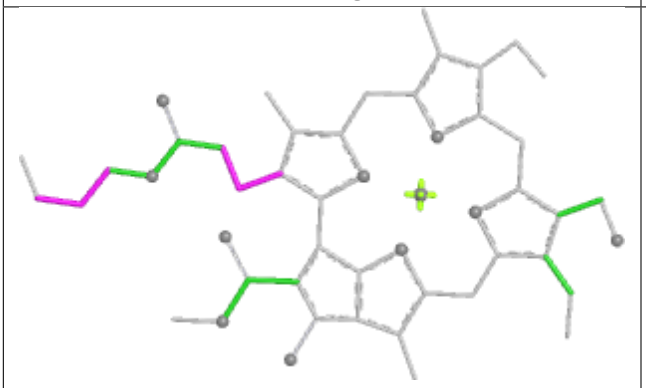
Ligand CHL g 606



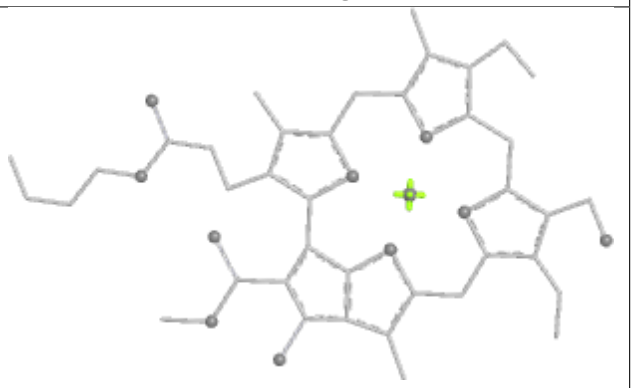
Bond lengths



Bond angles

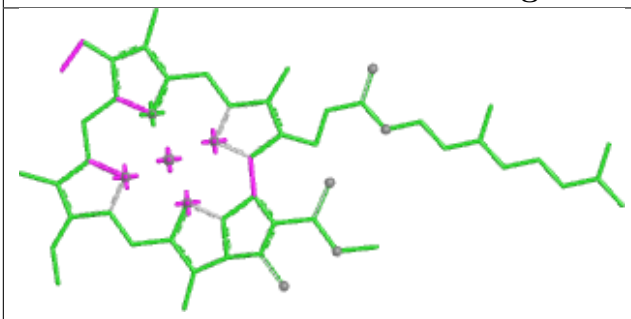


Torsions

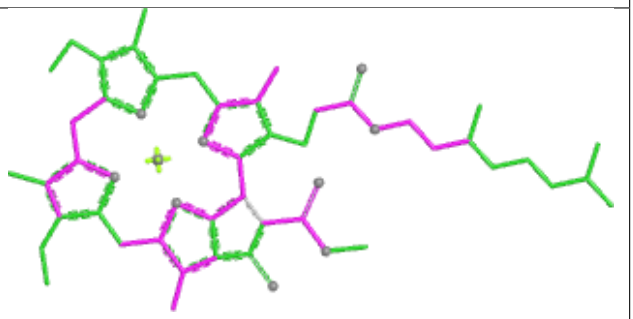


Rings

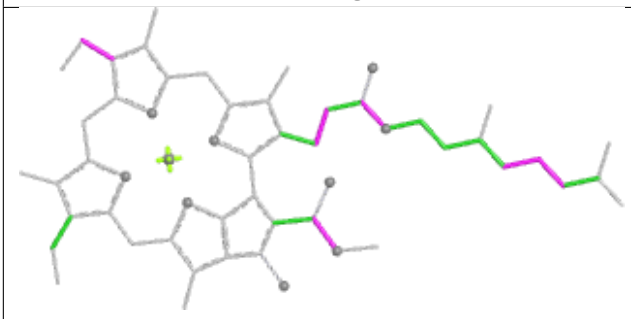
Ligand CLA s1 613



Bond lengths



Bond angles



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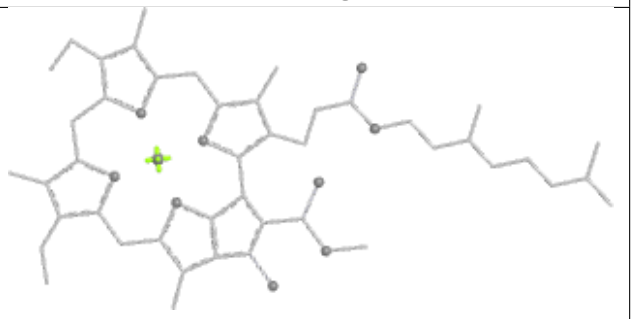
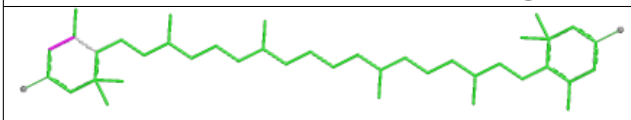


Rings

Ligand LUT g1 620



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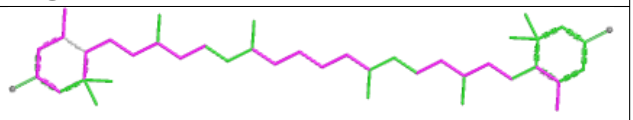
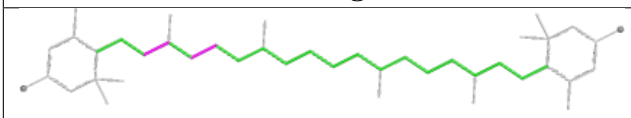


Bond angles



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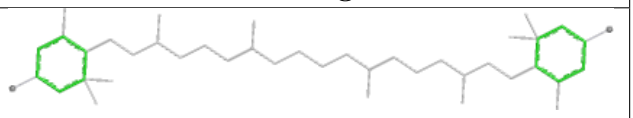
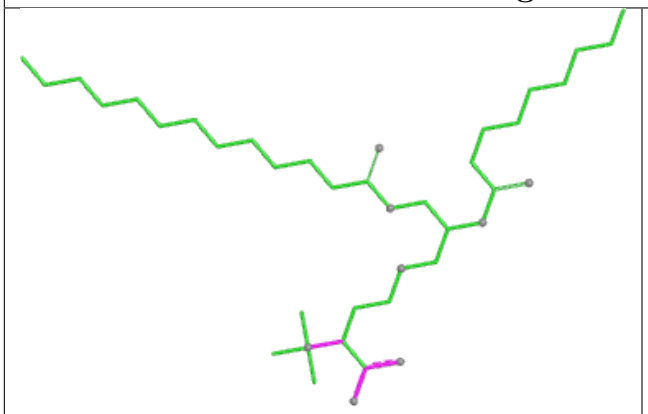
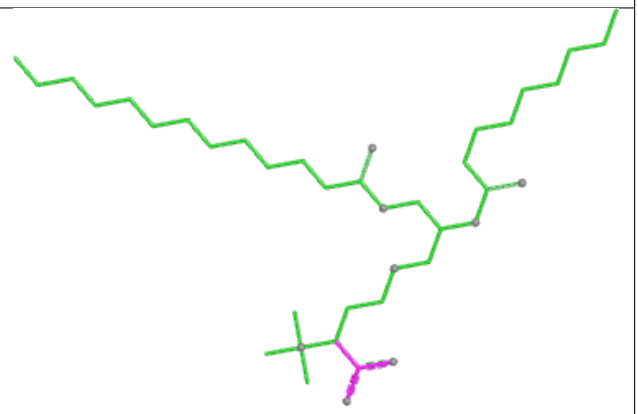


Rings

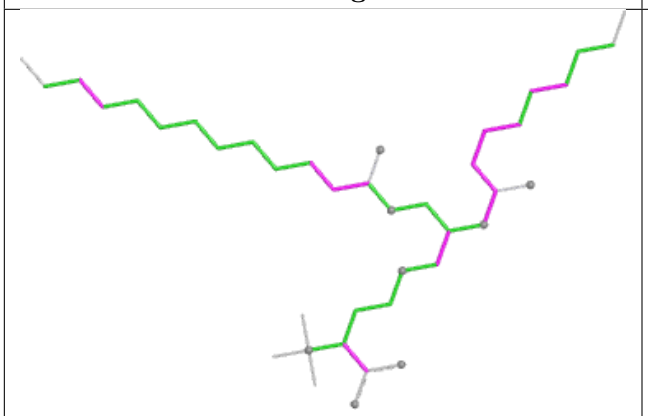
Ligand LMK c1 527



Bond lengths



Bond angles



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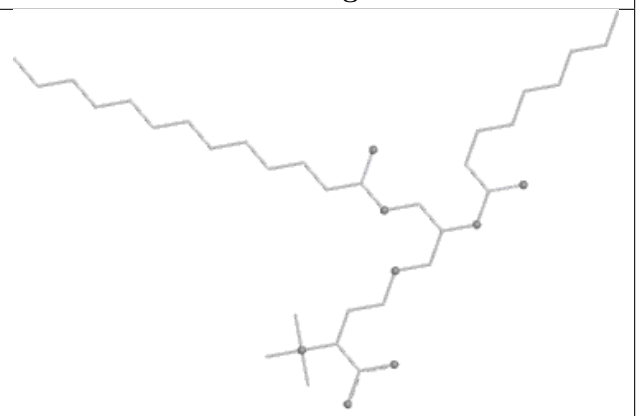
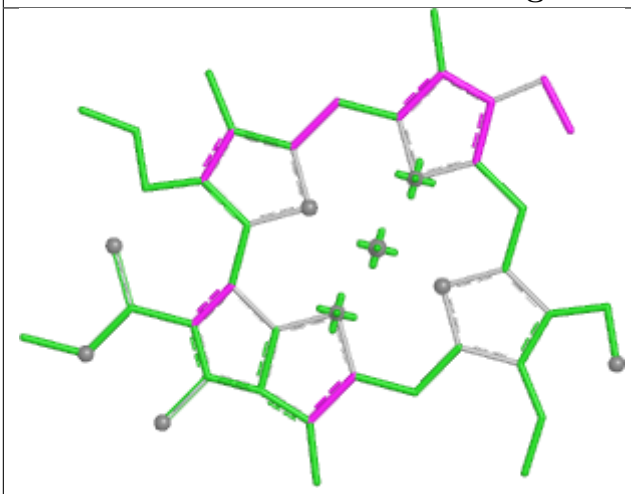


Rings

Ligand CHL S 606



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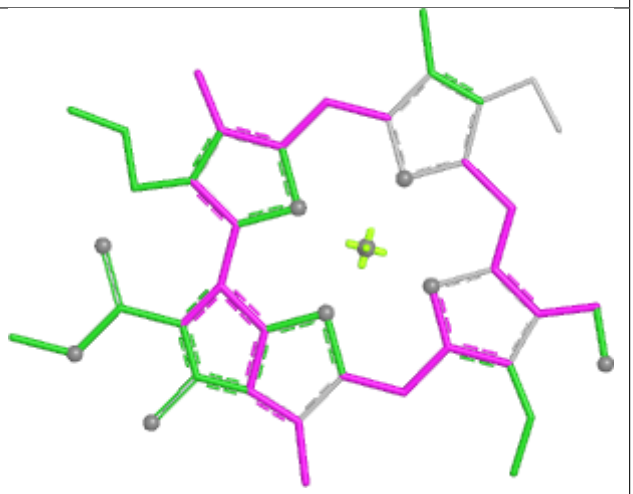
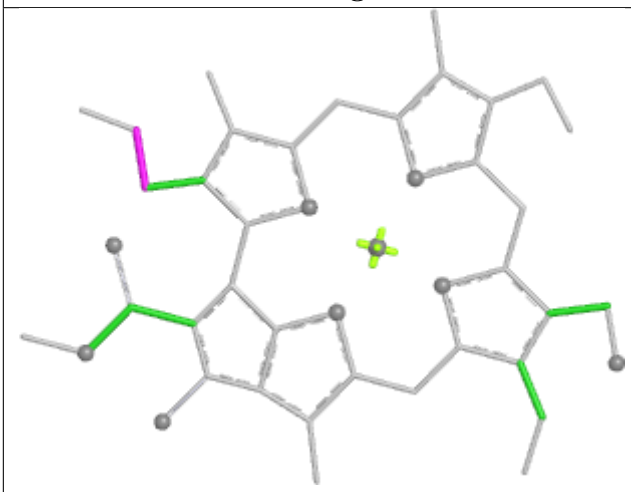
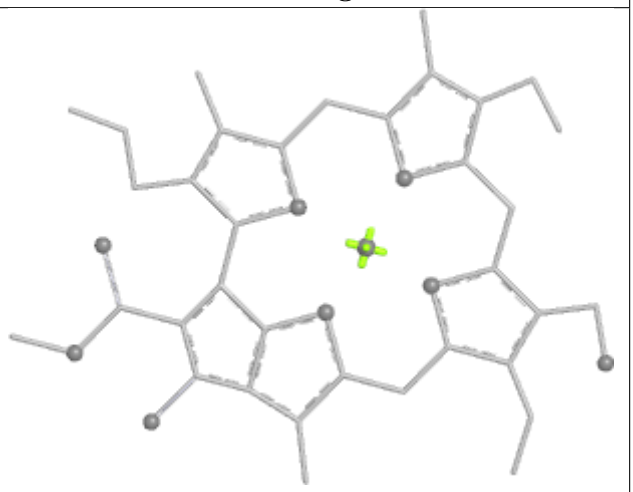


Bond angles

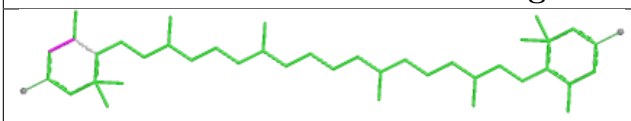


Torsions



Rings

Ligand LUT g 620



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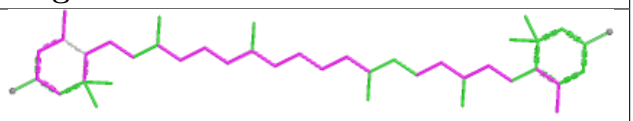
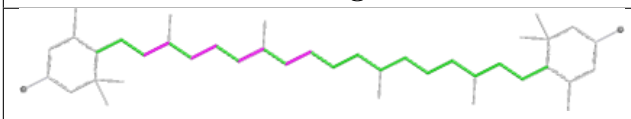


Bond angles



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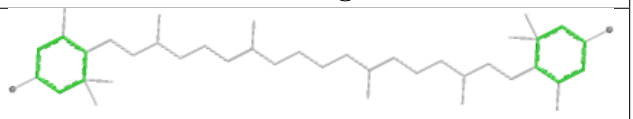
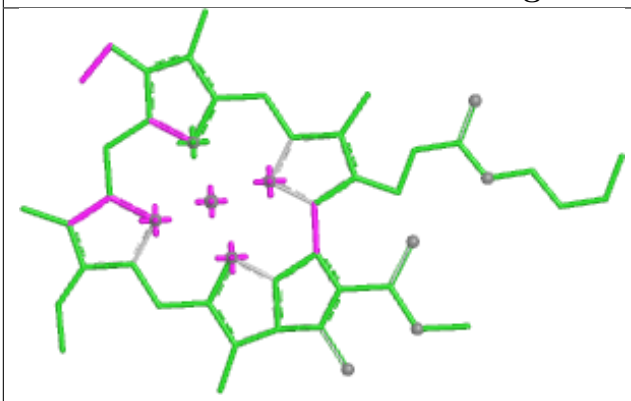


Rings

Ligand CLA N 611



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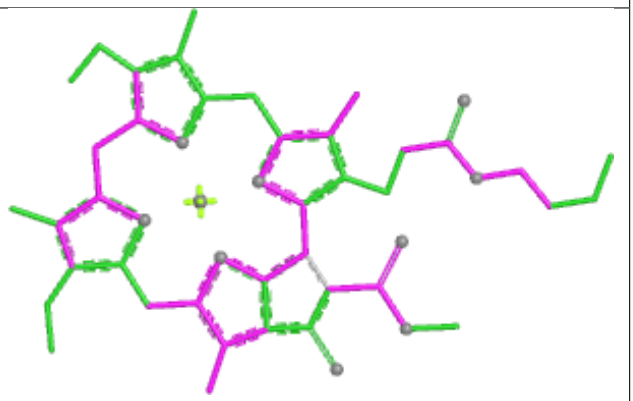
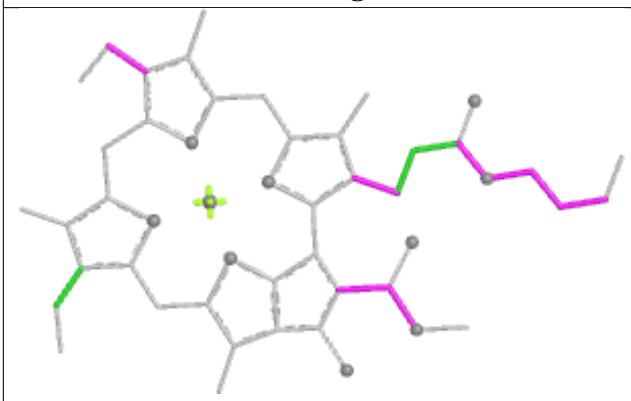


Bond angles



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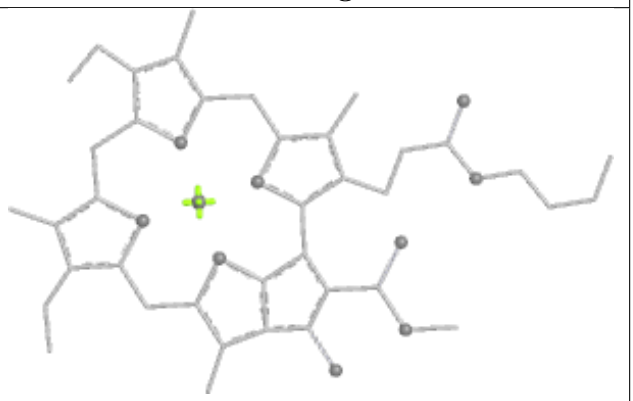
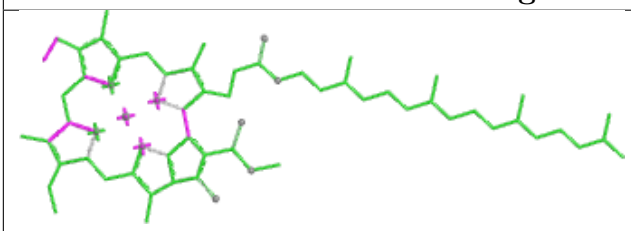


Rings

Ligand CLA b1 611



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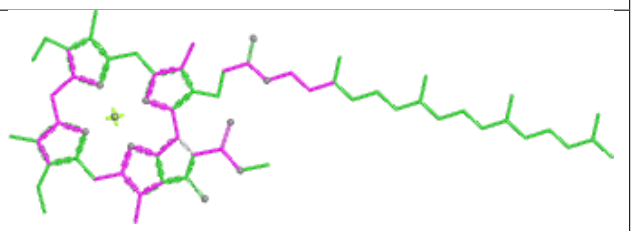
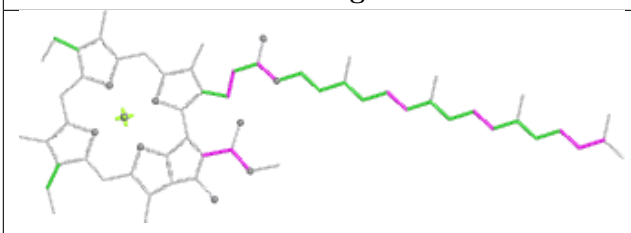
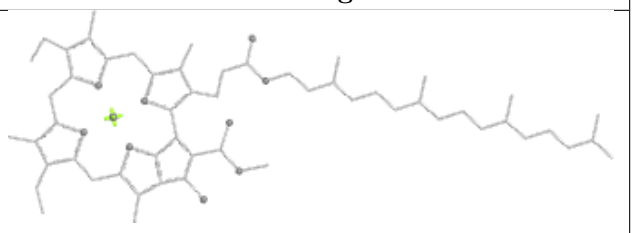


Bond angles

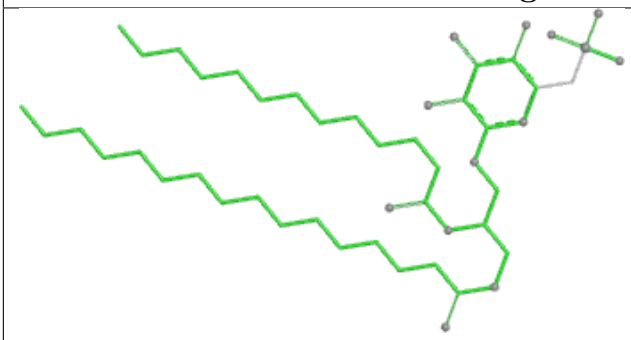


Torsions



Rings

Ligand SQD a1 412



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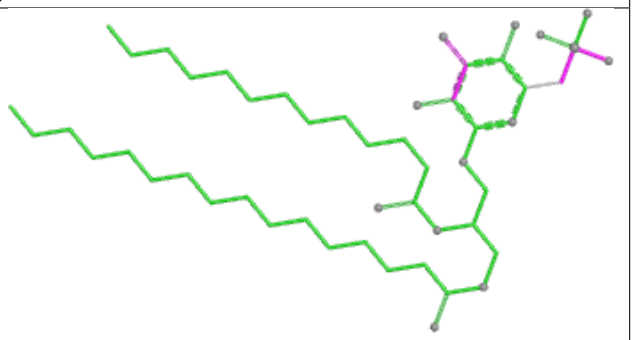
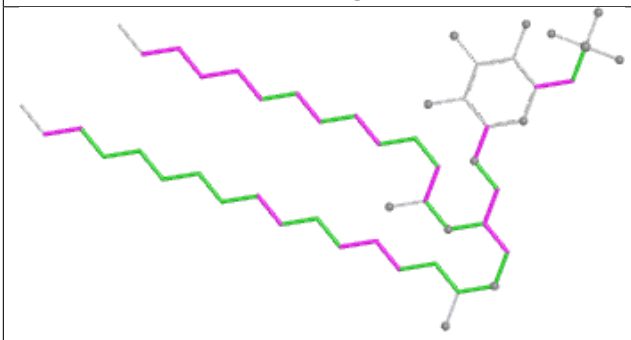


Bond angles



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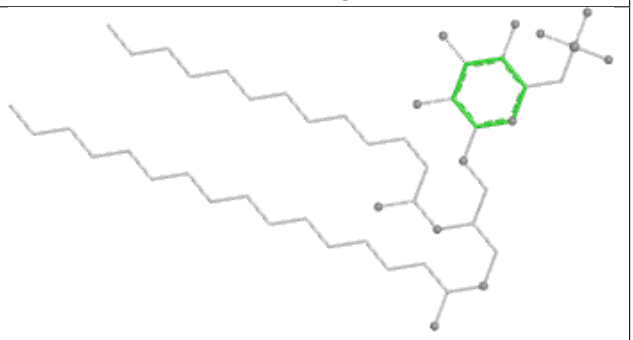
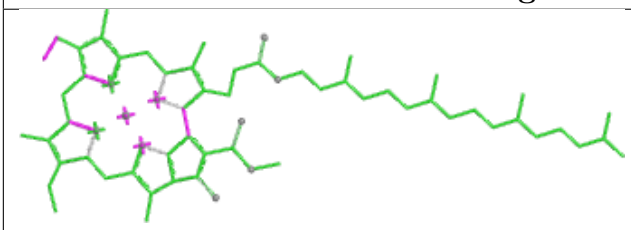


Rings

Ligand CLA n1 602



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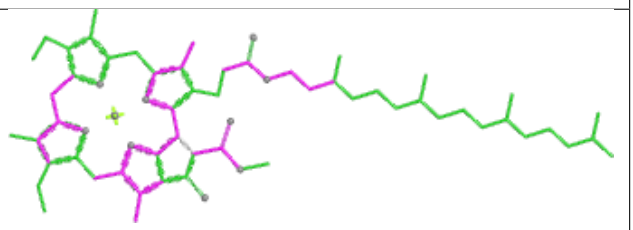
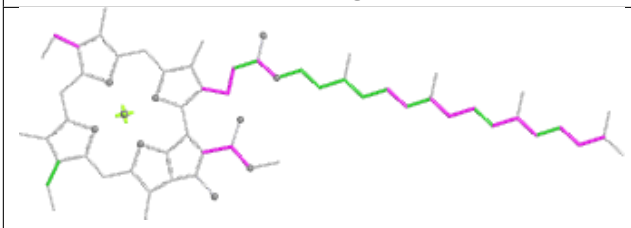
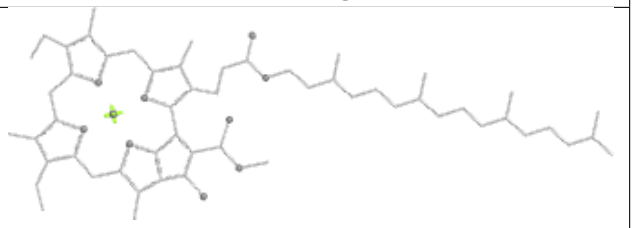


Bond angles

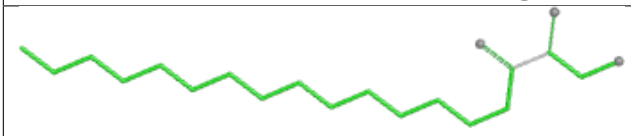


Torsions



Rings

Ligand SPH Y1 625



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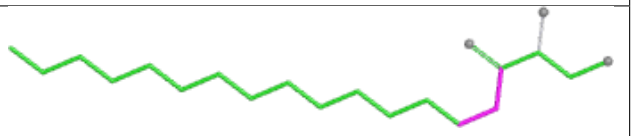
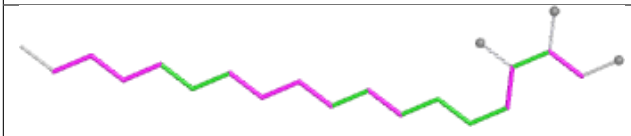


Bond angles



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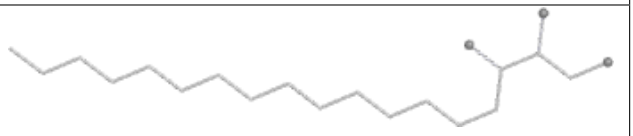
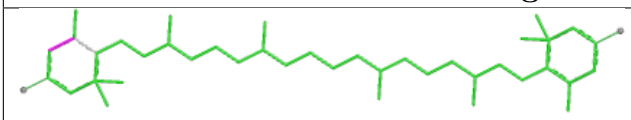


Rings

Ligand LUT s1 620



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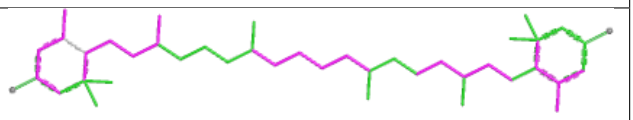
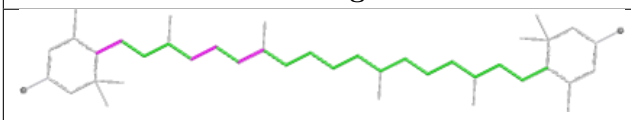
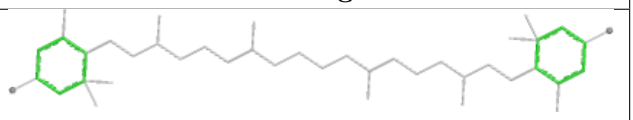


Bond angles

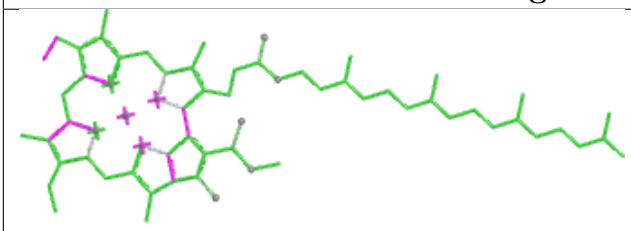


Torsions

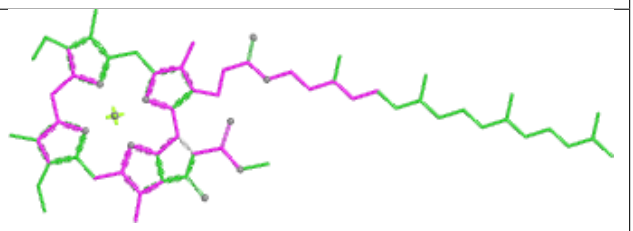


Rings

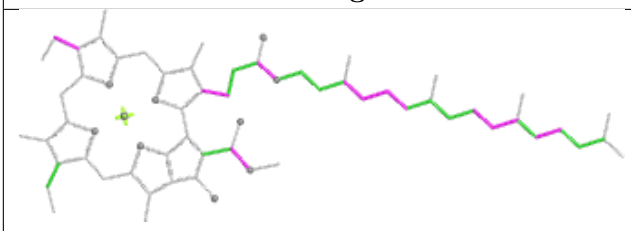
Ligand CLA c 511



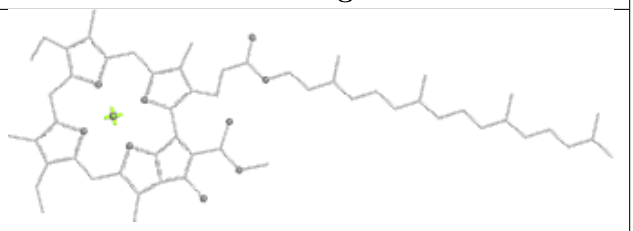
Bond lengths



Bond angles

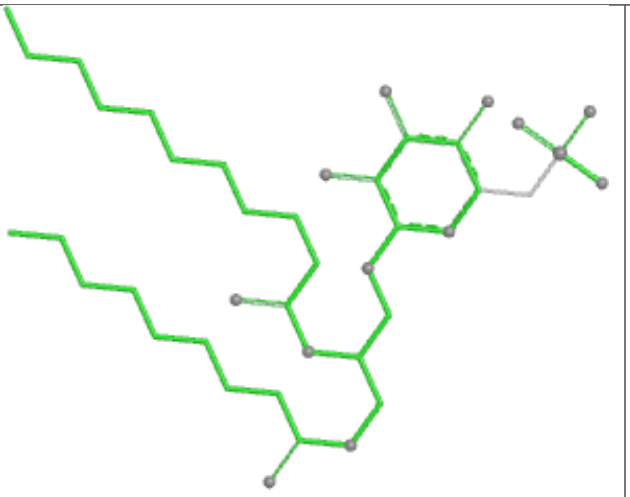


Torsions

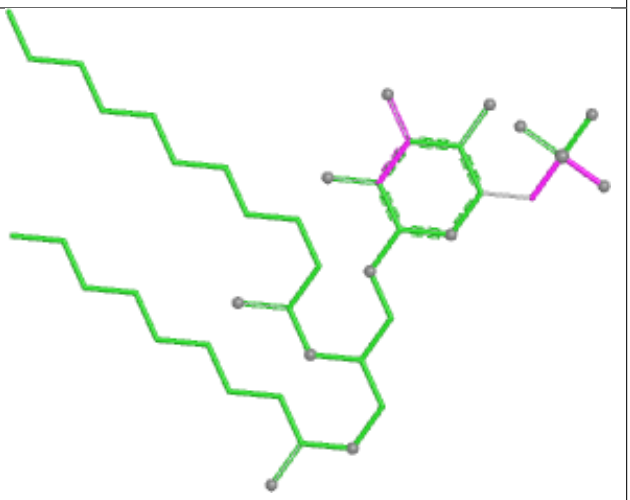


Rings

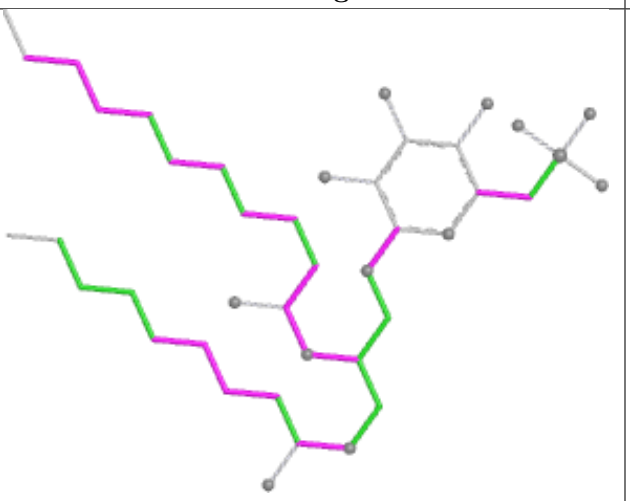
Ligand SQD b1 621



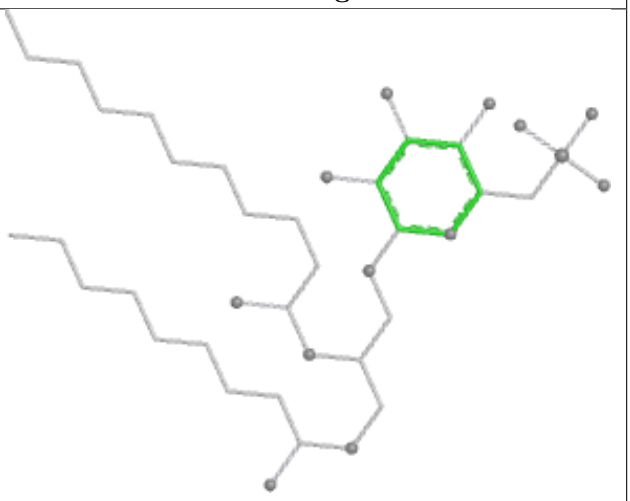
Bond lengths



Bond angles

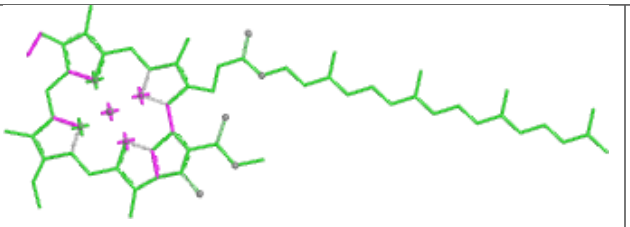


Torsions



Rings

Ligand CLA C 504



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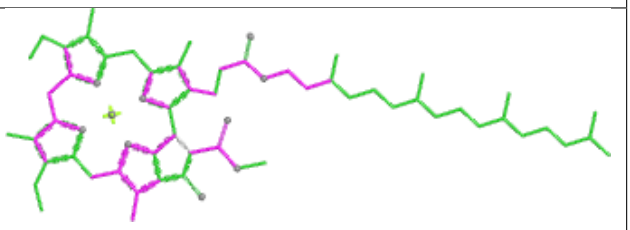
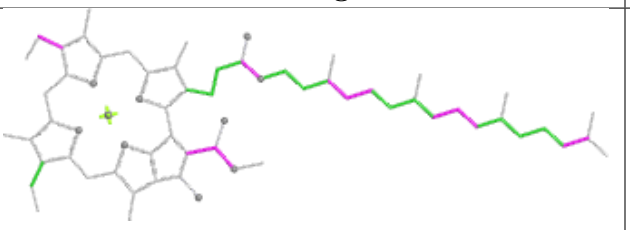


Bond angles



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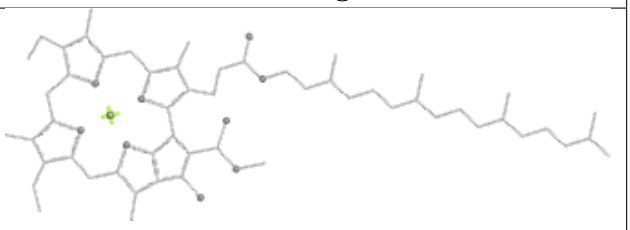
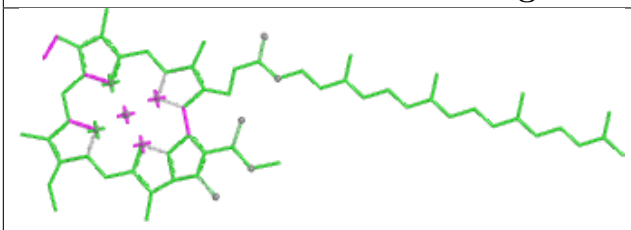


Rings

Ligand CLA n1 604



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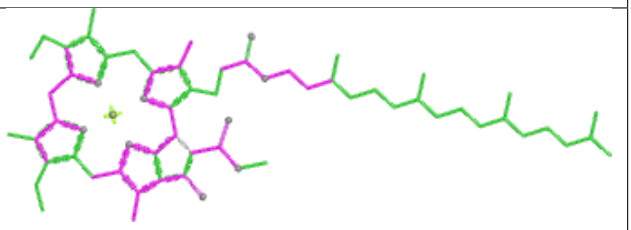

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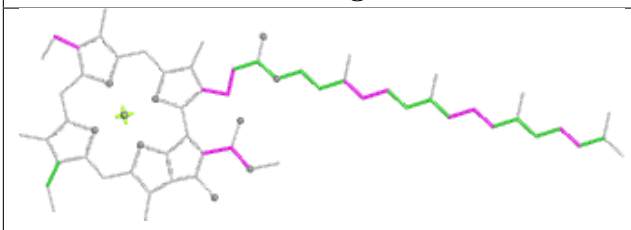

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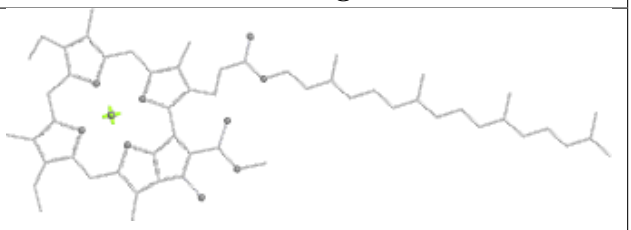
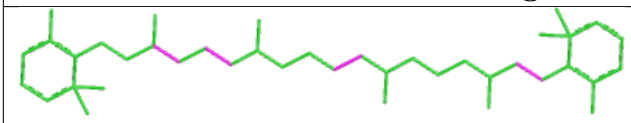
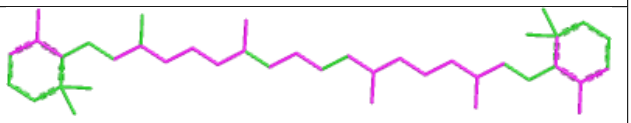


Rings

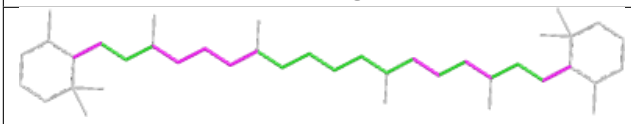
Ligand BCR D 404



Bond lengths



Bond angles



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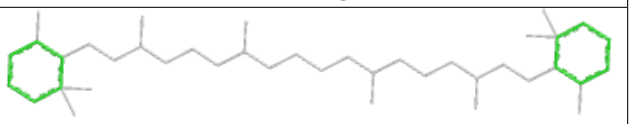
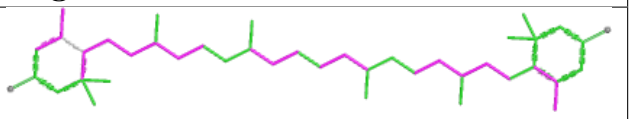


Rings

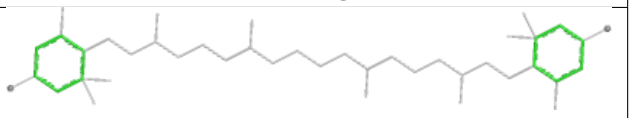
Ligand LUT g 621

Bond lengths



Bond angles

Torsions

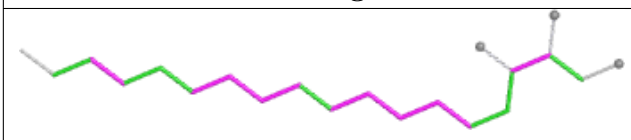


Rings

Ligand SPH a1 414

Bond lengths

Bond angles



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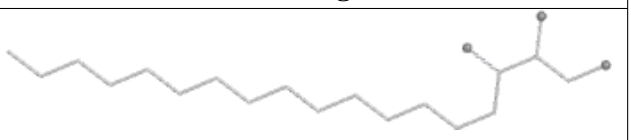
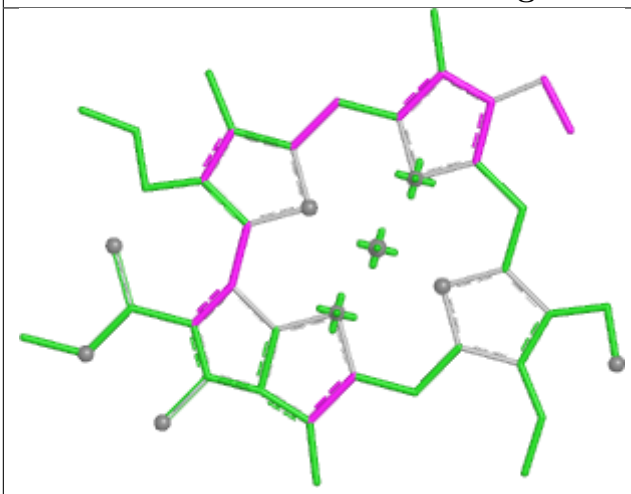
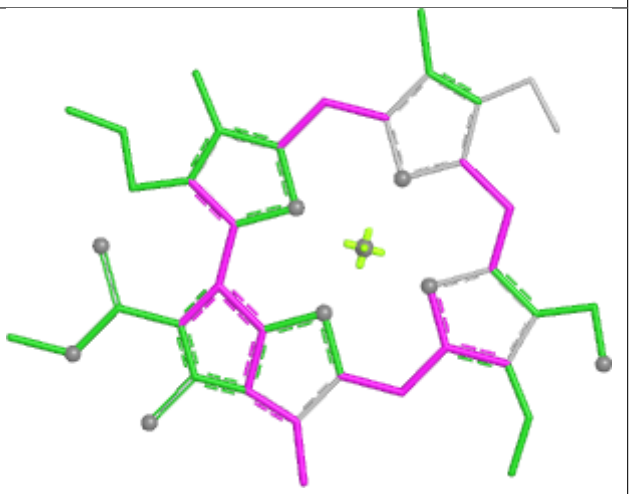
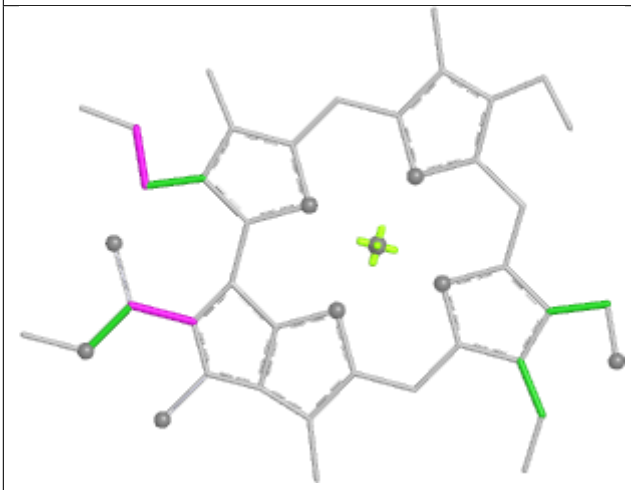
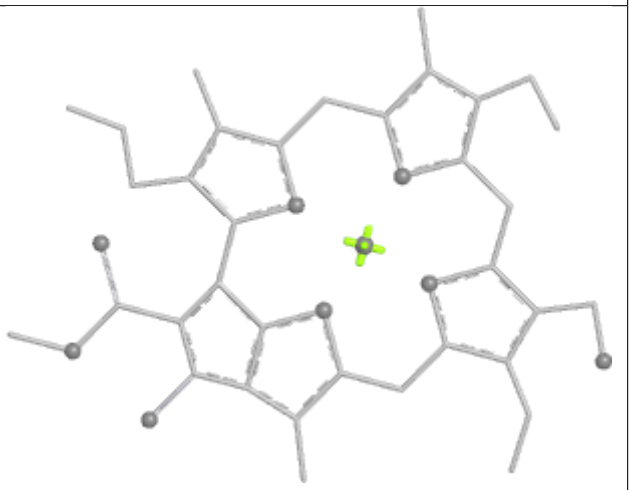
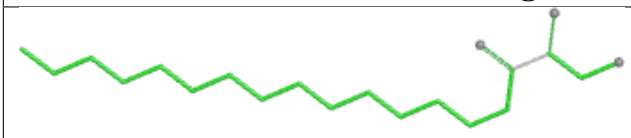
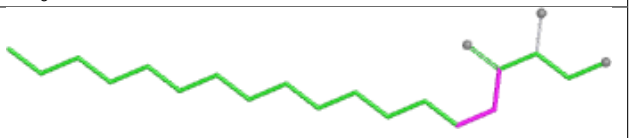
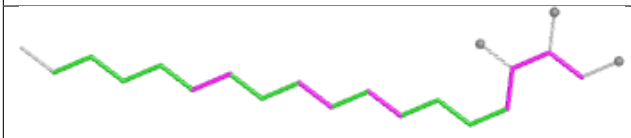
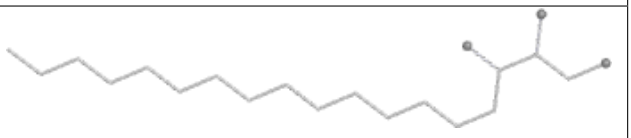
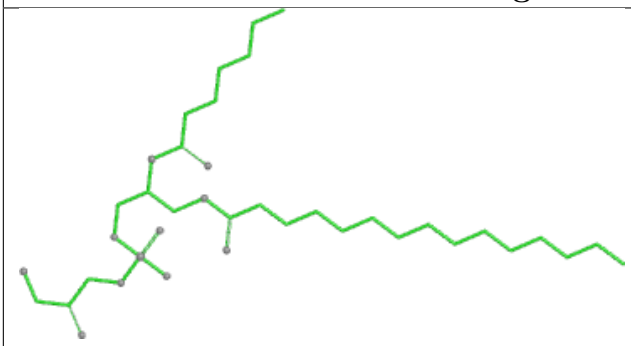


Rings

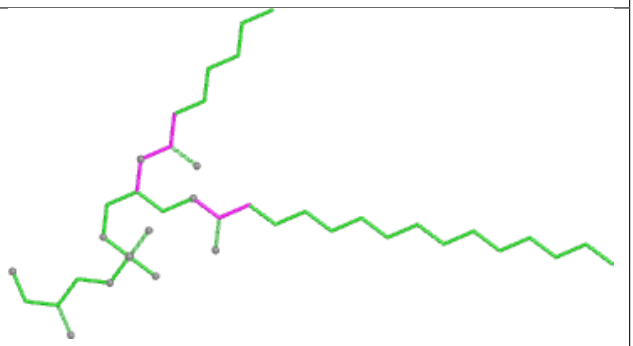
Ligand CHL S1 606	
 Bond lengths	 Bond angles
 Torsions	 Rings

Ligand SPH y1 625	
 Bond lengths	 Bond angles
 Torsions	 Rings

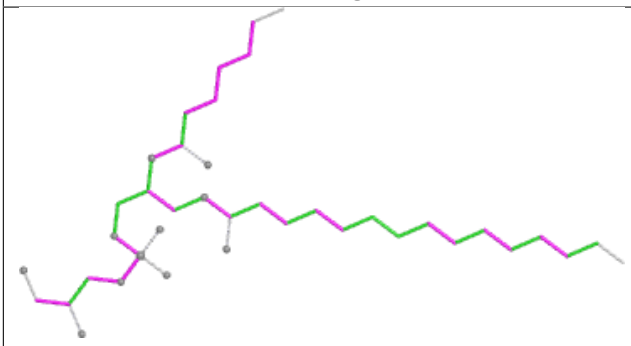
Ligand LHG D1 410



Bond lengths



Bond angles



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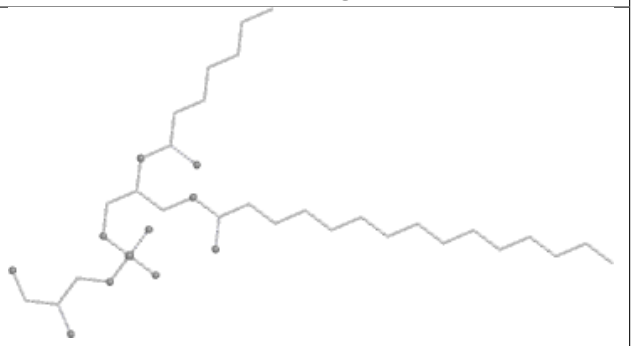
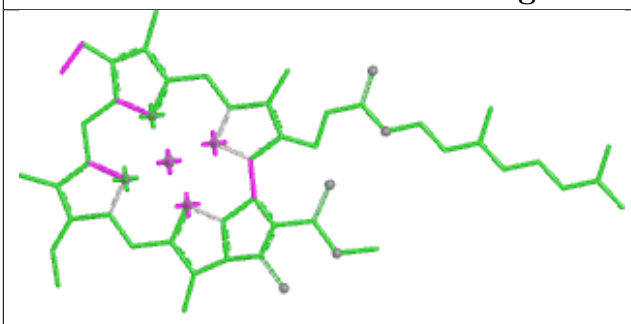


Rings

Ligand CLA S1 613



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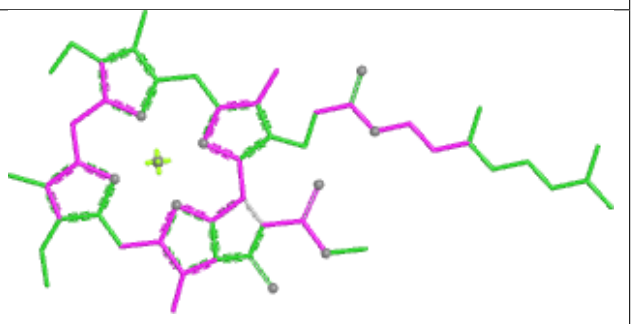
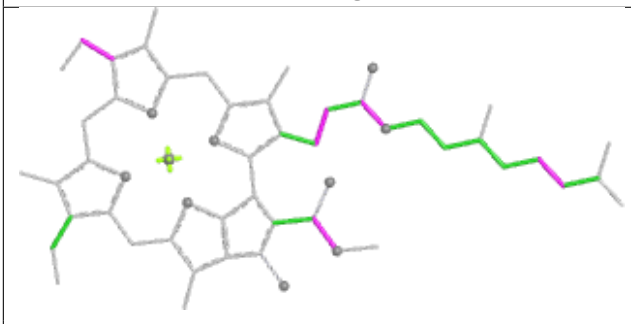


Bond angles



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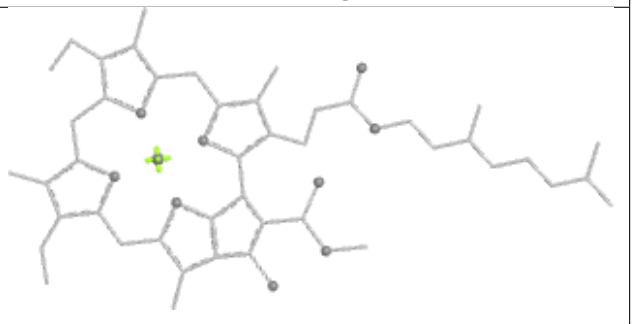
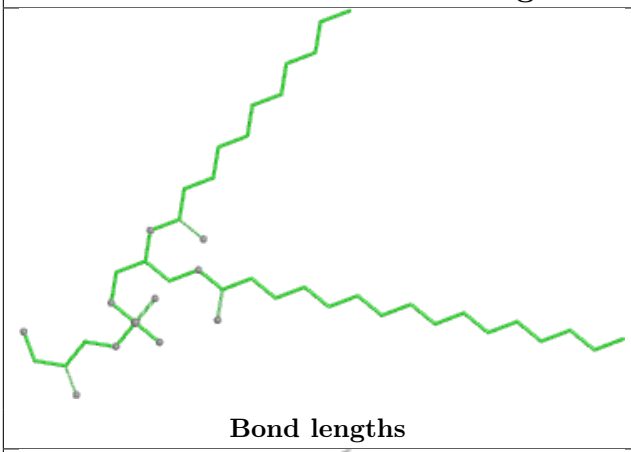


Rings

Ligand LHG d1 408



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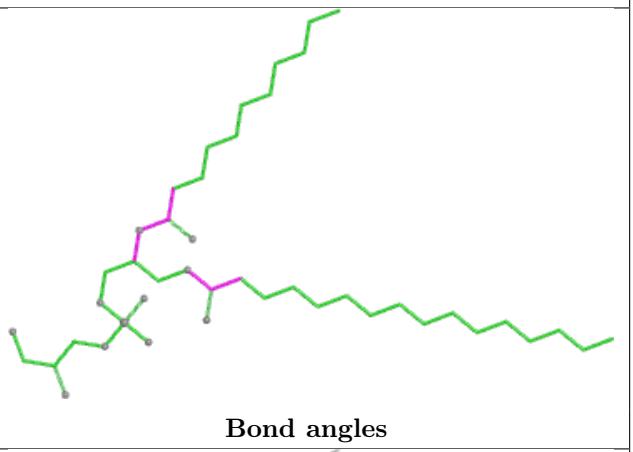

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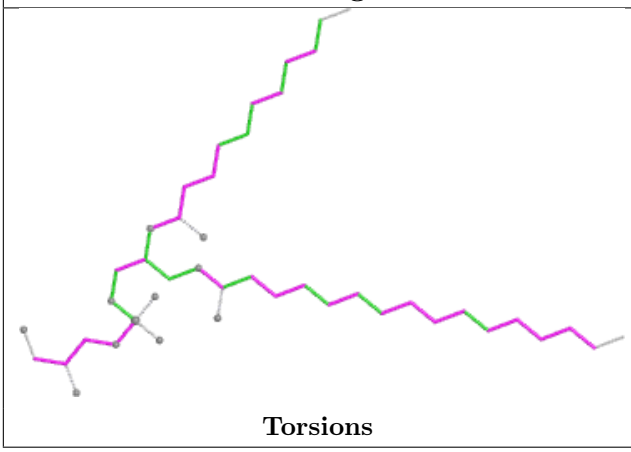

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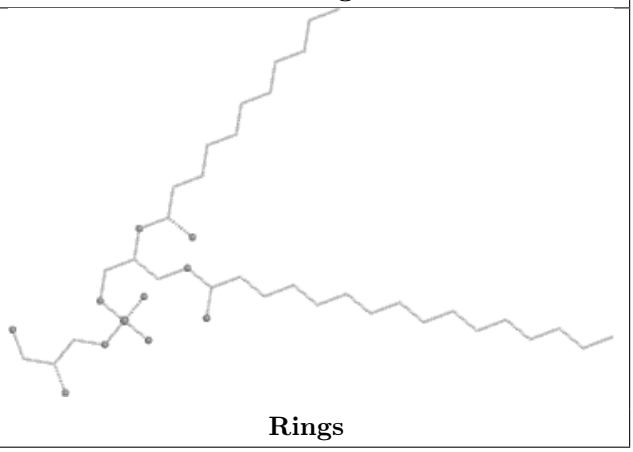
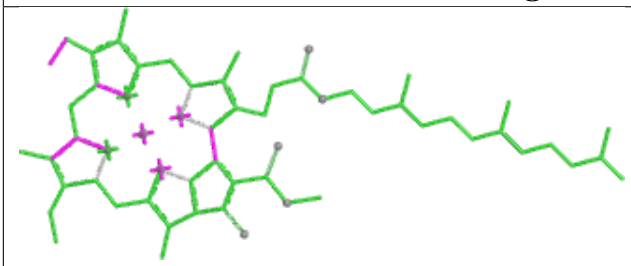


Rings

Ligand CLA R 609



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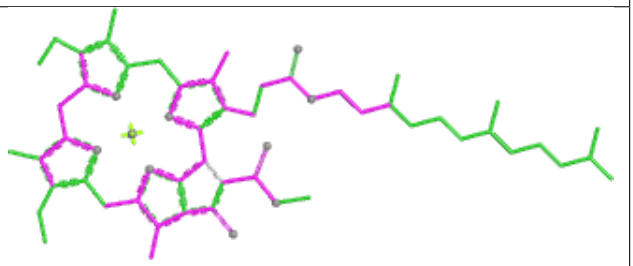
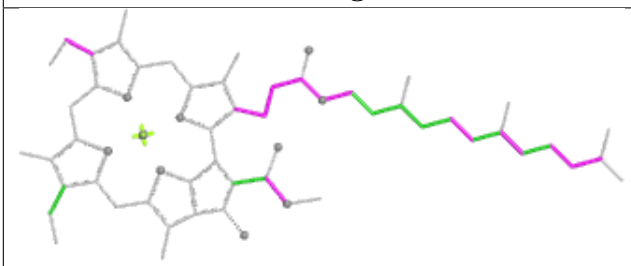


Bond angles



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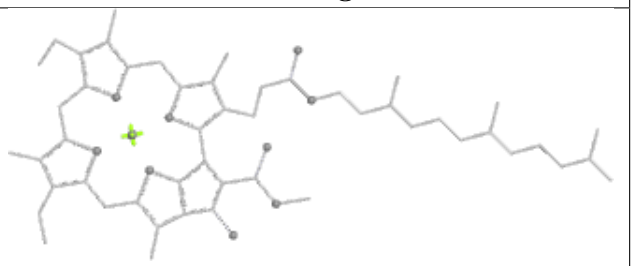
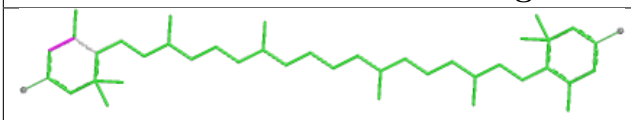


Rings

Ligand LUT Y1 620



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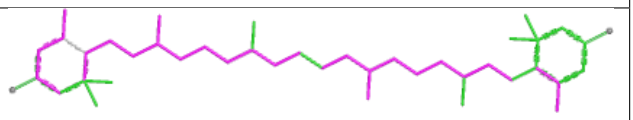
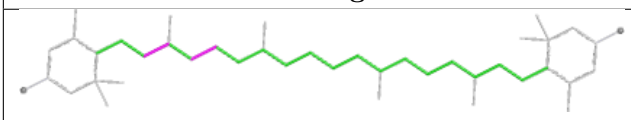


Bond angles



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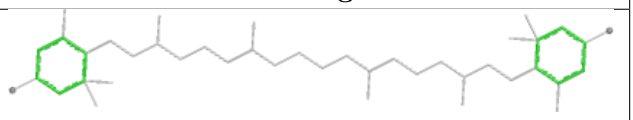
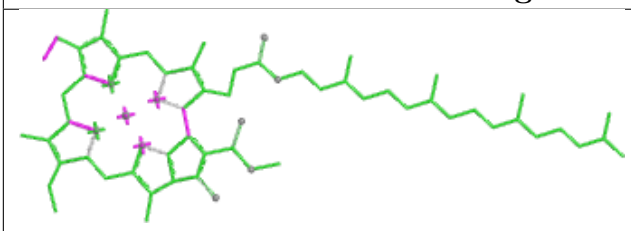


Rings

Ligand CLA Y1 611



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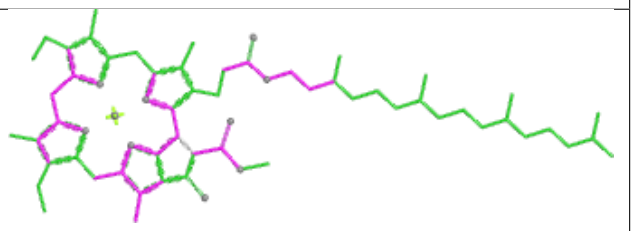
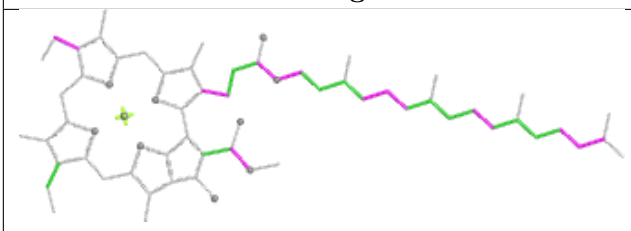
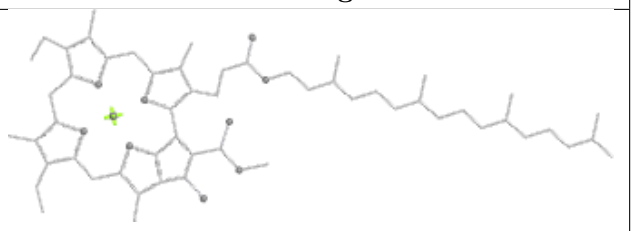


Bond angles

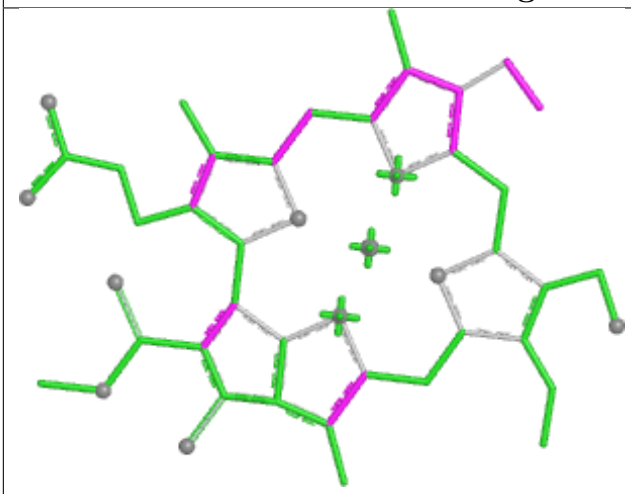


Torsions



Rings

Ligand CHL S1 601



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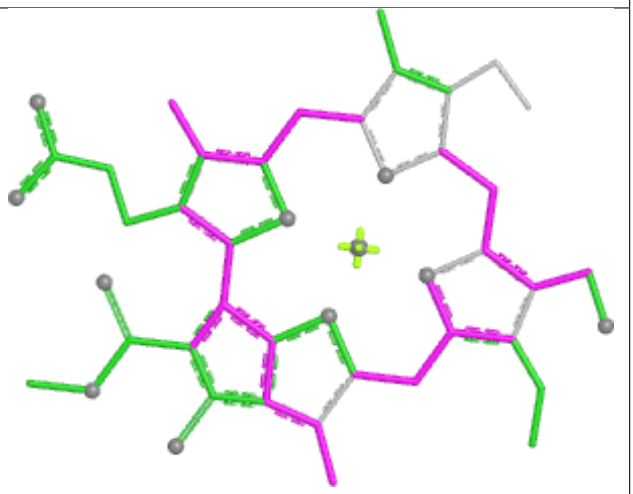
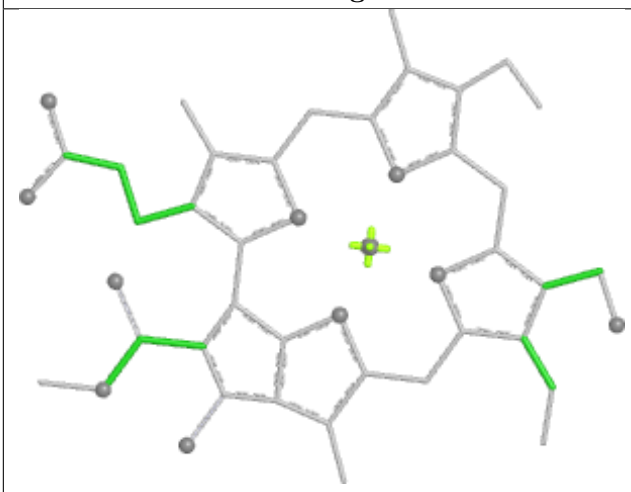
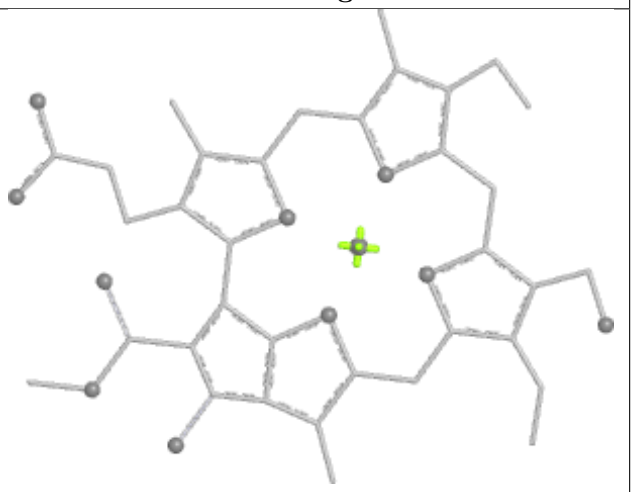


Bond angles

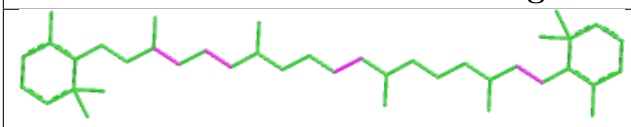


Torsions

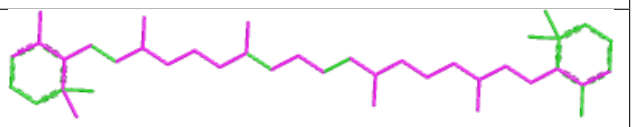


Rings

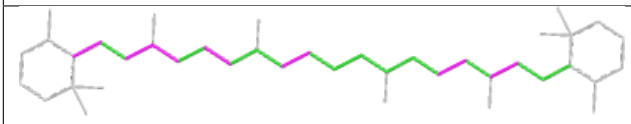
Ligand BCR c 516



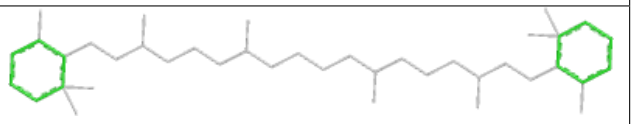
Bond lengths



Bond angles

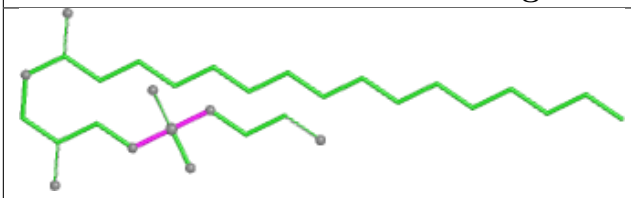


Torsions



Rings

Ligand LPX s1 625



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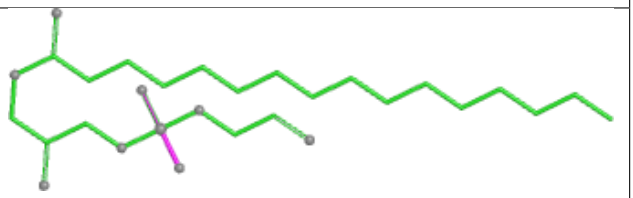
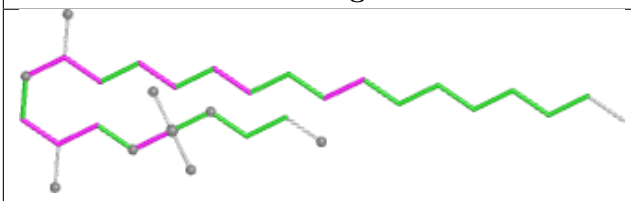


Bond angles



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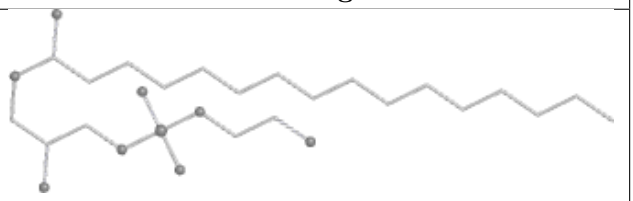
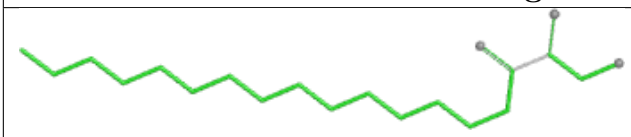


Rings

Ligand SPH Y 625



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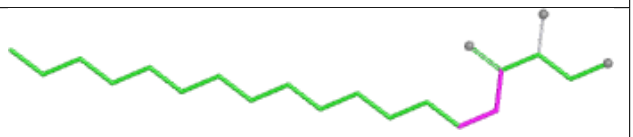

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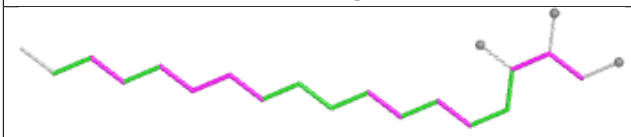

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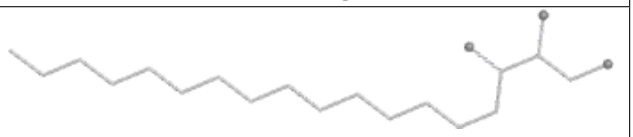
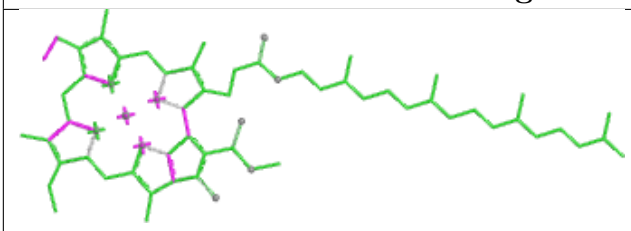


Rings

Ligand CLA C1 513



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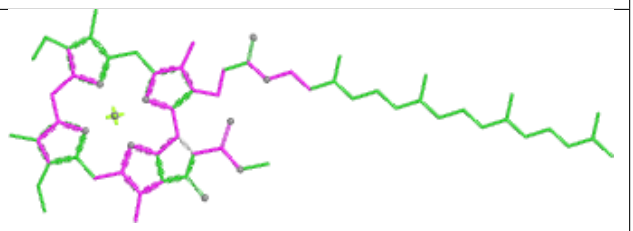
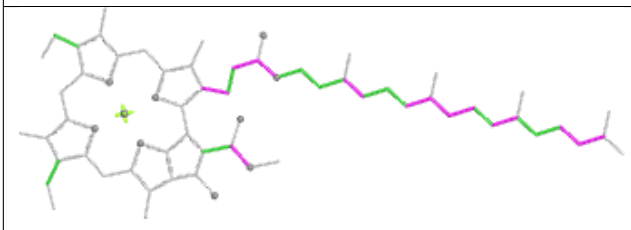


Bond angles



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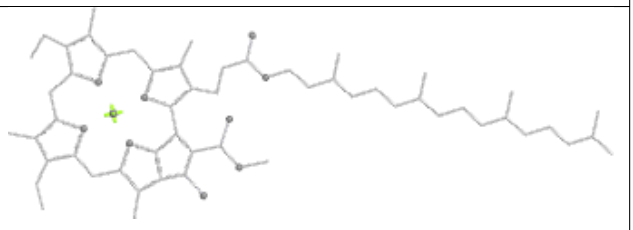
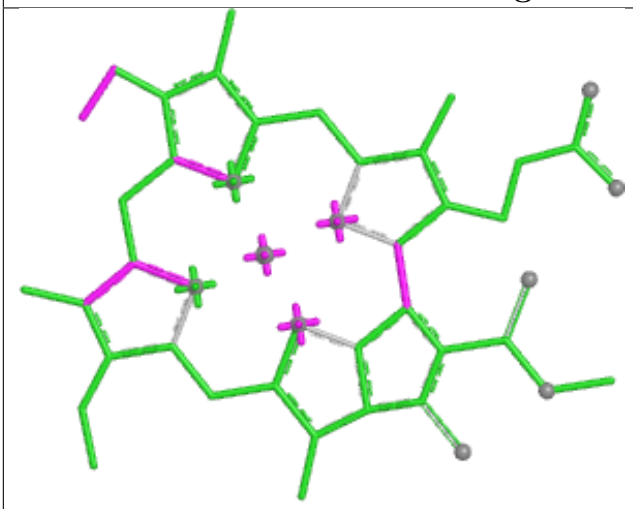


Rings

Ligand CLA N1 612



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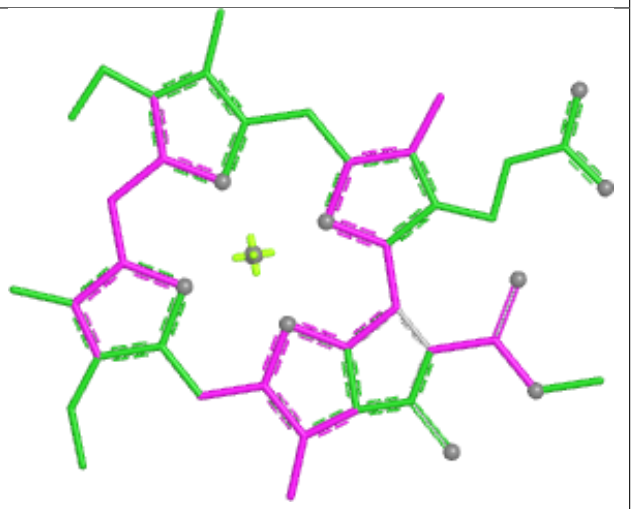

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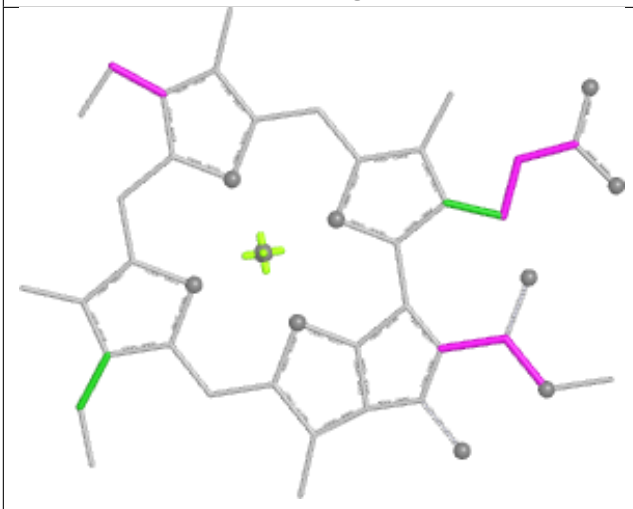
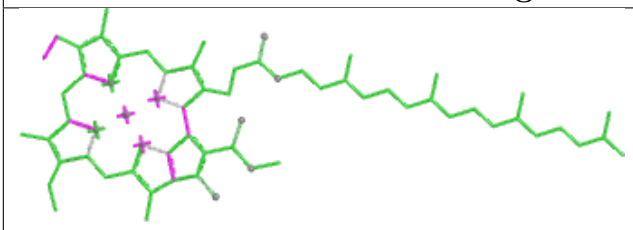


Torsions

Rings

Ligand CLA B1 607



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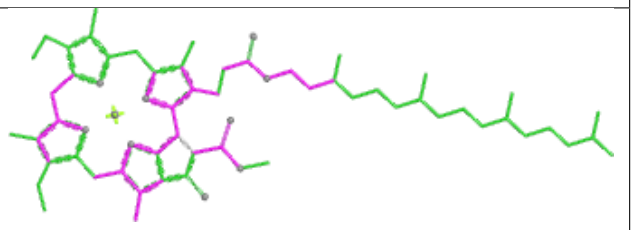

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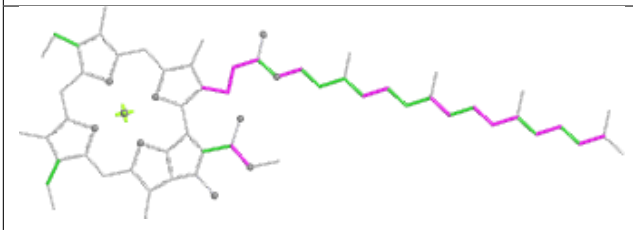

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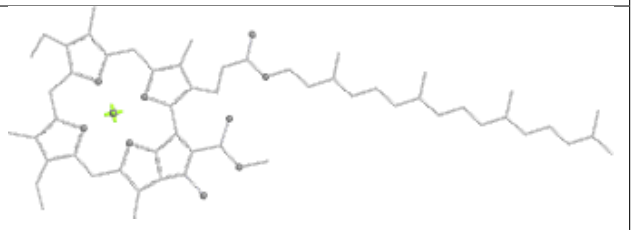
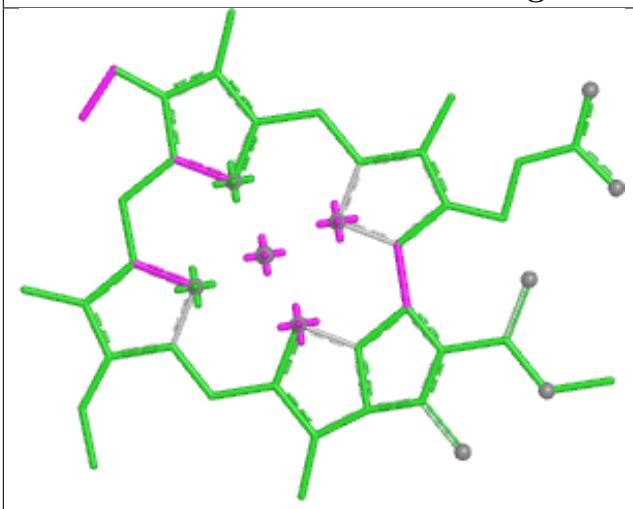


Rings

Ligand CLA S 612



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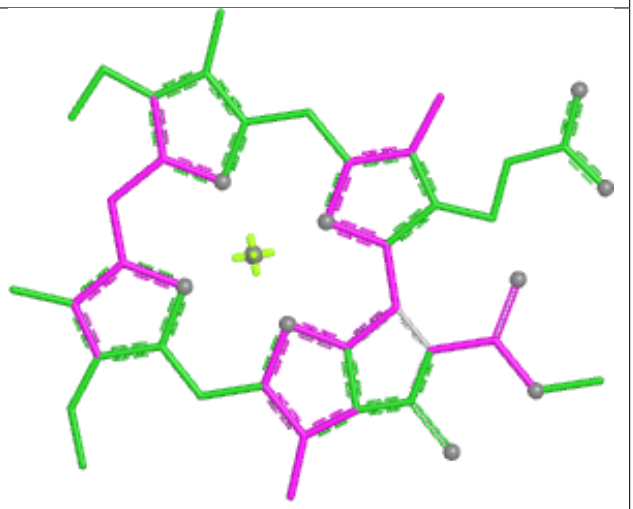
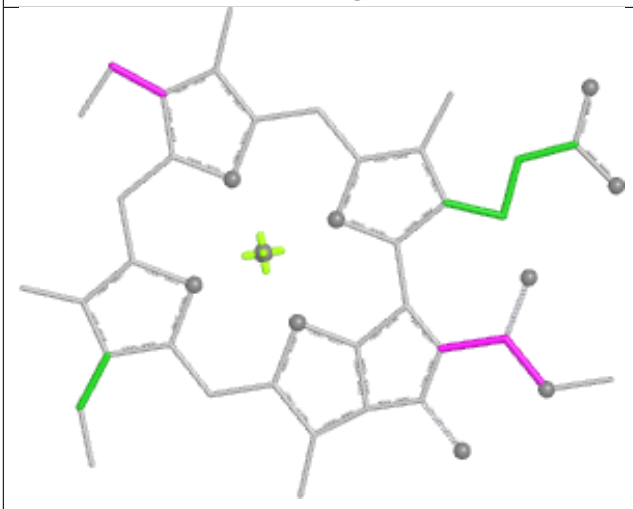


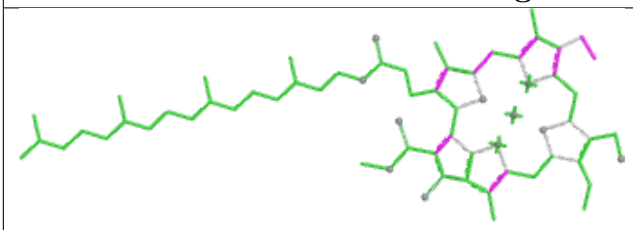
Bond angles



Torsions

Rings

Ligand CHL Y1 607



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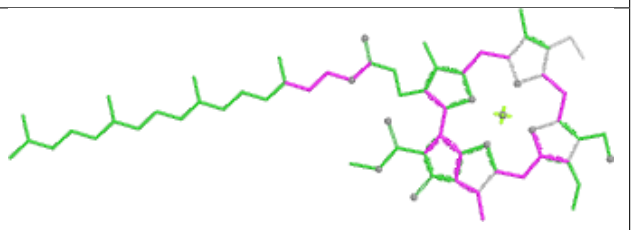

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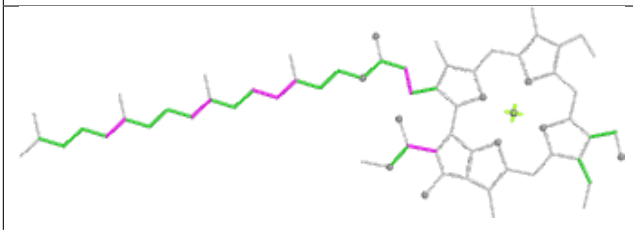

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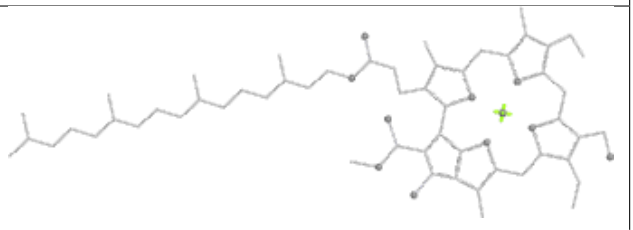
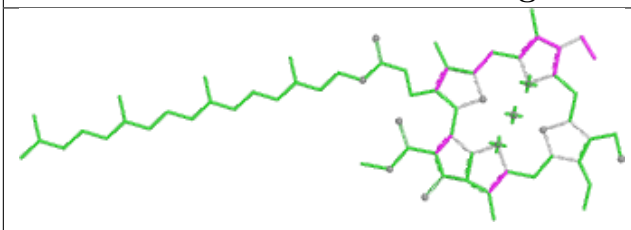


Rings

Ligand CHL g1 601



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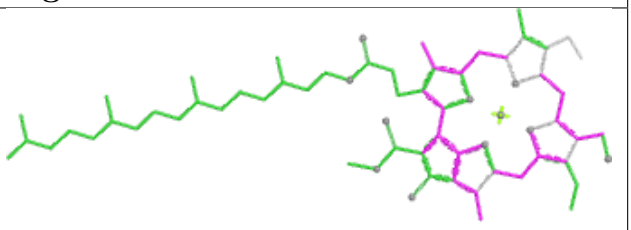
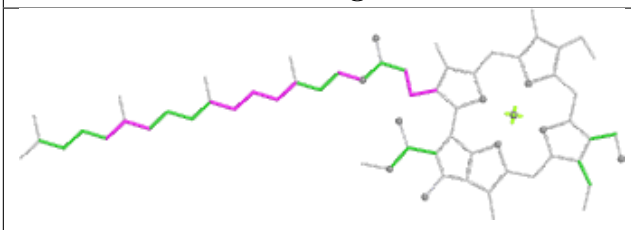


Bond angles



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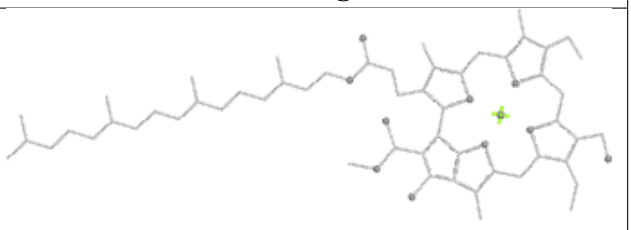
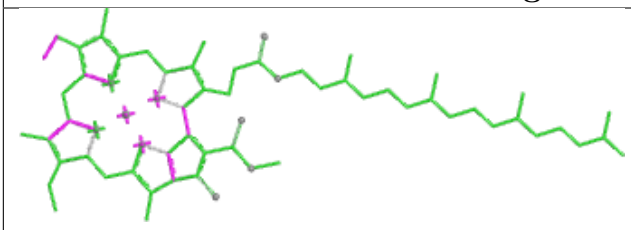


Rings

Ligand CLA N 602



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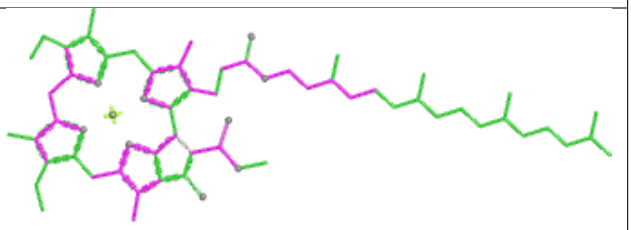

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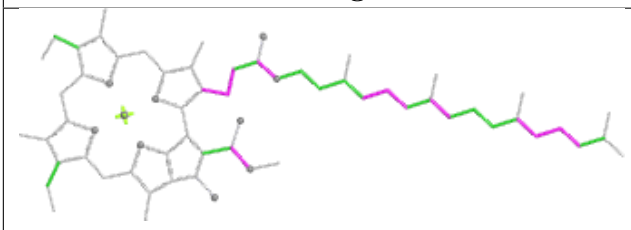

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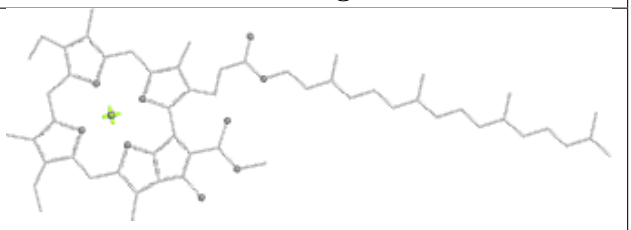
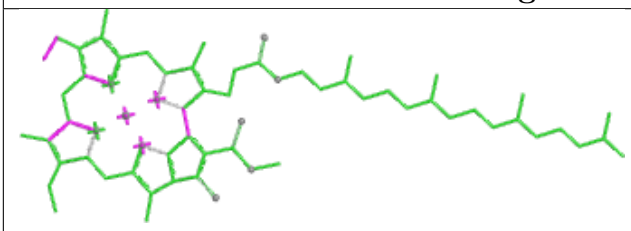


Rings

Ligand CLA b1 603



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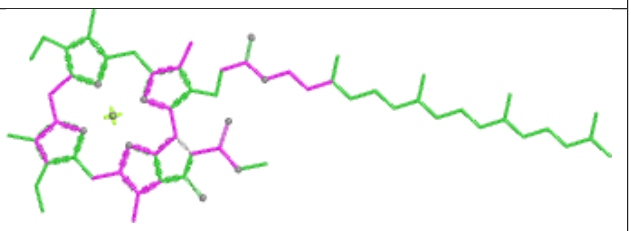

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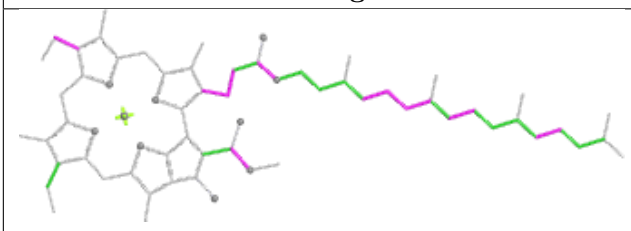

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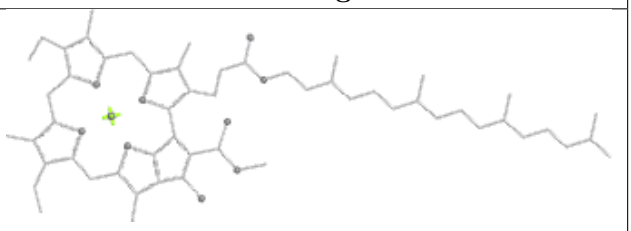
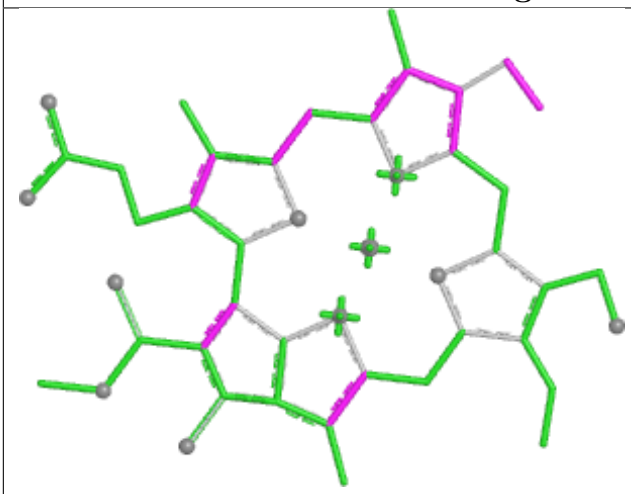


Rings

Ligand CHL Y1 605



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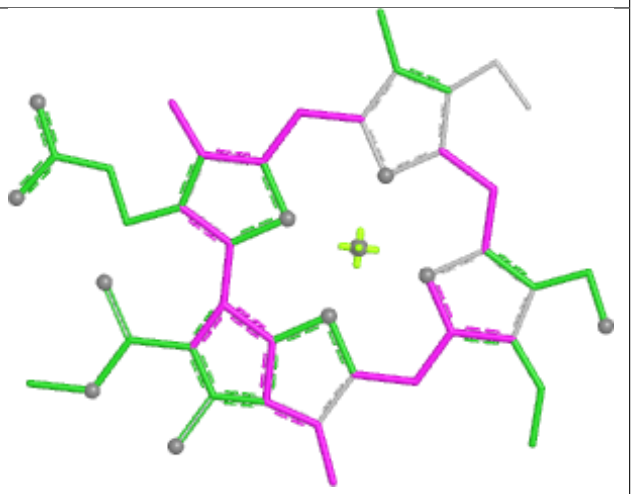
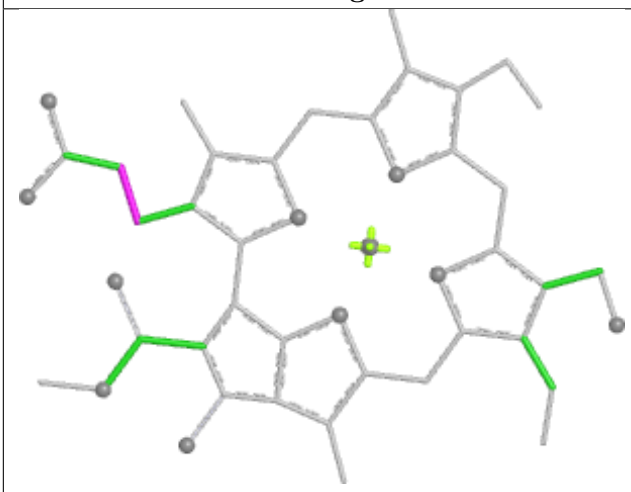


Bond angles



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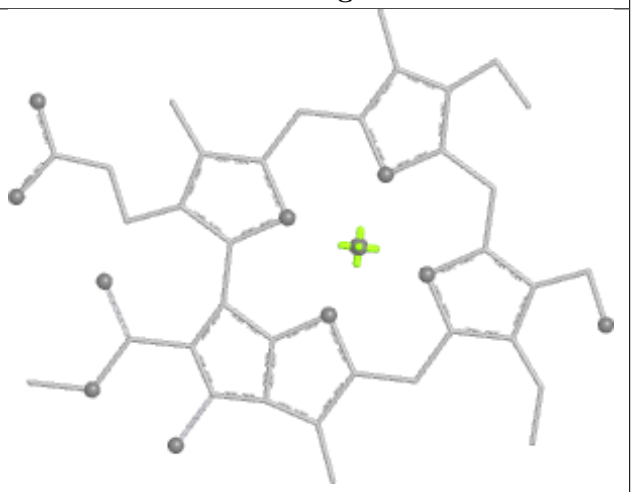
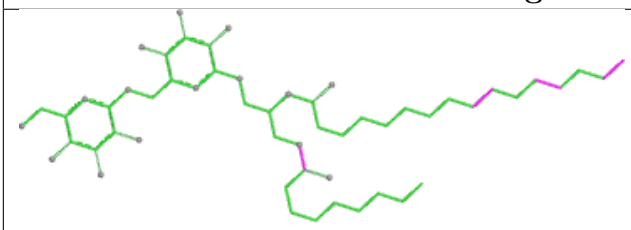


Rings

Ligand DGD c 518



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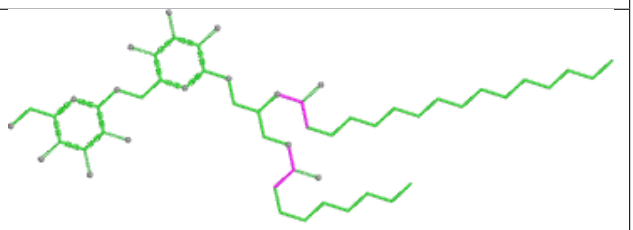
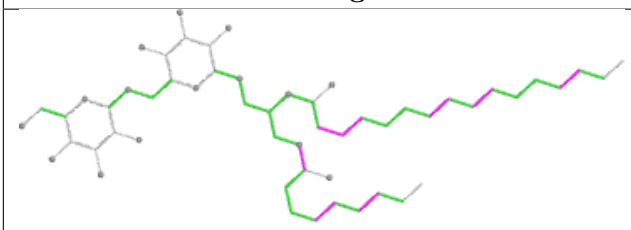


Bond angles



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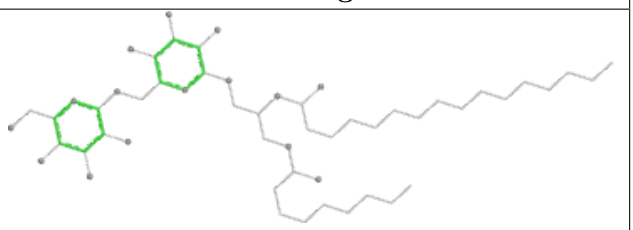
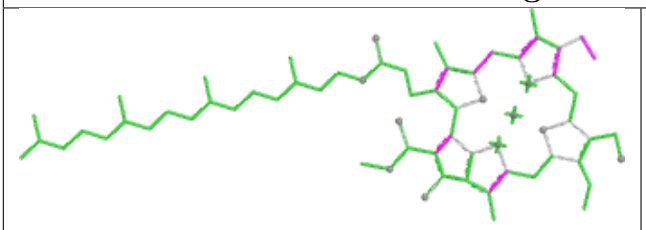


Rings

Ligand CHL Y 607



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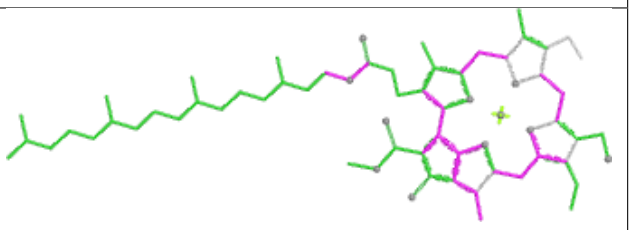
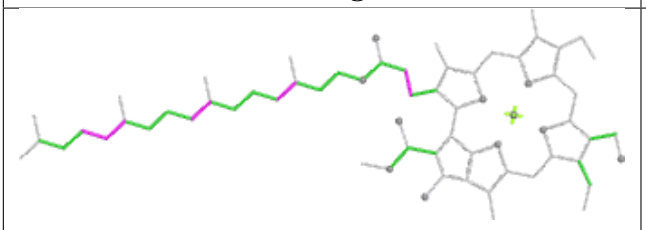


Bond angles



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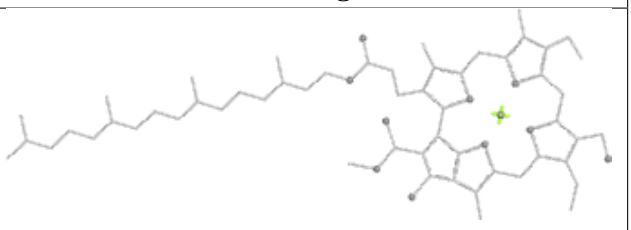
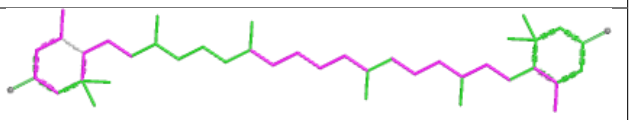


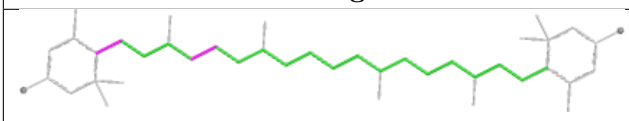
Rings

Ligand LUT Y1 621

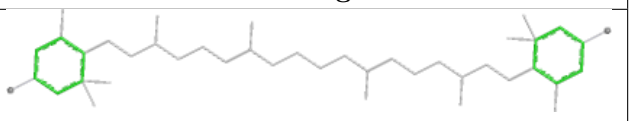
Bond lengths



Bond angles

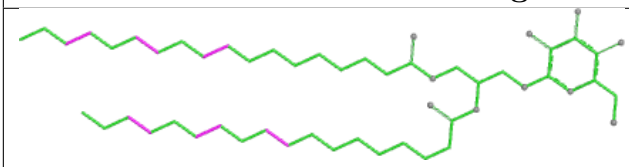


Torsions

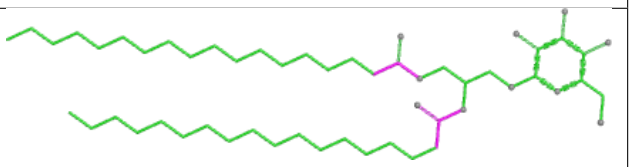


Rings

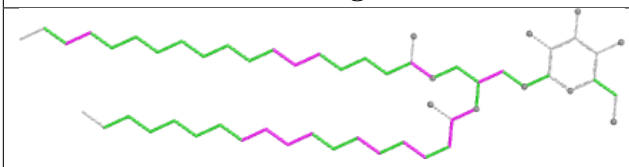
Ligand LMG C1 523



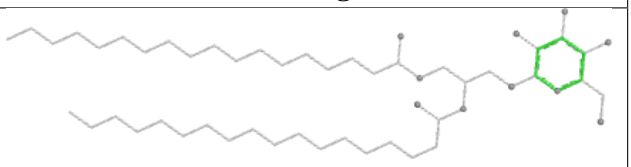
Bond lengths



Bond angles

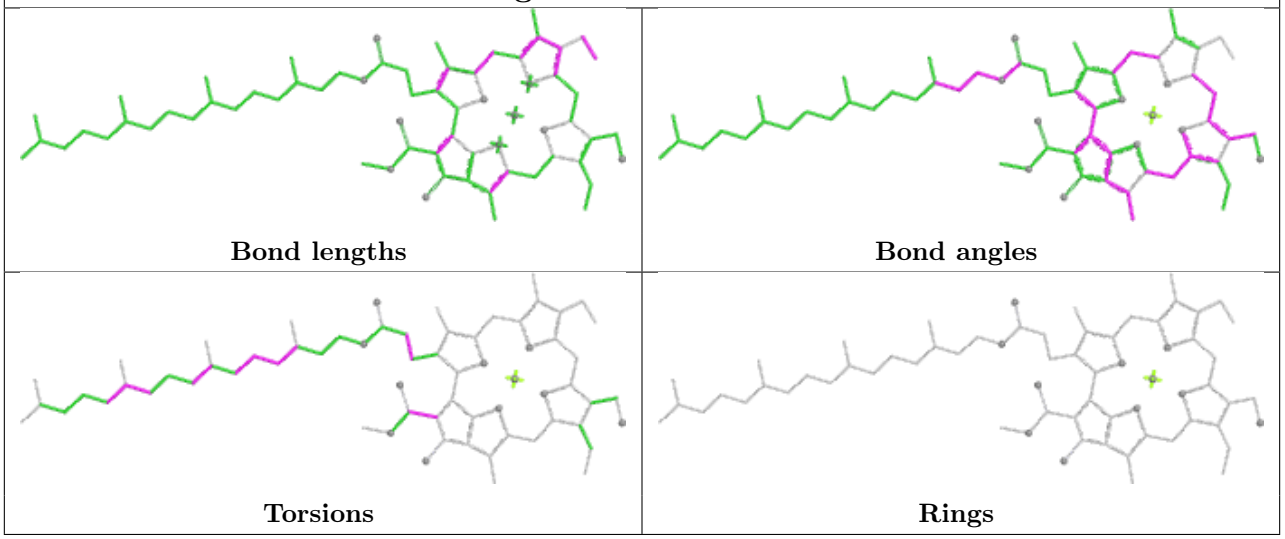


Torsions



Rings

Ligand CHL N1 606



5.7 Other polymers (i)

There are no such residues in this entry.

5.8 Polymer linkage issues (i)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	r	1
22	R	1
27	r1	1
27	R1	1
23	s	1
20	n1	1

All chain breaks are listed below:

Model	Chain	Residue-1	Atom-1	Residue-2	Atom-2	Distance (Å)
1	r	110:PRO	C	126:GLU	N	18.97
1	R	110:PRO	C	126:GLU	N	18.01
1	r1	110:PRO	C	126:GLU	N	12.33
1	R1	110:PRO	C	126:GLU	N	11.82
1	s	285:ARG	C	286:VAL	N	3.41
1	n1	57:PRO	C	58:PRO	N	3.28

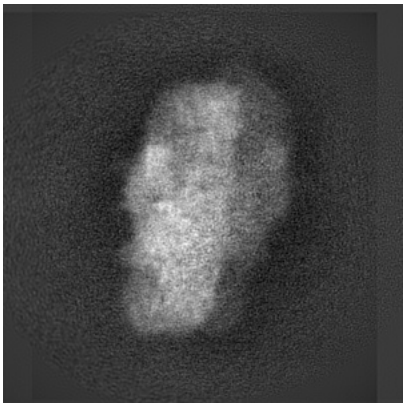
6 Map visualisation

This section contains visualisations of the EMDB entry EMD-13455. These allow visual inspection of the internal detail of the map and identification of artifacts.

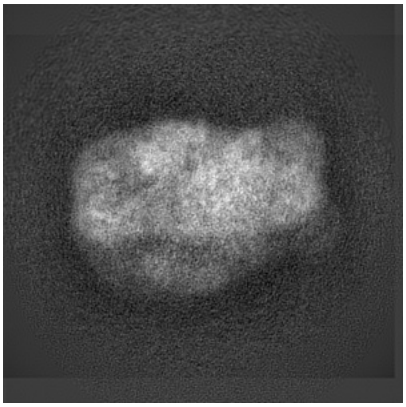
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections

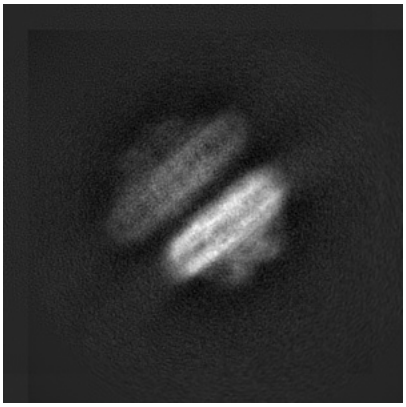
6.1.1 Primary map



X



Y

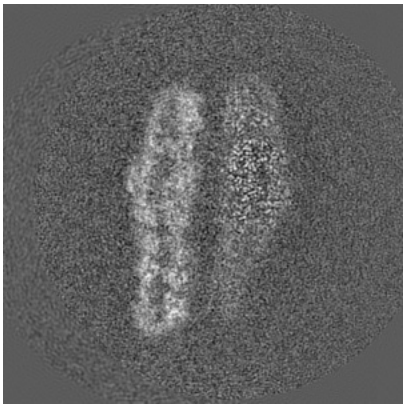


Z

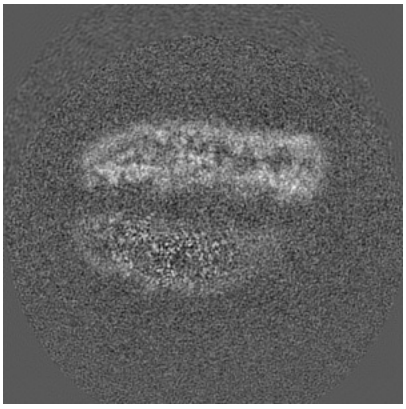
The images above show the map projected in three orthogonal directions.

6.2 Central slices

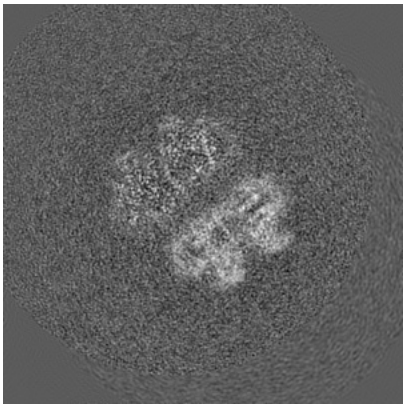
6.2.1 Primary map



X Index: 240



Y Index: 240

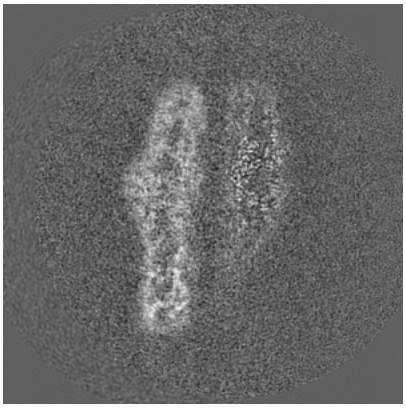


Z Index: 240

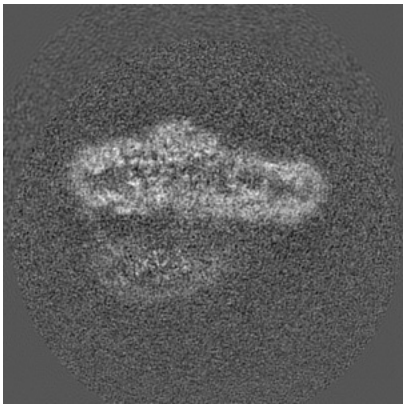
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices (i)

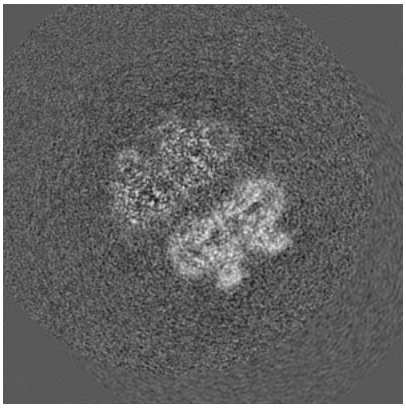
6.3.1 Primary map



X Index: 246



Y Index: 215

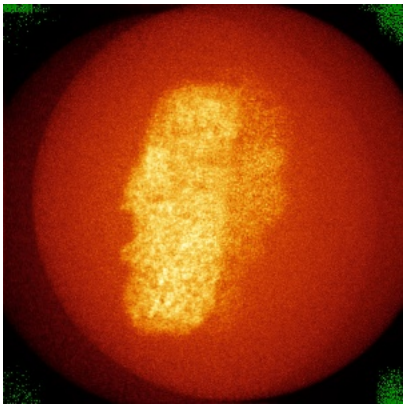


Z Index: 238

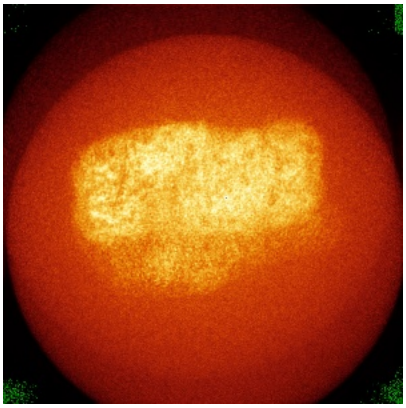
The images above show the largest variance slices of the map in three orthogonal directions.

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

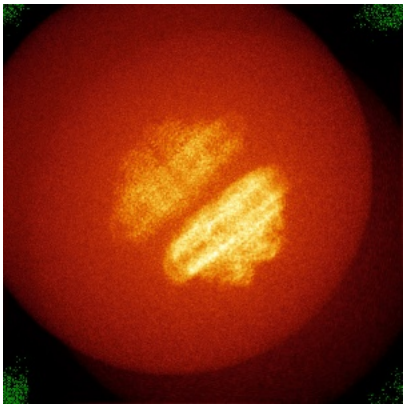
6.4.1 Primary map



X



Y



Z

The images above show the map standard deviation projections with false color in three orthogonal directions. Minimum values are shown in green, max in blue, and dark to light orange shades represent small to large values respectively.

6.5 Orthogonal surface views (i)

This section was not generated.

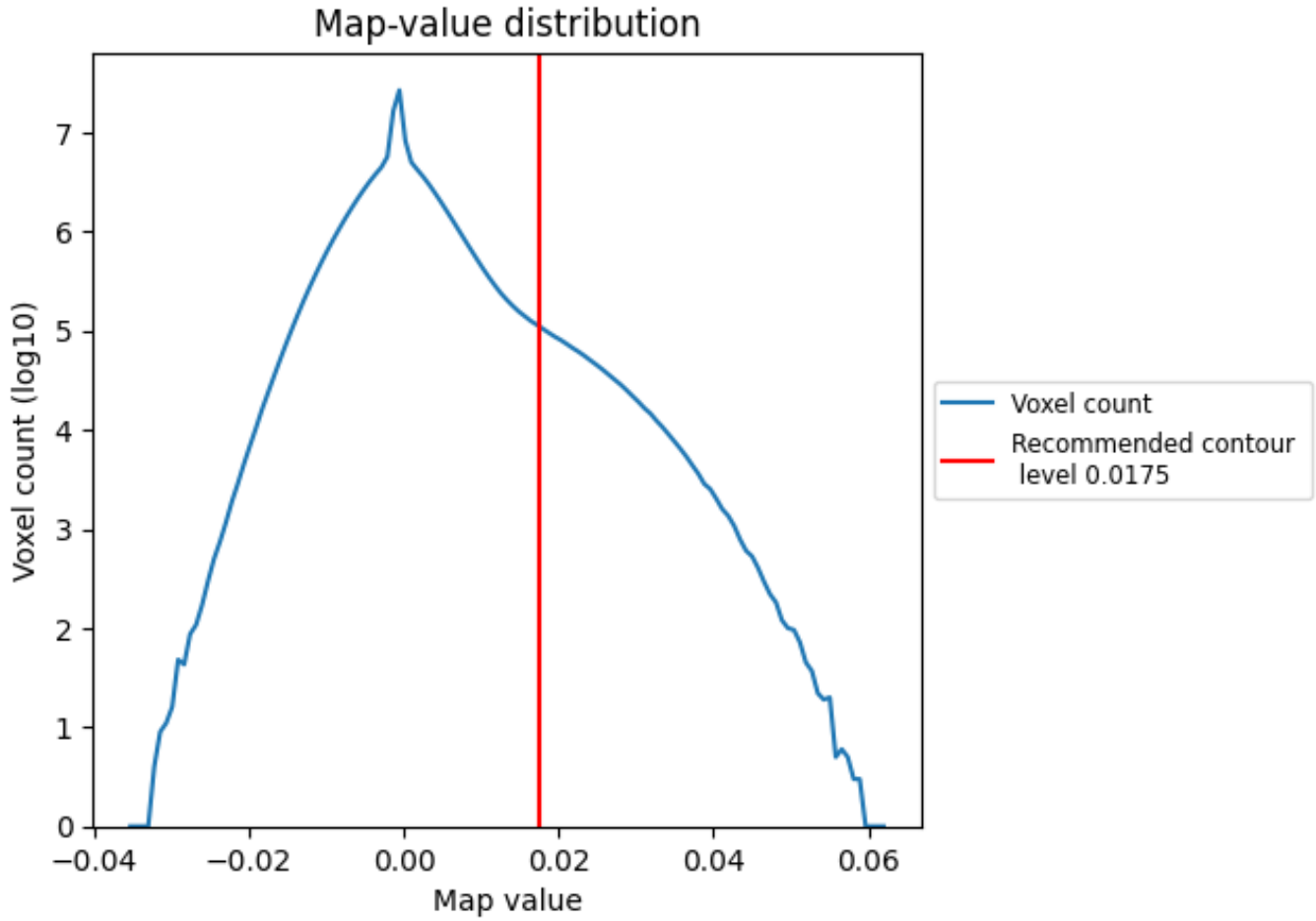
6.6 Mask visualisation (i)

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

7 Map analysis

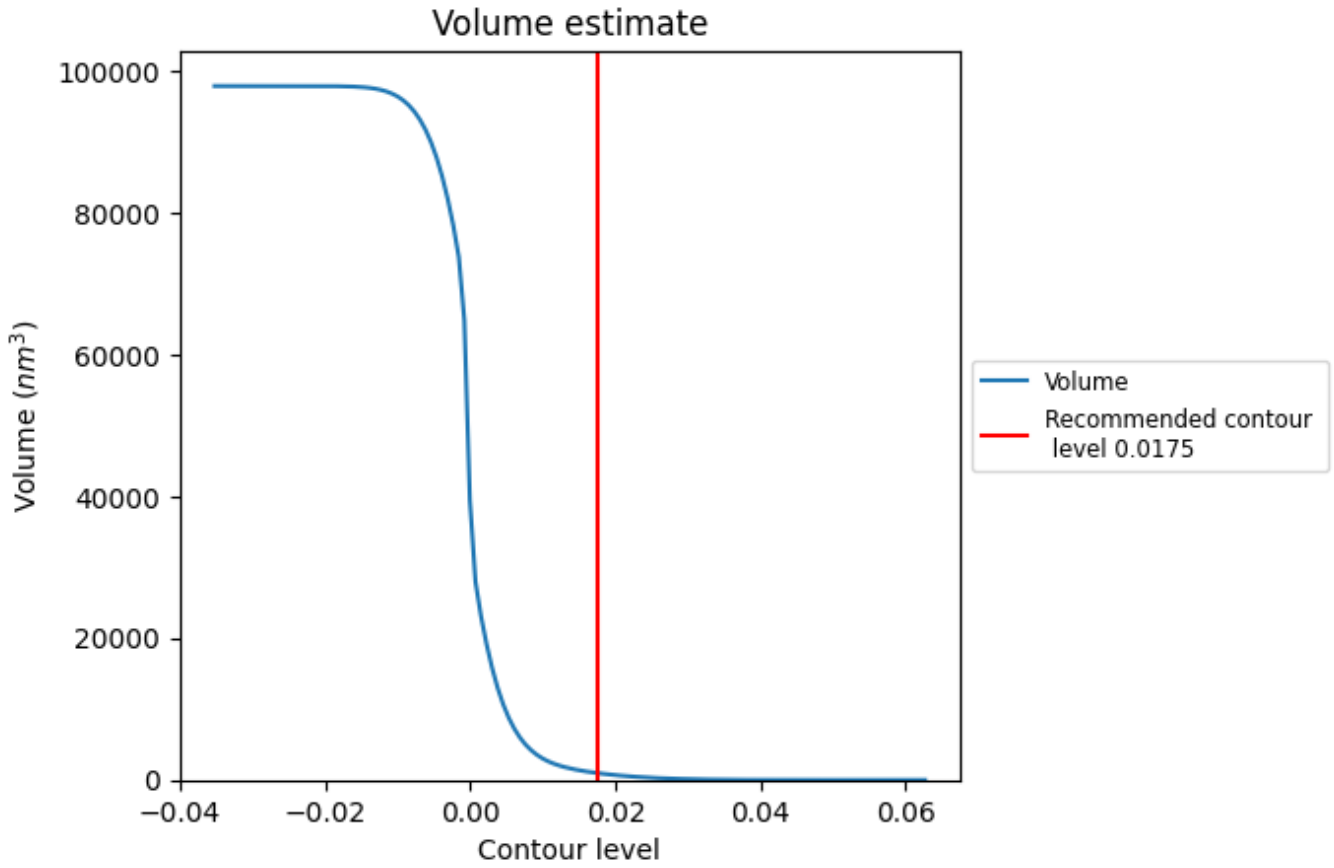
This section contains the results of statistical analysis of the map.

7.1 Map-value distribution



The map-value distribution is plotted in 128 intervals along the x-axis. The y-axis is logarithmic. A spike in this graph at zero usually indicates that the volume has been masked.

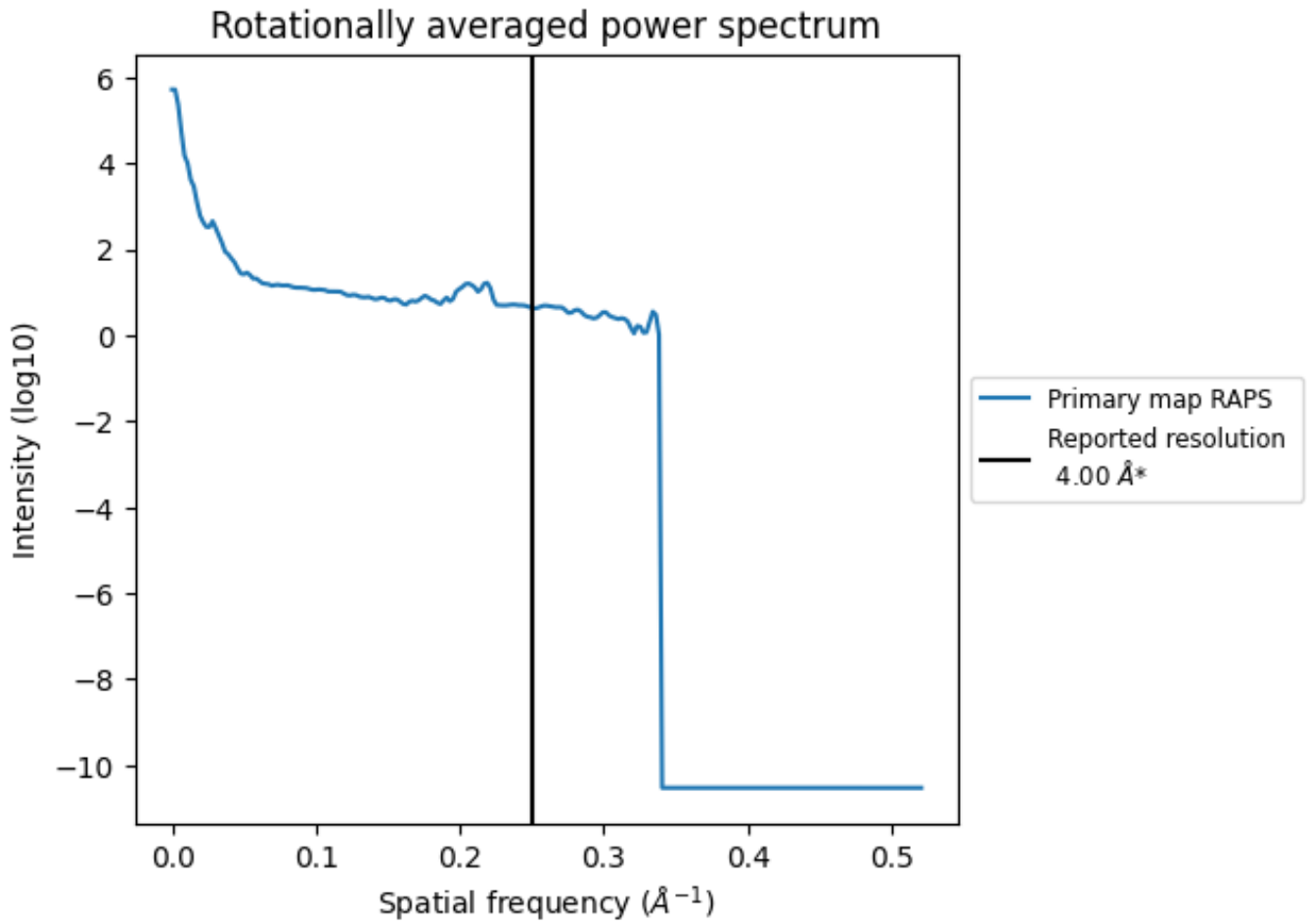
7.2 Volume estimate



The volume at the recommended contour level is 976 nm^3; this corresponds to an approximate mass of 881 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)

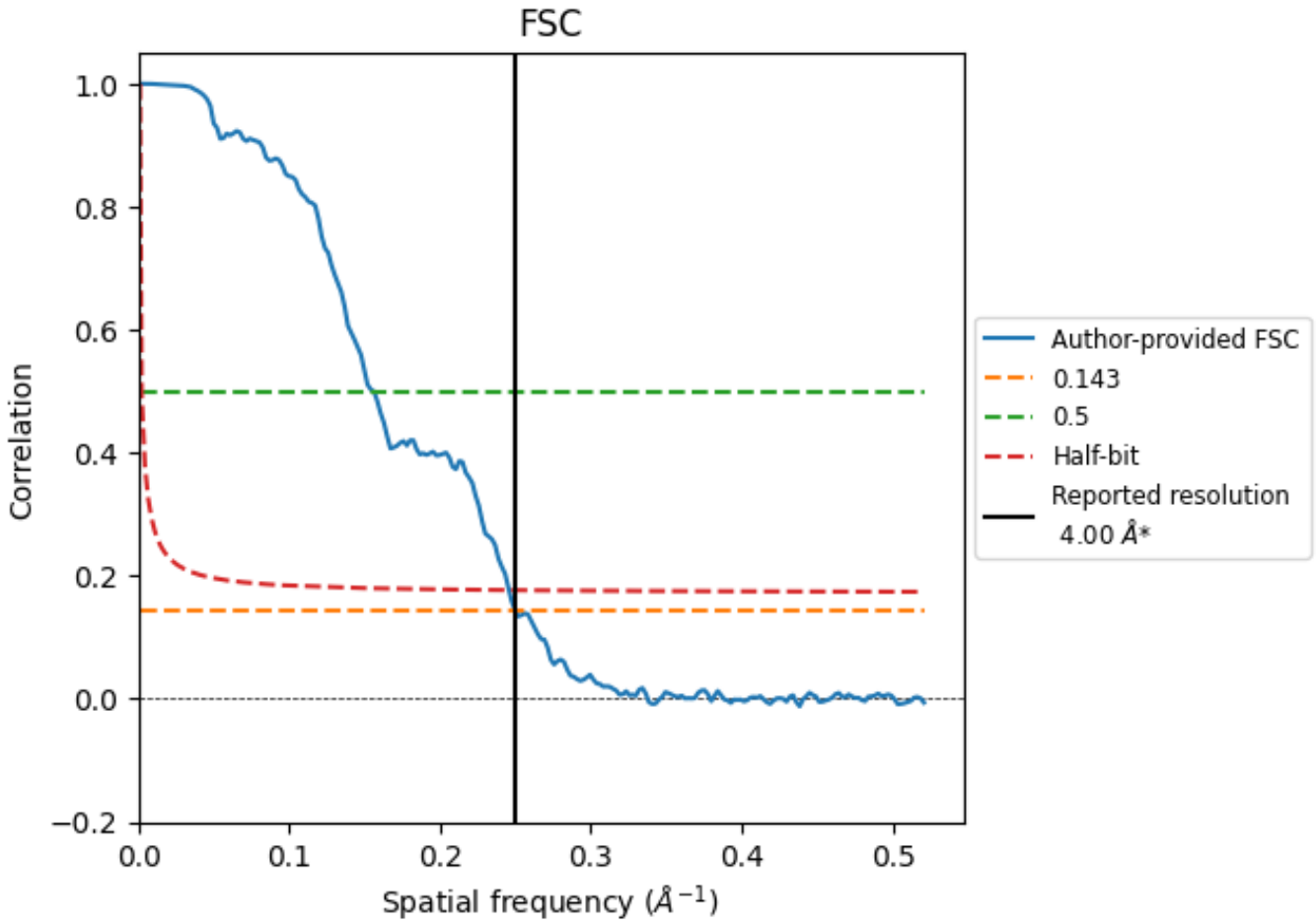


*Reported resolution corresponds to spatial frequency of 0.250 $Å^{-1}$

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 0.250 $Å^{-1}$

8.2 Resolution estimates (i)

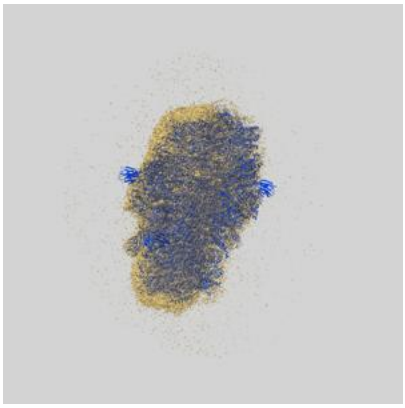
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	4.00	-	-
Author-provided FSC curve	4.00	6.41	4.07
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

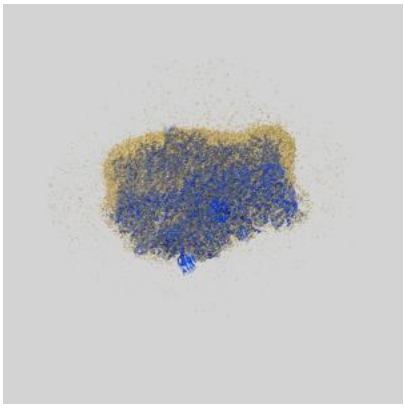
9 Map-model fit

This section contains information regarding the fit between EMDB map EMD-13455 and PDB model 7PIW. Per-residue inclusion information can be found in section 3 on page 74.

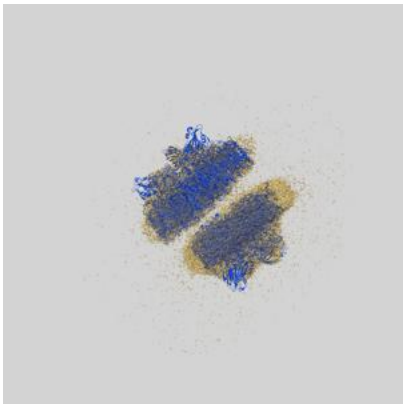
9.1 Map-model overlay



X



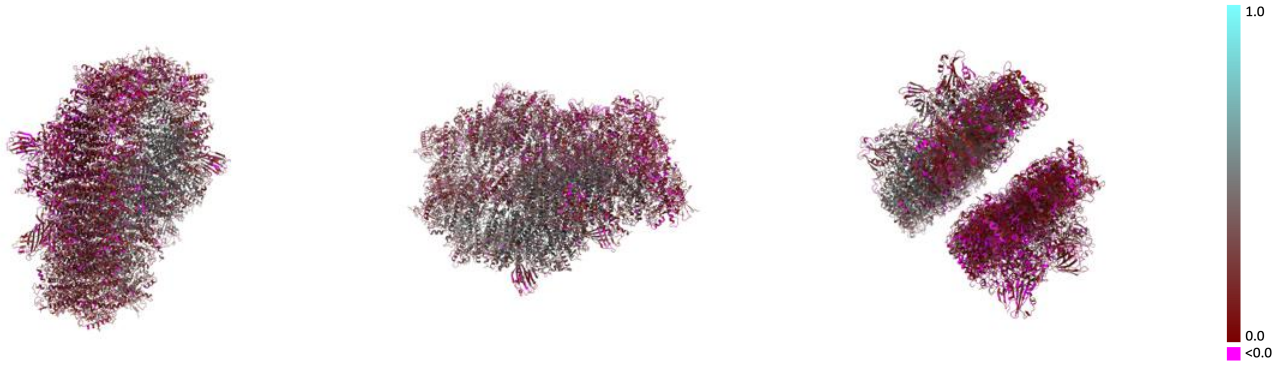
Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.0175 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model (i)



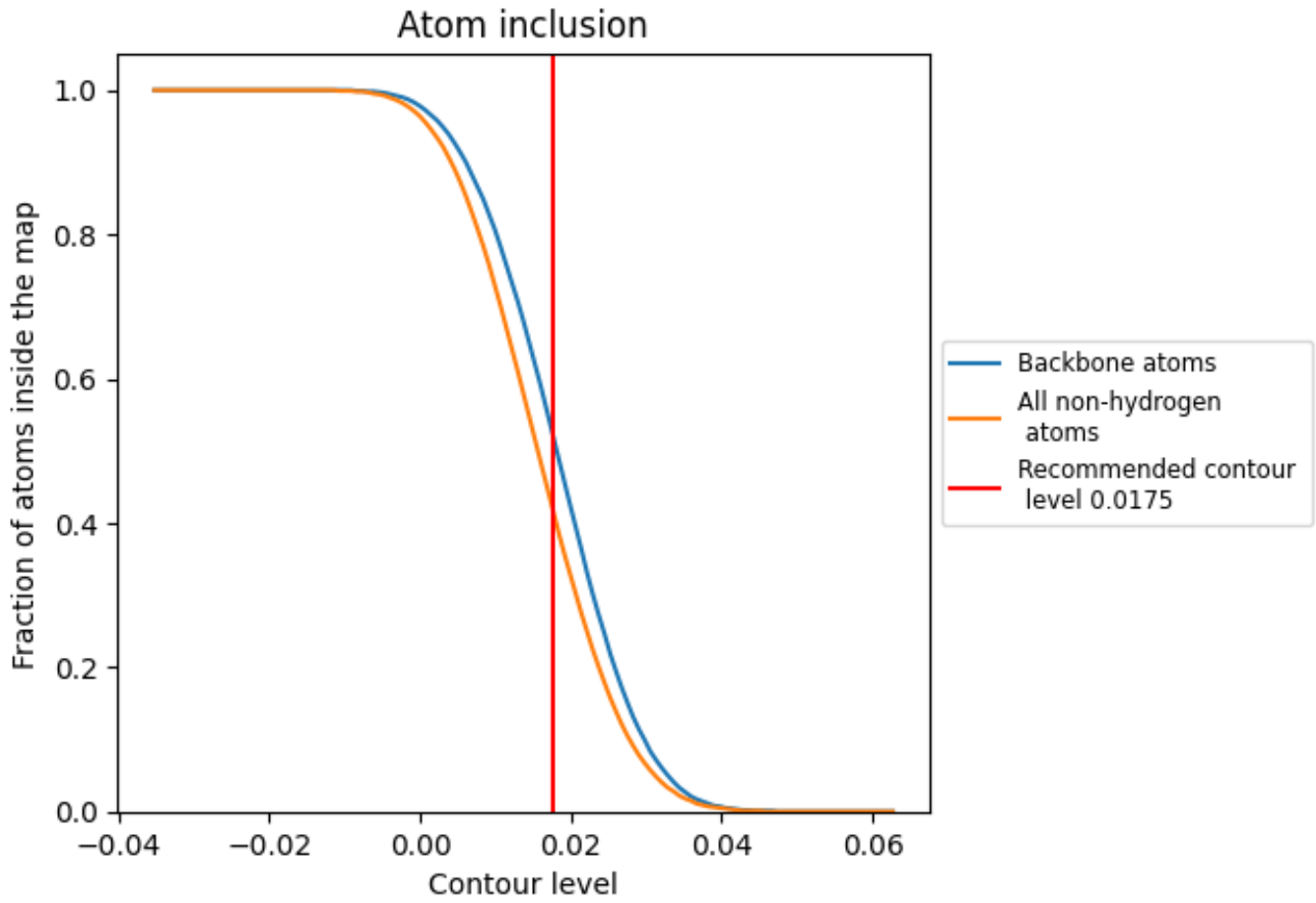
X Y Z

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

9.3 Atom inclusion mapped to coordinate model (i)

This section was not generated.

9.4 Atom inclusion (i)



At the recommended contour level, 53% of all backbone atoms, 42% 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 (0.0175) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	0.4230	0.2360
A	0.4920	0.4320
A1	0.6120	0.1910
B	0.3740	0.4030
B1	0.5830	0.1700
C	0.4930	0.4560
C1	0.6260	0.2020
D	0.4420	0.4380
D1	0.5980	0.1890
E	0.3810	0.3710
E1	0.7460	0.2080
F	0.4090	0.3800
F1	0.7590	0.2050
G	0.1980	0.2600
G1	0.6690	0.1600
H	0.2980	0.3500
H1	0.5310	0.1360
I	0.4670	0.4330
I1	0.5400	0.1970
J	0.3820	0.4050
J1	0.5240	0.1330
K	0.4160	0.4140
K1	0.6510	0.1960
L	0.3520	0.4110
L1	0.4340	0.1560
M	0.3310	0.3640
M1	0.3820	0.1470
N	0.2960	0.3340
N1	0.6720	0.1820
O	0.2270	0.3310
O1	0.6070	0.1800
P	0.0180	0.2020
P1	0.0950	0.1420
R	0.1040	0.1750
R1	0.4660	0.1110

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Chain	Atom inclusion	Q-score
S	0.2680	0.3030
S1	0.6810	0.1710
T	0.3590	0.4290
T1	0.3960	0.2160
U	0.2200	0.3330
U1	0.5410	0.2320
V	0.3600	0.3860
V1	0.6090	0.1950
W	0.3150	0.3650
W1	0.6040	0.2360
X	0.2690	0.2770
X1	0.6270	0.1450
Y	0.3620	0.3620
Y1	0.6270	0.1880
Z	0.2730	0.3710
Z1	0.6530	0.1750
a	0.4670	0.4160
a1	0.4720	0.1010
b	0.3610	0.3830
b1	0.4930	0.1120
c	0.4000	0.3630
c1	0.4770	0.0910
d	0.4390	0.4230
d1	0.4440	0.1090
e	0.2430	0.2560
e1	0.4650	0.1240
f	0.3670	0.3420
f1	0.5450	0.1770
g	0.1420	0.1520
g1	0.5720	0.0970
h	0.2440	0.3270
h1	0.4570	0.1090
i	0.4500	0.4350
i1	0.4140	0.1420
j	0.2450	0.3000
j1	0.4380	0.1210
k	0.3480	0.3170
k1	0.4060	0.0940
l	0.3920	0.4300
m	0.2480	0.3610
m1	0.3740	0.1220
n	0.1660	0.1610

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Chain	Atom inclusion	Q-score
n1	0.5480	0.1050
o	0.2180	0.2800
o1	0.5320	0.1330
p	0.0080	0.1570
p1	0.0860	0.0850
r	0.1200	0.1900
r1	0.4780	0.1150
s	0.1610	0.1410
s1	0.4600	0.0870
t	0.3590	0.3890
t1	0.3090	0.1070
u	0.2060	0.3570
u1	0.4130	0.1420
v	0.2090	0.2760
v1	0.3330	0.1020
w	0.3360	0.3470
w1	0.4700	0.1230
x	0.2590	0.2950
x1	0.3830	0.0660
y	0.3310	0.3270
y1	0.5280	0.1190
z	0.1600	0.1980
z1	0.4240	0.1280