



## Full wwPDB EM Validation Report ⓘ

Aug 10, 2022 – 05:18 am BST

PDB ID : 7PIN  
EMDB ID : EMD-13444  
Title : Stacked compact Dunaliella PSII  
Authors : Caspy, I.; Fadeeva, M.; Mazor, Y.; Nelson, N.  
Deposited on : 2021-08-22  
Resolution : 3.60 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](mailto: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>.

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

EMDB validation analysis : 0.0.1.dev8  
Mogul : 1.8.4, CSD as541be (2020)  
MolProbity : 4.02b-467  
buster-report : 1.1.7 (2018)  
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)  
Ideal geometry (proteins) : Engh & Huber (2001)  
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)  
Validation Pipeline (wwPDB-VP) : 2.29

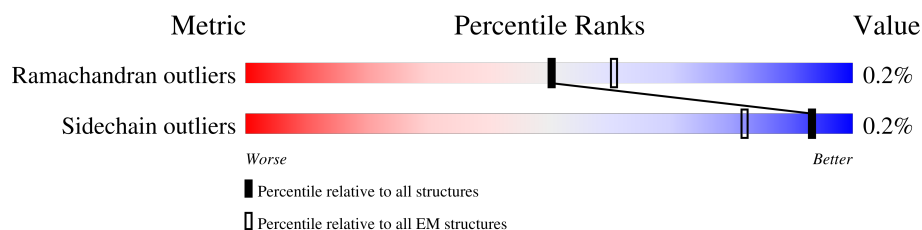
# 1 Overall quality at a glance

The following experimental techniques were used to determine the structure:

*ELECTRON MICROSCOPY*

The reported resolution of this entry is 3.60 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)
Ramachandran outliers	154571	4023
Sidechain outliers	154315	3826

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  $\geq 3$ , 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  $\leq 5\%$ . 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	100%
1	A1	336	100%
1	a	336	100%
1	a1	336	100%
2	B	484	100%
2	B1	484	99%
2	b	484	100%
2	b1	484	99%
3	V	32	100%

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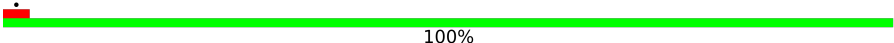
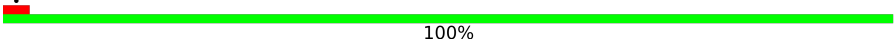
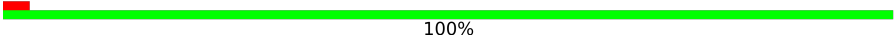
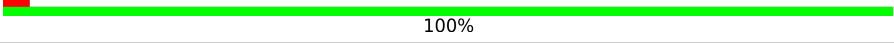
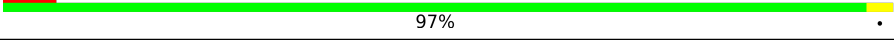
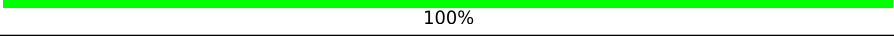
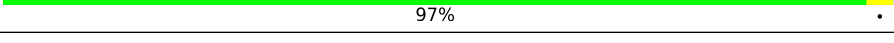
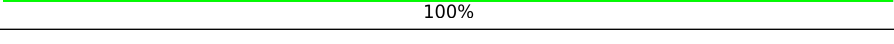
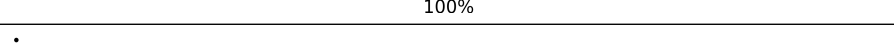
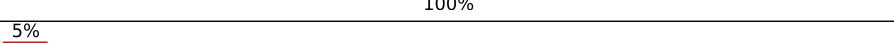
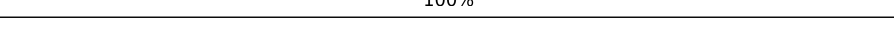
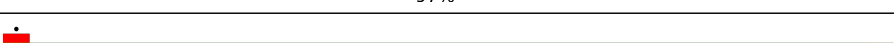






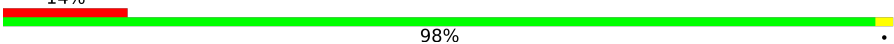
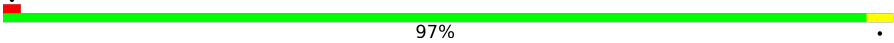
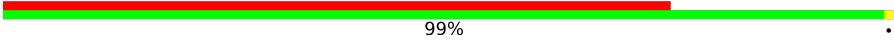
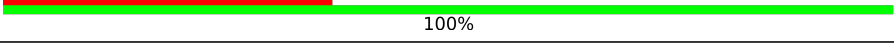
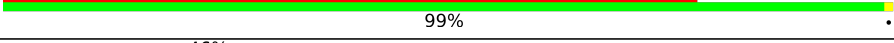
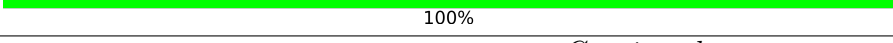



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Mol	Chain	Length	Quality of chain
3	V1	32	100%
3	v	32	100%
3	v1	32	12% 97%
4	C	449	100%
4	C1	449	100%
4	c	449	100%
4	c1	449	99%
5	D	348	99%
5	D1	348	100%
5	d	348	99%
5	d1	348	6% 99%
6	E	76	100%
6	E1	76	100%
6	e	76	5% 99%
6	e1	76	100%
7	F	31	6% 100%
7	F1	31	100%
7	f	31	100%
7	f1	31	10% 100%
8	H	67	97%
8	H1	67	99%
8	h	67	99%
8	h1	67	100%
9	I	35	100%
9	I1	35	100%

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Mol	Chain	Length	Quality of chain
9	i	35	 100%
9	i1	35	 100%
10	J	36	 100%
10	J1	36	 100%
10	j	36	 6% 97%
10	j1	36	 100%
11	K	37	 97%
11	K1	37	 100%
11	k	37	 100%
11	k1	37	 100%
12	L	38	 5% 100%
12	L1	38	 97%
12	l	38	 97%
13	M	31	 100%
13	M1	31	 100%
13	m	31	 13% 100%
13	m1	31	 6% 100%
14	O	238	 12% 98%
14	O1	238	 98%
14	o	238	 14% 98%
14	o1	238	 97%
15	P	187	 75% 99%
15	P1	187	 37% 100%
15	p	187	 78% 99%
15	p1	187	 46% 100%

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Mol	Chain	Length	Quality of chain
16	T	30	<div> <div>7%</div> <div>97%</div> <div>.</div> </div>
16	T1	30	<div> <div>.</div> <div>93%</div> <div>7%</div> </div>
16	t	30	<div> <div>.</div> <div>100%</div> </div>
16	t1	30	<div> <div>7%</div> <div>100%</div> </div>
17	W	44	<div> <div>11%</div> <div>100%</div> </div>
17	W1	44	<div> <div>100%</div> </div>
17	w	44	<div> <div>9%</div> <div>100%</div> </div>
17	w1	44	<div> <div>7%</div> <div>100%</div> </div>
18	X	30	<div> <div>23%</div> <div>100%</div> </div>
18	X1	30	<div> <div>.</div> <div>100%</div> </div>
18	x	30	<div> <div>17%</div> <div>100%</div> </div>
18	x1	30	<div> <div>10%</div> <div>100%</div> </div>
19	Z	61	<div> <div>100%</div> </div>
19	Z1	61	<div> <div>98%</div> <div>.</div> </div>
19	z	61	<div> <div>.</div> <div>100%</div> </div>
19	z1	61	<div> <div>10%</div> <div>100%</div> </div>
20	N	222	<div> <div>5%</div> <div>98%</div> <div>.</div> </div>
20	N1	222	<div> <div>99%</div> <div>.</div> </div>
20	n	222	<div> <div>8%</div> <div>99%</div> <div>.</div> </div>
20	n1	222	<div> <div>.</div> <div>98%</div> <div>.</div> </div>
21	G	221	<div> <div>9%</div> <div>100%</div> </div>
21	G1	221	<div> <div>.</div> <div>99%</div> <div>.</div> </div>
21	g	221	<div> <div>15%</div> <div>100%</div> </div>
21	g1	221	<div> <div>.</div> <div>100%</div> </div>
22	R	196	<div> <div>16%</div> <div>99%</div> <div>.</div> </div>

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Mol	Chain	Length	Quality of chain
22	R1	196	 99%
22	r	196	 99%
22	r1	196	 99%
23	S	243	 99%
23	S1	243	 99%
23	s	243	 98%
23	s1	243	 98%
24	Y	222	 99%
24	Y1	222	 99%
24	y	222	 99%
24	y1	222	 100%
25	U	27	 96%
25	U1	27	 100%
25	u	27	 96%
25	u1	27	 100%

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
29	CLA	A	405	X	-	-	-
29	CLA	A	406	X	-	-	-
29	CLA	A	407	X	-	-	-
29	CLA	A	410	X	-	-	-
29	CLA	A1	405	X	-	-	-
29	CLA	A1	406	X	-	-	-
29	CLA	A1	407	X	-	-	-
29	CLA	A1	410	X	-	-	-
29	CLA	B	602	X	-	-	-
29	CLA	B	603	X	-	-	-
29	CLA	B	604	X	-	-	-
29	CLA	B	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	B	606	X	-	-	-
29	CLA	B	607	X	-	-	-
29	CLA	B	608	X	-	-	-
29	CLA	B	609	X	-	-	-
29	CLA	B	610	X	-	-	-
29	CLA	B	611	X	-	-	-
29	CLA	B	612	X	-	-	-
29	CLA	B	613	X	-	-	-
29	CLA	B	614	X	-	-	-
29	CLA	B	615	X	-	-	-
29	CLA	B	616	X	-	-	-
29	CLA	B	617	X	-	-	-
29	CLA	B1	602	X	-	-	-
29	CLA	B1	603	X	-	-	-
29	CLA	B1	604	X	-	-	-
29	CLA	B1	605	X	-	-	-
29	CLA	B1	606	X	-	-	-
29	CLA	B1	607	X	-	-	-
29	CLA	B1	608	X	-	-	-
29	CLA	B1	609	X	-	-	-
29	CLA	B1	610	X	-	-	-
29	CLA	B1	611	X	-	-	-
29	CLA	B1	612	X	-	-	-
29	CLA	B1	613	X	-	-	-
29	CLA	B1	614	X	-	-	-
29	CLA	B1	615	X	-	-	-
29	CLA	B1	616	X	-	-	-
29	CLA	B1	617	X	-	-	-
29	CLA	C	501	X	-	-	-
29	CLA	C	502	X	-	-	-
29	CLA	C	503	X	-	-	-
29	CLA	C	504	X	-	-	-
29	CLA	C	505	X	-	-	-
29	CLA	C	506	X	-	-	-
29	CLA	C	507	X	-	-	-
29	CLA	C	508	X	-	-	-
29	CLA	C	509	X	-	-	-
29	CLA	C	510	X	-	-	-
29	CLA	C	511	X	-	-	-
29	CLA	C	512	X	-	-	-
29	CLA	C	513	X	-	-	-
29	CLA	C1	501	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	C1	502	X	-	-	-
29	CLA	C1	503	X	-	-	-
29	CLA	C1	504	X	-	-	-
29	CLA	C1	505	X	-	-	-
29	CLA	C1	506	X	-	-	-
29	CLA	C1	507	X	-	-	-
29	CLA	C1	508	X	-	-	-
29	CLA	C1	509	X	-	-	-
29	CLA	C1	510	X	-	-	-
29	CLA	C1	511	X	-	-	-
29	CLA	C1	512	X	-	-	-
29	CLA	C1	513	X	-	-	-
29	CLA	D	402	X	-	-	-
29	CLA	D	403	X	-	-	-
29	CLA	D1	402	X	-	-	-
29	CLA	D1	403	X	-	-	-
29	CLA	G	602	X	-	-	-
29	CLA	G	603	X	-	-	-
29	CLA	G	604	X	-	-	-
29	CLA	G	610	X	-	-	-
29	CLA	G	611	X	-	-	-
29	CLA	G	612	X	-	-	-
29	CLA	G	613	X	-	-	-
29	CLA	G	614	X	-	-	-
29	CLA	G1	602	X	-	-	-
29	CLA	G1	603	X	-	-	-
29	CLA	G1	604	X	-	-	-
29	CLA	G1	610	X	-	-	-
29	CLA	G1	611	X	-	-	-
29	CLA	G1	612	X	-	-	-
29	CLA	G1	613	X	-	-	-
29	CLA	G1	614	X	-	-	-
29	CLA	N	602	X	-	-	-
29	CLA	N	603	X	-	-	-
29	CLA	N	604	X	-	-	-
29	CLA	N	610	X	-	-	-
29	CLA	N	611	X	-	-	-
29	CLA	N	612	X	-	-	-
29	CLA	N	613	X	-	-	-
29	CLA	N	614	X	-	-	-
29	CLA	N1	602	X	-	-	-
29	CLA	N1	603	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	N1	604	X	-	-	-
29	CLA	N1	610	X	-	-	-
29	CLA	N1	611	X	-	-	-
29	CLA	N1	612	X	-	-	-
29	CLA	N1	613	X	-	-	-
29	CLA	N1	614	X	-	-	-
29	CLA	R	602	X	-	-	-
29	CLA	R	603	X	-	-	-
29	CLA	R	604	X	-	-	-
29	CLA	R	608	X	-	-	-
29	CLA	R	609	X	-	-	-
29	CLA	R	610	X	-	-	-
29	CLA	R	612	X	-	-	-
29	CLA	R1	602	X	-	-	-
29	CLA	R1	603	X	-	-	-
29	CLA	R1	604	X	-	-	-
29	CLA	R1	608	X	-	-	-
29	CLA	R1	609	X	-	-	-
29	CLA	R1	610	X	-	-	-
29	CLA	R1	612	X	-	-	-
29	CLA	S	602	X	-	-	-
29	CLA	S	603	X	-	-	-
29	CLA	S	604	X	-	-	-
29	CLA	S	605	X	-	-	-
29	CLA	S	609	X	-	-	-
29	CLA	S	610	X	-	-	-
29	CLA	S	611	X	-	-	-
29	CLA	S	612	X	-	-	-
29	CLA	S	613	X	-	-	-
29	CLA	S	614	X	-	-	-
29	CLA	S	617	X	-	-	-
29	CLA	S1	602	X	-	-	-
29	CLA	S1	603	X	-	-	-
29	CLA	S1	604	X	-	-	-
29	CLA	S1	605	X	-	-	-
29	CLA	S1	609	X	-	-	-
29	CLA	S1	610	X	-	-	-
29	CLA	S1	611	X	-	-	-
29	CLA	S1	612	X	-	-	-
29	CLA	S1	613	X	-	-	-
29	CLA	S1	614	X	-	-	-
29	CLA	S1	617	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	Y	602	X	-	-	-
29	CLA	Y	603	X	-	-	-
29	CLA	Y	604	X	-	-	-
29	CLA	Y	608	X	-	-	-
29	CLA	Y	610	X	-	-	-
29	CLA	Y	611	X	-	-	-
29	CLA	Y	612	X	-	-	-
29	CLA	Y	613	X	-	-	-
29	CLA	Y	614	X	-	-	-
29	CLA	Y1	602	X	-	-	-
29	CLA	Y1	603	X	-	-	-
29	CLA	Y1	604	X	-	-	-
29	CLA	Y1	608	X	-	-	-
29	CLA	Y1	610	X	-	-	-
29	CLA	Y1	611	X	-	-	-
29	CLA	Y1	612	X	-	-	-
29	CLA	Y1	613	X	-	-	-
29	CLA	Y1	614	X	-	-	-
29	CLA	a	405	X	-	-	-
29	CLA	a	406	X	-	-	-
29	CLA	a	407	X	-	-	-
29	CLA	a	410	X	-	-	-
29	CLA	a1	405	X	-	-	-
29	CLA	a1	406	X	-	-	-
29	CLA	a1	407	X	-	-	-
29	CLA	a1	410	X	-	-	-
29	CLA	b	602	X	-	-	-
29	CLA	b	603	X	-	-	-
29	CLA	b	604	X	-	-	-
29	CLA	b	605	X	-	-	-
29	CLA	b	606	X	-	-	-
29	CLA	b	607	X	-	-	-
29	CLA	b	608	X	-	-	-
29	CLA	b	609	X	-	-	-
29	CLA	b	610	X	-	-	-
29	CLA	b	611	X	-	-	-
29	CLA	b	612	X	-	-	-
29	CLA	b	613	X	-	-	-
29	CLA	b	614	X	-	-	-
29	CLA	b	615	X	-	-	-
29	CLA	b	616	X	-	-	-
29	CLA	b	617	X	-	-	-

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	d	402	X	-	-	-
29	CLA	d	403	X	-	-	-
29	CLA	d1	402	X	-	-	-
29	CLA	d1	403	X	-	-	-
29	CLA	g	602	X	-	-	-
29	CLA	g	603	X	-	-	-
29	CLA	g	604	X	-	-	-
29	CLA	g	610	X	-	-	-
29	CLA	g	611	X	-	-	-
29	CLA	g	612	X	-	-	-
29	CLA	g	613	X	-	-	-
29	CLA	g	614	X	-	-	-
29	CLA	g1	602	X	-	-	-
29	CLA	g1	603	X	-	-	-
29	CLA	g1	604	X	-	-	-
29	CLA	g1	610	X	-	-	-
29	CLA	g1	611	X	-	-	-
29	CLA	g1	612	X	-	-	-
29	CLA	g1	613	X	-	-	-
29	CLA	g1	614	X	-	-	-
29	CLA	n	602	X	-	-	-
29	CLA	n	603	X	-	-	-
29	CLA	n	604	X	-	-	-
29	CLA	n	610	X	-	-	-
29	CLA	n	611	X	-	-	-
29	CLA	n	612	X	-	-	-
29	CLA	n	613	X	-	-	-
29	CLA	n	614	X	-	-	-
29	CLA	n1	602	X	-	-	-
29	CLA	n1	603	X	-	-	-
29	CLA	n1	604	X	-	-	-
29	CLA	n1	610	X	-	-	-
29	CLA	n1	611	X	-	-	-
29	CLA	n1	612	X	-	-	-
29	CLA	n1	613	X	-	-	-
29	CLA	n1	614	X	-	-	-
29	CLA	r	602	X	-	-	-
29	CLA	r	603	X	-	-	-
29	CLA	r	604	X	-	-	-
29	CLA	r	608	X	-	-	-
29	CLA	r	609	X	-	-	-
29	CLA	r	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	r	612	X	-	-	-
29	CLA	r1	602	X	-	-	-
29	CLA	r1	603	X	-	-	-
29	CLA	r1	604	X	-	-	-
29	CLA	r1	608	X	-	-	-
29	CLA	r1	609	X	-	-	-
29	CLA	r1	610	X	-	-	-
29	CLA	r1	612	X	-	-	-
29	CLA	s	602	X	-	-	-
29	CLA	s	603	X	-	-	-
29	CLA	s	604	X	-	-	-
29	CLA	s	605	X	-	-	-
29	CLA	s	609	X	-	-	-
29	CLA	s	610	X	-	-	-
29	CLA	s	611	X	-	-	-
29	CLA	s	612	X	-	-	-
29	CLA	s	613	X	-	-	-
29	CLA	s	614	X	-	-	-
29	CLA	s	617	X	-	-	-
29	CLA	s1	602	X	-	-	-
29	CLA	s1	603	X	-	-	-
29	CLA	s1	604	X	-	-	-
29	CLA	s1	605	X	-	-	-
29	CLA	s1	609	X	-	-	-
29	CLA	s1	610	X	-	-	-
29	CLA	s1	611	X	-	-	-
29	CLA	s1	612	X	-	-	-
29	CLA	s1	613	X	-	-	-
29	CLA	s1	614	X	-	-	-
29	CLA	s1	617	X	-	-	-
29	CLA	y	602	X	-	-	-
29	CLA	y	603	X	-	-	-
29	CLA	y	604	X	-	-	-
29	CLA	y	608	X	-	-	-
29	CLA	y	610	X	-	-	-
29	CLA	y	611	X	-	-	-
29	CLA	y	612	X	-	-	-
29	CLA	y	613	X	-	-	-
29	CLA	y	614	X	-	-	-
29	CLA	y1	602	X	-	-	-
29	CLA	y1	603	X	-	-	-
29	CLA	y1	604	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
29	CLA	y1	608	X	-	-	-
29	CLA	y1	610	X	-	-	-
29	CLA	y1	611	X	-	-	-
29	CLA	y1	612	X	-	-	-
29	CLA	y1	613	X	-	-	-
29	CLA	y1	614	X	-	-	-
36	C7Z	B	620	X	-	-	-
36	C7Z	B1	620	X	-	-	-
36	C7Z	b	620	X	-	-	-
36	C7Z	b1	620	X	-	-	-
41	LMK	C	527	X	-	-	-
41	LMK	C1	527	X	-	-	-
41	LMK	c	527	X	-	-	-
41	LMK	c1	527	X	-	-	-
45	RRX	H	101	X	-	-	-
45	RRX	H1	101	X	-	-	-
45	RRX	h	101	X	-	-	-
45	RRX	h1	101	X	-	-	-
48	CHL	G	601	X	-	-	-
48	CHL	G	605	X	-	-	-
48	CHL	G	606	X	-	-	-
48	CHL	G	607	X	-	-	-
48	CHL	G	608	X	-	-	-
48	CHL	G	609	X	-	-	-
48	CHL	G1	601	X	-	-	-
48	CHL	G1	605	X	-	-	-
48	CHL	G1	606	X	-	-	-
48	CHL	G1	607	X	-	-	-
48	CHL	G1	608	X	-	-	-
48	CHL	G1	609	X	-	-	-
48	CHL	N	601	X	-	-	-
48	CHL	N	605	X	-	-	-
48	CHL	N	606	X	-	-	-
48	CHL	N	607	X	-	-	-
48	CHL	N	608	X	-	-	-
48	CHL	N	609	X	-	-	-
48	CHL	N1	601	X	-	-	-
48	CHL	N1	605	X	-	-	-
48	CHL	N1	606	X	-	-	-
48	CHL	N1	607	X	-	-	-
48	CHL	N1	608	X	-	-	-
48	CHL	N1	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
48	CHL	R	606	X	-	-	-
48	CHL	R	607	X	-	-	-
48	CHL	R1	606	X	-	-	-
48	CHL	R1	607	X	-	-	-
48	CHL	S	601	X	-	-	-
48	CHL	S	606	X	-	-	-
48	CHL	S	607	X	-	-	-
48	CHL	S	608	X	-	-	-
48	CHL	S1	601	X	-	-	-
48	CHL	S1	606	X	-	-	-
48	CHL	S1	607	X	-	-	-
48	CHL	S1	608	X	-	-	-
48	CHL	Y	601	X	-	-	-
48	CHL	Y	605	X	-	-	-
48	CHL	Y	606	X	-	-	-
48	CHL	Y	607	X	-	-	-
48	CHL	Y	609	X	-	-	-
48	CHL	Y1	601	X	-	-	-
48	CHL	Y1	605	X	-	-	-
48	CHL	Y1	606	X	-	-	-
48	CHL	Y1	607	X	-	-	-
48	CHL	Y1	609	X	-	-	-
48	CHL	g	601	X	-	-	-
48	CHL	g	605	X	-	-	-
48	CHL	g	606	X	-	-	-
48	CHL	g	607	X	-	-	-
48	CHL	g	608	X	-	-	-
48	CHL	g	609	X	-	-	-
48	CHL	g1	601	X	-	-	-
48	CHL	g1	605	X	-	-	-
48	CHL	g1	606	X	-	-	-
48	CHL	g1	607	X	-	-	-
48	CHL	g1	608	X	-	-	-
48	CHL	g1	609	X	-	-	-
48	CHL	n	601	X	-	-	-
48	CHL	n	605	X	-	-	-
48	CHL	n	606	X	-	-	-
48	CHL	n	607	X	-	-	-
48	CHL	n	608	X	-	-	-
48	CHL	n	609	X	-	-	-
48	CHL	n1	601	X	-	-	-
48	CHL	n1	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
48	CHL	n1	606	X	-	-	-
48	CHL	n1	607	X	-	-	-
48	CHL	n1	608	X	-	-	-
48	CHL	n1	609	X	-	-	-
48	CHL	r	606	X	-	-	-
48	CHL	r	607	X	-	-	-
48	CHL	r1	606	X	-	-	-
48	CHL	r1	607	X	-	-	-
48	CHL	s	601	X	-	-	-
48	CHL	s	606	X	-	-	-
48	CHL	s	607	X	-	-	-
48	CHL	s	608	X	-	-	-
48	CHL	s1	601	X	-	-	-
48	CHL	s1	606	X	-	-	-
48	CHL	s1	607	X	-	-	-
48	CHL	s1	608	X	-	-	-
48	CHL	y	601	X	-	-	-
48	CHL	y	605	X	-	-	-
48	CHL	y	606	X	-	-	-
48	CHL	y	607	X	-	-	-
48	CHL	y	609	X	-	-	-
48	CHL	y1	601	X	-	-	-
48	CHL	y1	605	X	-	-	-
48	CHL	y1	606	X	-	-	-
48	CHL	y1	607	X	-	-	-
48	CHL	y1	609	X	-	-	-
49	LUT	G	621	X	-	-	-
49	LUT	R	620	X	-	-	-
49	LUT	n1	621	X	-	-	-
50	XAT	G	622	X	-	-	-
50	XAT	G1	622	X	-	-	-
50	XAT	N	622	X	-	-	-
50	XAT	N1	622	X	-	-	-
50	XAT	Y1	622	X	-	-	-
50	XAT	g	622	X	-	-	-
50	XAT	g1	622	X	-	-	-
50	XAT	n	622	X	-	-	-
50	XAT	r	621	X	-	-	-
50	XAT	r1	621	X	-	-	-
51	NEX	g	623	X	-	-	-
51	NEX	g1	623	X	-	-	-
53	ERG	R	626	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
53	ERG	R1	626	X	-	-	-
53	ERG	r	626	X	-	-	-
53	ERG	r1	626	X	-	-	-

## 2 Entry composition [i](#)

There are 55 unique types of molecules in this entry. The entry contains 152240 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		

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

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

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



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

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

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

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

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

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

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

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

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

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

- 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 PsbJ.

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		

- 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		
11	k	37	Total	C	N	O	0	0
			297	207	43	47		
11	K1	37	Total	C	N	O	0	0
			297	207	43	47		
11	k1	37	Total	C	N	O	0	0
			297	207	43	47		

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

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

- Molecule 13 is a protein called PsbM.

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

- Molecule 14 is a protein called PsbO.

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

- 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	C	N	O	0	0
			201	132	32	37		

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

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

- Molecule 20 is a protein called LHCII M3.

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

- Molecule 21 is a protein called Chlorophyll a-b binding protein, chloroplastic.

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

There are 4 discrepancies between the modelled and reference sequences:

Chain	Residue	Modelled	Actual	Comment	Reference
G	180	ALA	PRO	conflict	UNP A1XKU7
g	180	ALA	PRO	conflict	UNP A1XKU7
G1	180	ALA	PRO	conflict	UNP A1XKU7
g1	180	ALA	PRO	conflict	UNP A1XKU7

- Molecule 22 is a protein called CP29.

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

- Molecule 23 is a protein called CP26.

Mol	Chain	Residues	Atoms					AltConf	Trace
23	S	243	Total	C	N	O	S	0	0
			1856	1200	298	355	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		

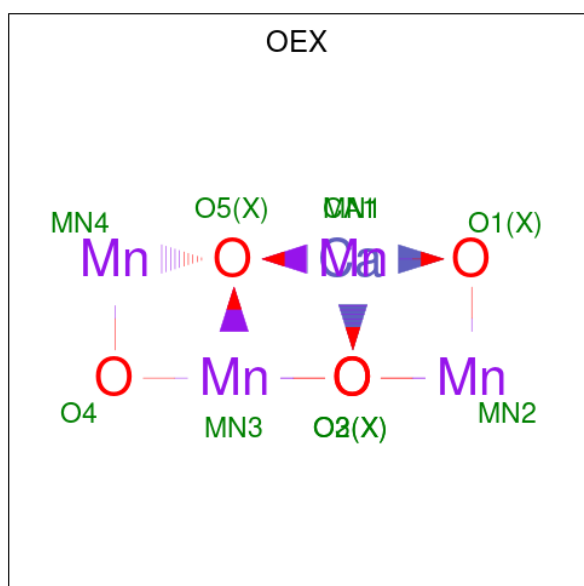
- Molecule 24 is a protein called LHCII M1.

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 CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula:  $\text{CaMn}_4\text{O}_5$ ).



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

- Molecule 27 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

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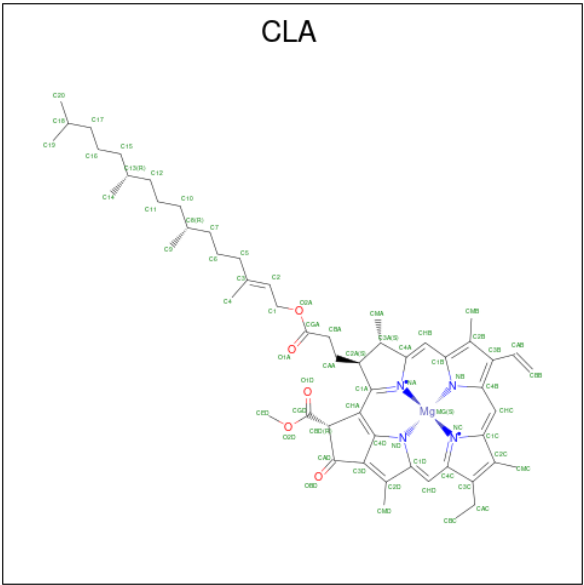
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Mol	Chain	Residues	Atoms		AltConf
27	A1	1	Total	Fe	0
			1	1	
27	a1	1	Total	Fe	0
			1	1	

- Molecule 28 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

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

- Molecule 29 is CHLOROPHYLL A (three-letter code: CLA) (formula: C<sub>55</sub>H<sub>72</sub>MgN<sub>4</sub>O<sub>5</sub>).



Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
29	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
29	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	

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Mol	Chain	Residues	Atoms					AltConf
29	A	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	

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Mol	Chain	Residues	Atoms					AltConf
29	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
29	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
29	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
29	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
29	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
29	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
29	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
29	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
29	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
29	D	1	Total 130	C 110	Mg 2	N 8	O 10	0
29	D	1	Total 130	C 110	Mg 2	N 8	O 10	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G	1	Total 466	C 388	Mg 8	N 32	O 38	0

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Mol	Chain	Residues	Atoms					AltConf
29	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	R	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	R	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	R	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	R	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	R	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	R	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	R	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	R	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	S	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S	1	Total 625	C 515	Mg 11	N 44	O 55	0

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Mol	Chain	Residues	Atoms					AltConf
29	S	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	a	1	Total 239	C 199	Mg 4	N 16	O 20	0
29	a	1	Total 239	C 199	Mg 4	N 16	O 20	0
29	a	1	Total 239	C 199	Mg 4	N 16	O 20	0
29	a	1	Total 239	C 199	Mg 4	N 16	O 20	0
29	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
29	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
29	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
29	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0
29	b	1	Total 1040	C 880	Mg 16	N 64	O 80	0

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Mol	Chain	Residues	Atoms					AltConf
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	

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Mol	Chain	Residues	Atoms					AltConf
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
29	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
29	n	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	g	1	Total	C	Mg	N	O	0
			466	388	8	32	38	
29	g	1	Total	C	Mg	N	O	0
			466	388	8	32	38	
29	g	1	Total	C	Mg	N	O	0
			466	388	8	32	38	
29	g	1	Total	C	Mg	N	O	0
			466	388	8	32	38	
29	g	1	Total	C	Mg	N	O	0
			466	388	8	32	38	
29	g	1	Total	C	Mg	N	O	0
			466	388	8	32	38	
29	g	1	Total	C	Mg	N	O	0
			466	388	8	32	38	

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Mol	Chain	Residues	Atoms					AltConf
29	r	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	r	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	r	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	r	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	r	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	r	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	r	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	y	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	y	1	Total 570	C 480	Mg 9	N 36	O 45	0

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Mol	Chain	Residues	Atoms					AltConf
29	y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	y	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	A1	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
29	A1	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
29	A1	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
29	A1	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	

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Mol	Chain	Residues	Atoms					AltConf
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	B1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	C1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	C1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	D1	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
29	D1	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
29	N1	1	Total	C	Mg	N	O	0
			468	388	8	32	40	

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Mol	Chain	Residues	Atoms					AltConf
29	N1	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N1	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N1	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N1	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N1	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N1	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N1	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	N1	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	G1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	G1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	R1	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	R1	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	R1	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	R1	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	R1	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	R1	1	Total 409	C 339	Mg 7	N 28	O 35	0

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Mol	Chain	Residues	Atoms					AltConf
29	R1	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	S1	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S1	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S1	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S1	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S1	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S1	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S1	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S1	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S1	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S1	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S1	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	S1	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	Y1	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y1	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y1	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y1	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y1	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y1	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y1	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y1	1	Total 570	C 480	Mg 9	N 36	O 45	0
29	Y1	1	Total 570	C 480	Mg 9	N 36	O 45	0

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Mol	Chain	Residues	Atoms					AltConf
29	a1	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
29	a1	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
29	a1	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
29	a1	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
29	b1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	b1	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
29	c1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	

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Mol	Chain	Residues	Atoms					AltConf
29	c1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	c1	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
29	d1	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
29	d1	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
29	n1	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n1	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n1	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n1	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n1	1	Total	C	Mg	N	O	0
			468	388	8	32	40	
29	n1	1	Total	C	Mg	N	O	0
			468	388	8	32	40	

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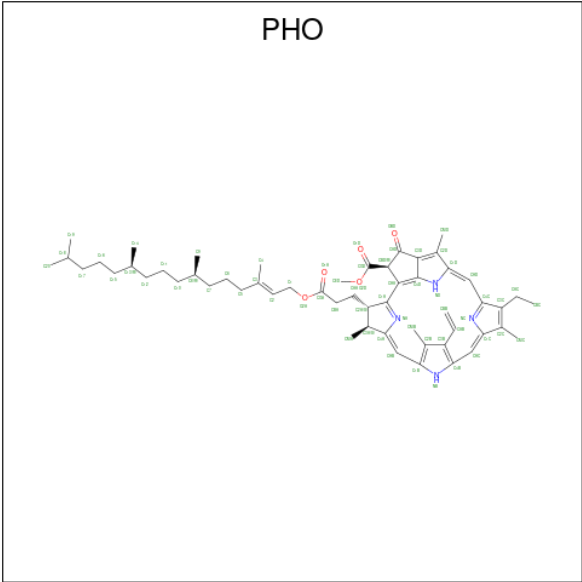
Mol	Chain	Residues	Atoms					AltConf
29	n1	1	Total 468	C 388	Mg 8	N 32	O 40	0
29	g1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	g1	1	Total 466	C 388	Mg 8	N 32	O 38	0
29	r1	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	r1	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	r1	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	r1	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	r1	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	r1	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	r1	1	Total 409	C 339	Mg 7	N 28	O 35	0
29	s1	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s1	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s1	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s1	1	Total 625	C 515	Mg 11	N 44	O 55	0
29	s1	1	Total 625	C 515	Mg 11	N 44	O 55	0

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Mol	Chain	Residues	Atoms					AltConf
29	s1	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	s1	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	s1	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	s1	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	s1	1	Total	C	Mg	N	O	0
			625	515	11	44	55	
29	y1	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	y1	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	y1	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	y1	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	y1	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	y1	1	Total	C	Mg	N	O	0
			570	480	9	36	45	
29	y1	1	Total	C	Mg	N	O	0
			570	480	9	36	45	

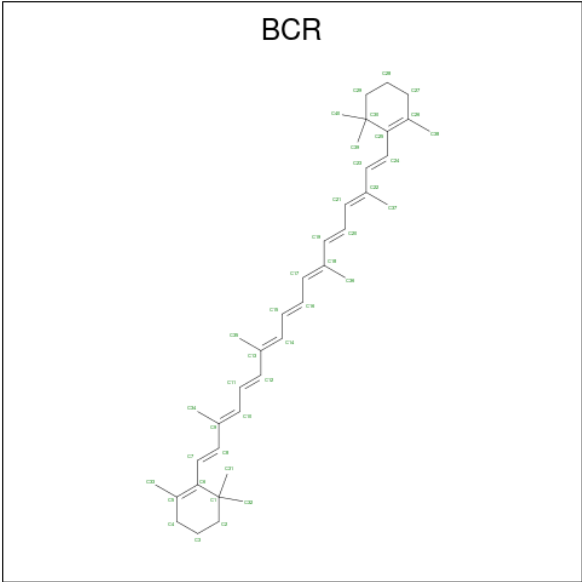
- Molecule 30 is PHEOPHYTIN A (three-letter code: PHO) (formula:  $C_{55}H_{74}N_4O_5$ ).



Mol	Chain	Residues	Atoms				AltConf
30	A	1	Total	C	N	O	0
			128	110	8	10	
30	A	1	Total	C	N	O	0
			128	110	8	10	
30	a	1	Total	C	N	O	0
			128	110	8	10	
30	a	1	Total	C	N	O	0
			128	110	8	10	
30	A1	1	Total	C	N	O	0
			128	110	8	10	
30	A1	1	Total	C	N	O	0
			128	110	8	10	
30	a1	1	Total	C	N	O	0
			128	110	8	10	
30	a1	1	Total	C	N	O	0
			128	110	8	10	

- Molecule 31 is BETA-CAROTENE (three-letter code: BCR) (formula: C<sub>40</sub>H<sub>56</sub>).





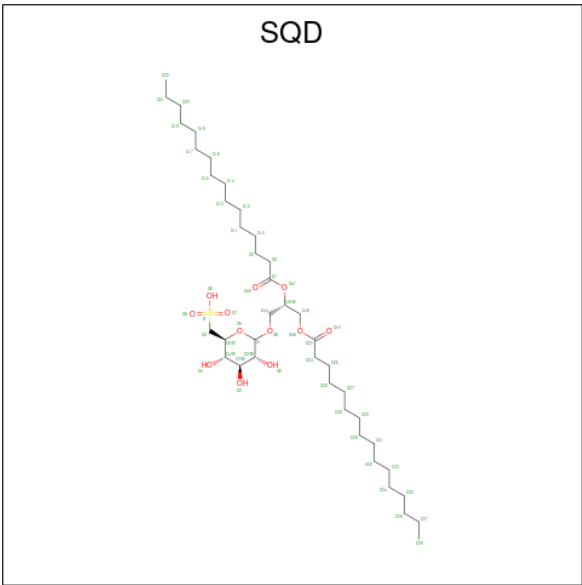
Mol	Chain	Residues	Atoms		AltConf
31	A	1	Total	C	0
			40	40	
31	B	1	Total	C	0
			80	80	
31	B	1	Total	C	0
			80	80	
31	C	1	Total	C	0
			160	160	
31	C	1	Total	C	0
			160	160	
31	C	1	Total	C	0
			160	160	
31	C	1	Total	C	0
			160	160	
31	D	1	Total	C	0
			40	40	
31	a	1	Total	C	0
			40	40	
31	b	1	Total	C	0
			80	80	
31	b	1	Total	C	0
			80	80	
31	c	1	Total	C	0
			160	160	
31	c	1	Total	C	0
			160	160	
31	c	1	Total	C	0
			160	160	

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Mol	Chain	Residues	Atoms	AltConf
31	c	1	Total C 160 160	0
31	d	1	Total C 40 40	0
31	A1	1	Total C 40 40	0
31	B1	1	Total C 80 80	0
31	B1	1	Total C 80 80	0
31	C1	1	Total C 160 160	0
31	C1	1	Total C 160 160	0
31	C1	1	Total C 160 160	0
31	C1	1	Total C 160 160	0
31	D1	1	Total C 40 40	0
31	a1	1	Total C 40 40	0
31	b1	1	Total C 80 80	0
31	b1	1	Total C 80 80	0
31	c1	1	Total C 160 160	0
31	c1	1	Total C 160 160	0
31	c1	1	Total C 160 160	0
31	c1	1	Total C 160 160	0
31	d1	1	Total C 40 40	0

- Molecule 32 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C<sub>41</sub>H<sub>78</sub>O<sub>12</sub>S).



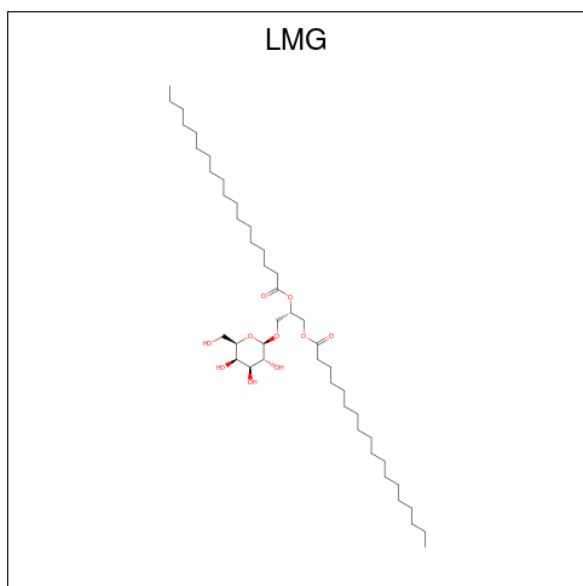
Mol	Chain	Residues	Atoms				AltConf
32	A	1	Total	C	O	S	0
			51	38	12	1	
32	B	1	Total	C	O	S	0
			96	70	24	2	
32	B	1	Total	C	O	S	0
			96	70	24	2	
32	C	1	Total	C	O	S	0
			54	41	12	1	
32	M	1	Total	C	O	S	0
			42	29	12	1	
32	a	1	Total	C	O	S	0
			51	38	12	1	
32	b	1	Total	C	O	S	0
			96	70	24	2	
32	b	1	Total	C	O	S	0
			96	70	24	2	
32	c	1	Total	C	O	S	0
			54	41	12	1	
32	m	1	Total	C	O	S	0
			42	29	12	1	
32	A1	1	Total	C	O	S	0
			51	38	12	1	
32	B1	1	Total	C	O	S	0
			96	70	24	2	
32	B1	1	Total	C	O	S	0
			96	70	24	2	
32	C1	1	Total	C	O	S	0
			54	41	12	1	

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Mol	Chain	Residues	Atoms				AltConf
32	M1	1	Total	C	O	S	0
			42	29	12	1	
32	a1	1	Total	C	O	S	0
			51	38	12	1	
32	b1	1	Total	C	O	S	0
			96	70	24	2	
32	b1	1	Total	C	O	S	0
			96	70	24	2	
32	c1	1	Total	C	O	S	0
			54	41	12	1	
32	m1	1	Total	C	O	S	0
			42	29	12	1	

- Molecule 33 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C<sub>45</sub>H<sub>86</sub>O<sub>10</sub>).



Mol	Chain	Residues	Atoms				AltConf
33	A	1	Total	C	O		0
			48	38	10		
33	B	1	Total	C	O		0
			44	34	10		
33	C	1	Total	C	O		0
			106	86	20		
33	C	1	Total	C	O		0
			106	86	20		
33	D	1	Total	C	O		0
			46	36	10		

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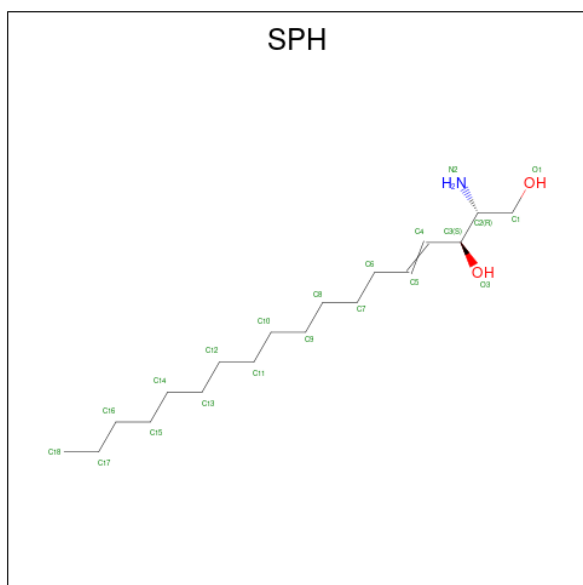
Mol	Chain	Residues	Atoms			AltConf
33	H	1	Total 48	C 38	O 10	0
33	W	1	Total 39	C 29	O 10	0
33	a	1	Total 48	C 38	O 10	0
33	b	1	Total 44	C 34	O 10	0
33	c	1	Total 106	C 86	O 20	0
33	c	1	Total 106	C 86	O 20	0
33	d	1	Total 46	C 36	O 10	0
33	h	1	Total 48	C 38	O 10	0
33	w	1	Total 39	C 29	O 10	0
33	A1	1	Total 48	C 38	O 10	0
33	B1	1	Total 44	C 34	O 10	0
33	C1	1	Total 106	C 86	O 20	0
33	C1	1	Total 106	C 86	O 20	0
33	D1	1	Total 46	C 36	O 10	0
33	H1	1	Total 48	C 38	O 10	0
33	W1	1	Total 39	C 29	O 10	0
33	a1	1	Total 48	C 38	O 10	0
33	b1	1	Total 44	C 34	O 10	0
33	c1	1	Total 106	C 86	O 20	0
33	c1	1	Total 106	C 86	O 20	0
33	d1	1	Total 46	C 36	O 10	0

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Mol	Chain	Residues	Atoms			AltConf
33	h1	1	Total	C	O	0
			48	38	10	
33	w1	1	Total	C	O	0
			39	29	10	

- Molecule 34 is SPHINGOSINE (three-letter code: SPH) (formula:  $C_{18}H_{37}NO_2$ ).

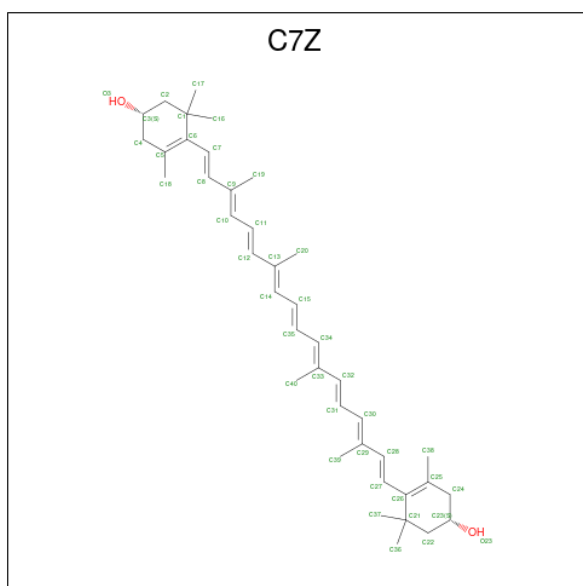


Mol	Chain	Residues	Atoms				AltConf
34	A	1	Total	C	N	O	0
			21	18	1	2	
34	Y	1	Total	C	N	O	0
			21	18	1	2	
34	a	1	Total	C	N	O	0
			21	18	1	2	
34	y	1	Total	C	N	O	0
			21	18	1	2	
34	A1	1	Total	C	N	O	0
			21	18	1	2	
34	Y1	1	Total	C	N	O	0
			21	18	1	2	
34	a1	1	Total	C	N	O	0
			21	18	1	2	
34	y1	1	Total	C	N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

- Molecule 35 is SODIUM ION (three-letter code: NA) (formula: Na).

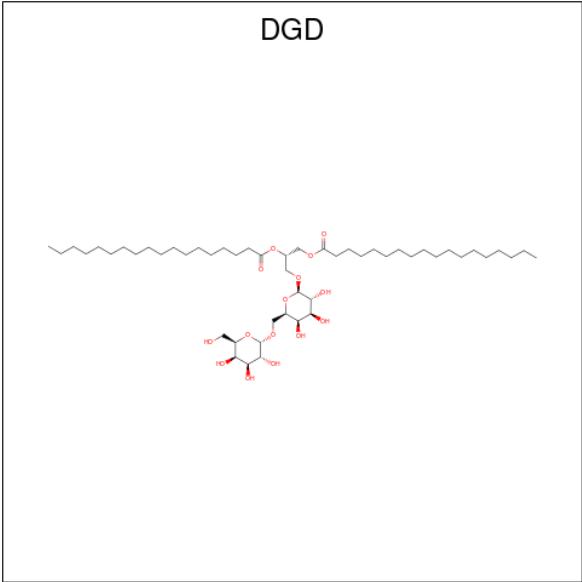
Mol	Chain	Residues	Atoms		AltConf
35	A	1	Total	Na	0
			1	1	
35	a	1	Total	Na	0
			1	1	
35	A1	1	Total	Na	0
			1	1	
35	a1	1	Total	Na	0
			1	1	

- Molecule 36 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 (three-letter code: C7Z) (formula:  $C_{40}H_{56}O_2$ ).



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

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



Mol	Chain	Residues	Atoms			AltConf
37	B	1	Total	C	O	0
			43	28	15	
37	C	1	Total	C	O	0
			176	131	45	
37	C	1	Total	C	O	0
			176	131	45	
37	C	1	Total	C	O	0
			176	131	45	
37	b	1	Total	C	O	0
			43	28	15	
37	c	1	Total	C	O	0
			176	131	45	
37	c	1	Total	C	O	0
			176	131	45	
37	c	1	Total	C	O	0
			176	131	45	
37	B1	1	Total	C	O	0
			43	28	15	
37	C1	1	Total	C	O	0
			176	131	45	
37	C1	1	Total	C	O	0
			176	131	45	
37	C1	1	Total	C	O	0
			176	131	45	
37	b1	1	Total	C	O	0
			43	28	15	
37	c1	1	Total	C	O	0
			176	131	45	

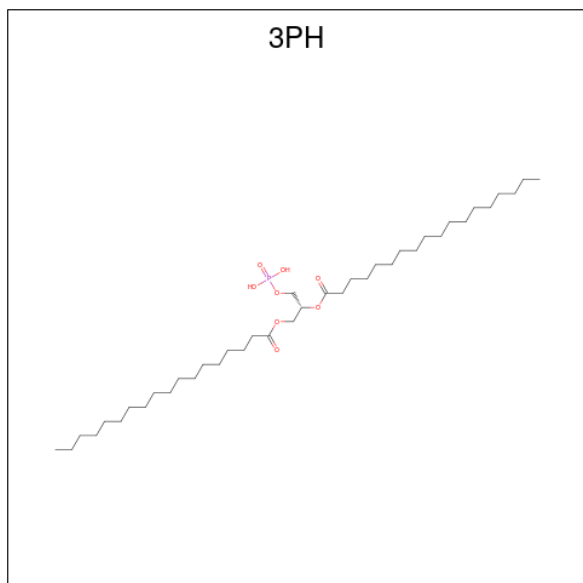
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Mol	Chain	Residues	Atoms			AltConf
37	c1	1	Total	C	O	0
			176	131	45	
37	c1	1	Total	C	O	0
			176	131	45	

- Molecule 38 is 1,2-DIACYL-GLYCEROL-3-SN-PHOSPHATE (three-letter code: 3PH) (formula: C<sub>39</sub>H<sub>77</sub>O<sub>8</sub>P).



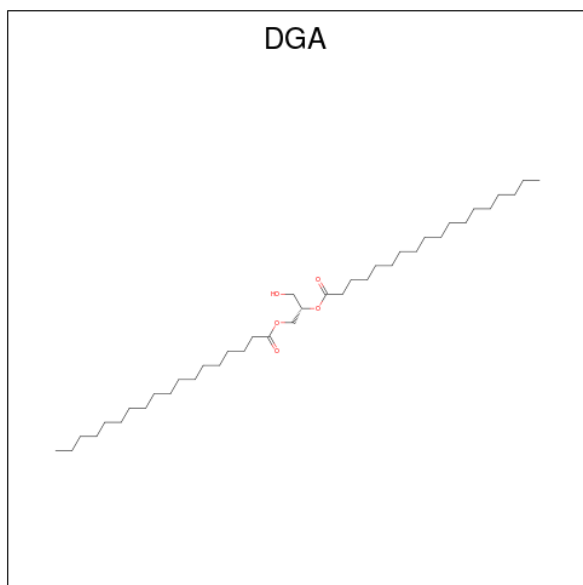
Mol	Chain	Residues	Atoms				AltConf
38	B	1	Total	C	O	P	0
			48	39	8	1	
38	T	1	Total	C	O	P	0
			48	39	8	1	
38	S	1	Total	C	O	P	0
			48	39	8	1	
38	b	1	Total	C	O	P	0
			48	39	8	1	
38	t	1	Total	C	O	P	0
			48	39	8	1	
38	s	1	Total	C	O	P	0
			48	39	8	1	
38	B1	1	Total	C	O	P	0
			48	39	8	1	
38	T1	1	Total	C	O	P	0
			48	39	8	1	
38	S1	1	Total	C	O	P	0
			48	39	8	1	

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Mol	Chain	Residues	Atoms				AltConf
38	b1	1	Total	C	O	P	0
			48	39	8	1	
38	t1	1	Total	C	O	P	0
			48	39	8	1	
38	s1	1	Total	C	O	P	0
			48	39	8	1	

- Molecule 39 is DIACYL GLYCEROL (three-letter code: DGA) (formula:  $C_{39}H_{76}O_5$ ).



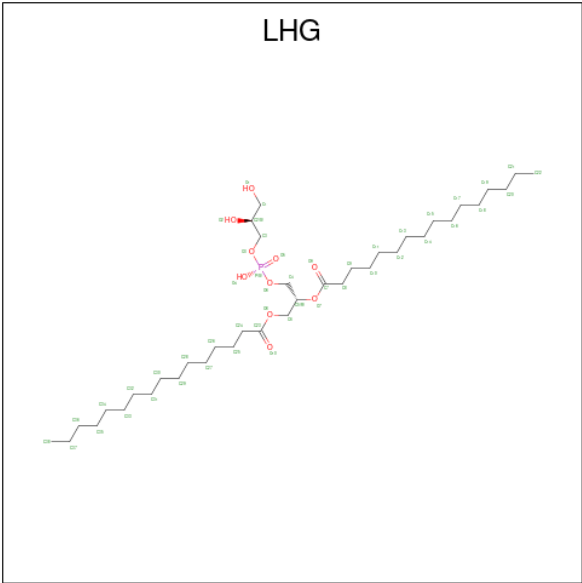
Mol	Chain	Residues	Atoms			AltConf
39	B	1	Total	C	O	0
			44	39	5	
39	C	1	Total	C	O	0
			44	39	5	
39	J	1	Total	C	O	0
			29	24	5	
39	b	1	Total	C	O	0
			44	39	5	
39	c	1	Total	C	O	0
			44	39	5	
39	j	1	Total	C	O	0
			29	24	5	
39	B1	1	Total	C	O	0
			44	39	5	
39	C1	1	Total	C	O	0
			44	39	5	

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Mol	Chain	Residues	Atoms			AltConf
39	J1	1	Total	C	O	0
			29	24	5	
39	b1	1	Total	C	O	0
			44	39	5	
39	c1	1	Total	C	O	0
			44	39	5	
39	j1	1	Total	C	O	0
			29	24	5	

- Molecule 40 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C<sub>38</sub>H<sub>75</sub>O<sub>10</sub>P).



Mol	Chain	Residues	Atoms				AltConf
40	C	1	Total	C	O	P	0
			47	36	10	1	
40	D	1	Total	C	O	P	0
			132	99	30	3	
40	D	1	Total	C	O	P	0
			132	99	30	3	
40	D	1	Total	C	O	P	0
			132	99	30	3	
40	L	1	Total	C	O	P	0
			49	38	10	1	
40	N	1	Total	C	O	P	0
			49	38	10	1	
40	G	1	Total	C	O	P	0
			49	38	10	1	

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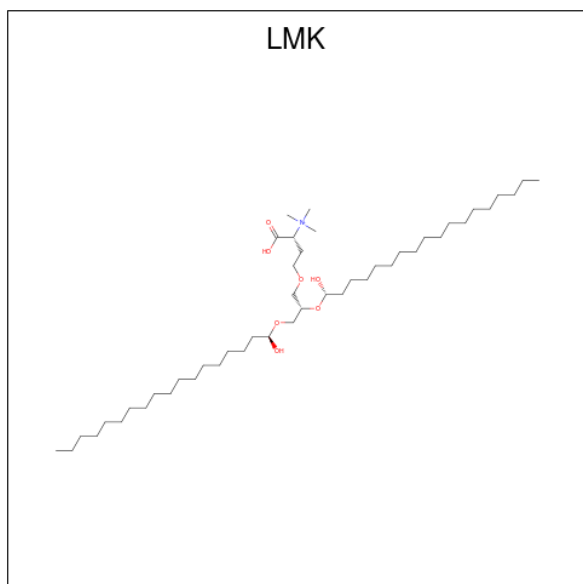
Mol	Chain	Residues	Atoms				AltConf
40	S	1	Total 45	C 34	O 10	P 1	0
40	Y	1	Total 49	C 38	O 10	P 1	0
40	c	1	Total 47	C 36	O 10	P 1	0
40	d	1	Total 132	C 99	O 30	P 3	0
40	d	1	Total 132	C 99	O 30	P 3	0
40	d	1	Total 132	C 99	O 30	P 3	0
40	l	1	Total 49	C 38	O 10	P 1	0
40	n	1	Total 49	C 38	O 10	P 1	0
40	g	1	Total 49	C 38	O 10	P 1	0
40	s	1	Total 45	C 34	O 10	P 1	0
40	y	1	Total 49	C 38	O 10	P 1	0
40	C1	1	Total 47	C 36	O 10	P 1	0
40	D1	1	Total 132	C 99	O 30	P 3	0
40	D1	1	Total 132	C 99	O 30	P 3	0
40	D1	1	Total 132	C 99	O 30	P 3	0
40	L1	1	Total 49	C 38	O 10	P 1	0
40	N1	1	Total 49	C 38	O 10	P 1	0
40	G1	1	Total 49	C 38	O 10	P 1	0
40	S1	1	Total 45	C 34	O 10	P 1	0
40	Y1	1	Total 49	C 38	O 10	P 1	0
40	c1	1	Total 47	C 36	O 10	P 1	0

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Mol	Chain	Residues	Atoms				AltConf
40	d1	1	Total	C	O	P	0
			132	99	30	3	
40	d1	1	Total	C	O	P	0
			132	99	30	3	
40	d1	1	Total	C	O	P	0
			132	99	30	3	
40	n1	1	Total	C	O	P	0
			49	38	10	1	
40	g1	1	Total	C	O	P	0
			49	38	10	1	
40	s1	1	Total	C	O	P	0
			45	34	10	1	
40	y1	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 41 is trimethyl-[(2 {R})-1-oxidanyl-1-oxidanylidene-4-[(2 {S})-2-[(1 {S})-1-oxidan-1-yl]octadecoxy]-3-[(1 {R})-1-oxidanyloctadecoxy]propoxy]butan-2-yl]azanum (three-letter code: LMK) (formula: C<sub>46</sub>H<sub>94</sub>NO<sub>7</sub>).



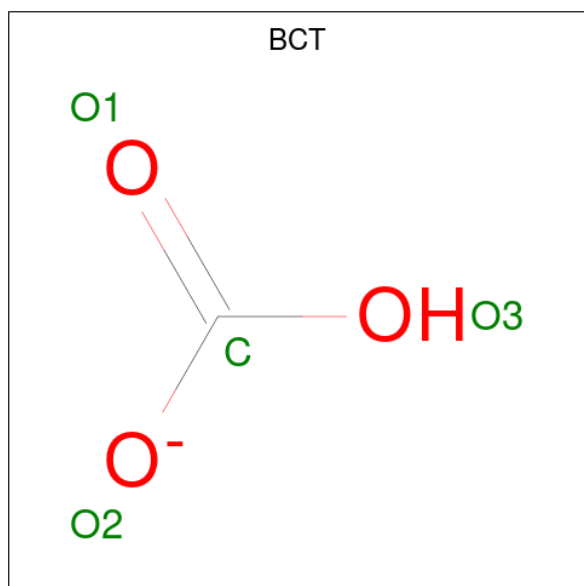
Mol	Chain	Residues	Atoms				AltConf
41	C	1	Total	C	N	O	0
			40	32	1	7	
41	c	1	Total	C	N	O	0
			40	32	1	7	
41	C1	1	Total	C	N	O	0
			40	32	1	7	

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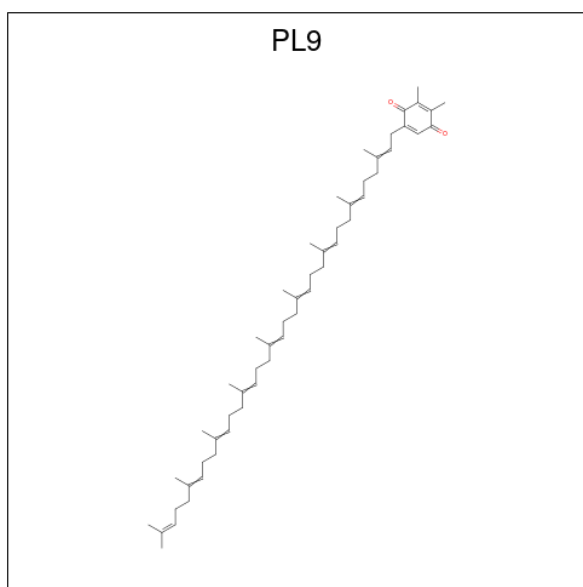
Mol	Chain	Residues	Atoms				AltConf
41	c1	1	Total	C	N	O	0
			40	32	1	7	

- Molecule 42 is BICARBONATE ION (three-letter code: BCT) (formula:  $\text{CHO}_3$ ).



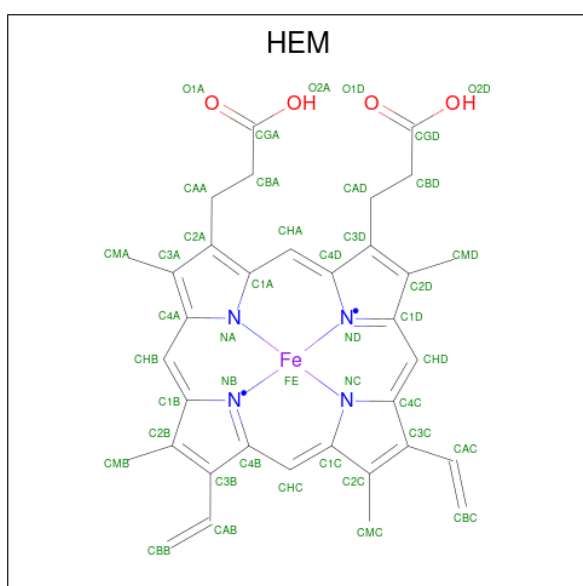
Mol	Chain	Residues	Atoms			AltConf
42	D	1	Total	C	O	0
			4	1	3	
42	d	1	Total	C	O	0
			4	1	3	
42	D1	1	Total	C	O	0
			4	1	3	
42	d1	1	Total	C	O	0
			4	1	3	

- Molecule 43 is 2,3-DIMETHYL-5-(3,7,11,15,19,23,27,31,35-NONAMETHYL-2,6,10,14,18,22,26,30,34-HEXATRIACONTANONAENYL-2,5-CYCLOHEXADIENE-1,4-DIONE-2,3-DIMETHYL-5-SOLANESYL-1,4-BENZOQUINONE (three-letter code: PL9) (formula:  $\text{C}_{53}\text{H}_{80}\text{O}_2$ ).



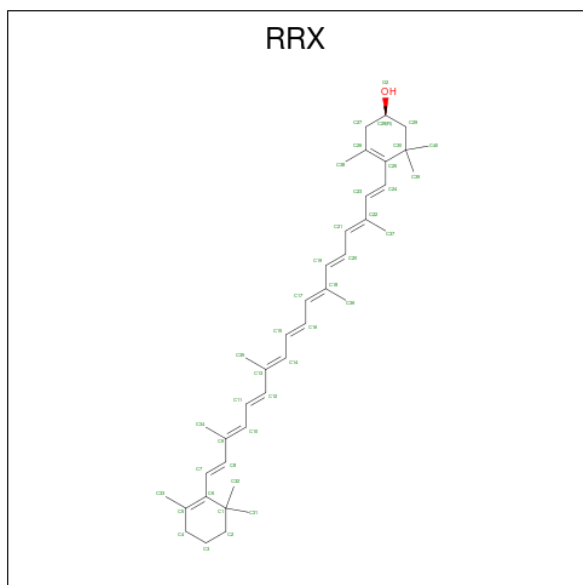
Mol	Chain	Residues	Atoms			AltConf
43	D	1	Total	C	O	0
			55	53	2	
43	d	1	Total	C	O	0
			55	53	2	
43	D1	1	Total	C	O	0
			55	53	2	
43	d1	1	Total	C	O	0
			55	53	2	

- Molecule 44 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula:  $C_{34}H_{32}FeN_4O_4$ ).



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

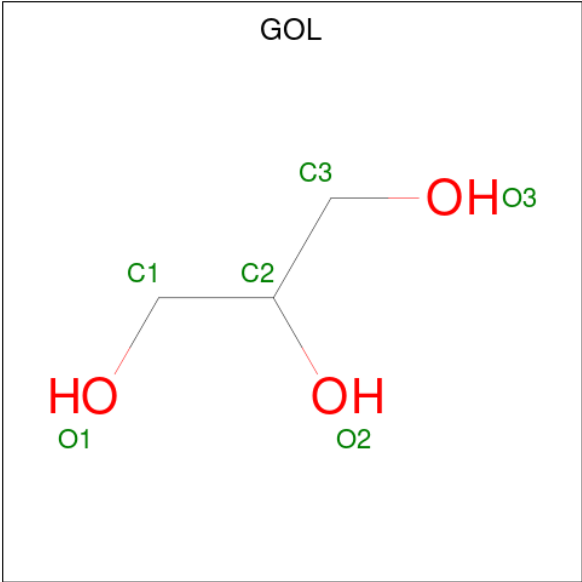
- Molecule 45 is (3R)-beta,beta-caroten-3-ol (three-letter code: RRX) (formula:  $C_{40}H_{56}O$ ).



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

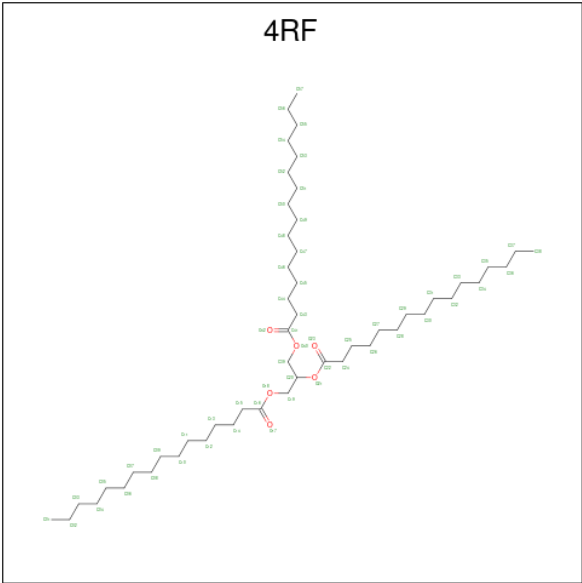
- Molecule 46 is GLYCEROL (three-letter code: GOL) (formula:  $C_3H_8O_3$ ).





Mol	Chain	Residues	Atoms			AltConf
46	I	1	Total	C	O	0
			6	3	3	
46	I1	1	Total	C	O	0
			6	3	3	

- Molecule 47 is Tripalmitoylglycerol (three-letter code: 4RF) (formula: C<sub>51</sub>H<sub>98</sub>O<sub>6</sub>).



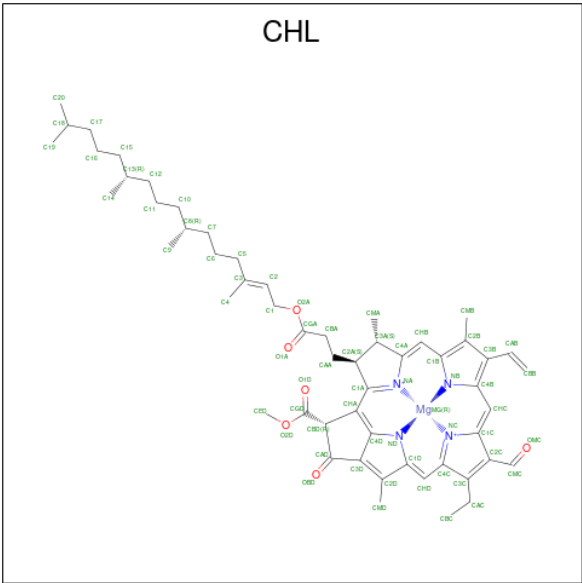
Mol	Chain	Residues	Atoms			AltConf
47	I	1	Total	C	O	0
			57	51	6	
47	K	1	Total	C	O	0
			57	51	6	

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

- Molecule 48 is CHLOROPHYLL B (three-letter code: CHL) (formula: C<sub>55</sub>H<sub>70</sub>MgN<sub>4</sub>O<sub>6</sub>).



Mol	Chain	Residues	Atoms					AltConf
48	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
48	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
48	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
48	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
48	N	1	Total	C	Mg	N	O	0
			380	314	6	24	36	

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Mol	Chain	Residues	Atoms					AltConf
48	N	1	Total 380	C 314	Mg 6	N 24	O 36	0
48	G	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	G	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	G	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	G	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	G	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	G	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	R	1	Total 94	C 74	Mg 2	N 8	O 10	0
48	R	1	Total 94	C 74	Mg 2	N 8	O 10	0
48	S	1	Total 194	C 154	Mg 4	N 16	O 20	0
48	S	1	Total 194	C 154	Mg 4	N 16	O 20	0
48	S	1	Total 194	C 154	Mg 4	N 16	O 20	0
48	S	1	Total 194	C 154	Mg 4	N 16	O 20	0
48	Y	1	Total 310	C 255	Mg 5	N 20	O 30	0
48	Y	1	Total 310	C 255	Mg 5	N 20	O 30	0
48	Y	1	Total 310	C 255	Mg 5	N 20	O 30	0
48	Y	1	Total 310	C 255	Mg 5	N 20	O 30	0
48	Y	1	Total 310	C 255	Mg 5	N 20	O 30	0
48	n	1	Total 380	C 314	Mg 6	N 24	O 36	0
48	n	1	Total 380	C 314	Mg 6	N 24	O 36	0
48	n	1	Total 380	C 314	Mg 6	N 24	O 36	0

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Mol	Chain	Residues	Atoms					AltConf
48	n	1	Total 380	C 314	Mg 6	N 24	O 36	0
48	n	1	Total 380	C 314	Mg 6	N 24	O 36	0
48	n	1	Total 380	C 314	Mg 6	N 24	O 36	0
48	g	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	g	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	g	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	g	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	g	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	g	1	Total 340	C 276	Mg 6	N 24	O 34	0
48	r	1	Total 94	C 74	Mg 2	N 8	O 10	0
48	r	1	Total 94	C 74	Mg 2	N 8	O 10	0
48	s	1	Total 194	C 154	Mg 4	N 16	O 20	0
48	s	1	Total 194	C 154	Mg 4	N 16	O 20	0
48	s	1	Total 194	C 154	Mg 4	N 16	O 20	0
48	s	1	Total 194	C 154	Mg 4	N 16	O 20	0
48	y	1	Total 310	C 255	Mg 5	N 20	O 30	0
48	y	1	Total 310	C 255	Mg 5	N 20	O 30	0
48	y	1	Total 310	C 255	Mg 5	N 20	O 30	0
48	y	1	Total 310	C 255	Mg 5	N 20	O 30	0
48	y	1	Total 310	C 255	Mg 5	N 20	O 30	0
48	N1	1	Total 380	C 314	Mg 6	N 24	O 36	0

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Mol	Chain	Residues	Atoms					AltConf
48	N1	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
48	N1	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
48	N1	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
48	N1	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
48	N1	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
48	G1	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
48	G1	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
48	G1	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
48	G1	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
48	G1	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
48	G1	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
48	R1	1	Total	C	Mg	N	O	0
			94	74	2	8	10	
48	R1	1	Total	C	Mg	N	O	0
			94	74	2	8	10	
48	S1	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
48	S1	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
48	S1	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
48	S1	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
48	Y1	1	Total	C	Mg	N	O	0
			310	255	5	20	30	
48	Y1	1	Total	C	Mg	N	O	0
			310	255	5	20	30	
48	Y1	1	Total	C	Mg	N	O	0
			310	255	5	20	30	
48	Y1	1	Total	C	Mg	N	O	0
			310	255	5	20	30	

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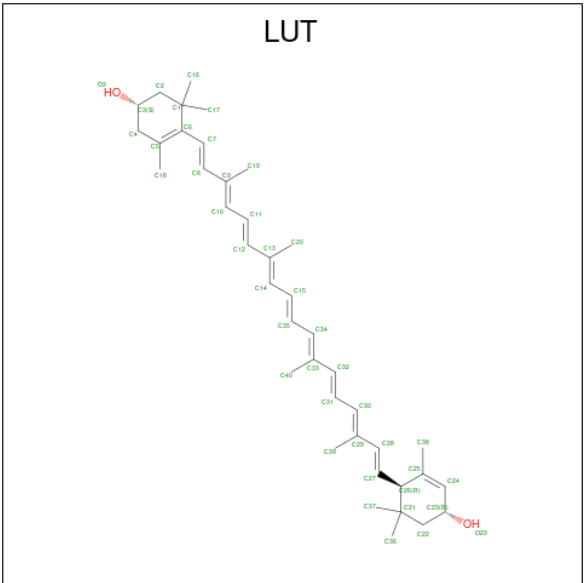
Mol	Chain	Residues	Atoms					AltConf
48	Y1	1	Total	C	Mg	N	O	0
			310	255	5	20	30	
48	n1	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
48	n1	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
48	n1	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
48	n1	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
48	n1	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
48	n1	1	Total	C	Mg	N	O	0
			380	314	6	24	36	
48	g1	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
48	g1	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
48	g1	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
48	g1	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
48	g1	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
48	g1	1	Total	C	Mg	N	O	0
			340	276	6	24	34	
48	r1	1	Total	C	Mg	N	O	0
			94	74	2	8	10	
48	r1	1	Total	C	Mg	N	O	0
			94	74	2	8	10	
48	s1	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
48	s1	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
48	s1	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
48	s1	1	Total	C	Mg	N	O	0
			194	154	4	16	20	
48	y1	1	Total	C	Mg	N	O	0
			310	255	5	20	30	
48	y1	1	Total	C	Mg	N	O	0
			310	255	5	20	30	

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Mol	Chain	Residues	Atoms					AltConf
48	y1	1	Total	C	Mg	N	O	0
			310	255	5	20	30	
48	y1	1	Total	C	Mg	N	O	0
			310	255	5	20	30	
48	y1	1	Total	C	Mg	N	O	0
			310	255	5	20	30	

- Molecule 49 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>2</sub>).



Mol	Chain	Residues	Atoms			AltConf
49	N	1	Total	C	O	0
			84	80	4	
49	N	1	Total	C	O	0
			84	80	4	
49	G	1	Total	C	O	0
			84	80	4	
49	G	1	Total	C	O	0
			84	80	4	
49	R	1	Total	C	O	0
			42	40	2	
49	S	1	Total	C	O	0
			84	80	4	
49	S	1	Total	C	O	0
			84	80	4	
49	Y	1	Total	C	O	0
			84	80	4	

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Mol	Chain	Residues	Atoms			AltConf
49	Y	1	Total	C	O	0
			84	80	4	
49	n	1	Total	C	O	0
			84	80	4	
49	n	1	Total	C	O	0
			84	80	4	
49	g	1	Total	C	O	0
			84	80	4	
49	g	1	Total	C	O	0
			84	80	4	
49	r	1	Total	C	O	0
			42	40	2	
49	s	1	Total	C	O	0
			84	80	4	
49	s	1	Total	C	O	0
			84	80	4	
49	y	1	Total	C	O	0
			84	80	4	
49	y	1	Total	C	O	0
			84	80	4	
49	N1	1	Total	C	O	0
			84	80	4	
49	N1	1	Total	C	O	0
			84	80	4	
49	G1	1	Total	C	O	0
			84	80	4	
49	G1	1	Total	C	O	0
			84	80	4	
49	R1	1	Total	C	O	0
			42	40	2	
49	S1	1	Total	C	O	0
			84	80	4	
49	S1	1	Total	C	O	0
			84	80	4	
49	Y1	1	Total	C	O	0
			84	80	4	
49	Y1	1	Total	C	O	0
			84	80	4	
49	n1	1	Total	C	O	0
			84	80	4	
49	n1	1	Total	C	O	0
			84	80	4	

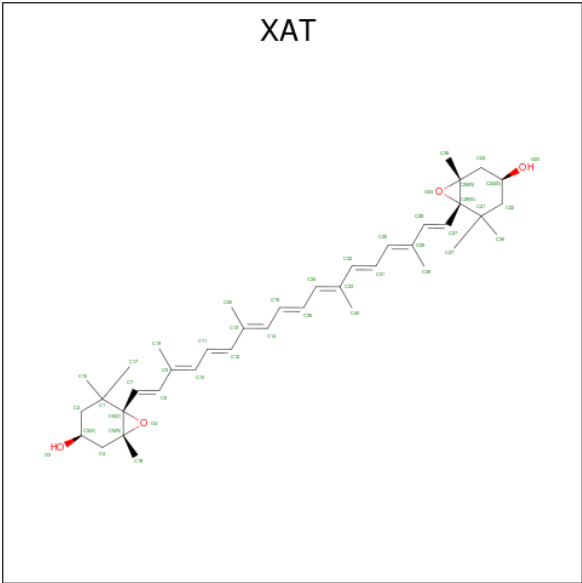
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Mol	Chain	Residues	Atoms			AltConf
49	g1	1	Total	C	O	0
			84	80	4	
49	g1	1	Total	C	O	0
			84	80	4	
49	r1	1	Total	C	O	0
			42	40	2	
49	s1	1	Total	C	O	0
			84	80	4	
49	s1	1	Total	C	O	0
			84	80	4	
49	y1	1	Total	C	O	0
			84	80	4	
49	y1	1	Total	C	O	0
			84	80	4	

- Molecule 50 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 (three-letter code: XAT) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



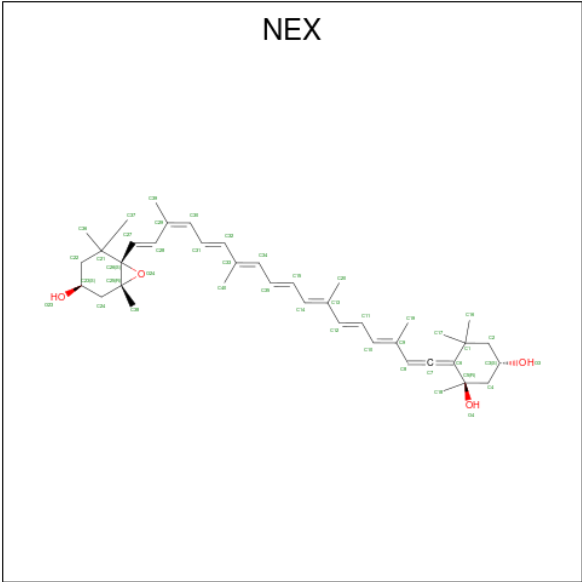
Mol	Chain	Residues	Atoms			AltConf
50	N	1	Total	C	O	0
			44	40	4	
50	G	1	Total	C	O	0
			44	40	4	
50	R	1	Total	C	O	0
			44	40	4	
50	Y	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
50	n	1	Total	C	O	0
			44	40	4	
50	g	1	Total	C	O	0
			44	40	4	
50	r	1	Total	C	O	0
			44	40	4	
50	y	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	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	y1	1	Total	C	O	0
			44	40	4	

- Molecule 51 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-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE}-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C<sub>40</sub>H<sub>56</sub>O<sub>4</sub>).



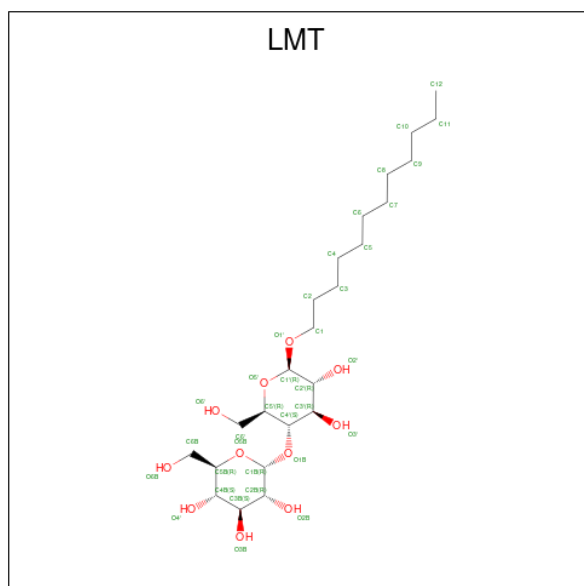
Mol	Chain	Residues	Atoms			AltConf
51	N	1	Total	C	O	0
			44	40	4	
51	G	1	Total	C	O	0
			44	40	4	
51	R	1	Total	C	O	0
			44	40	4	
51	S	1	Total	C	O	0
			44	40	4	
51	Y	1	Total	C	O	0
			44	40	4	
51	n	1	Total	C	O	0
			44	40	4	
51	g	1	Total	C	O	0
			44	40	4	
51	r	1	Total	C	O	0
			44	40	4	
51	s	1	Total	C	O	0
			44	40	4	
51	y	1	Total	C	O	0
			44	40	4	
51	N1	1	Total	C	O	0
			44	40	4	
51	G1	1	Total	C	O	0
			44	40	4	
51	R1	1	Total	C	O	0
			44	40	4	
51	S1	1	Total	C	O	0
			44	40	4	

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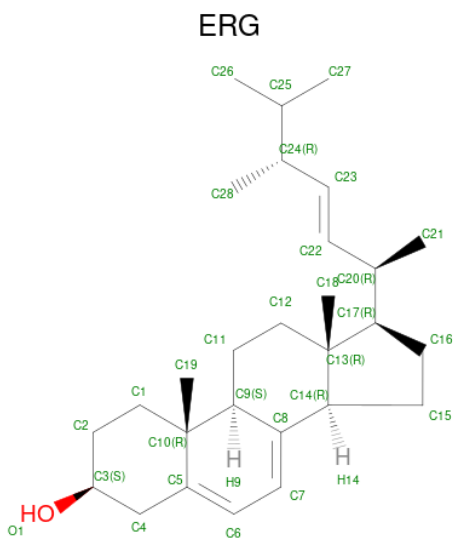
Mol	Chain	Residues	Atoms			AltConf
51	Y1	1	Total	C	O	0
			44	40	4	
51	n1	1	Total	C	O	0
			44	40	4	
51	g1	1	Total	C	O	0
			44	40	4	
51	r1	1	Total	C	O	0
			44	40	4	
51	s1	1	Total	C	O	0
			44	40	4	
51	y1	1	Total	C	O	0
			44	40	4	

- Molecule 52 is DODECYL-BETA-D-MALTOSIDE (three-letter code: LMT) (formula:  $C_{24}H_{46}O_{11}$ ).



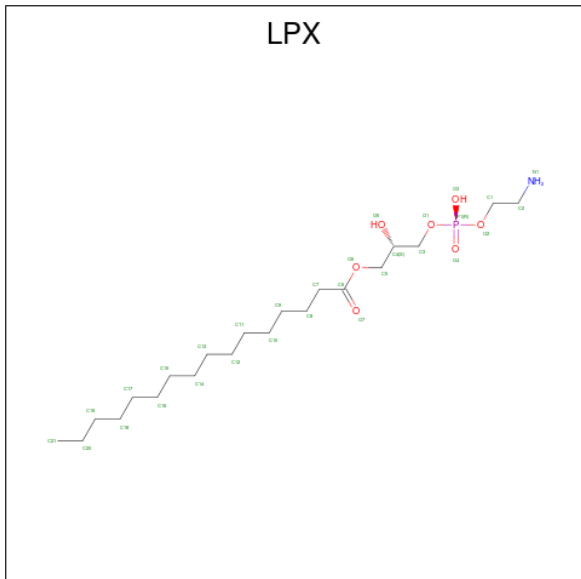
Mol	Chain	Residues	Atoms			AltConf
52	R	1	Total	C	O	0
			35	24	11	
52	r	1	Total	C	O	0
			35	24	11	
52	R1	1	Total	C	O	0
			35	24	11	
52	r1	1	Total	C	O	0
			35	24	11	

- Molecule 53 is ERGOSTEROL (three-letter code: ERG) (formula:  $C_{28}H_{44}O$ ).



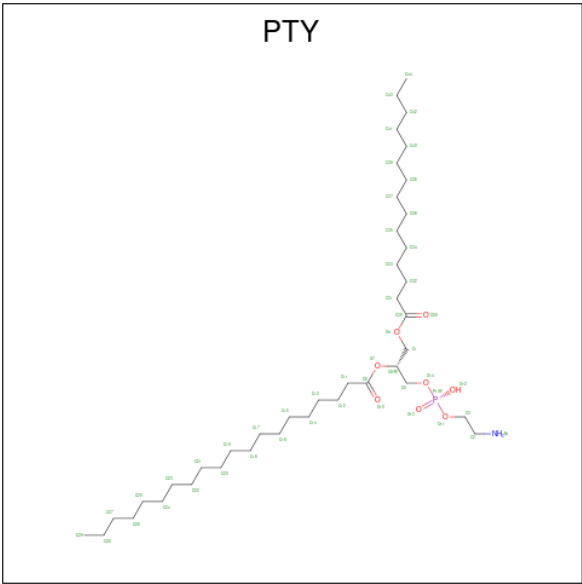
Mol	Chain	Residues	Atoms			AltConf
53	R	1	Total 29	C 28	O 1	0
53	r	1	Total 29	C 28	O 1	0
53	R1	1	Total 29	C 28	O 1	0
53	r1	1	Total 29	C 28	O 1	0

- Molecule 54 is (2S)-3-[(R)-(2-aminoethoxy)(hydroxy)phosphoryl]oxy}-2-hydroxypropyl hexadecanoate (three-letter code: LPX) (formula: C<sub>21</sub>H<sub>44</sub>NO<sub>7</sub>P).



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

- Molecule 55 is PHOSPHATIDYLETHANOLAMINE (three-letter code: PTY) (formula: C<sub>40</sub>H<sub>80</sub>NO<sub>8</sub>P).



Mol	Chain	Residues	Atoms					AltConf
55	Y	1	Total	C	N	O	P	0
			69	49	2	16	2	
55	Y	1	Total	C	N	O	P	0
			69	49	2	16	2	
55	y	1	Total	C	N	O	P	0
			69	49	2	16	2	
55	y	1	Total	C	N	O	P	0
			69	49	2	16	2	
55	Y1	1	Total	C	N	O	P	0
			69	49	2	16	2	
55	Y1	1	Total	C	N	O	P	0
			69	49	2	16	2	
55	y1	1	Total	C	N	O	P	0
			69	49	2	16	2	

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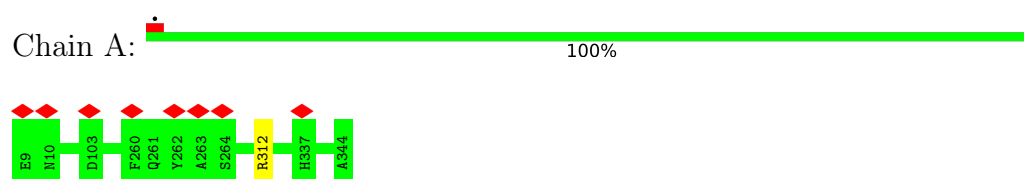
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	N	O	P	
55	y1	1	69	49	2	16	2	0

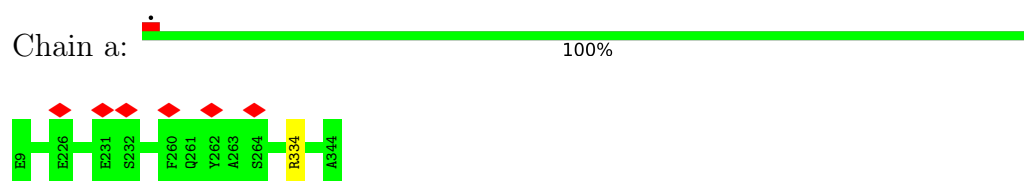
### 3 Residue-property plots [i](#)

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

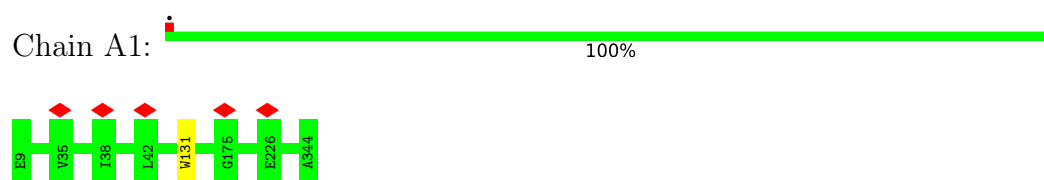
- Molecule 1: Photosystem II protein D1



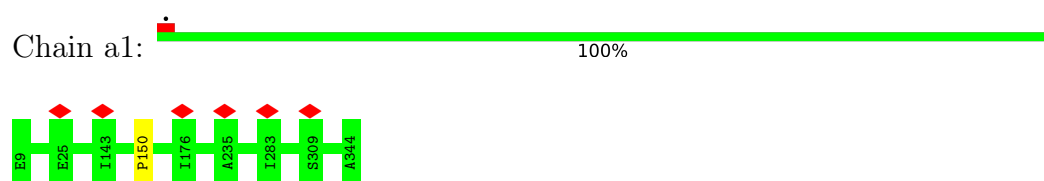
- Molecule 1: Photosystem II protein D1



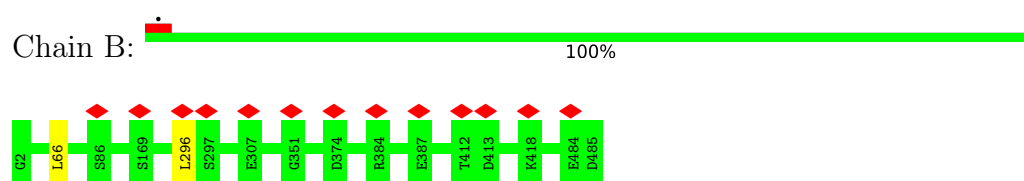
- Molecule 1: Photosystem II protein D1



- Molecule 1: Photosystem II protein D1



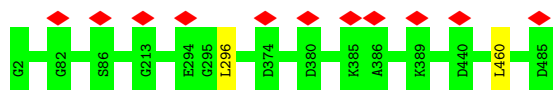
- Molecule 2: Photosystem II CP47 reaction center protein





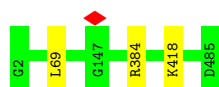
- Molecule 2: Photosystem II CP47 reaction center protein

Chain b:  100%



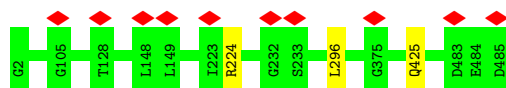
- Molecule 2: Photosystem II CP47 reaction center protein

Chain B1:  99%



- Molecule 2: Photosystem II CP47 reaction center protein

Chain b1:  99%



- Molecule 3: Photosystem II reaction center protein Ycf12

Chain V:  100%

There are no outlier residues recorded for this chain.

- Molecule 3: Photosystem II reaction center protein Ycf12

Chain v:  100%

There are no outlier residues recorded for this chain.

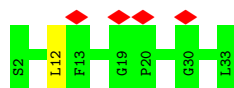
- Molecule 3: Photosystem II reaction center protein Ycf12

Chain V1:  100%

There are no outlier residues recorded for this chain.

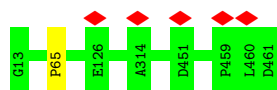
- Molecule 3: Photosystem II reaction center protein Ycf12

Chain v1:  12% 97%



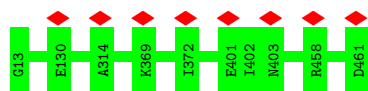
- Molecule 4: Photosystem II CP43 reaction center protein

Chain C:  100%



- Molecule 4: Photosystem II CP43 reaction center protein

Chain c: 100%



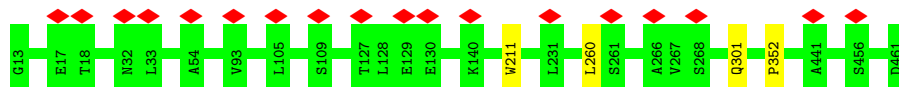
- Molecule 4: Photosystem II CP43 reaction center protein

Chain C1: 100%

There are no outlier residues recorded for this chain.

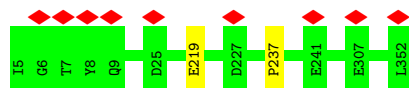
- Molecule 4: Photosystem II CP43 reaction center protein

Chain c1: 99%



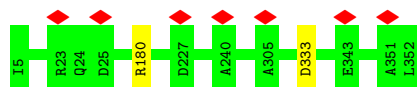
- Molecule 5: Photosystem II D2 protein

Chain D: 99%



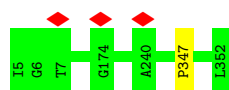
- Molecule 5: Photosystem II D2 protein

Chain d: 99%



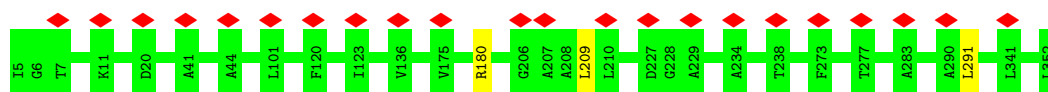
- Molecule 5: Photosystem II D2 protein

Chain D1: 100%



- Molecule 5: Photosystem II D2 protein

Chain d1: 99%



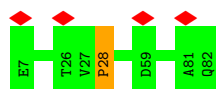
- Molecule 6: Cytochrome b559 subunit alpha

Chain E: 100%



- Molecule 6: Cytochrome b559 subunit alpha

Chain e: 99%



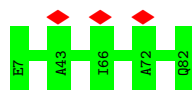
- Molecule 6: Cytochrome b559 subunit alpha

Chain E1: 100%

There are no outlier residues recorded for this chain.

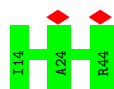
- Molecule 6: Cytochrome b559 subunit alpha

Chain e1: 100%



- Molecule 7: Cytochrome b559 subunit beta

Chain F: 100%



- Molecule 7: Cytochrome b559 subunit beta

Chain f: 100%

There are no outlier residues recorded for this chain.

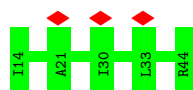
- Molecule 7: Cytochrome b559 subunit beta

Chain F1: 100%

There are no outlier residues recorded for this chain.

- Molecule 7: Cytochrome b559 subunit beta

Chain f1:  100%



- Molecule 8: Photosystem II reaction center protein H

Chain H:  97%



- Molecule 8: Photosystem II reaction center protein H

Chain h:  99%



- Molecule 8: Photosystem II reaction center protein H

Chain H1:  99%



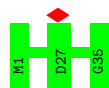
- Molecule 8: Photosystem II reaction center protein H

Chain h1:  100%

There are no outlier residues recorded for this chain.

- Molecule 9: Photosystem II reaction center protein I

Chain I:  100%



- Molecule 9: Photosystem II reaction center protein I

Chain i:  100%



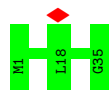
- Molecule 9: Photosystem II reaction center protein I

Chain I1:  100%

There are no outlier residues recorded for this chain.

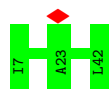
- Molecule 9: Photosystem II reaction center protein I

Chain i1:  100%



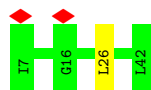
- Molecule 10: PsbJ

Chain J:  100%



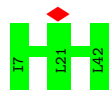
- Molecule 10: PsbJ

Chain j:  97%



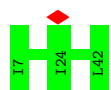
- Molecule 10: PsbJ

Chain J1:  100%



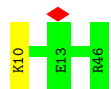
- Molecule 10: PsbJ

Chain j1:  100%



- Molecule 11: Photosystem II reaction center protein K

Chain K:  97%



- Molecule 11: Photosystem II reaction center protein K

Chain k:  100%

There are no outlier residues recorded for this chain.

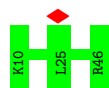
- Molecule 11: Photosystem II reaction center protein K

Chain K1:  100%

There are no outlier residues recorded for this chain.

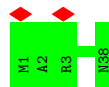
- Molecule 11: Photosystem II reaction center protein K

Chain k1:  100%



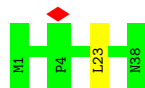
- Molecule 12: Photosystem II reaction center protein L

Chain L:  5% 100%



- Molecule 12: Photosystem II reaction center protein L

Chain l:  97%



- Molecule 12: Photosystem II reaction center protein L

Chain L1:  97%



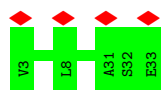
- Molecule 13: PsbM

Chain M:  100%

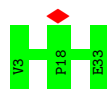


- Molecule 13: PsbM

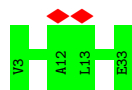
Chain m:  13% 100%



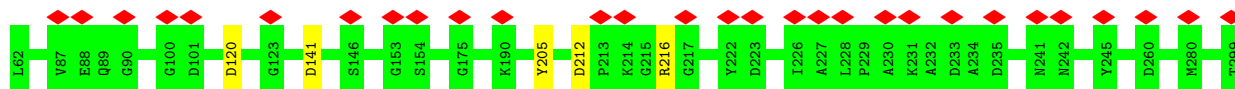
• Molecule 13: PsbM



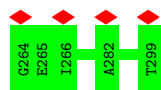
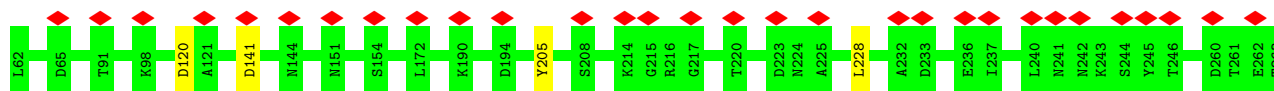
• Molecule 13: PsbM



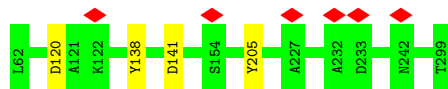
• Molecule 14: PsbO



• Molecule 14: PsbO

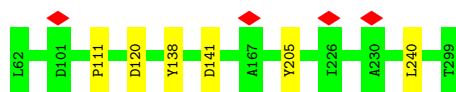


• Molecule 14: PsbO

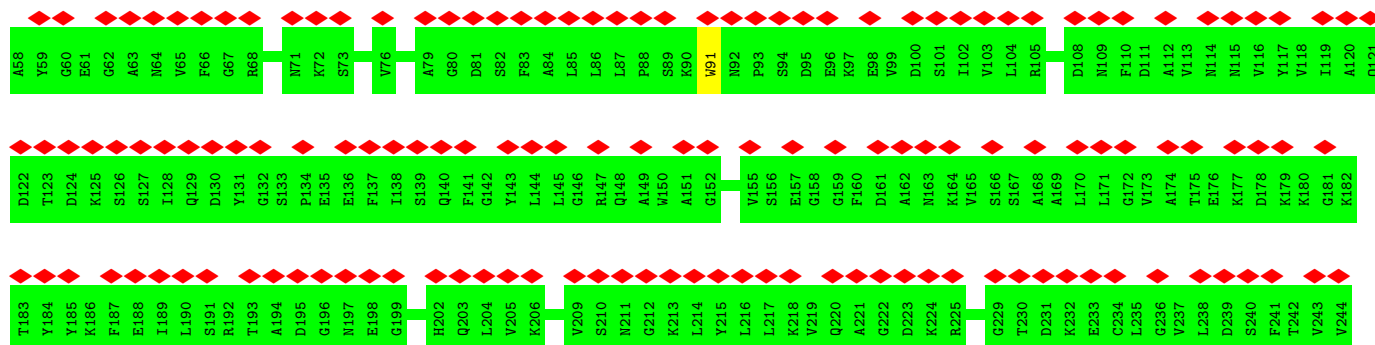
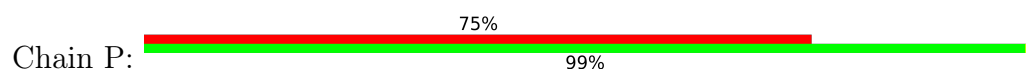


• Molecule 14: PsbO

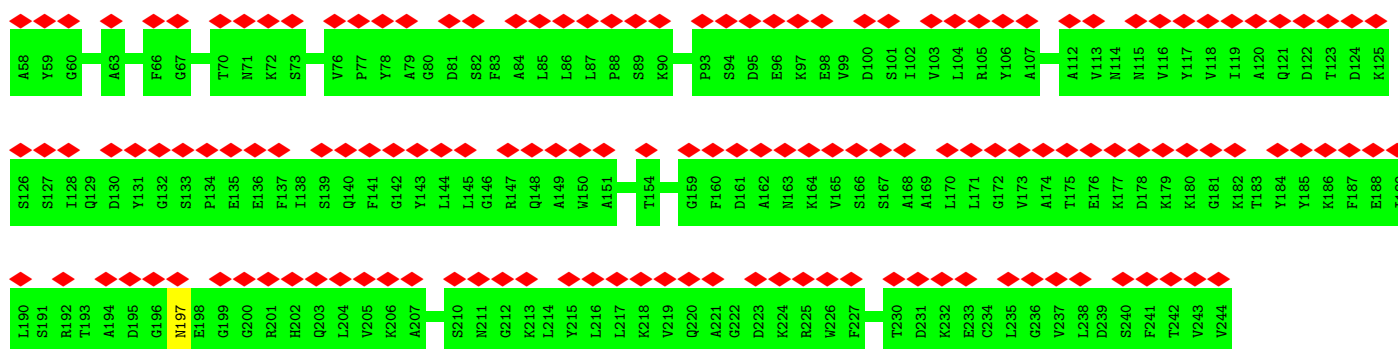
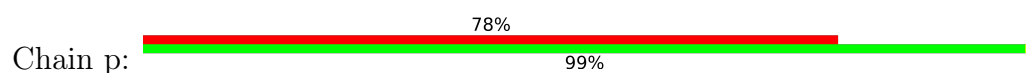




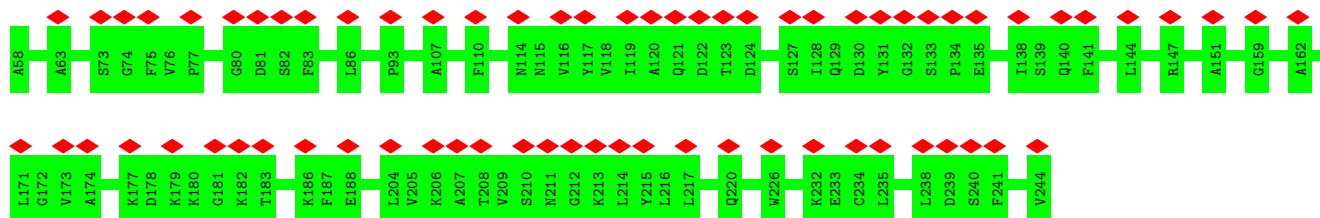
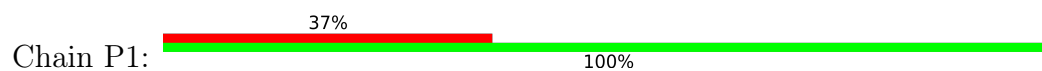
## ● Molecule 15: PsbP



## ● Molecule 15: PsbP



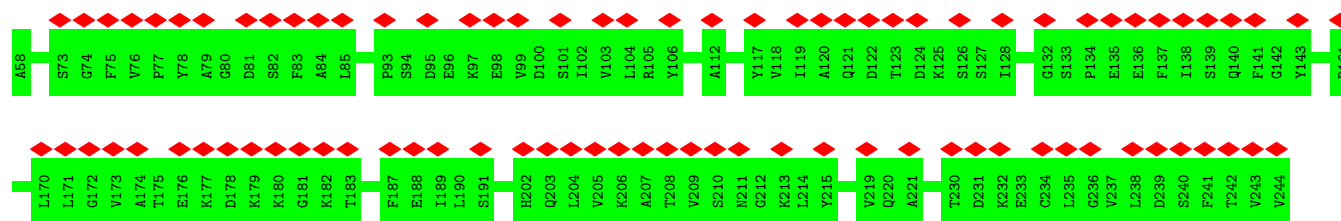
## ● Molecule 15: PsbP



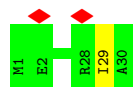
## ● Molecule 15: PsbP







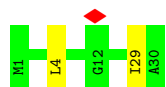
- Molecule 16: Photosystem II reaction center protein T



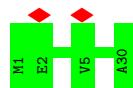
- Molecule 16: Photosystem II reaction center protein T



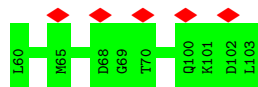
- Molecule 16: Photosystem II reaction center protein T



- Molecule 16: Photosystem II reaction center protein T

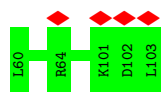


- Molecule 17: PsbW



- Molecule 17: PsbW





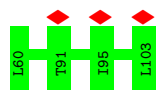
- Molecule 17: PsbW

Chain W1:  100%

There are no outlier residues recorded for this chain.

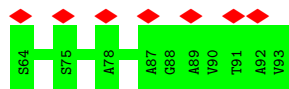
- Molecule 17: PsbW

Chain w1:  7%  100%



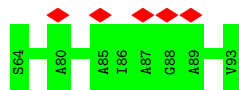
- Molecule 18: PsbX

Chain X:  23%  100%



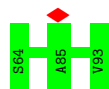
- Molecule 18: PsbX

Chain x:  17%  100%



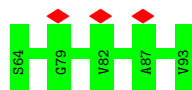
- Molecule 18: PsbX

Chain X1:  0%  100%



- Molecule 18: PsbX

Chain x1:  10%  100%



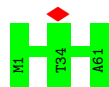
- Molecule 19: Photosystem II reaction center protein Z

Chain Z:  100%

There are no outlier residues recorded for this chain.

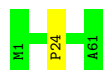
- Molecule 19: Photosystem II reaction center protein Z

Chain z:  100%



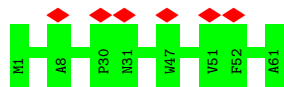
- Molecule 19: Photosystem II reaction center protein Z

Chain Z1:  98%



- Molecule 19: Photosystem II reaction center protein Z

Chain z1:  10%  100%



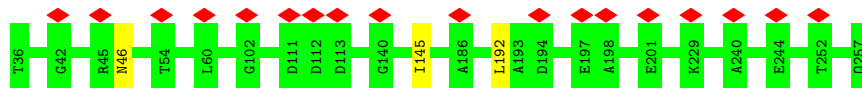
- Molecule 20: LHCII M3

Chain N:  5%  98%



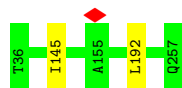
- Molecule 20: LHCII M3

Chain n:  8%  99%



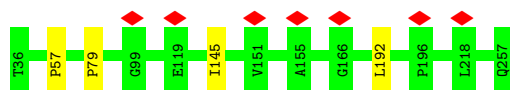
- Molecule 20: LHCII M3

Chain N1:  99%

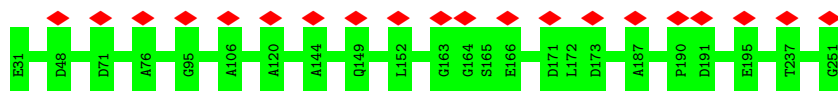


- Molecule 20: LHCII M3

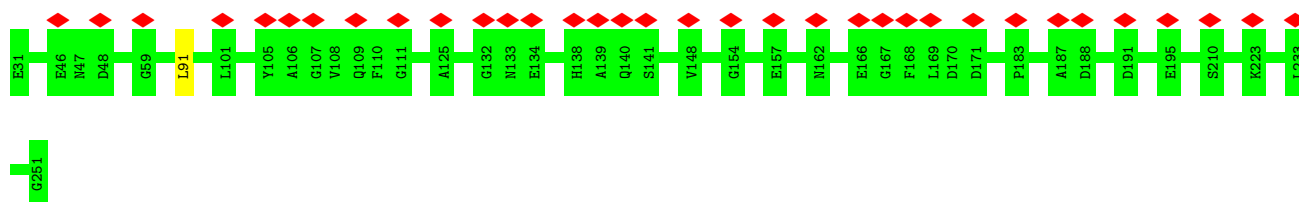
Chain n1:  98%



- Molecule 21: Chlorophyll a-b binding protein, chloroplastic



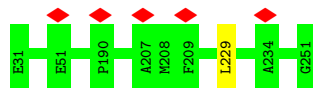
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic



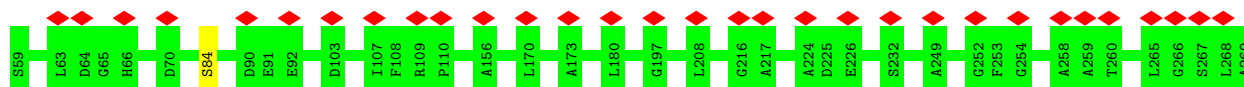
- Molecule 21: Chlorophyll a-b binding protein, chloroplastic



- Molecule 21: Chlorophyll a-b binding protein, chloroplastic

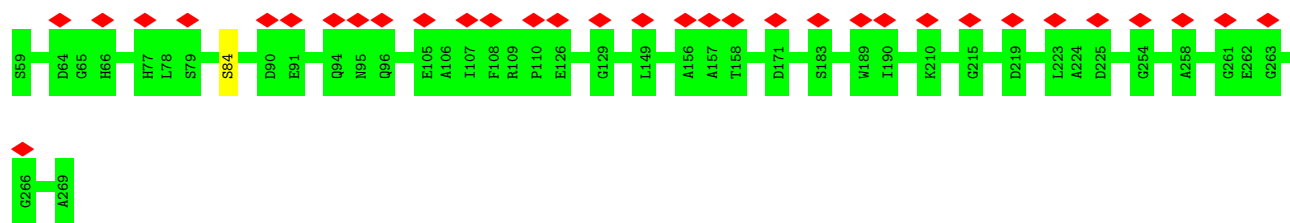


- Molecule 22: CP29



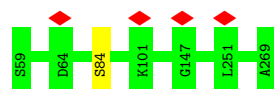
- Molecule 22: CP29





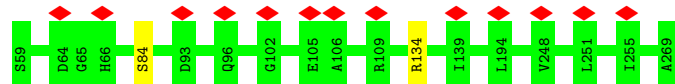
• Molecule 22: CP29

Chain R1: 99%



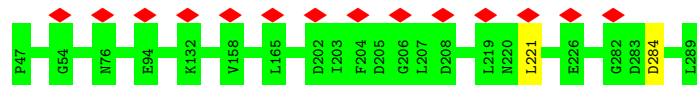
• Molecule 22: CP29

Chain r1: 7% 99%



• Molecule 23: CP26

Chain S: 6% 99%



• Molecule 23: CP26

Chain s: 98%



• Molecule 23: CP26

Chain S1: 99%



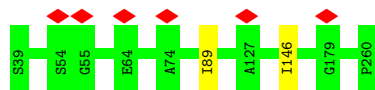
• Molecule 23: CP26

Chain s1: 9% 98%



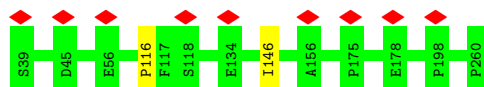
- Molecule 24: LHCII M1

Chain Y:  99%



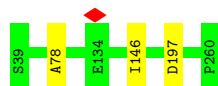
- Molecule 24: LHCII M1

Chain y:  99%



- Molecule 24: LHCII M1

Chain Y1:  99%



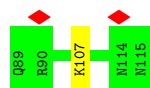
- Molecule 24: LHCII M1

Chain y1:  100%



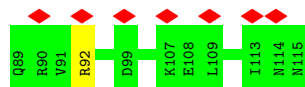
- Molecule 25: PsbU

Chain U:  96%



- Molecule 25: PsbU

Chain u:  96%



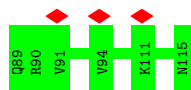
- Molecule 25: PsbU

Chain U1:  100%

There are no outlier residues recorded for this chain.

- Molecule 25: PsbU

Chain u1:  11% 100%



## 4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, Not provided	
Number of particles used	9567	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 ( $e^-/\text{\AA}^2$ )	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	0.102	Depositor
Minimum map value	-0.072	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.008	Depositor
Recommended contour level	0.013	Depositor
Map size ( $\text{\AA}$ )	460.8, 460.8, 460.8	wwPDB
Map dimensions	480, 480, 480	wwPDB
Map angles ( $^\circ$ )	90.0, 90.0, 90.0	wwPDB
Pixel spacing ( $\text{\AA}$ )	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: BCR, LMT, SPH, C7Z, GOL, 4RF, PL9, LPX, FE2, DGD, LHG, ERG, LMG, CHL, OEX, LMK, NA, HEM, NEX, DGA, BCT, XAT, PTY, PHO, CLA, SEP, RRX, LUT, CL, 3PH, SQD

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	$\# Z  > 5$	RMSZ	$\# Z  > 5$
1	A	0.41	0/2723	0.60	0/3715
1	A1	0.36	0/2723	0.61	0/3715
1	a	0.41	0/2723	0.61	0/3715
1	a1	0.36	0/2723	0.65	2/3715 (0.1%)
2	B	0.40	0/3912	0.63	2/5327 (0.0%)
2	B1	0.35	0/3912	0.61	1/5327 (0.0%)
2	b	0.39	0/3912	0.61	2/5327 (0.0%)
2	b1	0.33	0/3912	0.60	1/5327 (0.0%)
3	V	0.34	0/228	0.67	0/311
3	V1	0.26	0/228	0.54	0/311
3	v	0.30	0/228	0.66	0/311
3	v1	0.29	0/228	0.76	1/311 (0.3%)
4	C	0.46	2/3602 (0.1%)	0.70	4/4913 (0.1%)
4	C1	0.34	0/3602	0.59	0/4913
4	c	0.39	0/3602	0.59	0/4913
4	c1	0.40	2/3602 (0.1%)	0.67	4/4913 (0.1%)
5	D	0.45	1/2860 (0.0%)	0.64	2/3899 (0.1%)
5	D1	0.36	0/2860	0.62	2/3899 (0.1%)
5	d	0.41	0/2860	0.61	1/3899 (0.0%)
5	d1	0.36	0/2860	0.65	2/3899 (0.1%)
6	E	0.34	0/639	0.59	0/870
6	E1	0.33	0/639	0.63	0/870
6	e	0.55	1/639 (0.2%)	0.85	3/870 (0.3%)
6	e1	0.30	0/639	0.59	0/870
7	F	0.33	0/259	0.56	0/351
7	F1	0.31	0/259	0.58	0/351
7	f	0.38	0/259	0.68	0/351
7	f1	0.33	0/259	0.64	0/351
8	H	0.37	0/513	0.77	2/703 (0.3%)
8	H1	0.31	0/513	0.65	1/703 (0.1%)
8	h	0.36	0/513	0.68	1/703 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
8	h1	0.31	0/513	0.62	0/703
9	I	0.44	0/287	0.57	0/386
9	I1	0.34	0/287	0.60	0/386
9	i	0.38	0/287	0.55	0/386
9	i1	0.36	0/287	0.59	0/386
10	J	0.29	0/272	0.54	0/369
10	J1	0.31	0/272	0.58	0/369
10	j	0.35	0/272	0.69	1/369 (0.3%)
10	j1	0.29	0/272	0.61	0/369
11	K	0.40	0/308	0.64	0/423
11	K1	0.33	0/308	0.63	0/423
11	k	0.43	0/308	0.61	0/423
11	k1	0.36	0/308	0.66	0/423
12	L	0.37	0/321	0.53	0/435
12	L1	0.37	0/321	0.74	1/435 (0.2%)
12	l	0.43	0/321	0.71	1/435 (0.2%)
13	M	0.33	0/237	0.54	0/323
13	M1	0.29	0/237	0.54	0/323
13	m	0.36	0/237	0.66	0/323
13	m1	0.35	0/237	0.60	0/323
14	O	0.36	0/1855	0.70	3/2505 (0.1%)
14	O1	0.34	0/1855	0.68	2/2505 (0.1%)
14	o	0.36	0/1855	0.68	3/2505 (0.1%)
14	o1	0.48	1/1855 (0.1%)	0.82	7/2505 (0.3%)
15	P	0.28	0/1473	0.57	1/1988 (0.1%)
15	P1	0.30	0/1473	0.57	0/1988
15	p	0.31	0/1473	0.57	0/1988
15	p1	0.32	0/1473	0.58	0/1988
16	T	0.33	0/254	0.62	0/342
16	T1	0.39	0/254	0.72	1/342 (0.3%)
16	t	0.36	0/254	0.55	0/342
16	t1	0.32	0/254	0.60	0/342
17	W	0.32	0/339	0.63	0/460
17	W1	0.31	0/339	0.59	0/460
17	w	0.32	0/339	0.57	0/460
17	w1	0.29	0/339	0.60	0/460
18	X	0.32	0/202	0.55	0/276
18	X1	0.31	0/202	0.53	0/276
18	x	0.35	0/202	0.69	0/276
18	x1	0.27	0/202	0.58	0/276
19	Z	0.31	0/469	0.52	0/641
19	Z1	0.31	0/469	0.59	1/641 (0.2%)
19	z	0.33	0/469	0.53	0/641

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z  >5	RMSZ	# Z  >5
19	z1	0.28	0/469	0.52	0/641
20	N	0.36	0/1751	0.59	1/2386 (0.0%)
20	N1	0.35	0/1751	0.58	0/2386
20	n	0.37	0/1750	0.58	0/2382
20	n1	0.44	2/1750 (0.1%)	0.71	5/2382 (0.2%)
21	G	0.34	0/1725	0.59	0/2348
21	G1	0.38	1/1725 (0.1%)	0.64	2/2348 (0.1%)
21	g	0.34	0/1725	0.60	1/2348 (0.0%)
21	g1	0.33	0/1725	0.58	1/2348 (0.0%)
22	R	0.34	0/1506	0.61	0/2035
22	R1	0.30	0/1506	0.55	0/2035
22	r	0.31	0/1506	0.60	0/2035
22	r1	0.33	0/1506	0.62	0/2035
23	S	0.35	0/1903	0.64	1/2590 (0.0%)
23	S1	0.32	0/1903	0.63	2/2590 (0.1%)
23	s	0.34	0/1903	0.68	1/2590 (0.0%)
23	s1	0.37	1/1903 (0.1%)	0.73	4/2590 (0.2%)
24	Y	0.35	0/1715	0.58	1/2338 (0.0%)
24	Y1	0.35	0/1715	0.65	2/2338 (0.1%)
24	y	0.37	0/1715	0.55	1/2338 (0.0%)
24	y1	0.32	0/1715	0.57	0/2338
25	U	0.37	0/224	0.69	0/298
25	U1	0.36	0/224	0.67	0/298
25	u	0.38	0/224	0.76	0/298
25	u1	0.36	0/224	0.67	0/298
All	All	0.37	11/117985 (0.0%)	0.63	74/160485 (0.0%)

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

Mol	Chain	#Chirality outliers	#Planarity outliers
1	A	0	1
1	A1	0	1
2	B1	0	1
All	All	0	3

All (11) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
14	o1	111	PRO	CG-CD	-14.28	1.03	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	C	65	PRO	CG-CD	-13.03	1.07	1.50
6	e	28	PRO	CG-CD	-10.62	1.15	1.50
4	c1	352	PRO	CG-CD	-9.09	1.20	1.50
20	n1	57	PRO	CG-CD	-8.65	1.22	1.50
20	n1	79	PRO	CG-CD	-7.62	1.25	1.50
23	s1	155	PRO	CG-CD	-6.54	1.29	1.50
21	G1	56	GLU	C-N	-6.19	1.19	1.34
4	C	65	PRO	CB-CG	-5.11	1.24	1.50
5	D	219	GLU	CG-CD	-5.10	1.44	1.51
4	c1	352	PRO	N-CD	5.09	1.54	1.47

All (74) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
4	C	65	PRO	N-CD-CG	-18.59	75.32	103.20
14	o1	111	PRO	N-CD-CG	-18.29	75.77	103.20
6	e	28	PRO	N-CD-CG	-12.50	84.44	103.20
20	n1	57	PRO	N-CD-CG	-12.30	84.74	103.20
4	C	65	PRO	CA-CB-CG	-11.58	82.00	104.00
14	o1	111	PRO	CA-CB-CG	-11.00	83.11	104.00
5	D	237	PRO	CA-N-CD	-10.94	96.18	111.50
23	s1	155	PRO	CA-N-CD	-10.81	96.37	111.50
4	c1	352	PRO	N-CD-CG	-10.76	87.06	103.20
4	c1	352	PRO	CA-N-CD	-10.71	96.50	111.50
20	n1	79	PRO	N-CD-CG	-10.33	87.70	103.20
23	s1	155	PRO	N-CD-CG	-9.73	88.60	103.20
4	C	65	PRO	CB-CG-CD	9.66	144.16	106.50
6	e	28	PRO	CA-N-CD	-9.44	98.29	111.50
20	n1	57	PRO	CA-CB-CG	-9.19	86.53	104.00
2	b	296	LEU	CA-CB-CG	8.09	133.91	115.30
2	B	296	LEU	CA-CB-CG	7.93	133.54	115.30
2	b1	296	LEU	CA-CB-CG	7.78	133.18	115.30
5	d1	291	LEU	CA-CB-CG	7.54	132.64	115.30
21	G1	131	LEU	CA-CB-CG	7.51	132.58	115.30
23	S	221	LEU	CA-CB-CG	7.36	132.23	115.30
5	D	237	PRO	N-CD-CG	-7.33	92.20	103.20
21	G1	56	GLU	C-N-CA	7.23	139.77	121.70
1	a1	150	PRO	CA-N-CD	-7.19	101.43	111.50
14	o1	111	PRO	CA-N-CD	-7.04	101.65	111.50
23	s	221	LEU	CA-CB-CG	6.96	131.31	115.30
6	e	28	PRO	CA-CB-CG	-6.85	90.99	104.00
14	o1	111	PRO	CB-CG-CD	6.82	133.09	106.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
3	v1	12	LEU	CA-CB-CG	6.77	130.86	115.30
23	s1	221	LEU	CA-CB-CG	6.70	130.71	115.30
23	S1	221	LEU	CA-CB-CG	6.70	130.71	115.30
21	g	91	LEU	CA-CB-CG	6.62	130.53	115.30
24	y	116	PRO	CA-N-CD	-6.41	102.53	111.50
20	n1	57	PRO	N-CA-CB	-6.39	95.57	102.60
4	C	65	PRO	CA-N-CD	-6.35	102.61	111.50
24	Y	89	ILE	CG1-CB-CG2	-6.28	97.58	111.40
14	O	212	ASP	CB-CG-OD1	6.16	123.84	118.30
1	a1	150	PRO	N-CD-CG	-6.12	94.02	103.20
4	c1	352	PRO	CA-CB-CG	-6.12	92.38	104.00
15	P	91	TRP	C-N-CA	6.04	136.81	121.70
8	H	62	LEU	CA-CB-CG	5.97	129.02	115.30
14	o	228	LEU	CA-CB-CG	5.83	128.71	115.30
20	n1	79	PRO	CA-N-CD	-5.80	103.38	111.50
23	s1	280	LEU	CA-CB-CG	5.78	128.59	115.30
19	Z1	24	PRO	CA-N-CD	-5.74	103.46	111.50
24	Y1	197	ASP	CB-CG-OD1	5.69	123.42	118.30
8	H	55	LEU	CA-CB-CG	5.56	128.08	115.30
2	B1	69	LEU	CA-CB-CG	5.53	128.03	115.30
4	c1	260	LEU	CA-CB-CG	5.45	127.84	115.30
5	d	333	ASP	CB-CG-OD1	5.39	123.15	118.30
12	l	23	LEU	CA-CB-CG	5.37	127.65	115.30
5	d1	209	LEU	CA-CB-CG	5.30	127.49	115.30
23	S1	243	MET	CA-CB-CG	5.29	122.29	113.30
2	B	66	LEU	CA-CB-CG	5.26	127.40	115.30
14	o1	120	ASP	CB-CG-OD2	5.25	123.03	118.30
2	b	460	LEU	CB-CG-CD1	-5.25	102.08	111.00
12	L1	18	LEU	CB-CG-CD1	-5.25	102.08	111.00
14	O	141	ASP	CB-CG-OD2	5.22	123.00	118.30
14	O1	120	ASP	CB-CG-OD2	5.22	123.00	118.30
14	O1	141	ASP	CB-CG-OD2	5.21	122.98	118.30
10	j	26	LEU	CA-CB-CG	5.21	127.27	115.30
14	o	120	ASP	CB-CG-OD2	5.21	122.98	118.30
14	O	120	ASP	CB-CG-OD2	5.19	122.97	118.30
14	o	141	ASP	CB-CG-OD2	5.19	122.97	118.30
14	o1	141	ASP	CB-CG-OD2	5.19	122.97	118.30
5	D1	347	PRO	CA-N-CD	-5.12	104.33	111.50
21	g1	229	LEU	CA-CB-CG	5.11	127.05	115.30
14	o1	240	LEU	CA-CB-CG	5.09	127.02	115.30
5	D1	347	PRO	N-CD-CG	-5.08	95.57	103.20
24	Y1	78	ALA	C-N-CA	-5.04	109.10	121.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
20	N	136	LEU	CA-CB-CG	5.03	126.87	115.30
8	H1	55	LEU	CA-CB-CG	5.02	126.84	115.30
16	T1	4	LEU	CB-CG-CD2	-5.01	102.48	111.00
8	h	61	LEU	CA-CB-CG	5.01	126.81	115.30

There are no chirality outliers.

All (3) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
1	A	312	ARG	Sidechain
1	A1	131	TRP	Peptide
2	B1	384	ARG	Sidechain

## 5.2 Too-close contacts [i](#)

Due to software issues we are unable to calculate clashes - this section is therefore empty.

## 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%)	321 (96%)	14 (4%)	0	100	100
1	A1	335/336 (100%)	313 (93%)	22 (7%)	0	100	100
1	a	335/336 (100%)	318 (95%)	17 (5%)	0	100	100
1	a1	335/336 (100%)	314 (94%)	21 (6%)	0	100	100
2	B	482/484 (100%)	464 (96%)	18 (4%)	0	100	100
2	B1	482/484 (100%)	447 (93%)	35 (7%)	0	100	100
2	b	482/484 (100%)	464 (96%)	18 (4%)	0	100	100
2	b1	482/484 (100%)	454 (94%)	28 (6%)	0	100	100
3	V	30/32 (94%)	28 (93%)	2 (7%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
3	V1	30/32 (94%)	28 (93%)	2 (7%)	0	100	100
3	v	30/32 (94%)	30 (100%)	0	0	100	100
3	v1	30/32 (94%)	29 (97%)	1 (3%)	0	100	100
4	C	447/449 (100%)	430 (96%)	17 (4%)	0	100	100
4	C1	447/449 (100%)	421 (94%)	26 (6%)	0	100	100
4	c	447/449 (100%)	431 (96%)	16 (4%)	0	100	100
4	c1	447/449 (100%)	421 (94%)	25 (6%)	1 (0%)	47	79
5	D	346/348 (99%)	330 (95%)	16 (5%)	0	100	100
5	D1	346/348 (99%)	324 (94%)	22 (6%)	0	100	100
5	d	346/348 (99%)	331 (96%)	15 (4%)	0	100	100
5	d1	346/348 (99%)	324 (94%)	22 (6%)	0	100	100
6	E	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
6	E1	74/76 (97%)	68 (92%)	6 (8%)	0	100	100
6	e	74/76 (97%)	71 (96%)	3 (4%)	0	100	100
6	e1	74/76 (97%)	69 (93%)	5 (7%)	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%)	62 (95%)	3 (5%)	0	100	100
8	H1	65/67 (97%)	63 (97%)	2 (3%)	0	100	100
8	h	65/67 (97%)	62 (95%)	3 (5%)	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%)	29 (88%)	4 (12%)	0	100	100
9	i1	33/35 (94%)	31 (94%)	2 (6%)	0	100	100
10	J	34/36 (94%)	33 (97%)	1 (3%)	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
10	j1	34/36 (94%)	33 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
11	K	35/37 (95%)	33 (94%)	2 (6%)	0	100	100
11	K1	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	k	35/37 (95%)	34 (97%)	1 (3%)	0	100	100
11	k1	35/37 (95%)	35 (100%)	0	0	100	100
12	L	36/38 (95%)	36 (100%)	0	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	29/31 (94%)	29 (100%)	0	0	100	100
13	M1	29/31 (94%)	27 (93%)	2 (7%)	0	100	100
13	m	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
13	m1	29/31 (94%)	28 (97%)	1 (3%)	0	100	100
14	O	236/238 (99%)	215 (91%)	19 (8%)	2 (1%)	19	59
14	O1	236/238 (99%)	212 (90%)	23 (10%)	1 (0%)	34	71
14	o	236/238 (99%)	218 (92%)	17 (7%)	1 (0%)	34	71
14	o1	236/238 (99%)	210 (89%)	25 (11%)	1 (0%)	34	71
15	P	185/187 (99%)	176 (95%)	9 (5%)	0	100	100
15	P1	185/187 (99%)	175 (95%)	10 (5%)	0	100	100
15	p	185/187 (99%)	170 (92%)	15 (8%)	0	100	100
15	p1	185/187 (99%)	169 (91%)	16 (9%)	0	100	100
16	T	28/30 (93%)	27 (96%)	0	1 (4%)	3	29
16	T1	28/30 (93%)	25 (89%)	2 (7%)	1 (4%)	3	29
16	t	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
16	t1	28/30 (93%)	27 (96%)	1 (4%)	0	100	100
17	W	42/44 (96%)	38 (90%)	4 (10%)	0	100	100
17	W1	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
17	w	42/44 (96%)	39 (93%)	3 (7%)	0	100	100
17	w1	42/44 (96%)	39 (93%)	3 (7%)	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%)	28 (100%)	0	0	100	100
18	x1	28/30 (93%)	28 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
19	Z	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
19	Z1	59/61 (97%)	55 (93%)	4 (7%)	0	100	100
19	z	59/61 (97%)	59 (100%)	0	0	100	100
19	z1	59/61 (97%)	57 (97%)	2 (3%)	0	100	100
20	N	220/222 (99%)	202 (92%)	16 (7%)	2 (1%)	17	57
20	N1	220/222 (99%)	202 (92%)	16 (7%)	2 (1%)	17	57
20	n	218/222 (98%)	199 (91%)	17 (8%)	2 (1%)	17	57
20	n1	218/222 (98%)	202 (93%)	14 (6%)	2 (1%)	17	57
21	G	219/221 (99%)	196 (90%)	23 (10%)	0	100	100
21	G1	219/221 (99%)	195 (89%)	24 (11%)	0	100	100
21	g	219/221 (99%)	197 (90%)	22 (10%)	0	100	100
21	g1	219/221 (99%)	195 (89%)	24 (11%)	0	100	100
22	R	191/196 (97%)	177 (93%)	14 (7%)	0	100	100
22	R1	191/196 (97%)	176 (92%)	15 (8%)	0	100	100
22	r	191/196 (97%)	177 (93%)	14 (7%)	0	100	100
22	r1	191/196 (97%)	176 (92%)	15 (8%)	0	100	100
23	S	241/243 (99%)	219 (91%)	21 (9%)	1 (0%)	34	71
23	S1	241/243 (99%)	208 (86%)	32 (13%)	1 (0%)	34	71
23	s	241/243 (99%)	219 (91%)	20 (8%)	2 (1%)	19	59
23	s1	241/243 (99%)	214 (89%)	26 (11%)	1 (0%)	34	71
24	Y	220/222 (99%)	212 (96%)	7 (3%)	1 (0%)	29	68
24	Y1	220/222 (99%)	205 (93%)	14 (6%)	1 (0%)	29	68
24	y	220/222 (99%)	204 (93%)	15 (7%)	1 (0%)	29	68
24	y1	220/222 (99%)	204 (93%)	15 (7%)	1 (0%)	29	68
25	U	25/27 (93%)	23 (92%)	2 (8%)	0	100	100
25	U1	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
25	u	25/27 (93%)	24 (96%)	1 (4%)	0	100	100
25	u1	25/27 (93%)	25 (100%)	0	0	100	100
All	All	14636/14846 (99%)	13696 (94%)	915 (6%)	25 (0%)	50	79

All (25) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
14	O	205	TYR
20	N	192	LEU
14	o	205	TYR
20	n	192	LEU
23	s	284	ASP
14	O1	205	TYR
20	N1	192	LEU
23	s1	284	ASP
20	N	145	ILE
24	Y	146	ILE
24	y	146	ILE
14	o1	205	TYR
20	n1	192	LEU
20	n	145	ILE
23	s	92	LYS
24	Y1	146	ILE
23	S	284	ASP
24	y1	146	ILE
14	O	216	ARG
23	S1	92	LYS
4	c1	211	TRP
20	N1	145	ILE
20	n1	145	ILE
16	T	29	ILE
16	T1	29	ILE

### 5.3.2 Protein sidechains [i](#)

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

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

Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
1	A	276/275 (100%)	276 (100%)	0	100	100
1	A1	276/275 (100%)	276 (100%)	0	100	100
1	a	276/275 (100%)	275 (100%)	1 (0%)	91	97
1	a1	276/275 (100%)	276 (100%)	0	100	100
2	B	388/388 (100%)	388 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
2	B1	388/388 (100%)	387 (100%)	1 (0%)	92	97
2	b	388/388 (100%)	388 (100%)	0	100	100
2	b1	388/388 (100%)	386 (100%)	2 (0%)	88	95
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%)	349 (100%)	1 (0%)	92	97
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%)	278 (100%)	1 (0%)	91	97
5	d1	279/279 (100%)	278 (100%)	1 (0%)	91	97
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%)	67 (98%)	1 (2%)	65	84
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
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	32 (97%)	1 (3%)	41	71
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	26/26 (100%)	26 (100%)	0	100	100
13	M1	26/26 (100%)	26 (100%)	0	100	100
13	m	26/26 (100%)	26 (100%)	0	100	100
13	m1	26/26 (100%)	26 (100%)	0	100	100
14	O	195/195 (100%)	195 (100%)	0	100	100
14	O1	195/195 (100%)	194 (100%)	1 (0%)	88	95
14	o	195/195 (100%)	195 (100%)	0	100	100
14	o1	195/195 (100%)	194 (100%)	1 (0%)	88	95
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%)	150 (99%)	1 (1%)	84	93
15	p1	151/151 (100%)	151 (100%)	0	100	100
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

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
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%)	170 (99%)	1 (1%)	86	94
20	N1	171/171 (100%)	171 (100%)	0	100	100
20	n	171/171 (100%)	170 (99%)	1 (1%)	86	94
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	151/151 (100%)	151 (100%)	0	100	100
22	R1	151/151 (100%)	151 (100%)	0	100	100
22	r	151/151 (100%)	151 (100%)	0	100	100
22	r1	151/151 (100%)	150 (99%)	1 (1%)	84	93
23	S	190/190 (100%)	190 (100%)	0	100	100
23	S1	190/190 (100%)	190 (100%)	0	100	100
23	s	190/190 (100%)	189 (100%)	1 (0%)	88	95
23	s1	190/190 (100%)	188 (99%)	2 (1%)	73	88
24	Y	167/167 (100%)	167 (100%)	0	100	100
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%)	25 (96%)	1 (4%)	33	66
25	U1	26/26 (100%)	26 (100%)	0	100	100
25	u	26/26 (100%)	25 (96%)	1 (4%)	33	66

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
25	u1	26/26 (100%)	26 (100%)	0	100	100
All	All	11841/11837 (100%)	11821 (100%)	20 (0%)	93	98

All (20) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
11	K	10	LYS
20	N	170	ASN
25	U	107	LYS
1	a	334	ARG
5	d	180	ARG
6	e	28	PRO
15	p	197	ASN
20	n	46	ASN
23	s	132	LYS
25	u	92	ARG
2	B1	418	LYS
14	O1	138	TYR
2	b1	224	ARG
2	b1	425	GLN
4	c1	301	GLN
5	d1	180	ARG
14	o1	138	TYR
22	r1	134	ARG
23	s1	99	LYS
23	s1	132	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (50) such sidechains are listed below:

Mol	Chain	Res	Type
1	A	198	HIS
1	A	234	ASN
4	C	147	ASN
5	D	83	ASN
5	D	350	ASN
12	L	9	GLN
21	G	239	ASN
24	Y	149	GLN
5	d	164	GLN
5	d	186	GLN
5	d	322	ASN

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Mol	Chain	Res	Type
7	f	23	HIS
7	f	40	GLN
7	f	43	GLN
14	o	274	GLN
21	g	85	HIS
1	A1	108	ASN
1	A1	165	GLN
1	A1	191	ASN
1	A1	230	ASN
1	A1	322	ASN
1	A1	325	ASN
1	A1	335	ASN
2	B1	58	GLN
2	B1	281	GLN
4	C1	56	ASN
4	C1	301	GLN
4	C1	320	GLN
5	D1	117	HIS
5	D1	230	ASN
5	D1	350	ASN
12	L1	9	GLN
14	O1	82	ASN
14	O1	274	GLN
19	Z1	58	ASN
22	R1	174	GLN
2	b1	114	HIS
2	b1	317	ASN
4	c1	429	HIS
5	d1	129	GLN
5	d1	334	GLN
8	h1	69	ASN
8	h1	79	ASN
14	o1	82	ASN
20	n1	46	ASN
21	g1	121	GLN
22	r1	203	ASN
24	y1	113	ASN
24	y1	225	GLN
24	y1	236	ASN

### 5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

4 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
22	SEP	R1	84	22	8,9,10	1.52	1 (12%)	8,12,14	1.71	2 (25%)
22	SEP	r	84	22	8,9,10	1.51	1 (12%)	8,12,14	1.39	2 (25%)
22	SEP	R	84	22	8,9,10	1.58	1 (12%)	8,12,14	1.40	2 (25%)
22	SEP	r1	84	22	8,9,10	1.53	1 (12%)	8,12,14	1.69	2 (25%)

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
22	SEP	R1	84	22	-	4/5/8/10	-
22	SEP	r	84	22	-	2/5/8/10	-
22	SEP	R	84	22	-	2/5/8/10	-
22	SEP	r1	84	22	-	5/5/8/10	-

All (4) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
22	R	84	SEP	P-O1P	3.37	1.61	1.50
22	r1	84	SEP	P-O1P	3.30	1.61	1.50
22	R1	84	SEP	P-O1P	3.29	1.61	1.50
22	r	84	SEP	P-O1P	3.22	1.60	1.50

All (8) bond angle outliers are listed below:



Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
22	r1	84	SEP	P-OG-CB	-3.36	109.03	118.30
22	R1	84	SEP	OG-CB-CA	3.23	111.29	108.14
22	R1	84	SEP	P-OG-CB	-3.07	109.85	118.30
22	r1	84	SEP	OG-CB-CA	2.79	110.86	108.14
22	r	84	SEP	P-OG-CB	-2.56	111.25	118.30
22	R	84	SEP	OG-CB-CA	2.49	110.57	108.14
22	r	84	SEP	OG-CB-CA	2.30	110.39	108.14
22	R	84	SEP	P-OG-CB	-2.07	112.59	118.30

There are no chirality outliers.

All (13) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
22	R	84	SEP	N-CA-CB-OG
22	R1	84	SEP	N-CA-CB-OG
22	R1	84	SEP	CB-OG-P-O2P
22	R1	84	SEP	CB-OG-P-O3P
22	r1	84	SEP	N-CA-CB-OG
22	r1	84	SEP	CB-OG-P-O2P
22	R1	84	SEP	CB-OG-P-O1P
22	r1	84	SEP	CB-OG-P-O1P
22	r	84	SEP	CB-OG-P-O2P
22	r1	84	SEP	CB-OG-P-O3P
22	R	84	SEP	CA-CB-OG-P
22	r	84	SEP	N-CA-CB-OG
22	r1	84	SEP	CA-CB-OG-P

There are no ring outliers.

No monomer is involved in short contacts.

## 5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

## 5.6 Ligand geometry [i](#)

Of 721 ligands modelled in this entry, 16 are monoatomic - leaving 705 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	CHL	N1	606	-	66,74,74	0.94	4 (6%)	73,114,114	1.11	8 (10%)
50	XAT	R1	621	-	39,47,47	0.68	1 (2%)	54,74,74	1.91	18 (33%)
29	CLA	B	609	-	65,73,73	1.34	8 (12%)	76,113,113	2.24	18 (23%)
49	LUT	N1	620	-	42,43,43	2.37	1 (2%)	51,60,60	1.99	14 (27%)
29	CLA	N	603	-	65,73,73	1.33	8 (12%)	76,113,113	2.07	18 (23%)
33	LMG	W	201	-	39,39,55	0.85	2 (5%)	47,47,63	1.21	4 (8%)
29	CLA	y1	611	40	65,73,73	1.34	8 (12%)	76,113,113	2.05	17 (22%)
29	CLA	B	603	-	65,73,73	1.36	9 (13%)	76,113,113	1.96	17 (22%)
29	CLA	c	512	-	65,73,73	1.39	9 (13%)	76,113,113	2.00	19 (25%)
33	LMG	B	622	-	44,44,55	0.86	3 (6%)	52,52,63	1.24	2 (3%)
29	CLA	Y	612	-	65,73,73	1.36	8 (12%)	76,113,113	1.99	17 (22%)
37	DGD	B1	623	-	44,44,67	0.86	1 (2%)	58,58,81	1.21	6 (10%)
49	LUT	G1	621	-	42,43,43	2.23	1 (2%)	51,60,60	2.08	10 (19%)
49	LUT	s1	620	-	42,43,43	2.39	1 (2%)	51,60,60	2.02	16 (31%)
49	LUT	S	620	-	42,43,43	2.29	1 (2%)	51,60,60	2.12	18 (35%)
37	DGD	b	623	-	44,44,67	0.89	2 (4%)	58,58,81	1.26	6 (10%)
29	CLA	Y	613	24	65,73,73	1.38	8 (12%)	76,113,113	2.14	21 (27%)
29	CLA	r	604	-	49,57,73	1.56	8 (16%)	55,93,113	2.37	13 (23%)
40	LHG	S1	624	29	44,44,48	0.44	0	47,50,54	1.12	4 (8%)
29	CLA	n1	614	-	49,57,73	1.56	8 (16%)	55,93,113	2.40	15 (27%)
29	CLA	g1	612	21	43,51,73	1.67	10 (23%)	49,86,113	2.28	13 (26%)
30	PHO	a1	408	-	51,69,69	1.04	4 (7%)	47,99,99	1.17	6 (12%)
49	LUT	y	620	-	42,43,43	2.33	1 (2%)	51,60,60	1.92	15 (29%)
29	CLA	c1	513	-	65,73,73	1.39	9 (13%)	76,113,113	2.04	18 (23%)
29	CLA	A1	406	-	65,73,73	1.38	9 (13%)	76,113,113	2.04	20 (26%)
29	CLA	C1	513	-	65,73,73	1.35	7 (10%)	76,113,113	1.96	20 (26%)
29	CLA	a1	410	-	60,68,73	1.43	9 (15%)	70,107,113	2.17	19 (27%)
43	PL9	d	405	-	55,55,55	1.75	10 (18%)	68,69,69	1.54	11 (16%)
40	LHG	s	624	29	44,44,48	0.43	0	47,50,54	1.13	3 (6%)
29	CLA	b	605	-	65,73,73	1.40	7 (10%)	76,113,113	2.17	21 (27%)
33	LMG	d	411	-	46,46,55	0.93	3 (6%)	54,54,63	1.19	4 (7%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
50	XAT	r1	621	-	39,47,47	0.73	1 (2%)	54,74,74	2.16	18 (33%)
48	CHL	y	606	-	66,74,74	0.91	4 (6%)	73,114,114	1.21	10 (13%)
29	CLA	R1	612	-	60,68,73	1.44	7 (11%)	70,107,113	2.07	17 (24%)
29	CLA	d	403	-	65,73,73	1.36	8 (12%)	76,113,113	2.03	17 (22%)
31	BCR	b	619	-	41,41,41	1.83	5 (12%)	56,56,56	4.15	16 (28%)
31	BCR	c1	515	-	41,41,41	1.91	4 (9%)	56,56,56	4.38	13 (23%)
44	HEM	F	101	7,6	41,50,50	1.44	4 (9%)	45,82,82	1.30	3 (6%)
29	CLA	r1	604	-	49,57,73	1.56	7 (14%)	55,93,113	2.28	16 (29%)
29	CLA	b1	614	-	65,73,73	1.38	10 (15%)	76,113,113	1.89	17 (22%)
31	BCR	C	515	-	41,41,41	1.83	6 (14%)	56,56,56	4.20	16 (28%)
49	LUT	S1	620	-	42,43,43	2.32	1 (2%)	51,60,60	1.76	9 (17%)
29	CLA	S	609	-	60,68,73	1.43	8 (13%)	70,107,113	1.98	16 (22%)
29	CLA	C1	502	-	65,73,73	1.37	7 (10%)	76,113,113	1.98	17 (22%)
40	LHG	Y1	624	-	48,48,48	0.40	0	51,54,54	1.11	4 (7%)
45	RRX	h1	101	-	42,42,42	4.84	24 (57%)	57,58,58	2.65	25 (43%)
31	BCR	B1	618	-	41,41,41	1.88	4 (9%)	56,56,56	4.43	19 (33%)
39	DGA	J	101	-	28,28,43	1.31	3 (10%)	30,30,45	1.27	2 (6%)
51	NEX	y1	623	-	38,46,46	3.26	10 (26%)	50,70,70	2.03	18 (36%)
40	LHG	d	408	-	43,43,48	0.40	0	46,49,54	1.04	3 (6%)
29	CLA	b	615	-	65,73,73	1.34	7 (10%)	76,113,113	2.08	18 (23%)
29	CLA	g1	604	-	49,57,73	1.52	7 (14%)	55,93,113	2.31	18 (32%)
37	DGD	B	623	-	44,44,67	0.89	1 (2%)	58,58,81	1.36	6 (10%)
51	NEX	R1	622	-	38,46,46	3.31	9 (23%)	50,70,70	1.93	14 (28%)
29	CLA	y	602	24	65,73,73	1.40	8 (12%)	76,113,113	1.90	14 (18%)
36	C7Z	B	620	-	43,43,43	5.27	26 (60%)	58,60,60	2.44	22 (37%)
42	BCT	D	401	27	2,3,3	1.26	0	2,3,3	2.71	2 (100%)
29	CLA	C	512	-	65,73,73	1.34	6 (9%)	76,113,113	2.01	18 (23%)
29	CLA	s	604	-	55,63,73	1.48	7 (12%)	64,101,113	2.10	16 (25%)
29	CLA	Y1	614	-	65,73,73	1.37	7 (10%)	76,113,113	2.02	17 (22%)
37	DGD	c1	518	-	56,56,67	1.02	5 (8%)	70,70,81	1.11	4 (5%)
49	LUT	G	621	-	42,43,43	2.36	1 (2%)	51,60,60	1.94	12 (23%)
29	CLA	n	612	-	45,53,73	1.63	7 (15%)	52,89,113	2.07	13 (25%)
29	CLA	b	609	-	65,73,73	1.39	10 (15%)	76,113,113	2.04	19 (25%)
29	CLA	N1	603	-	65,73,73	1.37	7 (10%)	76,113,113	2.10	22 (28%)
29	CLA	Y1	610	-	65,73,73	1.35	7 (10%)	76,113,113	2.05	19 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
48	CHL	s	608	-	61,69,74	0.91	3 (4%)	67,108,114	1.30	11 (16%)
48	CHL	g1	609	-	66,74,74	0.88	3 (4%)	73,114,114	1.25	9 (12%)
29	CLA	G	610	21	65,73,73	1.35	8 (12%)	76,113,113	2.04	18 (23%)
29	CLA	c1	501	-	65,73,73	1.38	8 (12%)	76,113,113	2.05	18 (23%)
33	LMG	b	622	-	44,44,55	0.87	3 (6%)	52,52,63	1.15	2 (3%)
40	LHG	g1	624	-	48,48,48	0.41	0	51,54,54	1.11	3 (5%)
32	SQD	M	101	-	41,42,54	0.90	0	50,53,65	0.98	3 (6%)
29	CLA	b	604	-	65,73,73	1.39	8 (12%)	76,113,113	1.87	15 (19%)
38	3PH	B1	624	-	47,47,47	0.86	3 (6%)	51,52,52	1.11	2 (3%)
29	CLA	c	509	-	65,73,73	1.35	6 (9%)	76,113,113	1.94	16 (21%)
51	NEX	N1	623	-	38,46,46	3.26	10 (26%)	50,70,70	1.68	10 (20%)
55	PTY	Y	627	-	18,18,49	1.31	3 (16%)	21,23,54	1.40	2 (9%)
29	CLA	S	611	40	65,73,73	1.38	7 (10%)	76,113,113	1.94	16 (21%)
49	LUT	N1	621	-	42,43,43	2.33	2 (4%)	51,60,60	2.10	13 (25%)
29	CLA	g	612	-	43,51,73	1.70	7 (16%)	49,86,113	2.18	13 (26%)
32	SQD	b	626	-	53,54,54	0.82	0	62,65,65	0.91	3 (4%)
29	CLA	b1	615	-	65,73,73	1.34	8 (12%)	76,113,113	2.05	16 (21%)
39	DGA	b1	625	-	43,43,43	1.13	2 (4%)	45,45,45	1.50	3 (6%)
40	LHG	c1	525	-	46,46,48	0.39	0	49,52,54	1.01	2 (4%)
48	CHL	y1	606	-	66,74,74	0.83	2 (3%)	73,114,114	1.16	10 (13%)
29	CLA	N	610	-	65,73,73	1.36	7 (10%)	76,113,113	2.07	18 (23%)
40	LHG	G1	624	-	48,48,48	0.40	0	51,54,54	1.03	3 (5%)
32	SQD	c1	526	-	53,54,54	0.80	0	62,65,65	0.93	2 (3%)
32	SQD	C1	526	-	53,54,54	0.81	0	62,65,65	0.88	2 (3%)
51	NEX	G	623	-	38,46,46	3.37	11 (28%)	50,70,70	1.92	12 (24%)
33	LMG	a1	413	-	48,48,55	0.99	5 (10%)	56,56,63	1.31	4 (7%)
29	CLA	c	504	-	65,73,73	1.33	8 (12%)	76,113,113	2.05	16 (21%)
48	CHL	S	608	-	61,69,74	0.89	3 (4%)	67,108,114	1.27	11 (16%)
48	CHL	G	605	21	48,56,74	0.96	3 (6%)	51,92,114	1.32	8 (15%)
31	BCR	c1	516	-	41,41,41	1.91	4 (9%)	56,56,56	4.43	13 (23%)
48	CHL	N1	608	-	50,58,74	0.96	2 (4%)	52,94,114	1.51	8 (15%)
29	CLA	y1	613	-	65,73,73	1.33	7 (10%)	76,113,113	2.06	17 (22%)
26	OEX	A1	401	1,4	0,15,15	-	-	-	-	-
37	DGD	c1	520	-	60,60,67	1.09	6 (10%)	74,74,81	1.00	3 (4%)
38	3PH	b	624	-	47,47,47	0.86	4 (8%)	51,52,52	1.18	3 (5%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	y1	612	-	65,73,73	1.34	8 (12%)	76,113,113	2.05	20 (26%)
29	CLA	G1	602	-	65,73,73	1.40	8 (12%)	76,113,113	2.08	21 (27%)
29	CLA	a1	405	-	65,73,73	1.30	6 (9%)	76,113,113	2.12	19 (25%)
29	CLA	s1	609	-	60,68,73	1.40	9 (15%)	70,107,113	2.18	15 (21%)
29	CLA	B	616	-	65,73,73	1.36	9 (13%)	76,113,113	1.95	19 (25%)
29	CLA	b	606	-	65,73,73	1.33	8 (12%)	76,113,113	2.11	17 (22%)
29	CLA	B	608	-	65,73,73	1.34	7 (10%)	76,113,113	2.02	16 (21%)
29	CLA	g1	613	-	65,73,73	1.38	8 (12%)	76,113,113	2.03	16 (21%)
48	CHL	N	605	20	66,74,74	0.92	4 (6%)	73,114,114	1.24	11 (15%)
29	CLA	Y	611	-	65,73,73	1.34	9 (13%)	76,113,113	1.91	13 (17%)
29	CLA	S1	617	23	50,58,73	1.54	8 (16%)	58,95,113	2.32	19 (32%)
29	CLA	b	603	-	65,73,73	1.38	8 (12%)	76,113,113	2.04	18 (23%)
42	BCT	D1	401	27	2,3,3	1.29	0	2,3,3	3.02	2 (100%)
47	4RF	I	102	-	56,56,56	1.05	4 (7%)	59,59,59	0.97	3 (5%)
49	LUT	Y1	620	-	42,43,43	2.39	1 (2%)	51,60,60	1.87	14 (27%)
29	CLA	c	506	-	65,73,73	1.38	9 (13%)	76,113,113	2.07	19 (25%)
29	CLA	R1	608	-	60,68,73	1.42	8 (13%)	70,107,113	2.08	16 (22%)
29	CLA	c	508	-	65,73,73	1.37	8 (12%)	76,113,113	1.98	17 (22%)
48	CHL	Y1	609	-	66,74,74	0.84	2 (3%)	73,114,114	1.28	10 (13%)
33	LMG	w	201	-	39,39,55	0.89	2 (5%)	47,47,63	1.29	4 (8%)
52	LMT	r1	625	-	36,36,36	1.18	4 (11%)	47,47,47	1.08	4 (8%)
31	BCR	D	404	-	41,41,41	1.86	4 (9%)	56,56,56	4.18	16 (28%)
37	DGD	b1	623	-	44,44,67	0.92	2 (4%)	58,58,81	1.32	5 (8%)
48	CHL	G	609	21	66,74,74	0.90	3 (4%)	73,114,114	1.18	12 (16%)
29	CLA	C	507	-	65,73,73	1.38	8 (12%)	76,113,113	2.04	17 (22%)
49	LUT	S1	621	-	42,43,43	2.39	2 (4%)	51,60,60	1.99	19 (37%)
29	CLA	C	504	-	65,73,73	1.34	8 (12%)	76,113,113	1.96	13 (17%)
33	LMG	C1	523	-	55,55,55	1.12	6 (10%)	63,63,63	1.15	6 (9%)
29	CLA	N1	602	-	65,73,73	1.36	7 (10%)	76,113,113	1.98	18 (23%)
29	CLA	R	612	-	60,68,73	1.44	10 (16%)	70,107,113	2.14	18 (25%)
29	CLA	b1	609	-	65,73,73	1.36	8 (12%)	76,113,113	2.05	15 (19%)
33	LMG	c	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.12	3 (4%)
29	CLA	G	614	-	49,57,73	1.55	7 (14%)	55,93,113	2.35	20 (36%)
29	CLA	n1	612	-	45,53,73	1.67	9 (20%)	52,89,113	2.05	13 (25%)
53	ERG	r1	626	-	31,32,32	7.77	19 (61%)	47,50,50	2.72	18 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	y1	608	-	50,58,73	1.55	10 (20%)	58,95,113	2.21	17 (29%)
48	CHL	S	607	-	43,51,74	1.07	3 (6%)	45,86,114	1.46	7 (15%)
49	LUT	N	620	-	42,43,43	2.34	1 (2%)	51,60,60	1.92	15 (29%)
33	LMG	A	413	-	48,48,55	1.01	5 (10%)	56,56,63	1.20	4 (7%)
39	DGA	B1	625	-	43,43,43	1.14	3 (6%)	45,45,45	1.46	3 (6%)
40	LHG	D	409	-	48,48,48	0.40	0	51,54,54	1.06	3 (5%)
33	LMG	c1	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.13	3 (4%)
45	RRX	H	101	-	42,42,42	4.84	24 (57%)	57,58,58	2.85	22 (38%)
29	CLA	Y	608	-	50,58,73	1.54	9 (18%)	58,95,113	2.29	17 (29%)
29	CLA	s	614	-	55,63,73	1.48	7 (12%)	64,101,113	2.12	15 (23%)
31	BCR	c	516	-	41,41,41	1.87	4 (9%)	56,56,56	4.24	12 (21%)
29	CLA	A1	407	-	50,58,73	1.56	8 (16%)	58,95,113	2.22	18 (31%)
40	LHG	D	410	-	38,38,48	0.42	0	41,44,54	1.16	4 (9%)
37	DGD	c	520	-	60,60,67	1.05	4 (6%)	74,74,81	1.03	3 (4%)
37	DGD	C	518	-	56,56,67	0.98	4 (7%)	70,70,81	0.95	2 (2%)
39	DGA	C	524	-	43,43,43	1.13	3 (6%)	45,45,45	1.50	3 (6%)
29	CLA	n	610	-	65,73,73	1.38	9 (13%)	76,113,113	2.12	20 (26%)
51	NEX	R	622	-	38,46,46	3.42	11 (28%)	50,70,70	1.98	12 (24%)
49	LUT	g	620	-	42,43,43	2.32	1 (2%)	51,60,60	2.16	16 (31%)
50	XAT	g	622	-	39,47,47	0.80	1 (2%)	54,74,74	2.22	16 (29%)
29	CLA	N1	612	-	45,53,73	1.64	8 (17%)	52,89,113	2.16	12 (23%)
29	CLA	C1	508	-	65,73,73	1.37	9 (13%)	76,113,113	1.92	14 (18%)
51	NEX	G1	623	-	38,46,46	3.38	10 (26%)	50,70,70	1.77	11 (22%)
29	CLA	C1	505	-	65,73,73	1.34	7 (10%)	76,113,113	2.01	17 (22%)
29	CLA	S1	611	40	65,73,73	1.41	9 (13%)	76,113,113	1.94	14 (18%)
48	CHL	n1	605	-	66,74,74	0.90	3 (4%)	73,114,114	1.29	11 (15%)
29	CLA	c1	512	-	65,73,73	1.38	7 (10%)	76,113,113	2.03	19 (25%)
48	CHL	S	606	-	44,52,74	1.10	3 (6%)	46,87,114	1.48	10 (21%)
29	CLA	R	603	-	60,68,73	1.48	9 (15%)	70,107,113	2.00	17 (24%)
43	PL9	d1	405	-	55,55,55	1.13	3 (5%)	68,69,69	1.57	14 (20%)
29	CLA	B1	604	-	65,73,73	1.37	7 (10%)	76,113,113	1.86	16 (21%)
29	CLA	B	611	-	65,73,73	1.37	8 (12%)	76,113,113	2.01	19 (25%)
29	CLA	C1	503	-	65,73,73	1.38	9 (13%)	76,113,113	2.01	21 (27%)
32	SQD	b1	626	-	53,54,54	0.80	0	62,65,65	0.93	2 (3%)
29	CLA	y	611	40	65,73,73	1.35	7 (10%)	76,113,113	1.88	15 (19%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	Y1	608	-	50,58,73	1.57	8 (16%)	58,95,113	2.24	16 (27%)
29	CLA	g1	603	-	65,73,73	1.38	8 (12%)	76,113,113	1.88	16 (21%)
29	CLA	y	613	-	65,73,73	1.36	7 (10%)	76,113,113	2.04	18 (23%)
48	CHL	s1	601	23	46,54,74	1.07	3 (6%)	49,90,114	1.46	12 (24%)
29	CLA	s1	610	-	65,73,73	1.38	7 (10%)	76,113,113	2.01	19 (25%)
29	CLA	c	511	4	65,73,73	1.36	8 (12%)	76,113,113	2.01	19 (25%)
29	CLA	R1	610	-	60,68,73	1.43	9 (15%)	70,107,113	2.28	18 (25%)
47	4RF	i1	101	-	56,56,56	1.06	3 (5%)	59,59,59	0.92	3 (5%)
29	CLA	s	603	-	65,73,73	1.38	8 (12%)	76,113,113	2.02	17 (22%)
29	CLA	S	604	-	55,63,73	1.45	8 (14%)	64,101,113	2.22	17 (26%)
50	XAT	r	621	-	39,47,47	0.73	1 (2%)	54,74,74	2.02	13 (24%)
48	CHL	n1	609	-	66,74,74	0.78	2 (3%)	73,114,114	1.32	12 (16%)
29	CLA	S	602	-	60,68,73	1.45	8 (13%)	70,107,113	2.17	18 (25%)
48	CHL	Y1	607	-	66,74,74	0.86	3 (4%)	73,114,114	1.19	9 (12%)
29	CLA	g	614	-	49,57,73	1.57	9 (18%)	55,93,113	2.23	15 (27%)
29	CLA	C1	512	-	65,73,73	1.35	7 (10%)	76,113,113	2.09	21 (27%)
51	NEX	n1	623	-	38,46,46	3.26	9 (23%)	50,70,70	1.71	11 (22%)
29	CLA	C	506	-	65,73,73	1.43	8 (12%)	76,113,113	2.05	18 (23%)
31	BCR	B	619	-	41,41,41	1.85	4 (9%)	56,56,56	3.81	21 (37%)
48	CHL	Y	605	24	46,54,74	1.07	3 (6%)	49,90,114	1.51	10 (20%)
48	CHL	G1	608	-	44,52,74	1.10	3 (6%)	46,87,114	1.43	7 (15%)
38	3PH	S	626	-	47,47,47	0.87	2 (4%)	51,52,52	4.41	4 (7%)
48	CHL	g1	606	-	50,58,74	1.06	4 (8%)	52,94,114	1.28	9 (17%)
55	PTY	Y1	627	-	18,18,49	1.28	2 (11%)	21,23,54	1.41	2 (9%)
37	DGD	C	520	-	60,60,67	1.06	6 (10%)	74,74,81	1.07	3 (4%)
29	CLA	S1	613	-	55,63,73	1.45	7 (12%)	64,101,113	2.15	15 (23%)
33	LMG	w1	201	-	39,39,55	0.85	2 (5%)	47,47,63	1.17	3 (6%)
49	LUT	R1	620	-	42,43,43	2.36	1 (2%)	51,60,60	1.94	10 (19%)
40	LHG	G	624	29	48,48,48	0.37	0	51,54,54	1.06	3 (5%)
49	LUT	s	620	-	42,43,43	2.37	1 (2%)	51,60,60	1.91	15 (29%)
29	CLA	Y	610	-	65,73,73	1.36	9 (13%)	76,113,113	2.14	18 (23%)
29	CLA	c1	506	-	65,73,73	1.30	6 (9%)	76,113,113	2.09	20 (26%)
48	CHL	n	607	-	66,74,74	0.81	2 (3%)	73,114,114	1.27	12 (16%)
29	CLA	n	604	-	65,73,73	1.35	8 (12%)	76,113,113	2.01	17 (22%)
48	CHL	R1	606	-	44,52,74	1.07	3 (6%)	46,87,114	1.30	8 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	C	503	-	65,73,73	1.35	8 (12%)	76,113,113	1.99	17 (22%)
48	CHL	s	606	-	44,52,74	1.04	3 (6%)	46,87,114	1.46	7 (15%)
29	CLA	S1	609	-	60,68,73	1.39	8 (13%)	70,107,113	2.09	17 (24%)
42	BCT	d	401	-	2,3,3	1.27	0	2,3,3	2.80	2 (100%)
37	DGD	C1	519	-	63,63,67	1.10	7 (11%)	77,77,81	1.05	3 (3%)
29	CLA	S1	602	23	60,68,73	1.39	9 (15%)	70,107,113	2.13	17 (24%)
33	LMG	h1	102	-	48,48,55	1.00	4 (8%)	56,56,63	1.23	4 (7%)
29	CLA	A1	410	-	60,68,73	1.40	7 (11%)	70,107,113	2.13	20 (28%)
29	CLA	N1	604	-	65,73,73	1.36	8 (12%)	76,113,113	2.15	17 (22%)
51	NEX	r	622	-	38,46,46	3.31	9 (23%)	50,70,70	1.78	11 (22%)
33	LMG	C1	521	-	51,51,55	1.07	5 (9%)	59,59,63	1.14	2 (3%)
29	CLA	c	502	-	65,73,73	1.37	7 (10%)	76,113,113	2.06	16 (21%)
29	CLA	B1	602	-	65,73,73	1.39	9 (13%)	76,113,113	2.02	17 (22%)
29	CLA	S1	604	-	55,63,73	1.49	9 (16%)	64,101,113	2.20	18 (28%)
48	CHL	Y	609	-	66,74,74	0.91	4 (6%)	73,114,114	1.43	14 (19%)
48	CHL	g	607	-	66,74,74	0.85	2 (3%)	73,114,114	1.27	11 (15%)
48	CHL	Y1	606	-	66,74,74	0.90	4 (6%)	73,114,114	1.25	10 (13%)
50	XAT	G	622	-	39,47,47	0.71	1 (2%)	54,74,74	2.11	15 (27%)
48	CHL	s	601	-	46,54,74	1.15	4 (8%)	49,90,114	1.43	8 (16%)
29	CLA	C	511	-	65,73,73	1.34	8 (12%)	76,113,113	1.98	18 (23%)
32	SQD	B	626	-	53,54,54	0.79	0	62,65,65	0.91	2 (3%)
55	PTY	y	627	-	18,18,49	1.29	3 (16%)	21,23,54	1.50	2 (9%)
37	DGD	c	518	-	56,56,67	0.98	4 (7%)	70,70,81	1.14	4 (5%)
33	LMG	H1	102	-	48,48,55	1.02	5 (10%)	56,56,63	1.16	3 (5%)
55	PTY	y1	626	-	49,49,49	0.87	4 (8%)	52,54,54	1.08	2 (3%)
34	SPH	A1	414	-	19,20,20	0.67	1 (5%)	18,21,21	1.17	1 (5%)
48	CHL	R	606	-	44,52,74	1.20	4 (9%)	46,87,114	1.30	7 (15%)
48	CHL	n	601	20	66,74,74	0.91	3 (4%)	73,114,114	1.26	9 (12%)
52	LMT	R	625	-	36,36,36	1.22	6 (16%)	47,47,47	1.14	3 (6%)
52	LMT	R1	625	-	36,36,36	1.27	8 (22%)	47,47,47	1.15	4 (8%)
29	CLA	s	609	-	60,68,73	1.42	9 (15%)	70,107,113	2.03	15 (21%)
31	BCR	b1	618	-	41,41,41	2.03	4 (9%)	56,56,56	4.25	19 (33%)
49	LUT	S	621	-	42,43,43	2.25	1 (2%)	51,60,60	2.10	19 (37%)
48	CHL	g1	605	-	48,56,74	0.95	2 (4%)	51,92,114	1.50	10 (19%)
29	CLA	C	510	-	65,73,73	1.37	7 (10%)	76,113,113	1.97	18 (23%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	S1	612	-	45,53,73	1.59	6 (13%)	52,89,113	2.18	15 (28%)
48	CHL	Y1	601	-	66,74,74	0.91	3 (4%)	73,114,114	1.23	10 (13%)
31	BCR	C	516	-	41,41,41	1.84	4 (9%)	56,56,56	4.25	16 (28%)
29	CLA	S	605	23	50,58,73	1.59	9 (18%)	58,95,113	2.42	16 (27%)
29	CLA	y1	603	-	65,73,73	1.36	8 (12%)	76,113,113	1.93	16 (21%)
41	LMK	C1	527	-	38,39,53	1.50	2 (5%)	41,46,60	1.47	2 (4%)
49	LUT	N	621	-	42,43,43	2.39	1 (2%)	51,60,60	1.97	12 (23%)
50	XAT	R	621	-	39,47,47	0.73	1 (2%)	54,74,74	2.02	18 (33%)
29	CLA	n1	602	20	65,73,73	1.31	8 (12%)	76,113,113	2.04	20 (26%)
38	3PH	S1	626	-	47,47,47	0.87	4 (8%)	51,52,52	4.40	4 (7%)
29	CLA	A	405	-	65,73,73	1.35	6 (9%)	76,113,113	2.09	17 (22%)
42	BCT	d1	401	-	2,3,3	1.18	0	2,3,3	4.36	2 (100%)
49	LUT	y1	620	-	42,43,43	2.35	1 (2%)	51,60,60	1.97	10 (19%)
29	CLA	y1	614	-	65,73,73	1.40	9 (13%)	76,113,113	1.90	19 (25%)
48	CHL	g	601	21	66,74,74	0.88	4 (6%)	73,114,114	1.25	10 (13%)
49	LUT	y	621	-	42,43,43	2.36	1 (2%)	51,60,60	1.98	14 (27%)
29	CLA	n	603	-	65,73,73	1.36	8 (12%)	76,113,113	2.03	20 (26%)
38	3PH	T1	101	-	47,47,47	0.85	4 (8%)	51,52,52	1.09	2 (3%)
29	CLA	N1	614	-	49,57,73	1.54	7 (14%)	55,93,113	2.33	17 (30%)
49	LUT	Y1	621	-	42,43,43	2.32	1 (2%)	51,60,60	2.33	13 (25%)
29	CLA	B1	607	-	65,73,73	1.36	8 (12%)	76,113,113	2.08	19 (25%)
48	CHL	N	607	-	66,74,74	0.82	2 (3%)	73,114,114	1.23	12 (16%)
29	CLA	G1	611	-	65,73,73	1.35	7 (10%)	76,113,113	2.01	15 (19%)
29	CLA	G	603	-	65,73,73	1.33	8 (12%)	76,113,113	2.03	20 (26%)
29	CLA	y	610	24	65,73,73	1.33	7 (10%)	76,113,113	2.03	17 (22%)
40	LHG	s1	624	29	44,44,48	0.43	0	47,50,54	1.08	4 (8%)
29	CLA	g	610	-	65,73,73	1.33	8 (12%)	76,113,113	2.12	20 (26%)
29	CLA	B1	617	-	65,73,73	1.37	8 (12%)	76,113,113	1.98	16 (21%)
29	CLA	c	507	-	65,73,73	1.39	9 (13%)	76,113,113	2.02	16 (21%)
49	LUT	g1	620	-	42,43,43	2.33	1 (2%)	51,60,60	1.93	11 (21%)
31	BCR	c	515	-	41,41,41	1.88	5 (12%)	56,56,56	4.18	16 (28%)
29	CLA	g	603	-	65,73,73	1.37	9 (13%)	76,113,113	2.03	17 (22%)
26	OEX	A	401	1,4	0,15,15	-	-	-	-	-
29	CLA	D1	403	-	65,73,73	1.36	9 (13%)	76,113,113	2.05	22 (28%)
29	CLA	b1	604	-	65,73,73	1.38	9 (13%)	76,113,113	2.03	17 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
34	SPH	a	414	-	19,20,20	0.70	1 (5%)	18,21,21	1.10	1 (5%)
32	SQD	c	526	-	53,54,54	0.79	0	62,65,65	0.92	2 (3%)
33	LMG	A1	413	-	48,48,55	1.00	5 (10%)	56,56,63	1.20	5 (8%)
45	RRX	H1	101	-	42,42,42	4.95	24 (57%)	57,58,58	2.34	19 (33%)
48	CHL	s	607	-	43,51,74	1.09	3 (6%)	45,86,114	1.49	8 (17%)
31	BCR	b1	619	-	41,41,41	1.91	4 (9%)	56,56,56	4.36	15 (26%)
47	4RF	K	101	-	56,56,56	1.08	3 (5%)	59,59,59	0.91	3 (5%)
29	CLA	n1	603	-	65,73,73	1.34	7 (10%)	76,113,113	2.02	16 (21%)
31	BCR	C	514	-	41,41,41	1.87	5 (12%)	56,56,56	4.28	14 (25%)
48	CHL	n	606	-	66,74,74	0.92	4 (6%)	73,114,114	1.25	12 (16%)
29	CLA	a	407	-	49,57,73	1.55	7 (14%)	55,93,113	2.52	18 (32%)
33	LMG	W1	201	-	39,39,55	0.87	2 (5%)	47,47,63	1.37	6 (12%)
40	LHG	d	409	-	48,48,48	0.41	0	51,54,54	1.06	3 (5%)
39	DGA	C1	524	-	43,43,43	1.17	3 (6%)	45,45,45	1.54	4 (8%)
48	CHL	y1	607	-	66,74,74	0.77	2 (3%)	73,114,114	1.29	10 (13%)
30	PHO	A1	408	-	51,69,69	1.06	4 (7%)	47,99,99	1.15	4 (8%)
29	CLA	R	610	-	60,68,73	1.49	10 (16%)	70,107,113	2.14	21 (30%)
29	CLA	G1	604	-	49,57,73	1.57	7 (14%)	55,93,113	2.34	18 (32%)
29	CLA	s1	602	-	60,68,73	1.40	7 (11%)	70,107,113	2.30	21 (30%)
29	CLA	B1	606	-	65,73,73	1.38	9 (13%)	76,113,113	2.03	18 (23%)
48	CHL	Y	607	-	66,74,74	0.77	2 (3%)	73,114,114	1.28	9 (12%)
50	XAT	n1	622	-	39,47,47	0.71	1 (2%)	54,74,74	2.04	14 (25%)
29	CLA	A	406	-	65,73,73	1.32	7 (10%)	76,113,113	2.12	17 (22%)
29	CLA	c1	503	-	65,73,73	1.37	9 (13%)	76,113,113	2.06	19 (25%)
48	CHL	g	606	-	50,58,74	0.99	2 (4%)	52,94,114	1.55	9 (17%)
29	CLA	y	608	-	50,58,73	1.57	9 (18%)	58,95,113	2.25	17 (29%)
31	BCR	b	618	-	41,41,41	1.89	5 (12%)	56,56,56	4.48	20 (35%)
48	CHL	N	606	-	66,74,74	0.96	3 (4%)	73,114,114	1.21	13 (17%)
29	CLA	B1	603	-	65,73,73	1.39	9 (13%)	76,113,113	2.13	20 (26%)
49	LUT	Y	620	-	42,43,43	2.31	1 (2%)	51,60,60	1.81	13 (25%)
40	LHG	n1	624	-	48,48,48	0.41	0	51,54,54	1.07	3 (5%)
36	C7Z	b	620	-	43,43,43	5.32	27 (62%)	58,60,60	2.48	19 (32%)
31	BCR	A1	411	-	41,41,41	1.88	4 (9%)	56,56,56	4.17	15 (26%)
26	OEX	a	401	1,4	0,15,15	-	-	-	-	-
29	CLA	G1	613	-	65,73,73	1.32	7 (10%)	76,113,113	2.19	21 (27%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
37	DGD	c	519	-	63,63,67	1.12	5 (7%)	77,77,81	1.01	2 (2%)
49	LUT	n	621	-	42,43,43	2.39	1 (2%)	51,60,60	1.78	12 (23%)
29	CLA	B	606	-	65,73,73	1.33	8 (12%)	76,113,113	2.14	17 (22%)
48	CHL	y1	601	24	66,74,74	0.79	2 (3%)	73,114,114	1.28	9 (12%)
29	CLA	y1	610	24	65,73,73	1.39	9 (13%)	76,113,113	2.02	21 (27%)
32	SQD	C	526	-	53,54,54	0.81	1 (1%)	62,65,65	0.94	3 (4%)
29	CLA	N	613	-	65,73,73	1.38	7 (10%)	76,113,113	2.01	13 (17%)
29	CLA	G1	612	-	43,51,73	1.71	9 (20%)	49,86,113	2.15	12 (24%)
33	LMG	c	521	-	51,51,55	1.06	5 (9%)	59,59,63	1.16	4 (6%)
48	CHL	n1	607	-	66,74,74	0.77	2 (3%)	73,114,114	1.29	10 (13%)
29	CLA	R1	609	-	60,68,73	1.40	9 (15%)	70,107,113	4.53	19 (27%)
48	CHL	s1	607	-	43,51,74	1.02	3 (6%)	45,86,114	1.45	8 (17%)
33	LMG	H	102	-	48,48,55	1.01	5 (10%)	56,56,63	1.10	2 (3%)
40	LHG	D1	408	-	43,43,48	0.41	0	46,49,54	1.03	2 (4%)
40	LHG	D1	410	-	38,38,48	0.43	0	41,44,54	1.09	3 (7%)
46	GOL	I	101	-	5,5,5	0.54	0	5,5,5	0.39	0
29	CLA	B1	611	-	65,73,73	1.37	7 (10%)	76,113,113	2.09	16 (21%)
39	DGA	j1	101	-	28,28,43	1.32	3 (10%)	30,30,45	1.26	2 (6%)
49	LUT	s1	621	-	42,43,43	2.25	1 (2%)	51,60,60	2.37	13 (25%)
29	CLA	B1	613	-	65,73,73	1.37	8 (12%)	76,113,113	1.97	14 (18%)
29	CLA	b1	611	-	65,73,73	1.42	6 (9%)	76,113,113	2.02	18 (23%)
29	CLA	c1	510	-	65,73,73	1.39	8 (12%)	76,113,113	1.92	16 (21%)
53	ERG	R	626	-	31,32,32	7.79	18 (58%)	47,50,50	3.10	19 (40%)
29	CLA	S1	614	-	55,63,73	1.49	7 (12%)	64,101,113	2.12	17 (26%)
38	3PH	t	101	-	47,47,47	0.85	4 (8%)	51,52,52	1.19	2 (3%)
29	CLA	r	610	-	60,68,73	1.41	9 (15%)	70,107,113	2.20	20 (28%)
29	CLA	D	403	-	65,73,73	1.35	9 (13%)	76,113,113	2.08	19 (25%)
29	CLA	Y1	602	-	65,73,73	1.38	9 (13%)	76,113,113	2.07	17 (22%)
48	CHL	n1	601	-	66,74,74	0.82	2 (3%)	73,114,114	1.29	9 (12%)
34	SPH	Y1	625	-	19,20,20	0.64	0	18,21,21	1.03	1 (5%)
40	LHG	y	624	29	48,48,48	0.40	0	51,54,54	1.06	3 (5%)
49	LUT	n	620	-	42,43,43	2.35	1 (2%)	51,60,60	2.09	17 (33%)
50	XAT	n	622	-	39,47,47	0.78	1 (2%)	54,74,74	2.09	13 (24%)
40	LHG	l	101	-	48,48,48	0.38	0	51,54,54	4.45	4 (7%)
29	CLA	r1	608	-	60,68,73	1.45	7 (11%)	70,107,113	2.03	16 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	s	611	40	65,73,73	1.37	8 (12%)	76,113,113	1.91	13 (17%)
31	BCR	c1	517	-	41,41,41	1.91	5 (12%)	56,56,56	4.37	19 (33%)
29	CLA	d1	403	-	65,73,73	1.34	7 (10%)	76,113,113	2.04	19 (25%)
29	CLA	B1	608	-	65,73,73	1.38	8 (12%)	76,113,113	1.97	16 (21%)
40	LHG	c	525	-	46,46,48	0.40	0	49,52,54	1.12	3 (6%)
36	C7Z	b1	620	-	43,43,43	5.40	26 (60%)	58,60,60	2.51	22 (37%)
29	CLA	b1	616	-	65,73,73	1.38	7 (10%)	76,113,113	1.94	14 (18%)
29	CLA	r1	602	-	60,68,73	1.40	7 (11%)	70,107,113	2.09	19 (27%)
33	LMG	b1	622	-	44,44,55	0.86	2 (4%)	52,52,63	1.17	3 (5%)
31	BCR	d	404	-	41,41,41	1.84	4 (9%)	56,56,56	4.25	16 (28%)
33	LMG	d1	411	-	46,46,55	0.93	3 (6%)	54,54,63	1.11	3 (5%)
29	CLA	c	505	-	65,73,73	1.40	8 (12%)	76,113,113	2.00	16 (21%)
51	NEX	s1	623	-	38,46,46	3.40	12 (31%)	50,70,70	2.71	15 (30%)
51	NEX	S	623	-	38,46,46	3.42	10 (26%)	50,70,70	1.71	12 (24%)
29	CLA	b1	608	-	65,73,73	1.36	8 (12%)	76,113,113	2.04	19 (25%)
32	SQD	m1	101	-	41,42,54	0.88	0	50,53,65	0.99	3 (6%)
29	CLA	N1	611	-	49,57,73	1.59	8 (16%)	55,93,113	2.29	16 (29%)
50	XAT	y	622	-	39,47,47	0.73	1 (2%)	54,74,74	3.68	19 (35%)
29	CLA	N1	613	-	65,73,73	1.35	8 (12%)	76,113,113	2.02	17 (22%)
49	LUT	g1	621	-	42,43,43	2.36	1 (2%)	51,60,60	2.33	14 (27%)
29	CLA	C1	506	-	65,73,73	1.36	7 (10%)	76,113,113	2.01	17 (22%)
29	CLA	R1	603	-	60,68,73	1.45	8 (13%)	70,107,113	1.89	14 (20%)
50	XAT	N	622	-	39,47,47	0.70	1 (2%)	54,74,74	2.21	13 (24%)
29	CLA	d1	402	-	65,73,73	1.39	9 (13%)	76,113,113	1.95	17 (22%)
41	LMK	c1	527	-	38,39,53	1.51	3 (7%)	41,46,60	1.24	2 (4%)
39	DGA	c	524	-	43,43,43	1.10	3 (6%)	45,45,45	1.55	3 (6%)
29	CLA	R1	604	-	49,57,73	1.56	8 (16%)	55,93,113	2.34	15 (27%)
29	CLA	Y1	603	-	65,73,73	1.39	10 (15%)	76,113,113	1.95	16 (21%)
29	CLA	b	613	-	65,73,73	1.37	8 (12%)	76,113,113	1.95	11 (14%)
29	CLA	n	613	-	65,73,73	1.36	6 (9%)	76,113,113	2.12	18 (23%)
29	CLA	G	613	-	65,73,73	1.35	8 (12%)	76,113,113	2.04	20 (26%)
29	CLA	r	608	-	60,68,73	1.40	9 (15%)	70,107,113	2.00	18 (25%)
47	4RF	i	101	-	56,56,56	1.07	3 (5%)	59,59,59	0.93	3 (5%)
29	CLA	a	406	-	65,73,73	1.34	8 (12%)	76,113,113	2.25	20 (26%)
44	HEM	f	101	7,6	41,50,50	1.45	4 (9%)	45,82,82	1.35	6 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
48	CHL	Y	601	24	66,74,74	0.91	3 (4%)	73,114,114	1.21	9 (12%)
48	CHL	s1	608	-	61,69,74	1.04	5 (8%)	67,108,114	1.38	11 (16%)
45	RRX	h	101	-	42,42,42	4.74	24 (57%)	57,58,58	3.10	25 (43%)
40	LHG	d1	408	-	43,43,48	0.40	0	46,49,54	1.05	2 (4%)
40	LHG	L	101	-	48,48,48	0.38	0	51,54,54	4.46	5 (9%)
29	CLA	G	612	-	43,51,73	1.66	6 (13%)	49,86,113	2.20	14 (28%)
29	CLA	a	410	-	60,68,73	1.39	9 (15%)	70,107,113	2.17	18 (25%)
29	CLA	r1	612	-	60,68,73	1.42	7 (11%)	70,107,113	2.05	19 (27%)
29	CLA	n	614	-	49,57,73	1.56	9 (18%)	55,93,113	2.36	20 (36%)
40	LHG	N	624	-	48,48,48	0.40	0	51,54,54	1.08	3 (5%)
48	CHL	g1	607	-	66,74,74	0.81	2 (3%)	73,114,114	1.23	9 (12%)
50	XAT	y1	622	-	39,47,47	0.74	1 (2%)	54,74,74	3.88	20 (37%)
49	LUT	s	621	-	42,43,43	2.30	1 (2%)	51,60,60	1.98	16 (31%)
33	LMG	a	413	-	48,48,55	0.99	5 (10%)	56,56,63	1.19	4 (7%)
29	CLA	b	602	-	65,73,73	1.38	8 (12%)	76,113,113	1.98	18 (23%)
29	CLA	s1	605	-	50,58,73	1.60	11 (22%)	58,95,113	2.28	18 (31%)
51	NEX	Y	623	-	38,46,46	3.34	9 (23%)	50,70,70	1.85	12 (24%)
49	LUT	Y	621	-	42,43,43	2.32	1 (2%)	51,60,60	2.00	15 (29%)
29	CLA	r1	603	-	60,68,73	1.41	8 (13%)	70,107,113	2.11	17 (24%)
29	CLA	g	613	-	65,73,73	1.33	7 (10%)	76,113,113	2.04	18 (23%)
39	DGA	j	101	-	28,28,43	1.28	3 (10%)	30,30,45	1.28	2 (6%)
51	NEX	S1	623	-	38,46,46	3.20	9 (23%)	50,70,70	1.79	10 (20%)
40	LHG	C	525	-	46,46,48	0.42	0	49,52,54	1.04	2 (4%)
44	HEM	f1	101	7	41,50,50	1.52	7 (17%)	45,82,82	1.19	4 (8%)
40	LHG	y1	624	29	48,48,48	0.41	0	51,54,54	0.98	2 (3%)
40	LHG	L1	101	-	48,48,48	0.37	0	51,54,54	1.11	3 (5%)
48	CHL	N1	605	20	66,74,74	0.90	3 (4%)	73,114,114	1.31	13 (17%)
43	PL9	D1	405	-	55,55,55	1.18	5 (9%)	68,69,69	1.72	15 (22%)
47	4RF	k	101	-	56,56,56	1.06	5 (8%)	59,59,59	0.83	3 (5%)
29	CLA	n	611	-	49,57,73	1.58	7 (14%)	55,93,113	2.30	17 (30%)
29	CLA	y	604	-	65,73,73	1.33	7 (10%)	76,113,113	2.09	19 (25%)
29	CLA	r	612	-	60,68,73	1.43	8 (13%)	70,107,113	2.03	16 (22%)
48	CHL	R	607	-	50,58,74	1.00	3 (6%)	52,94,114	1.44	9 (17%)
48	CHL	S1	608	-	61,69,74	0.84	2 (3%)	67,108,114	1.33	13 (19%)
29	CLA	C	505	-	65,73,73	1.40	8 (12%)	76,113,113	2.00	16 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	C1	501	-	65,73,73	1.35	8 (12%)	76,113,113	2.15	19 (25%)
51	NEX	Y1	623	-	38,46,46	3.15	10 (26%)	50,70,70	1.99	13 (26%)
29	CLA	r	603	-	60,68,73	1.45	8 (13%)	70,107,113	1.95	16 (22%)
30	PHO	a	408	-	51,69,69	1.08	6 (11%)	47,99,99	1.23	5 (10%)
29	CLA	g	611	-	65,73,73	1.34	7 (10%)	76,113,113	2.10	17 (22%)
29	CLA	B1	610	-	65,73,73	1.36	8 (12%)	76,113,113	1.91	14 (18%)
34	SPH	y1	625	-	19,20,20	0.62	0	18,21,21	1.27	2 (11%)
29	CLA	s	602	-	60,68,73	1.41	8 (13%)	70,107,113	2.10	21 (30%)
29	CLA	B	610	-	65,73,73	1.35	8 (12%)	76,113,113	1.98	17 (22%)
48	CHL	N1	609	-	66,74,74	0.77	2 (3%)	73,114,114	1.44	13 (17%)
31	BCR	C1	517	-	41,41,41	1.87	4 (9%)	56,56,56	4.45	16 (28%)
54	LPX	S1	625	-	29,29,29	1.02	2 (6%)	31,33,33	0.93	1 (3%)
44	HEM	F1	101	7	41,50,50	1.48	3 (7%)	45,82,82	1.47	9 (20%)
29	CLA	B	615	-	65,73,73	1.35	8 (12%)	76,113,113	2.03	19 (25%)
29	CLA	b	617	-	65,73,73	1.35	8 (12%)	76,113,113	2.02	16 (21%)
32	SQD	B1	626	-	53,54,54	0.80	0	62,65,65	0.92	2 (3%)
37	DGD	c1	519	-	63,63,67	1.14	6 (9%)	77,77,81	1.04	3 (3%)
48	CHL	N	609	-	66,74,74	0.79	3 (4%)	73,114,114	1.22	11 (15%)
29	CLA	C1	507	-	65,73,73	1.38	8 (12%)	76,113,113	1.92	17 (22%)
29	CLA	b1	606	-	65,73,73	1.35	7 (10%)	76,113,113	2.05	18 (23%)
33	LMG	D	411	-	46,46,55	0.91	4 (8%)	54,54,63	0.99	2 (3%)
37	DGD	C	519	-	63,63,67	1.13	7 (11%)	77,77,81	1.01	2 (2%)
51	NEX	n	623	-	38,46,46	3.48	11 (28%)	50,70,70	1.66	11 (22%)
51	NEX	N	623	-	38,46,46	3.40	9 (23%)	50,70,70	1.64	11 (22%)
48	CHL	n	605	20	66,74,74	0.93	5 (7%)	73,114,114	1.24	8 (10%)
29	CLA	y	614	-	65,73,73	1.35	7 (10%)	76,113,113	2.00	18 (23%)
47	4RF	I1	102	-	56,56,56	1.06	4 (7%)	59,59,59	0.98	3 (5%)
48	CHL	G1	606	-	50,58,74	0.99	2 (4%)	52,94,114	1.39	11 (21%)
49	LUT	R	620	-	42,43,43	2.33	1 (2%)	51,60,60	2.03	17 (33%)
29	CLA	Y1	611	-	65,73,73	1.36	8 (12%)	76,113,113	1.95	17 (22%)
29	CLA	c1	511	-	65,73,73	1.36	7 (10%)	76,113,113	2.06	17 (22%)
48	CHL	y	607	-	66,74,74	0.82	3 (4%)	73,114,114	1.31	12 (16%)
29	CLA	C1	511	-	65,73,73	1.37	8 (12%)	76,113,113	2.13	19 (25%)
29	CLA	B	617	-	65,73,73	1.37	8 (12%)	76,113,113	2.04	15 (19%)
31	BCR	c1	514	-	41,41,41	1.85	4 (9%)	56,56,56	4.49	17 (30%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	Y	602	-	65,73,73	1.38	9 (13%)	76,113,113	2.06	19 (25%)
32	SQD	A	412	-	50,51,54	0.81	0	59,62,65	0.94	3 (5%)
38	3PH	s	626	-	47,47,47	0.87	3 (6%)	51,52,52	4.40	4 (7%)
31	BCR	C1	514	-	41,41,41	1.84	5 (12%)	56,56,56	4.05	13 (23%)
38	3PH	s1	626	-	47,47,47	0.86	3 (6%)	51,52,52	4.37	4 (7%)
29	CLA	D	402	-	65,73,73	1.38	8 (12%)	76,113,113	1.90	13 (17%)
40	LHG	d1	410	-	38,38,48	0.44	0	41,44,54	1.04	2 (4%)
36	C7Z	B1	620	-	43,43,43	5.38	26 (60%)	58,60,60	2.39	22 (37%)
29	CLA	y	603	-	65,73,73	1.39	10 (15%)	76,113,113	2.10	16 (21%)
31	BCR	c	514	-	41,41,41	1.84	4 (9%)	56,56,56	4.25	14 (25%)
32	SQD	B	621	-	41,42,54	0.88	0	50,53,65	1.01	3 (6%)
29	CLA	A	407	-	50,58,73	1.54	9 (18%)	58,95,113	2.32	18 (31%)
51	NEX	g	623	-	38,46,46	3.48	11 (28%)	50,70,70	1.86	15 (30%)
29	CLA	R1	602	-	60,68,73	1.45	9 (15%)	70,107,113	2.05	17 (24%)
29	CLA	N1	610	-	65,73,73	1.31	7 (10%)	76,113,113	1.99	18 (23%)
34	SPH	A	414	-	19,20,20	0.66	0	18,21,21	1.13	2 (11%)
51	NEX	y	623	-	38,46,46	3.41	9 (23%)	50,70,70	1.96	15 (30%)
29	CLA	S1	610	-	65,73,73	1.35	7 (10%)	76,113,113	2.02	18 (23%)
39	DGA	c1	524	-	43,43,43	1.14	3 (6%)	45,45,45	1.51	3 (6%)
29	CLA	G1	614	-	49,57,73	1.53	7 (14%)	55,93,113	2.37	17 (30%)
30	PHO	a1	409	-	51,69,69	1.03	3 (5%)	47,99,99	1.21	6 (12%)
48	CHL	Y	606	-	66,74,74	0.90	4 (6%)	73,114,114	1.14	8 (10%)
29	CLA	c	503	-	65,73,73	1.35	8 (12%)	76,113,113	1.98	21 (27%)
48	CHL	n	609	-	66,74,74	0.77	2 (3%)	73,114,114	1.40	12 (16%)
29	CLA	S	610	-	65,73,73	1.37	9 (13%)	76,113,113	1.92	21 (27%)
29	CLA	G	611	40	65,73,73	1.37	7 (10%)	76,113,113	2.01	17 (22%)
49	LUT	y1	621	-	42,43,43	2.37	1 (2%)	51,60,60	2.41	16 (31%)
48	CHL	y	601	24	66,74,74	0.86	3 (4%)	73,114,114	1.32	12 (16%)
49	LUT	g	621	-	42,43,43	2.37	2 (4%)	51,60,60	1.91	12 (23%)
29	CLA	R	609	-	60,68,73	1.45	8 (13%)	70,107,113	4.48	18 (25%)
48	CHL	g1	601	-	66,74,74	0.82	2 (3%)	73,114,114	1.29	11 (15%)
29	CLA	c	513	-	65,73,73	1.37	8 (12%)	76,113,113	2.12	18 (23%)
29	CLA	B	604	-	65,73,73	1.38	7 (10%)	76,113,113	1.94	14 (18%)
29	CLA	b	607	-	65,73,73	1.36	8 (12%)	76,113,113	2.02	20 (26%)
32	SQD	a	412	-	50,51,54	0.81	0	59,62,65	0.92	2 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	s1	604	-	55,63,73	1.46	5 (9%)	64,101,113	2.22	18 (28%)
33	LMG	C	521	-	51,51,55	1.06	5 (9%)	59,59,63	1.19	3 (5%)
40	LHG	S	624	29	44,44,48	0.43	0	47,50,54	1.05	3 (6%)
48	CHL	n	608	-	50,58,74	1.01	3 (6%)	52,94,114	1.28	10 (19%)
29	CLA	Y	603	-	65,73,73	1.38	8 (12%)	76,113,113	2.01	18 (23%)
48	CHL	G	601	21	66,74,74	0.87	3 (4%)	73,114,114	1.24	11 (15%)
29	CLA	A	410	-	60,68,73	1.43	9 (15%)	70,107,113	2.17	18 (25%)
48	CHL	y1	605	24	46,54,74	1.03	3 (6%)	49,90,114	1.31	8 (16%)
29	CLA	S1	603	-	65,73,73	1.38	8 (12%)	76,113,113	2.01	16 (21%)
40	LHG	C1	525	-	46,46,48	0.39	0	49,52,54	1.04	3 (6%)
29	CLA	C	502	-	65,73,73	1.37	8 (12%)	76,113,113	2.00	15 (19%)
48	CHL	G1	605	21	48,56,74	0.96	3 (6%)	51,92,114	1.38	9 (17%)
33	LMG	h	102	-	48,48,55	1.01	5 (10%)	56,56,63	1.22	4 (7%)
32	SQD	B1	621	-	41,42,54	0.89	0	50,53,65	0.96	2 (4%)
48	CHL	g	609	-	66,74,74	0.91	3 (4%)	73,114,114	1.25	8 (10%)
29	CLA	S	613	-	55,63,73	1.47	7 (12%)	64,101,113	2.18	16 (25%)
29	CLA	b1	617	-	65,73,73	1.36	6 (9%)	76,113,113	1.97	18 (23%)
29	CLA	n1	613	-	65,73,73	1.36	9 (13%)	76,113,113	2.16	17 (22%)
31	BCR	a1	411	-	41,41,41	1.92	5 (12%)	56,56,56	4.06	15 (26%)
32	SQD	b	621	-	41,42,54	0.87	0	50,53,65	1.02	3 (6%)
29	CLA	B1	614	-	65,73,73	1.38	9 (13%)	76,113,113	1.98	14 (18%)
48	CHL	r	606	-	44,52,74	1.05	3 (6%)	46,87,114	1.34	7 (15%)
48	CHL	g	608	-	44,52,74	1.07	3 (6%)	46,87,114	1.47	12 (26%)
32	SQD	b1	621	-	41,42,54	0.89	0	50,53,65	0.98	3 (6%)
52	LMT	r	625	-	36,36,36	1.22	5 (13%)	47,47,47	1.16	3 (6%)
29	CLA	c1	505	-	65,73,73	1.35	10 (15%)	76,113,113	2.07	17 (22%)
31	BCR	A	411	-	41,41,41	1.86	4 (9%)	56,56,56	4.22	14 (25%)
29	CLA	a	405	-	65,73,73	1.34	6 (9%)	76,113,113	2.08	18 (23%)
29	CLA	B1	616	-	65,73,73	1.35	8 (12%)	76,113,113	2.00	15 (19%)
31	BCR	B	618	-	41,41,41	1.88	5 (12%)	56,56,56	4.32	18 (32%)
29	CLA	b	611	-	65,73,73	1.36	7 (10%)	76,113,113	2.01	18 (23%)
51	NEX	s	623	-	38,46,46	3.52	11 (28%)	50,70,70	2.12	14 (28%)
29	CLA	r	609	-	60,68,73	1.42	7 (11%)	70,107,113	2.05	17 (24%)
48	CHL	N	608	-	50,58,74	0.97	3 (6%)	52,94,114	1.35	9 (17%)
48	CHL	n1	608	-	50,58,74	0.92	2 (4%)	52,94,114	1.38	10 (19%)



Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
40	LHG	d1	409	-	48,48,48	0.40	0	51,54,54	1.03	2 (3%)
53	ERG	R1	626	-	31,32,32	7.67	19 (61%)	47,50,50	2.83	19 (40%)
29	CLA	g1	610	-	65,73,73	1.30	6 (9%)	76,113,113	2.29	20 (26%)
29	CLA	r	602	22	60,68,73	1.44	8 (13%)	70,107,113	2.03	19 (27%)
29	CLA	c	501	-	65,73,73	1.36	8 (12%)	76,113,113	2.06	16 (21%)
48	CHL	y1	609	-	66,74,74	0.82	2 (3%)	73,114,114	1.29	10 (13%)
29	CLA	d	402	-	65,73,73	1.38	8 (12%)	76,113,113	1.94	16 (21%)
33	LMG	D1	411	-	46,46,55	0.91	4 (8%)	54,54,63	1.12	3 (5%)
40	LHG	N1	624	-	48,48,48	0.39	0	51,54,54	1.07	3 (5%)
29	CLA	B	607	-	65,73,73	1.36	8 (12%)	76,113,113	2.00	17 (22%)
29	CLA	s1	614	-	55,63,73	1.49	10 (18%)	64,101,113	2.16	16 (25%)
29	CLA	c1	508	-	65,73,73	1.36	7 (10%)	76,113,113	1.97	19 (25%)
48	CHL	G1	609	-	66,74,74	0.90	3 (4%)	73,114,114	1.20	11 (15%)
40	LHG	Y	624	-	48,48,48	0.39	0	51,54,54	1.06	3 (5%)
29	CLA	C	508	-	65,73,73	1.42	7 (10%)	76,113,113	2.06	19 (25%)
29	CLA	b	614	-	65,73,73	1.34	8 (12%)	76,113,113	2.14	16 (21%)
39	DGA	B	625	-	43,43,43	1.09	2 (4%)	45,45,45	1.52	3 (6%)
55	PTY	Y1	626	-	49,49,49	0.89	4 (8%)	52,54,54	1.04	2 (3%)
49	LUT	n1	621	-	42,43,43	2.34	1 (2%)	51,60,60	2.13	18 (35%)
29	CLA	b1	610	-	65,73,73	1.36	9 (13%)	76,113,113	1.93	17 (22%)
48	CHL	S1	607	-	43,51,74	1.01	2 (4%)	45,86,114	1.53	9 (20%)
29	CLA	D1	402	-	65,73,73	1.37	7 (10%)	76,113,113	2.04	18 (23%)
29	CLA	r1	609	-	60,68,73	1.41	8 (13%)	70,107,113	2.05	18 (25%)
41	LMK	C	527	-	38,39,53	1.47	2 (5%)	41,46,60	1.56	4 (9%)
29	CLA	G1	610	-	65,73,73	1.36	9 (13%)	76,113,113	2.06	20 (26%)
31	BCR	c	517	-	41,41,41	1.84	4 (9%)	56,56,56	4.29	17 (30%)
29	CLA	n	602	-	65,73,73	1.43	8 (12%)	76,113,113	1.92	19 (25%)
29	CLA	R	604	-	49,57,73	1.54	8 (16%)	55,93,113	2.35	17 (30%)
48	CHL	N	601	20	66,74,74	0.87	3 (4%)	73,114,114	1.34	9 (12%)
39	DGA	J1	101	-	28,28,43	1.27	2 (7%)	30,30,45	1.34	2 (6%)
29	CLA	B	613	-	65,73,73	1.37	8 (12%)	76,113,113	2.04	16 (21%)
51	NEX	r1	622	-	38,46,46	3.37	9 (23%)	50,70,70	1.83	12 (24%)
29	CLA	Y1	604	-	65,73,73	1.39	6 (9%)	76,113,113	1.95	15 (19%)
34	SPH	Y	625	-	19,20,20	0.63	0	18,21,21	1.00	0
29	CLA	G	604	-	49,57,73	1.58	8 (16%)	55,93,113	2.28	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
29	CLA	N	612	-	45,53,73	1.66	9 (20%)	52,89,113	2.05	12 (23%)
32	SQD	a1	412	-	50,51,54	0.82	0	59,62,65	0.95	2 (3%)
29	CLA	B	612	-	65,73,73	1.38	7 (10%)	76,113,113	1.98	16 (21%)
30	PHO	a	409	-	51,69,69	0.97	3 (5%)	47,99,99	1.38	8 (17%)
50	XAT	N1	622	-	39,47,47	0.72	1 (2%)	54,74,74	2.10	15 (27%)
46	GOL	I1	101	-	5,5,5	0.56	0	5,5,5	0.31	0
29	CLA	S	603	-	65,73,73	1.38	9 (13%)	76,113,113	1.85	17 (22%)
29	CLA	B1	605	-	65,73,73	1.34	8 (12%)	76,113,113	2.06	18 (23%)
29	CLA	n1	611	-	49,57,73	1.57	7 (14%)	55,93,113	2.29	15 (27%)
29	CLA	C1	509	-	65,73,73	1.34	8 (12%)	76,113,113	2.07	17 (22%)
54	LPX	s1	625	-	29,29,29	1.01	2 (6%)	31,33,33	1.05	2 (6%)
54	LPX	S	625	-	29,29,29	1.02	2 (6%)	31,33,33	0.94	1 (3%)
50	XAT	Y	622	-	39,47,47	0.70	1 (2%)	54,74,74	3.77	16 (29%)
47	4RF	k1	101	-	56,56,56	1.04	3 (5%)	59,59,59	0.88	3 (5%)
29	CLA	N	602	-	65,73,73	1.34	8 (12%)	76,113,113	2.01	21 (27%)
29	CLA	y	612	-	65,73,73	1.37	8 (12%)	76,113,113	1.99	16 (21%)
47	4RF	K1	101	-	56,56,56	1.07	3 (5%)	59,59,59	0.84	3 (5%)
48	CHL	R1	607	-	50,58,74	0.94	2 (4%)	52,94,114	1.37	9 (17%)
29	CLA	s1	611	40	65,73,73	1.40	8 (12%)	76,113,113	2.00	18 (23%)
29	CLA	g	602	-	65,73,73	1.35	8 (12%)	76,113,113	2.04	22 (28%)
49	LUT	r1	620	-	42,43,43	2.36	2 (4%)	51,60,60	2.32	15 (29%)
29	CLA	s1	617	-	50,58,73	1.51	8 (16%)	58,95,113	2.27	19 (32%)
49	LUT	G1	620	-	42,43,43	2.26	1 (2%)	51,60,60	1.86	13 (25%)
34	SPH	a1	414	-	19,20,20	0.73	1 (5%)	18,21,21	0.98	1 (5%)
29	CLA	S	617	23	50,58,73	1.52	8 (16%)	58,95,113	2.29	17 (29%)
48	CHL	N1	607	-	66,74,74	0.81	2 (3%)	73,114,114	1.28	11 (15%)
40	LHG	n	624	-	48,48,48	0.38	0	51,54,54	1.08	2 (3%)
29	CLA	Y1	613	-	65,73,73	1.33	8 (12%)	76,113,113	2.12	17 (22%)
29	CLA	s1	603	-	65,73,73	1.37	8 (12%)	76,113,113	2.05	17 (22%)
29	CLA	y1	602	-	65,73,73	1.33	9 (13%)	76,113,113	2.03	21 (27%)
48	CHL	G	606	-	50,58,74	1.08	3 (6%)	52,94,114	1.45	11 (21%)
48	CHL	r1	606	-	44,52,74	1.10	3 (6%)	46,87,114	1.12	4 (8%)
53	ERG	r	626	-	31,32,32	7.80	18 (58%)	47,50,50	3.01	16 (34%)
49	LUT	G	620	-	42,43,43	2.25	1 (2%)	51,60,60	1.99	17 (33%)
29	CLA	R	608	-	60,68,73	1.46	10 (16%)	70,107,113	2.07	16 (22%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	BCR	a	411	-	41,41,41	1.83	4 (9%)	56,56,56	4.25	14 (25%)
48	CHL	g	605	21	48,56,74	0.98	3 (6%)	51,92,114	1.62	12 (23%)
29	CLA	g1	611	-	65,73,73	1.37	8 (12%)	76,113,113	1.88	16 (21%)
29	CLA	y1	604	-	65,73,73	1.35	8 (12%)	76,113,113	2.07	17 (22%)
29	CLA	B1	609	-	65,73,73	1.38	8 (12%)	76,113,113	1.99	17 (22%)
40	LHG	g	624	-	48,48,48	0.39	0	51,54,54	0.97	2 (3%)
29	CLA	R	602	-	60,68,73	1.44	9 (15%)	70,107,113	1.99	19 (27%)
29	CLA	c1	502	-	65,73,73	1.43	8 (12%)	76,113,113	1.84	13 (17%)
29	CLA	C	509	-	65,73,73	1.36	8 (12%)	76,113,113	2.07	19 (25%)
33	LMG	B1	622	-	44,44,55	0.88	3 (6%)	52,52,63	1.08	4 (7%)
41	LMK	c	527	-	38,39,53	1.50	2 (5%)	41,46,60	1.25	2 (4%)
29	CLA	C	513	-	65,73,73	1.36	7 (10%)	76,113,113	1.97	17 (22%)
29	CLA	Y	614	-	65,73,73	1.38	10 (15%)	76,113,113	2.01	18 (23%)
29	CLA	b1	613	-	65,73,73	1.36	8 (12%)	76,113,113	2.06	16 (21%)
48	CHL	n1	606	-	66,74,74	0.86	4 (6%)	73,114,114	1.23	11 (15%)
38	3PH	T	101	-	47,47,47	0.85	3 (6%)	51,52,52	1.19	2 (3%)
43	PL9	D	405	-	55,55,55	1.56	5 (9%)	68,69,69	1.47	12 (17%)
38	3PH	B	624	-	47,47,47	0.86	4 (8%)	51,52,52	1.12	2 (3%)
29	CLA	c1	504	-	65,73,73	1.38	8 (12%)	76,113,113	2.10	14 (18%)
29	CLA	g1	602	-	65,73,73	1.36	8 (12%)	76,113,113	1.97	19 (25%)
29	CLA	C1	504	-	65,73,73	1.37	7 (10%)	76,113,113	2.02	17 (22%)
29	CLA	Y1	612	-	65,73,73	1.38	8 (12%)	76,113,113	1.96	18 (23%)
33	LMG	c1	521	-	51,51,55	1.06	5 (9%)	59,59,63	1.10	3 (5%)
48	CHL	Y1	605	-	46,54,74	0.97	2 (4%)	49,90,114	1.40	7 (14%)
29	CLA	G	602	-	65,73,73	1.34	7 (10%)	76,113,113	2.10	21 (27%)
26	OEX	a1	401	1	0,15,15	-	-	-	-	-
50	XAT	g1	622	-	39,47,47	0.75	1 (2%)	54,74,74	1.88	16 (29%)
29	CLA	s	617	-	50,58,73	1.54	7 (14%)	58,95,113	2.35	18 (31%)
31	BCR	D1	404	-	41,41,41	1.85	4 (9%)	56,56,56	4.33	16 (28%)
34	SPH	y	625	-	19,20,20	0.61	0	18,21,21	1.21	2 (11%)
48	CHL	N1	601	-	66,74,74	0.87	3 (4%)	73,114,114	1.42	12 (16%)
29	CLA	g	604	-	49,57,73	1.57	9 (18%)	55,93,113	2.21	17 (30%)
29	CLA	b1	602	-	65,73,73	1.39	10 (15%)	76,113,113	1.93	18 (23%)
48	CHL	r	607	-	50,58,74	1.02	3 (6%)	52,94,114	1.45	9 (17%)
54	LPX	s	625	-	29,29,29	1.02	2 (6%)	31,33,33	0.94	1 (3%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
31	BCR	d1	404	-	41,41,41	1.88	4 (9%)	56,56,56	4.27	22 (39%)
29	CLA	B1	615	-	65,73,73	1.34	7 (10%)	76,113,113	1.99	19 (25%)
29	CLA	b	610	-	65,73,73	1.32	7 (10%)	76,113,113	2.03	17 (22%)
40	LHG	D	408	-	43,43,48	0.41	0	46,49,54	1.10	2 (4%)
29	CLA	b	612	-	65,73,73	1.37	8 (12%)	76,113,113	2.10	17 (22%)
32	SQD	M1	101	-	41,42,54	0.90	0	50,53,65	0.97	2 (4%)
49	LUT	r	620	-	42,43,43	2.34	1 (2%)	51,60,60	2.12	14 (27%)
55	PTY	y	626	-	49,49,49	0.88	3 (6%)	52,54,54	1.12	3 (5%)
37	DGD	C1	518	-	56,56,67	0.98	4 (7%)	70,70,81	1.07	6 (8%)
29	CLA	N	604	-	65,73,73	1.36	7 (10%)	76,113,113	2.08	19 (25%)
29	CLA	n1	604	-	65,73,73	1.34	7 (10%)	76,113,113	1.99	16 (21%)
29	CLA	B1	612	-	65,73,73	1.35	6 (9%)	76,113,113	2.12	21 (27%)
38	3PH	b1	624	-	47,47,47	0.86	4 (8%)	51,52,52	1.15	2 (3%)
31	BCR	C1	516	-	41,41,41	1.89	4 (9%)	56,56,56	4.66	17 (30%)
29	CLA	A1	405	-	65,73,73	1.34	8 (12%)	76,113,113	2.00	17 (22%)
30	PHO	A	408	-	51,69,69	1.01	4 (7%)	47,99,99	1.20	5 (10%)
30	PHO	A	409	-	51,69,69	1.02	4 (7%)	47,99,99	1.33	6 (12%)
48	CHL	S1	606	-	44,52,74	1.05	3 (6%)	46,87,114	1.46	8 (17%)
32	SQD	m	101	-	41,42,54	0.91	0	50,53,65	0.99	3 (6%)
29	CLA	b1	612	-	65,73,73	1.35	8 (12%)	76,113,113	2.17	19 (25%)
31	BCR	C1	515	-	41,41,41	1.93	4 (9%)	56,56,56	3.77	16 (28%)
48	CHL	s1	606	-	44,52,74	0.95	2 (4%)	46,87,114	1.40	8 (17%)
29	CLA	a1	406	-	65,73,73	1.36	8 (12%)	76,113,113	2.09	21 (27%)
55	PTY	Y	626	-	49,49,49	0.88	3 (6%)	52,54,54	1.02	2 (3%)
33	LMG	C	523	-	55,55,55	1.13	6 (10%)	63,63,63	1.13	2 (3%)
29	CLA	s	610	-	65,73,73	1.42	9 (13%)	76,113,113	1.96	17 (22%)
32	SQD	A1	412	-	50,51,54	0.81	0	59,62,65	0.98	4 (6%)
29	CLA	s1	612	-	45,53,73	1.66	10 (22%)	52,89,113	2.01	11 (21%)
29	CLA	b1	603	-	65,73,73	1.38	7 (10%)	76,113,113	2.00	19 (25%)
48	CHL	S	601	23	46,54,74	1.21	5 (10%)	49,90,114	1.37	9 (18%)
55	PTY	y1	627	-	18,18,49	1.27	2 (11%)	21,23,54	1.45	2 (9%)
29	CLA	b	616	-	65,73,73	1.35	8 (12%)	76,113,113	1.87	15 (19%)
39	DGA	b	625	-	43,43,43	1.11	2 (4%)	45,45,45	1.45	3 (6%)
29	CLA	b1	607	-	65,73,73	1.38	8 (12%)	76,113,113	1.97	17 (22%)
31	BCR	B1	619	-	41,41,41	1.82	4 (9%)	56,56,56	4.44	18 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
40	LHG	d	410	-	38,38,48	0.43	0	41,44,54	1.11	3 (7%)
29	CLA	S	614	-	55,63,73	1.48	7 (12%)	64,101,113	2.14	16 (25%)
48	CHL	G	607	-	66,74,74	0.88	2 (3%)	73,114,114	1.21	10 (13%)
29	CLA	s1	613	-	55,63,73	1.51	10 (18%)	64,101,113	2.12	17 (26%)
29	CLA	b	608	-	65,73,73	1.32	7 (10%)	76,113,113	2.02	17 (22%)
48	CHL	G	608	-	44,52,74	1.08	3 (6%)	46,87,114	1.41	7 (15%)
29	CLA	a1	407	-	49,57,73	1.55	7 (14%)	55,93,113	2.44	18 (32%)
48	CHL	g1	608	-	44,52,74	1.01	3 (6%)	46,87,114	1.40	6 (13%)
29	CLA	Y	604	-	65,73,73	1.33	6 (9%)	76,113,113	2.02	18 (23%)
29	CLA	N	614	-	49,57,73	1.57	7 (14%)	55,93,113	2.34	15 (27%)
29	CLA	C	501	-	65,73,73	1.36	8 (12%)	76,113,113	2.03	18 (23%)
50	XAT	G1	622	-	39,47,47	0.76	1 (2%)	54,74,74	1.88	17 (31%)
48	CHL	S1	601	23	46,54,74	1.08	5 (10%)	49,90,114	1.41	9 (18%)
29	CLA	G1	603	-	65,73,73	1.34	7 (10%)	76,113,113	2.05	17 (22%)
29	CLA	C1	510	-	65,73,73	1.35	9 (13%)	76,113,113	1.94	15 (19%)
48	CHL	y	605	24	46,54,74	0.99	2 (4%)	49,90,114	1.48	10 (20%)
29	CLA	B	602	-	65,73,73	1.34	7 (10%)	76,113,113	1.96	15 (19%)
29	CLA	S1	605	-	50,58,73	1.57	9 (18%)	58,95,113	2.22	17 (29%)
48	CHL	G1	607	-	66,74,74	0.87	2 (3%)	73,114,114	1.16	8 (10%)
29	CLA	b1	605	-	65,73,73	1.30	7 (10%)	76,113,113	2.11	19 (25%)
29	CLA	c	510	-	65,73,73	1.37	7 (10%)	76,113,113	2.05	17 (22%)
29	CLA	B	605	-	65,73,73	1.40	8 (12%)	76,113,113	2.06	18 (23%)
37	DGD	C1	520	-	60,60,67	1.08	5 (8%)	74,74,81	0.95	2 (2%)
29	CLA	s	605	-	50,58,73	1.57	8 (16%)	58,95,113	2.30	16 (27%)
50	XAT	Y1	622	-	39,47,47	0.69	1 (2%)	54,74,74	3.83	20 (37%)
30	PHO	A1	409	-	51,69,69	0.99	3 (5%)	47,99,99	1.31	6 (12%)
29	CLA	B	614	-	65,73,73	1.32	8 (12%)	76,113,113	2.06	18 (23%)
51	NEX	g1	623	-	38,46,46	3.26	10 (26%)	50,70,70	1.91	15 (30%)
40	LHG	D1	409	-	48,48,48	0.41	0	51,54,54	1.07	3 (5%)
31	BCR	C	517	-	41,41,41	1.87	5 (12%)	56,56,56	4.32	18 (32%)
29	CLA	r1	610	-	60,68,73	1.44	8 (13%)	70,107,113	1.96	16 (22%)
49	LUT	n1	620	-	42,43,43	2.36	1 (2%)	51,60,60	1.77	10 (19%)
29	CLA	c1	507	-	65,73,73	1.35	7 (10%)	76,113,113	2.06	20 (26%)
29	CLA	S	612	-	45,53,73	1.62	8 (17%)	52,89,113	2.23	14 (26%)
29	CLA	s	612	-	45,53,73	1.60	8 (17%)	52,89,113	2.21	15 (28%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z  > 2	Counts	RMSZ	# Z  > 2
38	3PH	t1	101	-	47,47,47	0.87	3 (6%)	51,52,52	1.05	2 (3%)
29	CLA	N	611	-	49,57,73	1.57	7 (14%)	55,93,113	2.24	15 (27%)
29	CLA	g1	614	-	49,57,73	1.61	10 (20%)	55,93,113	2.31	17 (30%)
48	CHL	r1	607	-	50,58,74	0.99	3 (6%)	52,94,114	1.64	12 (23%)
48	CHL	y	609	-	66,74,74	0.87	4 (6%)	73,114,114	1.24	10 (13%)
29	CLA	c1	509	-	65,73,73	1.37	8 (12%)	76,113,113	1.82	16 (21%)
48	CHL	G1	601	21	66,74,74	0.89	3 (4%)	73,114,114	1.33	13 (17%)
29	CLA	s	613	-	55,63,73	1.45	7 (12%)	64,101,113	2.25	18 (28%)
29	CLA	n1	610	-	65,73,73	1.35	6 (9%)	76,113,113	1.98	16 (21%)

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	CHL	N1	606	-	4/4/20/26	12/39/137/137	-
50	XAT	R1	621	-	-	4/31/93/93	0/4/4/4
29	CLA	B	609	-	1/1/15/20	12/37/115/115	-
49	LUT	N1	620	-	-	8/29/67/67	0/2/2/2
29	CLA	N	603	-	1/1/15/20	17/37/115/115	-
33	LMG	W	201	-	-	14/34/54/70	0/1/1/1
29	CLA	y1	611	40	1/1/15/20	19/37/115/115	-
29	CLA	B	603	-	1/1/15/20	21/37/115/115	-
29	CLA	c	512	-	1/1/15/20	18/37/115/115	-
33	LMG	B	622	-	-	20/39/59/70	0/1/1/1
29	CLA	Y	612	-	1/1/15/20	13/37/115/115	-
37	DGD	B1	623	-	-	11/32/72/95	0/2/2/2
49	LUT	G1	621	-	-	3/29/67/67	0/2/2/2
49	LUT	s1	620	-	-	6/29/67/67	0/2/2/2
49	LUT	S	620	-	-	3/29/67/67	0/2/2/2
37	DGD	b	623	-	-	13/32/72/95	0/2/2/2
29	CLA	Y	613	24	1/1/15/20	22/37/115/115	-
29	CLA	r	604	-	1/1/11/20	9/18/96/115	-
40	LHG	S1	624	29	-	32/49/49/53	-
29	CLA	n1	614	-	1/1/11/20	9/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	g1	612	21	1/1/10/20	4/11/89/115	-
30	PHO	a1	408	-	-	17/37/103/103	0/5/6/6
49	LUT	y	620	-	-	4/29/67/67	0/2/2/2
29	CLA	c1	513	-	1/1/15/20	23/37/115/115	-
29	CLA	A1	406	-	1/1/15/20	21/37/115/115	-
29	CLA	C1	513	-	1/1/15/20	16/37/115/115	-
29	CLA	a1	410	-	1/1/14/20	13/31/109/115	-
43	PL9	d	405	-	-	9/53/73/73	0/1/1/1
40	LHG	s	624	29	-	26/49/49/53	-
29	CLA	b	605	-	1/1/15/20	19/37/115/115	-
33	LMG	d	411	-	-	19/41/61/70	0/1/1/1
50	XAT	r1	621	-	1/1/12/26	2/31/93/93	0/4/4/4
48	CHL	y	606	-	4/4/20/26	12/39/137/137	-
29	CLA	R1	612	-	1/1/14/20	19/31/109/115	-
29	CLA	d	403	-	1/1/15/20	16/37/115/115	-
31	BCR	b	619	-	-	6/29/63/63	0/2/2/2
31	BCR	c1	515	-	-	11/29/63/63	0/2/2/2
44	HEM	F	101	7,6	-	1/12/54/54	-
29	CLA	r1	604	-	1/1/11/20	10/18/96/115	-
29	CLA	b1	614	-	1/1/15/20	10/37/115/115	-
31	BCR	C	515	-	-	9/29/63/63	0/2/2/2
49	LUT	S1	620	-	-	4/29/67/67	0/2/2/2
29	CLA	S	609	-	1/1/14/20	10/31/109/115	-
29	CLA	C1	502	-	1/1/15/20	12/37/115/115	-
45	RRX	h1	101	-	1/1/11/25	10/29/65/65	0/2/2/2
40	LHG	Y1	624	-	-	18/53/53/53	-
31	BCR	B1	618	-	-	15/29/63/63	0/2/2/2
39	DGA	J	101	-	-	12/30/30/45	-
51	NEX	y1	623	-	-	10/27/83/83	0/3/3/3
40	LHG	d	408	-	-	26/48/48/53	-
29	CLA	b	615	-	1/1/15/20	19/37/115/115	-
29	CLA	g1	604	-	1/1/11/20	9/18/96/115	-
37	DGD	B	623	-	-	15/32/72/95	0/2/2/2
51	NEX	R1	622	-	-	14/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	y	602	24	1/1/15/20	15/37/115/115	-
36	C7Z	B	620	-	1/1/12/26	9/29/67/67	0/2/2/2
29	CLA	C	512	-	1/1/15/20	15/37/115/115	-
29	CLA	s	604	-	1/1/13/20	11/25/103/115	-
29	CLA	Y1	614	-	1/1/15/20	14/37/115/115	-
49	LUT	G	621	-	1/1/12/27	4/29/67/67	0/2/2/2
37	DGD	c1	518	-	-	14/44/84/95	0/2/2/2
29	CLA	n	612	-	1/1/11/20	5/13/91/115	-
29	CLA	b	609	-	1/1/15/20	13/37/115/115	-
29	CLA	N1	603	-	1/1/15/20	15/37/115/115	-
29	CLA	Y1	610	-	1/1/15/20	12/37/115/115	-
48	CHL	s	608	-	4/4/19/26	5/33/131/137	-
48	CHL	g1	609	-	4/4/20/26	7/39/137/137	-
29	CLA	G	610	21	1/1/15/20	16/37/115/115	-
29	CLA	c1	501	-	1/1/15/20	17/37/115/115	-
33	LMG	b	622	-	-	17/39/59/70	0/1/1/1
40	LHG	g1	624	-	-	35/53/53/53	-
32	SQD	M	101	-	-	24/37/57/69	0/1/1/1
29	CLA	b	604	-	1/1/15/20	14/37/115/115	-
38	3PH	B1	624	-	-	27/49/49/49	-
29	CLA	c	509	-	1/1/15/20	16/37/115/115	-
51	NEX	N1	623	-	-	6/27/83/83	0/3/3/3
55	PTY	Y	627	-	-	15/20/20/53	-
29	CLA	S	611	40	1/1/15/20	16/37/115/115	-
49	LUT	N1	621	-	-	4/29/67/67	0/2/2/2
29	CLA	g	612	-	1/1/10/20	6/11/89/115	-
32	SQD	b	626	-	-	17/49/69/69	0/1/1/1
29	CLA	b1	615	-	1/1/15/20	17/37/115/115	-
39	DGA	b1	625	-	-	22/45/45/45	-
40	LHG	c1	525	-	-	33/51/51/53	-
48	CHL	y1	606	-	4/4/20/26	6/39/137/137	-
29	CLA	N	610	-	1/1/15/20	19/37/115/115	-
40	LHG	G1	624	-	-	29/53/53/53	-
32	SQD	c1	526	-	-	22/49/69/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
32	SQD	C1	526	-	-	25/49/69/69	0/1/1/1
51	NEX	G	623	-	-	5/27/83/83	0/3/3/3
33	LMG	a1	413	-	-	20/43/63/70	0/1/1/1
29	CLA	c	504	-	1/1/15/20	18/37/115/115	-
48	CHL	S	608	-	4/4/19/26	7/33/131/137	-
48	CHL	G	605	21	4/4/16/26	6/18/116/137	-
48	CHL	N1	608	-	3/3/16/26	5/20/118/137	-
31	BCR	c1	516	-	-	12/29/63/63	0/2/2/2
29	CLA	y1	613	-	1/1/15/20	18/37/115/115	-
37	DGD	c1	520	-	-	11/48/88/95	0/2/2/2
38	3PH	b	624	-	-	23/49/49/49	-
29	CLA	y1	612	-	1/1/15/20	17/37/115/115	-
29	CLA	G1	602	-	1/1/15/20	21/37/115/115	-
29	CLA	a1	405	-	1/1/15/20	17/37/115/115	-
29	CLA	s1	609	-	1/1/14/20	17/31/109/115	-
29	CLA	B	616	-	1/1/15/20	7/37/115/115	-
29	CLA	b	606	-	1/1/15/20	15/37/115/115	-
29	CLA	B	608	-	1/1/15/20	27/37/115/115	-
29	CLA	g1	613	-	1/1/15/20	22/37/115/115	-
48	CHL	N	605	20	4/4/20/26	9/39/137/137	-
29	CLA	Y	611	-	1/1/15/20	12/37/115/115	-
29	CLA	S1	617	23	1/1/12/20	7/19/97/115	-
29	CLA	b	603	-	1/1/15/20	21/37/115/115	-
47	4RF	I	102	-	-	30/59/59/59	-
49	LUT	Y1	620	-	-	8/29/67/67	0/2/2/2
29	CLA	c	506	-	1/1/15/20	17/37/115/115	-
29	CLA	R1	608	-	1/1/14/20	11/31/109/115	-
29	CLA	c	508	-	1/1/15/20	12/37/115/115	-
48	CHL	Y1	609	-	4/4/20/26	8/39/137/137	-
33	LMG	w	201	-	-	17/34/54/70	0/1/1/1
52	LMT	r1	625	-	-	10/21/61/61	0/2/2/2
31	BCR	D	404	-	-	13/29/63/63	0/2/2/2
48	CHL	G	609	21	4/4/20/26	10/39/137/137	-
37	DGD	b1	623	-	-	14/32/72/95	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	C	507	-	1/1/15/20	14/37/115/115	-
49	LUT	S1	621	-	-	7/29/67/67	0/2/2/2
29	CLA	C	504	-	1/1/15/20	16/37/115/115	-
33	LMG	C1	523	-	-	19/50/70/70	0/1/1/1
29	CLA	N1	602	-	1/1/15/20	17/37/115/115	-
29	CLA	R	612	-	1/1/14/20	10/31/109/115	-
29	CLA	b1	609	-	1/1/15/20	16/37/115/115	-
33	LMG	c	523	-	-	21/50/70/70	0/1/1/1
29	CLA	G	614	-	1/1/11/20	10/18/96/115	-
29	CLA	n1	612	-	1/1/11/20	5/13/91/115	-
53	ERG	r1	626	-	5/5/11/15	8/13/71/71	0/4/4/4
29	CLA	y1	608	-	1/1/12/20	9/19/97/115	-
48	CHL	S	607	-	3/3/15/26	1/12/110/137	-
49	LUT	N	620	-	-	2/29/67/67	0/2/2/2
33	LMG	A	413	-	-	15/43/63/70	0/1/1/1
39	DGA	B1	625	-	-	26/45/45/45	-
40	LHG	D	409	-	-	25/53/53/53	-
33	LMG	c1	523	-	-	18/50/70/70	0/1/1/1
45	RRX	H	101	-	1/1/11/25	7/29/65/65	0/2/2/2
29	CLA	Y	608	-	1/1/12/20	7/19/97/115	-
29	CLA	s	614	-	1/1/13/20	4/25/103/115	-
31	BCR	c	516	-	-	15/29/63/63	0/2/2/2
29	CLA	A1	407	-	1/1/12/20	9/19/97/115	-
40	LHG	D	410	-	-	26/43/43/53	-
37	DGD	c	520	-	-	9/48/88/95	0/2/2/2
37	DGD	C	518	-	-	18/44/84/95	0/2/2/2
39	DGA	C	524	-	-	18/45/45/45	-
29	CLA	n	610	-	1/1/15/20	18/37/115/115	-
51	NEX	R	622	-	-	8/27/83/83	0/3/3/3
49	LUT	g	620	-	-	4/29/67/67	0/2/2/2
50	XAT	g	622	-	2/2/12/26	3/31/93/93	0/4/4/4
29	CLA	N1	612	-	1/1/11/20	4/13/91/115	-
29	CLA	C1	508	-	1/1/15/20	13/37/115/115	-
51	NEX	G1	623	-	-	12/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	C1	505	-	1/1/15/20	19/37/115/115	-
29	CLA	S1	611	40	1/1/15/20	16/37/115/115	-
48	CHL	n1	605	-	4/4/20/26	7/39/137/137	-
29	CLA	c1	512	-	1/1/15/20	17/37/115/115	-
48	CHL	S	606	-	3/3/15/26	2/13/111/137	-
29	CLA	R	603	-	1/1/14/20	16/31/109/115	-
43	PL9	d1	405	-	-	20/53/73/73	0/1/1/1
29	CLA	B1	604	-	1/1/15/20	14/37/115/115	-
29	CLA	B	611	-	1/1/15/20	13/37/115/115	-
29	CLA	C1	503	-	1/1/15/20	19/37/115/115	-
32	SQD	b1	626	-	-	26/49/69/69	0/1/1/1
29	CLA	y	611	40	1/1/15/20	16/37/115/115	-
29	CLA	Y1	608	-	1/1/12/20	7/19/97/115	-
29	CLA	g1	603	-	1/1/15/20	18/37/115/115	-
29	CLA	y	613	-	1/1/15/20	24/37/115/115	-
48	CHL	s1	601	23	3/3/16/26	4/15/113/137	-
29	CLA	s1	610	-	1/1/15/20	18/37/115/115	-
29	CLA	c	511	4	1/1/15/20	9/37/115/115	-
29	CLA	R1	610	-	1/1/14/20	17/31/109/115	-
47	4RF	i1	101	-	-	30/59/59/59	-
29	CLA	s	603	-	1/1/15/20	15/37/115/115	-
29	CLA	S	604	-	1/1/13/20	9/25/103/115	-
50	XAT	r	621	-	2/2/12/26	2/31/93/93	0/4/4/4
48	CHL	n1	609	-	4/4/20/26	5/39/137/137	-
29	CLA	S	602	-	1/1/14/20	16/31/109/115	-
48	CHL	Y1	607	-	4/4/20/26	11/39/137/137	-
29	CLA	g	614	-	1/1/11/20	11/18/96/115	-
29	CLA	C1	512	-	1/1/15/20	16/37/115/115	-
51	NEX	n1	623	-	-	5/27/83/83	0/3/3/3
29	CLA	C	506	-	1/1/15/20	13/37/115/115	-
31	BCR	B	619	-	-	8/29/63/63	0/2/2/2
48	CHL	Y	605	24	3/3/16/26	3/15/113/137	-
48	CHL	G1	608	-	2/2/15/26	1/13/111/137	-
38	3PH	S	626	-	-	24/49/49/49	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	CHL	g1	606	-	3/3/16/26	3/20/118/137	-
55	PTY	Y1	627	-	-	12/20/20/53	-
37	DGD	C	520	-	-	14/48/88/95	0/2/2/2
29	CLA	S1	613	-	1/1/13/20	9/25/103/115	-
33	LMG	w1	201	-	-	17/34/54/70	0/1/1/1
49	LUT	R1	620	-	-	9/29/67/67	0/2/2/2
40	LHG	G	624	29	-	33/53/53/53	-
49	LUT	s	620	-	-	1/29/67/67	0/2/2/2
29	CLA	Y	610	-	1/1/15/20	12/37/115/115	-
29	CLA	c1	506	-	1/1/15/20	16/37/115/115	-
48	CHL	n	607	-	4/4/20/26	8/39/137/137	-
29	CLA	n	604	-	1/1/15/20	13/37/115/115	-
48	CHL	R1	606	-	3/3/15/26	4/13/111/137	-
29	CLA	C	503	-	1/1/15/20	18/37/115/115	-
48	CHL	s	606	-	3/3/15/26	2/13/111/137	-
29	CLA	S1	609	-	1/1/14/20	10/31/109/115	-
37	DGD	C1	519	-	-	22/51/91/95	0/2/2/2
29	CLA	S1	602	23	1/1/14/20	17/31/109/115	-
33	LMG	h1	102	-	-	22/43/63/70	0/1/1/1
29	CLA	A1	410	-	1/1/14/20	12/31/109/115	-
29	CLA	N1	604	-	1/1/15/20	18/37/115/115	-
51	NEX	r	622	-	-	9/27/83/83	0/3/3/3
33	LMG	C1	521	-	-	12/46/66/70	0/1/1/1
29	CLA	c	502	-	1/1/15/20	12/37/115/115	-
29	CLA	B1	602	-	1/1/15/20	24/37/115/115	-
29	CLA	S1	604	-	1/1/13/20	10/25/103/115	-
48	CHL	Y	609	-	4/4/20/26	6/39/137/137	-
48	CHL	g	607	-	4/4/20/26	10/39/137/137	-
48	CHL	Y1	606	-	4/4/20/26	7/39/137/137	-
50	XAT	G	622	-	1/1/12/26	2/31/93/93	0/4/4/4
48	CHL	s	601	-	3/3/16/26	4/15/113/137	-
29	CLA	C	511	-	1/1/15/20	14/37/115/115	-
32	SQD	B	626	-	-	23/49/69/69	0/1/1/1
55	PTY	y	627	-	-	15/20/20/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	DGD	c	518	-	-	9/44/84/95	0/2/2/2
33	LMG	H1	102	-	-	17/43/63/70	0/1/1/1
55	PTY	y1	626	-	-	33/53/53/53	-
48	CHL	R	606	-	3/3/15/26	1/13/111/137	-
48	CHL	n	601	20	4/4/20/26	4/39/137/137	-
34	SPH	A1	414	-	-	16/21/21/21	-
52	LMT	R	625	-	-	9/21/61/61	0/2/2/2
52	LMT	R1	625	-	-	10/21/61/61	0/2/2/2
29	CLA	s	609	-	1/1/14/20	16/31/109/115	-
31	BCR	b1	618	-	-	11/29/63/63	0/2/2/2
49	LUT	S	621	-	-	4/29/67/67	0/2/2/2
48	CHL	g1	605	-	4/4/16/26	7/18/116/137	-
29	CLA	C	510	-	1/1/15/20	13/37/115/115	-
29	CLA	S1	612	-	1/1/11/20	6/13/91/115	-
48	CHL	Y1	601	-	4/4/20/26	7/39/137/137	-
31	BCR	C	516	-	-	13/29/63/63	0/2/2/2
29	CLA	S	605	23	1/1/12/20	9/19/97/115	-
29	CLA	y1	603	-	1/1/15/20	18/37/115/115	-
41	LMK	C1	527	-	2/2/6/6	19/46/46/60	-
49	LUT	N	621	-	-	4/29/67/67	0/2/2/2
50	XAT	R	621	-	-	2/31/93/93	0/4/4/4
29	CLA	n1	602	20	1/1/15/20	17/37/115/115	-
38	3PH	S1	626	-	-	30/49/49/49	-
29	CLA	A	405	-	1/1/15/20	14/37/115/115	-
49	LUT	y1	620	-	-	3/29/67/67	0/2/2/2
29	CLA	y1	614	-	1/1/15/20	16/37/115/115	-
48	CHL	g	601	21	4/4/20/26	16/39/137/137	-
49	LUT	y	621	-	-	2/29/67/67	0/2/2/2
29	CLA	n	603	-	1/1/15/20	23/37/115/115	-
38	3PH	T1	101	-	-	29/49/49/49	-
29	CLA	N1	614	-	1/1/11/20	7/18/96/115	-
49	LUT	Y1	621	-	-	6/29/67/67	0/2/2/2
29	CLA	B1	607	-	1/1/15/20	14/37/115/115	-
48	CHL	N	607	-	4/4/20/26	7/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	G1	611	-	1/1/15/20	19/37/115/115	-
29	CLA	G	603	-	1/1/15/20	14/37/115/115	-
29	CLA	y	610	24	1/1/15/20	13/37/115/115	-
40	LHG	s1	624	29	-	27/49/49/53	-
29	CLA	g	610	-	1/1/15/20	19/37/115/115	-
29	CLA	B1	617	-	1/1/15/20	16/37/115/115	-
29	CLA	c	507	-	1/1/15/20	15/37/115/115	-
49	LUT	g1	620	-	-	6/29/67/67	0/2/2/2
31	BCR	c	515	-	-	10/29/63/63	0/2/2/2
29	CLA	g	603	-	1/1/15/20	21/37/115/115	-
29	CLA	D1	403	-	1/1/15/20	17/37/115/115	-
29	CLA	b1	604	-	1/1/15/20	18/37/115/115	-
34	SPH	a	414	-	-	11/21/21/21	-
45	RRX	H1	101	-	1/1/11/25	9/29/65/65	0/2/2/2
32	SQD	c	526	-	-	20/49/69/69	0/1/1/1
48	CHL	s	607	-	3/3/15/26	0/12/110/137	-
33	LMG	A1	413	-	-	18/43/63/70	0/1/1/1
31	BCR	b1	619	-	-	9/29/63/63	0/2/2/2
47	4RF	K	101	-	-	32/59/59/59	-
29	CLA	n1	603	-	1/1/15/20	14/37/115/115	-
31	BCR	C	514	-	-	17/29/63/63	0/2/2/2
48	CHL	n	606	-	4/4/20/26	7/39/137/137	-
29	CLA	a	407	-	1/1/11/20	7/18/96/115	-
33	LMG	W1	201	-	-	16/34/54/70	0/1/1/1
40	LHG	d	409	-	-	26/53/53/53	-
39	DGA	C1	524	-	-	23/45/45/45	-
48	CHL	y1	607	-	4/4/20/26	4/39/137/137	-
30	PHO	A1	408	-	-	6/37/103/103	0/5/6/6
29	CLA	R	610	-	1/1/14/20	14/31/109/115	-
29	CLA	G1	604	-	1/1/11/20	8/18/96/115	-
29	CLA	s1	602	-	1/1/14/20	13/31/109/115	-
29	CLA	B1	606	-	1/1/15/20	18/37/115/115	-
48	CHL	Y	607	-	4/4/20/26	6/39/137/137	-
50	XAT	n1	622	-	-	4/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	A	406	-	1/1/15/20	14/37/115/115	-
29	CLA	c1	503	-	1/1/15/20	18/37/115/115	-
48	CHL	g	606	-	3/3/16/26	4/20/118/137	-
29	CLA	y	608	-	1/1/12/20	10/19/97/115	-
31	BCR	b	618	-	-	9/29/63/63	0/2/2/2
48	CHL	N	606	-	4/4/20/26	10/39/137/137	-
29	CLA	B1	603	-	1/1/15/20	21/37/115/115	-
49	LUT	Y	620	-	-	5/29/67/67	0/2/2/2
40	LHG	n1	624	-	-	29/53/53/53	-
36	C7Z	b	620	-	1/1/12/26	13/29/67/67	0/2/2/2
31	BCR	A1	411	-	-	9/29/63/63	0/2/2/2
29	CLA	G1	613	-	1/1/15/20	15/37/115/115	-
37	DGD	c	519	-	-	23/51/91/95	0/2/2/2
49	LUT	n	621	-	-	2/29/67/67	0/2/2/2
29	CLA	B	606	-	1/1/15/20	20/37/115/115	-
48	CHL	y1	601	24	4/4/20/26	5/39/137/137	-
29	CLA	y1	610	24	1/1/15/20	13/37/115/115	-
32	SQD	C	526	-	-	23/49/69/69	0/1/1/1
29	CLA	N	613	-	1/1/15/20	17/37/115/115	-
29	CLA	G1	612	-	1/1/10/20	7/11/89/115	-
33	LMG	c	521	-	-	14/46/66/70	0/1/1/1
48	CHL	n1	607	-	4/4/20/26	7/39/137/137	-
29	CLA	R1	609	-	1/1/14/20	14/31/109/115	-
48	CHL	s1	607	-	3/3/15/26	0/12/110/137	-
33	LMG	H	102	-	-	14/43/63/70	0/1/1/1
40	LHG	D1	408	-	-	26/48/48/53	-
40	LHG	D1	410	-	-	25/43/43/53	-
46	GOL	I	101	-	-	2/4/4/4	-
29	CLA	B1	611	-	1/1/15/20	13/37/115/115	-
39	DGA	j1	101	-	-	20/30/30/45	-
49	LUT	s1	621	-	-	5/29/67/67	0/2/2/2
29	CLA	B1	613	-	1/1/15/20	19/37/115/115	-
29	CLA	b1	611	-	1/1/15/20	10/37/115/115	-
29	CLA	c1	510	-	1/1/15/20	12/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
53	ERG	R	626	-	5/5/11/15	6/13/71/71	0/4/4/4
29	CLA	S1	614	-	1/1/13/20	8/25/103/115	-
38	3PH	t	101	-	-	27/49/49/49	-
29	CLA	r	610	-	1/1/14/20	11/31/109/115	-
29	CLA	D	403	-	1/1/15/20	16/37/115/115	-
29	CLA	Y1	602	-	1/1/15/20	20/37/115/115	-
48	CHL	n1	601	-	4/4/20/26	11/39/137/137	-
34	SPH	Y1	625	-	-	9/21/21/21	-
40	LHG	y	624	29	-	30/53/53/53	-
49	LUT	n	620	-	-	3/29/67/67	0/2/2/2
50	XAT	n	622	-	1/1/12/26	4/31/93/93	0/4/4/4
40	LHG	l	101	-	-	38/53/53/53	-
29	CLA	r1	608	-	1/1/14/20	16/31/109/115	-
29	CLA	s	611	40	1/1/15/20	15/37/115/115	-
31	BCR	c1	517	-	-	9/29/63/63	0/2/2/2
29	CLA	d1	403	-	1/1/15/20	12/37/115/115	-
29	CLA	B1	608	-	1/1/15/20	26/37/115/115	-
40	LHG	c	525	-	-	30/51/51/53	-
36	C7Z	b1	620	-	1/1/12/26	11/29/67/67	0/2/2/2
29	CLA	b1	616	-	1/1/15/20	9/37/115/115	-
29	CLA	r1	602	-	1/1/14/20	11/31/109/115	-
33	LMG	b1	622	-	-	19/39/59/70	0/1/1/1
31	BCR	d	404	-	-	13/29/63/63	0/2/2/2
33	LMG	d1	411	-	-	19/41/61/70	0/1/1/1
29	CLA	c	505	-	1/1/15/20	19/37/115/115	-
51	NEX	s1	623	-	-	3/27/83/83	0/3/3/3
51	NEX	S	623	-	-	8/27/83/83	0/3/3/3
29	CLA	b1	608	-	1/1/15/20	25/37/115/115	-
32	SQD	m1	101	-	-	22/37/57/69	0/1/1/1
29	CLA	N1	611	-	1/1/11/20	10/18/96/115	-
50	XAT	y	622	-	-	8/31/93/93	0/4/4/4
29	CLA	N1	613	-	1/1/15/20	14/37/115/115	-
49	LUT	g1	621	-	-	6/29/67/67	0/2/2/2
29	CLA	C1	506	-	1/1/15/20	19/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	R1	603	-	1/1/14/20	17/31/109/115	-
50	XAT	N	622	-	1/1/12/26	2/31/93/93	0/4/4/4
29	CLA	d1	402	-	1/1/15/20	10/37/115/115	-
41	LMK	c1	527	-	2/2/6/6	14/46/46/60	-
39	DGA	c	524	-	-	31/45/45/45	-
29	CLA	R1	604	-	1/1/11/20	10/18/96/115	-
29	CLA	Y1	603	-	1/1/15/20	14/37/115/115	-
29	CLA	b	613	-	1/1/15/20	19/37/115/115	-
29	CLA	n	613	-	1/1/15/20	18/37/115/115	-
29	CLA	G	613	-	1/1/15/20	19/37/115/115	-
29	CLA	r	608	-	1/1/14/20	17/31/109/115	-
48	CHL	Y	601	24	4/4/20/26	7/39/137/137	-
29	CLA	a	406	-	1/1/15/20	17/37/115/115	-
44	HEM	f	101	7,6	-	1/12/54/54	-
47	4RF	i	101	-	-	31/59/59/59	-
48	CHL	s1	608	-	4/4/19/26	5/33/131/137	-
45	RRX	h	101	-	1/1/11/25	4/29/65/65	0/2/2/2
40	LHG	d1	408	-	-	30/48/48/53	-
40	LHG	L	101	-	-	38/53/53/53	-
29	CLA	G	612	-	1/1/10/20	5/11/89/115	-
29	CLA	a	410	-	1/1/14/20	15/31/109/115	-
29	CLA	r1	612	-	1/1/14/20	16/31/109/115	-
29	CLA	n	614	-	1/1/11/20	4/18/96/115	-
48	CHL	g1	607	-	4/4/20/26	7/39/137/137	-
40	LHG	N	624	-	-	31/53/53/53	-
50	XAT	y1	622	-	-	7/31/93/93	0/4/4/4
49	LUT	s	621	-	-	3/29/67/67	0/2/2/2
33	LMG	a	413	-	-	20/43/63/70	0/1/1/1
29	CLA	b	602	-	1/1/15/20	21/37/115/115	-
29	CLA	s1	605	-	1/1/12/20	9/19/97/115	-
51	NEX	Y	623	-	-	7/27/83/83	0/3/3/3
49	LUT	Y	621	-	-	4/29/67/67	0/2/2/2
29	CLA	r1	603	-	1/1/14/20	20/31/109/115	-
29	CLA	g	613	-	1/1/15/20	19/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	DGA	j	101	-	-	20/30/30/45	-
51	NEX	S1	623	-	-	4/27/83/83	0/3/3/3
40	LHG	C	525	-	-	32/51/51/53	-
44	HEM	f1	101	7	-	2/12/54/54	-
40	LHG	y1	624	29	-	25/53/53/53	-
40	LHG	L1	101	-	-	36/53/53/53	-
48	CHL	N1	605	20	4/4/20/26	9/39/137/137	-
43	PL9	D1	405	-	-	18/53/73/73	0/1/1/1
47	4RF	k	101	-	-	31/59/59/59	-
29	CLA	n	611	-	1/1/11/20	8/18/96/115	-
29	CLA	y	604	-	1/1/15/20	15/37/115/115	-
29	CLA	r	612	-	1/1/14/20	14/31/109/115	-
48	CHL	R	607	-	3/3/16/26	7/20/118/137	-
48	CHL	S1	608	-	4/4/19/26	10/33/131/137	-
29	CLA	C	505	-	1/1/15/20	16/37/115/115	-
29	CLA	C1	501	-	1/1/15/20	15/37/115/115	-
51	NEX	Y1	623	-	-	8/27/83/83	0/3/3/3
29	CLA	r	603	-	1/1/14/20	17/31/109/115	-
30	PHO	a	408	-	-	12/37/103/103	0/5/6/6
29	CLA	g	611	-	1/1/15/20	15/37/115/115	-
29	CLA	B1	610	-	1/1/15/20	23/37/115/115	-
34	SPH	y1	625	-	-	12/21/21/21	-
29	CLA	s	602	-	1/1/14/20	16/31/109/115	-
29	CLA	B	610	-	1/1/15/20	21/37/115/115	-
48	CHL	N1	609	-	4/4/20/26	10/39/137/137	-
31	BCR	C1	517	-	-	11/29/63/63	0/2/2/2
54	LPX	S1	625	-	-	15/31/31/31	-
44	HEM	F1	101	7	-	1/12/54/54	-
29	CLA	B	615	-	1/1/15/20	15/37/115/115	-
29	CLA	b	617	-	1/1/15/20	13/37/115/115	-
48	CHL	N	609	-	4/4/20/26	11/39/137/137	-
32	SQD	B1	626	-	-	17/49/69/69	0/1/1/1
37	DGD	c1	519	-	-	24/51/91/95	0/2/2/2
29	CLA	C1	507	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	b1	606	-	1/1/15/20	13/37/115/115	-
33	LMG	D	411	-	-	11/41/61/70	0/1/1/1
37	DGD	C	519	-	-	26/51/91/95	0/2/2/2
51	NEX	n	623	-	-	5/27/83/83	1/3/3/3
51	NEX	N	623	-	-	4/27/83/83	1/3/3/3
48	CHL	n	605	20	4/4/20/26	8/39/137/137	-
29	CLA	y	614	-	1/1/15/20	15/37/115/115	-
48	CHL	G1	606	-	3/3/16/26	4/20/118/137	-
47	4RF	I1	102	-	-	24/59/59/59	-
49	LUT	R	620	-	1/1/12/27	2/29/67/67	0/2/2/2
29	CLA	Y1	611	-	1/1/15/20	16/37/115/115	-
29	CLA	c1	511	-	1/1/15/20	18/37/115/115	-
48	CHL	y	607	-	4/4/20/26	9/39/137/137	-
29	CLA	C1	511	-	1/1/15/20	10/37/115/115	-
29	CLA	B	617	-	1/1/15/20	17/37/115/115	-
31	BCR	c1	514	-	-	12/29/63/63	0/2/2/2
29	CLA	Y	602	-	1/1/15/20	18/37/115/115	-
32	SQD	A	412	-	-	24/46/66/69	0/1/1/1
38	3PH	s	626	-	-	22/49/49/49	-
31	BCR	C1	514	-	-	12/29/63/63	0/2/2/2
38	3PH	s1	626	-	-	27/49/49/49	-
29	CLA	D	402	-	1/1/15/20	19/37/115/115	-
40	LHG	d1	410	-	-	33/43/43/53	-
36	C7Z	B1	620	-	1/1/12/26	7/29/67/67	0/2/2/2
29	CLA	y	603	-	1/1/15/20	18/37/115/115	-
51	NEX	g	623	-	1/1/12/25	9/27/83/83	0/3/3/3
31	BCR	c	514	-	-	14/29/63/63	0/2/2/2
29	CLA	A	407	-	1/1/12/20	9/19/97/115	-
32	SQD	B	621	-	-	20/37/57/69	0/1/1/1
29	CLA	R1	602	-	1/1/14/20	12/31/109/115	-
29	CLA	N1	610	-	1/1/15/20	21/37/115/115	-
34	SPH	A	414	-	-	12/21/21/21	-
51	NEX	y	623	-	-	6/27/83/83	0/3/3/3
29	CLA	S1	610	-	1/1/15/20	22/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	DGA	c1	524	-	-	28/45/45/45	-
29	CLA	G1	614	-	1/1/11/20	8/18/96/115	-
30	PHO	a1	409	-	-	12/37/103/103	0/5/6/6
48	CHL	Y	606	-	4/4/20/26	7/39/137/137	-
29	CLA	c	503	-	1/1/15/20	20/37/115/115	-
48	CHL	n	609	-	4/4/20/26	5/39/137/137	-
29	CLA	S	610	-	1/1/15/20	20/37/115/115	-
29	CLA	G	611	40	1/1/15/20	17/37/115/115	-
49	LUT	y1	621	-	-	4/29/67/67	0/2/2/2
48	CHL	y	601	24	4/4/20/26	9/39/137/137	-
49	LUT	g	621	-	-	4/29/67/67	0/2/2/2
29	CLA	R	609	-	1/1/14/20	13/31/109/115	-
48	CHL	g1	601	-	4/4/20/26	12/39/137/137	-
29	CLA	c	513	-	1/1/15/20	23/37/115/115	-
29	CLA	B	604	-	1/1/15/20	16/37/115/115	-
29	CLA	b	607	-	1/1/15/20	16/37/115/115	-
32	SQD	a	412	-	-	14/46/66/69	0/1/1/1
29	CLA	s1	604	-	1/1/13/20	8/25/103/115	-
33	LMG	C	521	-	-	16/46/66/70	0/1/1/1
40	LHG	S	624	29	-	27/49/49/53	-
48	CHL	n	608	-	3/3/16/26	6/20/118/137	-
29	CLA	Y	603	-	1/1/15/20	17/37/115/115	-
48	CHL	G	601	21	4/4/20/26	11/39/137/137	-
29	CLA	A	410	-	1/1/14/20	14/31/109/115	-
48	CHL	y1	605	24	3/3/16/26	4/15/113/137	-
29	CLA	S1	603	-	1/1/15/20	12/37/115/115	-
40	LHG	C1	525	-	-	30/51/51/53	-
29	CLA	C	502	-	1/1/15/20	13/37/115/115	-
48	CHL	G1	605	21	4/4/16/26	4/18/116/137	-
33	LMG	h	102	-	-	11/43/63/70	0/1/1/1
32	SQD	B1	621	-	-	11/37/57/69	0/1/1/1
48	CHL	g	609	-	4/4/20/26	10/39/137/137	-
29	CLA	S	613	-	1/1/13/20	12/25/103/115	-
29	CLA	b1	617	-	1/1/15/20	14/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	n1	613	-	1/1/15/20	20/37/115/115	-
31	BCR	a1	411	-	-	6/29/63/63	0/2/2/2
32	SQD	b	621	-	-	19/37/57/69	0/1/1/1
29	CLA	B1	614	-	1/1/15/20	14/37/115/115	-
48	CHL	r	606	-	3/3/15/26	3/13/111/137	-
48	CHL	g	608	-	3/3/15/26	3/13/111/137	-
32	SQD	b1	621	-	-	17/37/57/69	0/1/1/1
52	LMT	r	625	-	-	13/21/61/61	0/2/2/2
29	CLA	c1	505	-	1/1/15/20	16/37/115/115	-
31	BCR	A	411	-	-	12/29/63/63	0/2/2/2
29	CLA	a	405	-	1/1/15/20	15/37/115/115	-
29	CLA	B1	616	-	1/1/15/20	18/37/115/115	-
31	BCR	B	618	-	-	11/29/63/63	0/2/2/2
29	CLA	b	611	-	1/1/15/20	7/37/115/115	-
51	NEX	s	623	-	-	4/27/83/83	0/3/3/3
29	CLA	r	609	-	1/1/14/20	12/31/109/115	-
48	CHL	N	608	-	3/3/16/26	3/20/118/137	-
48	CHL	n1	608	-	3/3/16/26	8/20/118/137	-
53	ERG	R1	626	-	5/5/11/15	9/13/71/71	0/4/4/4
40	LHG	d1	409	-	-	30/53/53/53	-
29	CLA	g1	610	-	1/1/15/20	18/37/115/115	-
29	CLA	r	602	22	1/1/14/20	14/31/109/115	-
29	CLA	c	501	-	1/1/15/20	19/37/115/115	-
48	CHL	y1	609	-	4/4/20/26	8/39/137/137	-
29	CLA	d	402	-	1/1/15/20	13/37/115/115	-
33	LMG	D1	411	-	-	10/41/61/70	0/1/1/1
40	LHG	N1	624	-	-	34/53/53/53	-
29	CLA	B	607	-	1/1/15/20	18/37/115/115	-
29	CLA	s1	614	-	1/1/13/20	15/25/103/115	-
29	CLA	c1	508	-	1/1/15/20	12/37/115/115	-
48	CHL	G1	609	-	4/4/20/26	10/39/137/137	-
40	LHG	Y	624	-	-	29/53/53/53	-
29	CLA	C	508	-	1/1/15/20	12/37/115/115	-
29	CLA	b	614	-	1/1/15/20	13/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	DGA	B	625	-	-	23/45/45/45	-
55	PTY	Y1	626	-	-	26/53/53/53	-
49	LUT	n1	621	-	1/1/12/27	5/29/67/67	0/2/2/2
29	CLA	b1	610	-	1/1/15/20	19/37/115/115	-
48	CHL	S1	607	-	3/3/15/26	1/12/110/137	-
29	CLA	D1	402	-	1/1/15/20	13/37/115/115	-
29	CLA	r1	609	-	1/1/14/20	17/31/109/115	-
41	LMK	C	527	-	2/2/6/6	21/46/46/60	-
29	CLA	G1	610	-	1/1/15/20	15/37/115/115	-
31	BCR	c	517	-	-	10/29/63/63	0/2/2/2
29	CLA	n	602	-	1/1/15/20	14/37/115/115	-
29	CLA	R	604	-	1/1/11/20	10/18/96/115	-
48	CHL	N	601	20	4/4/20/26	5/39/137/137	-
39	DGA	J1	101	-	-	15/30/30/45	-
29	CLA	B	613	-	1/1/15/20	18/37/115/115	-
51	NEX	r1	622	-	-	8/27/83/83	0/3/3/3
29	CLA	Y1	604	-	1/1/15/20	13/37/115/115	-
34	SPH	Y	625	-	-	10/21/21/21	-
29	CLA	G	604	-	1/1/11/20	8/18/96/115	-
29	CLA	N	612	-	1/1/11/20	4/13/91/115	-
32	SQD	a1	412	-	-	19/46/66/69	0/1/1/1
29	CLA	B	612	-	1/1/15/20	16/37/115/115	-
30	PHO	a	409	-	-	11/37/103/103	0/5/6/6
50	XAT	N1	622	-	1/1/12/26	1/31/93/93	0/4/4/4
46	GOL	I1	101	-	-	2/4/4/4	-
29	CLA	S	603	-	1/1/15/20	17/37/115/115	-
29	CLA	B1	605	-	1/1/15/20	15/37/115/115	-
29	CLA	n1	611	-	1/1/11/20	9/18/96/115	-
29	CLA	C1	509	-	1/1/15/20	10/37/115/115	-
54	LPX	s1	625	-	-	18/31/31/31	-
54	LPX	S	625	-	-	14/31/31/31	-
50	XAT	Y	622	-	-	7/31/93/93	0/4/4/4
47	4RF	k1	101	-	-	37/59/59/59	-
29	CLA	N	602	-	1/1/15/20	15/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	y	612	-	1/1/15/20	17/37/115/115	-
48	CHL	R1	607	-	3/3/16/26	4/20/118/137	-
47	4RF	K1	101	-	-	32/59/59/59	-
29	CLA	s1	611	40	1/1/15/20	20/37/115/115	-
29	CLA	g	602	-	1/1/15/20	22/37/115/115	-
49	LUT	r1	620	-	-	4/29/67/67	0/2/2/2
29	CLA	s1	617	-	1/1/12/20	11/19/97/115	-
49	LUT	G1	620	-	-	5/29/67/67	0/2/2/2
34	SPH	a1	414	-	-	10/21/21/21	-
29	CLA	S	617	23	1/1/12/20	7/19/97/115	-
48	CHL	N1	607	-	4/4/20/26	10/39/137/137	-
40	LHG	n	624	-	-	35/53/53/53	-
29	CLA	Y1	613	-	1/1/15/20	19/37/115/115	-
29	CLA	s1	603	-	1/1/15/20	15/37/115/115	-
29	CLA	y1	602	-	1/1/15/20	15/37/115/115	-
48	CHL	G	606	-	3/3/16/26	5/20/118/137	-
48	CHL	r1	606	-	3/3/15/26	4/13/111/137	-
53	ERG	r	626	-	5/5/11/15	8/13/71/71	0/4/4/4
49	LUT	G	620	-	-	3/29/67/67	0/2/2/2
29	CLA	R	608	-	1/1/14/20	19/31/109/115	-
31	BCR	a	411	-	-	11/29/63/63	0/2/2/2
48	CHL	g	605	21	4/4/16/26	5/18/116/137	-
29	CLA	g1	611	-	1/1/15/20	18/37/115/115	-
29	CLA	y1	604	-	1/1/15/20	13/37/115/115	-
29	CLA	B1	609	-	1/1/15/20	15/37/115/115	-
40	LHG	g	624	-	-	27/53/53/53	-
29	CLA	R	602	-	1/1/14/20	11/31/109/115	-
29	CLA	c1	502	-	1/1/15/20	16/37/115/115	-
29	CLA	C	509	-	1/1/15/20	20/37/115/115	-
33	LMG	B1	622	-	-	19/39/59/70	0/1/1/1
41	LMK	c	527	-	2/2/6/6	13/46/46/60	-
29	CLA	C	513	-	1/1/15/20	20/37/115/115	-
29	CLA	Y	614	-	1/1/15/20	17/37/115/115	-
29	CLA	b1	613	-	1/1/15/20	16/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
48	CHL	n1	606	-	4/4/20/26	7/39/137/137	-
38	3PH	T	101	-	-	26/49/49/49	-
43	PL9	D	405	-	-	9/53/73/73	0/1/1/1
38	3PH	B	624	-	-	34/49/49/49	-
29	CLA	c1	504	-	1/1/15/20	19/37/115/115	-
29	CLA	g1	602	-	1/1/15/20	19/37/115/115	-
29	CLA	C1	504	-	1/1/15/20	18/37/115/115	-
29	CLA	Y1	612	-	1/1/15/20	18/37/115/115	-
33	LMG	c1	521	-	-	14/46/66/70	0/1/1/1
48	CHL	Y1	605	-	3/3/16/26	3/15/113/137	-
29	CLA	G	602	-	1/1/15/20	17/37/115/115	-
50	XAT	g1	622	-	1/1/12/26	7/31/93/93	0/4/4/4
29	CLA	s	617	-	1/1/12/20	8/19/97/115	-
48	CHL	N1	601	-	4/4/20/26	9/39/137/137	-
31	BCR	D1	404	-	-	14/29/63/63	0/2/2/2
34	SPH	y	625	-	-	8/21/21/21	-
29	CLA	g	604	-	1/1/11/20	7/18/96/115	-
29	CLA	b1	602	-	1/1/15/20	22/37/115/115	-
48	CHL	r	607	-	3/3/16/26	4/20/118/137	-
54	LPX	s	625	-	-	15/31/31/31	-
31	BCR	d1	404	-	-	12/29/63/63	0/2/2/2
29	CLA	B1	615	-	1/1/15/20	14/37/115/115	-
29	CLA	b	610	-	1/1/15/20	15/37/115/115	-
40	LHG	D	408	-	-	23/48/48/53	-
29	CLA	b	612	-	1/1/15/20	16/37/115/115	-
32	SQD	M1	101	-	-	17/37/57/69	0/1/1/1
49	LUT	r	620	-	-	6/29/67/67	0/2/2/2
55	PTY	y	626	-	-	27/53/53/53	-
37	DGD	C1	518	-	-	12/44/84/95	0/2/2/2
29	CLA	N	604	-	1/1/15/20	19/37/115/115	-
29	CLA	n1	604	-	1/1/15/20	14/37/115/115	-
29	CLA	B1	612	-	1/1/15/20	15/37/115/115	-
38	3PH	b1	624	-	-	24/49/49/49	-
31	BCR	C1	516	-	-	15/29/63/63	0/2/2/2

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	A1	405	-	1/1/15/20	12/37/115/115	-
30	PHO	A	408	-	-	8/37/103/103	0/5/6/6
30	PHO	A	409	-	-	14/37/103/103	0/5/6/6
48	CHL	S1	606	-	3/3/15/26	2/13/111/137	-
32	SQD	m	101	-	-	20/37/57/69	0/1/1/1
29	CLA	b1	612	-	1/1/15/20	18/37/115/115	-
48	CHL	s1	606	-	3/3/15/26	0/13/111/137	-
31	BCR	C1	515	-	-	12/29/63/63	0/2/2/2
29	CLA	a1	406	-	1/1/15/20	16/37/115/115	-
55	PTY	Y	626	-	-	31/53/53/53	-
33	LMG	C	523	-	-	21/50/70/70	0/1/1/1
29	CLA	s	610	-	1/1/15/20	18/37/115/115	-
32	SQD	A1	412	-	-	15/46/66/69	0/1/1/1
29	CLA	s1	612	-	1/1/11/20	6/13/91/115	-
29	CLA	b1	603	-	1/1/15/20	19/37/115/115	-
48	CHL	S	601	23	3/3/16/26	3/15/113/137	-
55	PTY	y1	627	-	-	11/20/20/53	-
29	CLA	b	616	-	1/1/15/20	15/37/115/115	-
39	DGA	b	625	-	-	26/45/45/45	-
29	CLA	b1	607	-	1/1/15/20	12/37/115/115	-
31	BCR	B1	619	-	-	6/29/63/63	0/2/2/2
40	LHG	d	410	-	-	20/43/43/53	-
29	CLA	S	614	-	1/1/13/20	8/25/103/115	-
48	CHL	G	607	-	4/4/20/26	11/39/137/137	-
29	CLA	s1	613	-	1/1/13/20	11/25/103/115	-
29	CLA	b	608	-	1/1/15/20	28/37/115/115	-
48	CHL	G	608	-	3/3/15/26	1/13/111/137	-
29	CLA	a1	407	-	1/1/11/20	7/18/96/115	-
48	CHL	g1	608	-	3/3/15/26	1/13/111/137	-
29	CLA	Y	604	-	1/1/15/20	17/37/115/115	-
29	CLA	N	614	-	1/1/11/20	5/18/96/115	-
29	CLA	C	501	-	1/1/15/20	18/37/115/115	-
50	XAT	G1	622	-	1/1/12/26	2/31/93/93	0/4/4/4
48	CHL	S1	601	23	3/3/16/26	3/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	CLA	G1	603	-	1/1/15/20	23/37/115/115	-
29	CLA	C1	510	-	1/1/15/20	17/37/115/115	-
48	CHL	y	605	24	3/3/16/26	3/15/113/137	-
29	CLA	B	602	-	1/1/15/20	20/37/115/115	-
29	CLA	S1	605	-	1/1/12/20	8/19/97/115	-
48	CHL	G1	607	-	4/4/20/26	11/39/137/137	-
29	CLA	b1	605	-	1/1/15/20	18/37/115/115	-
29	CLA	c	510	-	1/1/15/20	14/37/115/115	-
29	CLA	B	605	-	1/1/15/20	19/37/115/115	-
50	XAT	Y1	622	-	1/1/12/26	4/31/93/93	0/4/4/4
29	CLA	s	605	-	1/1/12/20	11/19/97/115	-
37	DGD	C1	520	-	-	16/48/88/95	0/2/2/2
30	PHO	A1	409	-	-	11/37/103/103	0/5/6/6
29	CLA	B	614	-	1/1/15/20	14/37/115/115	-
51	NEX	g1	623	-	1/1/12/25	7/27/83/83	0/3/3/3
40	LHG	D1	409	-	-	31/53/53/53	-
31	BCR	C	517	-	-	13/29/63/63	0/2/2/2
29	CLA	r1	610	-	1/1/14/20	13/31/109/115	-
49	LUT	n1	620	-	-	5/29/67/67	0/2/2/2
29	CLA	c1	507	-	1/1/15/20	16/37/115/115	-
29	CLA	S	612	-	1/1/11/20	6/13/91/115	-
29	CLA	s	612	-	1/1/11/20	5/13/91/115	-
38	3PH	t1	101	-	-	30/49/49/49	-
29	CLA	N	611	-	1/1/11/20	7/18/96/115	-
29	CLA	g1	614	-	1/1/11/20	11/18/96/115	-
48	CHL	r1	607	-	3/3/16/26	4/20/118/137	-
48	CHL	y	609	-	4/4/20/26	6/39/137/137	-
29	CLA	c1	509	-	1/1/15/20	20/37/115/115	-
48	CHL	G1	601	21	4/4/20/26	13/39/137/137	-
29	CLA	s	613	-	1/1/13/20	9/25/103/115	-
29	CLA	n1	610	-	1/1/15/20	20/37/115/115	-

All (3829) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
53	R	626	ERG	C1-C10	-23.16	1.10	1.54
53	r	626	ERG	C1-C10	-22.96	1.10	1.54
53	R1	626	ERG	C1-C10	-22.89	1.10	1.54
53	r1	626	ERG	C1-C10	-22.73	1.11	1.54
53	r	626	ERG	C10-C9	-20.15	1.28	1.55
53	r1	626	ERG	C10-C9	-20.12	1.28	1.55
53	R	626	ERG	C10-C9	-19.91	1.29	1.55
53	R1	626	ERG	C10-C9	-19.17	1.30	1.55
36	b1	620	C7Z	C25-C26	16.02	1.62	1.34
36	B1	620	C7Z	C25-C26	15.63	1.61	1.34
45	H1	101	RRX	C26-C25	15.53	1.61	1.34
45	H	101	RRX	C26-C25	15.52	1.61	1.34
45	h	101	RRX	C26-C25	15.42	1.61	1.34
45	h1	101	RRX	C26-C25	15.41	1.61	1.34
36	B	620	C7Z	C25-C26	15.22	1.60	1.34
36	b	620	C7Z	C5-C6	15.22	1.60	1.34
36	b	620	C7Z	C25-C26	15.11	1.60	1.34
45	H1	101	RRX	C5-C6	14.93	1.60	1.34
36	B1	620	C7Z	C5-C6	14.92	1.60	1.34
36	b1	620	C7Z	C5-C6	14.80	1.60	1.34
45	h1	101	RRX	C5-C6	14.61	1.59	1.34
49	s1	620	LUT	C24-C25	14.59	1.51	1.33
36	B	620	C7Z	C5-C6	14.59	1.59	1.34
49	N	621	LUT	C24-C25	14.58	1.51	1.33
49	n1	620	LUT	C24-C25	14.58	1.51	1.33
49	Y1	620	LUT	C24-C25	14.57	1.51	1.33
49	y1	621	LUT	C24-C25	14.55	1.51	1.33
49	N1	620	LUT	C24-C25	14.53	1.51	1.33
45	H	101	RRX	C5-C6	14.51	1.59	1.34
49	g1	621	LUT	C24-C25	14.50	1.51	1.33
49	g	621	LUT	C24-C25	14.44	1.51	1.33
49	n	621	LUT	C24-C25	14.43	1.51	1.33
49	s	620	LUT	C24-C25	14.43	1.51	1.33
49	S1	621	LUT	C24-C25	14.39	1.51	1.33
49	y1	620	LUT	C24-C25	14.36	1.51	1.33
49	r	620	LUT	C24-C25	14.36	1.51	1.33
49	G	621	LUT	C24-C25	14.35	1.51	1.33
49	R1	620	LUT	C24-C25	14.34	1.51	1.33
49	n1	621	LUT	C24-C25	14.29	1.50	1.33
49	N	620	LUT	C24-C25	14.26	1.50	1.33
49	y	621	LUT	C24-C25	14.24	1.50	1.33
49	r1	620	LUT	C24-C25	14.24	1.50	1.33
49	n	620	LUT	C24-C25	14.24	1.50	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	g1	620	LUT	C24-C25	14.22	1.50	1.33
49	S1	620	LUT	C24-C25	14.19	1.50	1.33
49	R	620	LUT	C24-C25	14.19	1.50	1.33
49	Y1	621	LUT	C24-C25	14.19	1.50	1.33
49	g	620	LUT	C24-C25	14.13	1.50	1.33
49	N1	621	LUT	C24-C25	14.10	1.50	1.33
49	y	620	LUT	C24-C25	14.09	1.50	1.33
49	Y	621	LUT	C24-C25	14.09	1.50	1.33
49	Y	620	LUT	C24-C25	14.00	1.50	1.33
45	h	101	RRX	C5-C6	13.99	1.58	1.34
53	R	626	ERG	C10-C5	-13.96	1.25	1.52
53	R1	626	ERG	C10-C5	-13.92	1.25	1.52
53	r	626	ERG	C4-C3	-13.88	1.27	1.52
49	G1	620	LUT	C24-C25	13.85	1.50	1.33
49	s	621	LUT	C24-C25	13.84	1.50	1.33
53	r1	626	ERG	C4-C3	-13.82	1.28	1.52
49	s1	621	LUT	C24-C25	13.78	1.50	1.33
53	r1	626	ERG	C10-C5	-13.77	1.25	1.52
49	S	620	LUT	C24-C25	13.73	1.50	1.33
49	G	620	LUT	C24-C25	13.69	1.50	1.33
53	r	626	ERG	C10-C5	-13.64	1.25	1.52
53	R	626	ERG	C4-C3	-13.62	1.28	1.52
49	G1	621	LUT	C24-C25	13.62	1.50	1.33
49	S	621	LUT	C24-C25	13.59	1.50	1.33
53	R1	626	ERG	C4-C3	-13.30	1.28	1.52
36	B1	620	C7Z	C24-C23	12.05	1.73	1.52
36	b1	620	C7Z	C24-C23	12.04	1.73	1.52
53	r	626	ERG	C2-C3	-11.64	1.23	1.51
36	B	620	C7Z	C24-C23	11.64	1.72	1.52
53	r1	626	ERG	C2-C3	-11.30	1.24	1.51
36	b	620	C7Z	C24-C23	11.27	1.71	1.52
36	b	620	C7Z	C2-C3	-11.04	1.36	1.52
53	R	626	ERG	C2-C3	-10.99	1.25	1.51
53	R1	626	ERG	C2-C3	-10.68	1.26	1.51
36	b	620	C7Z	C22-C23	-10.65	1.37	1.52
45	H	101	RRX	C29-C28	-10.54	1.37	1.52
36	B1	620	C7Z	C2-C3	-10.44	1.37	1.52
45	h	101	RRX	C29-C28	-10.44	1.37	1.52
45	H1	101	RRX	C29-C28	-10.35	1.37	1.52
36	b1	620	C7Z	C22-C23	-10.28	1.37	1.52
45	h1	101	RRX	C29-C28	-10.21	1.37	1.52
36	B	620	C7Z	C2-C3	-10.10	1.37	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	B1	620	C7Z	C22-C23	-10.08	1.37	1.52
36	B	620	C7Z	C22-C23	-10.05	1.37	1.52
36	b1	620	C7Z	C2-C3	-10.00	1.37	1.52
53	R	626	ERG	C12-C13	9.14	1.70	1.54
53	R	626	ERG	O1-C3	9.12	1.70	1.43
53	r1	626	ERG	O1-C3	9.11	1.70	1.43
53	R1	626	ERG	O1-C3	9.08	1.70	1.43
53	r	626	ERG	O1-C3	9.03	1.70	1.43
53	R1	626	ERG	C6-C5	8.97	1.54	1.33
53	r	626	ERG	C6-C5	8.94	1.54	1.33
36	b1	620	C7Z	C4-C3	8.92	1.67	1.52
53	R	626	ERG	C6-C5	8.89	1.54	1.33
53	r1	626	ERG	C6-C5	8.81	1.54	1.33
53	r	626	ERG	C12-C13	8.79	1.69	1.54
53	R1	626	ERG	C12-C13	8.67	1.69	1.54
53	r1	626	ERG	C12-C13	8.63	1.69	1.54
31	C1	515	BCR	C10-C9	8.52	1.47	1.35
31	b1	618	BCR	C10-C9	8.45	1.47	1.35
36	B1	620	C7Z	C4-C3	8.41	1.66	1.52
36	B	620	C7Z	C4-C3	8.29	1.66	1.52
36	b	620	C7Z	C4-C3	8.29	1.66	1.52
51	n	623	NEX	C14-C13	-8.18	1.24	1.35
51	s	623	NEX	C14-C13	-8.10	1.25	1.35
31	c1	517	BCR	C10-C9	8.03	1.46	1.35
51	y	623	NEX	C34-C33	-8.01	1.25	1.35
45	H1	101	RRX	C27-C28	7.97	1.66	1.52
45	h1	101	RRX	C27-C28	7.93	1.66	1.52
51	g	623	NEX	C10-C9	-7.92	1.25	1.35
51	y	623	NEX	C14-C13	-7.90	1.25	1.35
51	s	623	NEX	C34-C33	-7.89	1.25	1.35
51	n	623	NEX	C10-C9	-7.88	1.25	1.35
51	s	623	NEX	C10-C9	-7.88	1.25	1.35
51	N	623	NEX	C10-C9	-7.86	1.25	1.35
51	g	623	NEX	C14-C13	-7.86	1.25	1.35
51	N	623	NEX	C30-C29	-7.86	1.25	1.35
51	R	622	NEX	C34-C33	-7.85	1.25	1.35
51	G1	623	NEX	C34-C33	-7.82	1.25	1.35
51	g	623	NEX	C34-C33	-7.80	1.25	1.35
51	n	623	NEX	C34-C33	-7.78	1.25	1.35
51	G1	623	NEX	C10-C9	-7.78	1.25	1.35
45	H	101	RRX	C27-C28	7.77	1.65	1.52
51	R	622	NEX	C14-C13	-7.77	1.25	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	R1	622	NEX	C10-C9	-7.75	1.25	1.35
51	n	623	NEX	C30-C29	-7.75	1.25	1.35
51	G	623	NEX	C14-C13	-7.72	1.25	1.35
31	C1	516	BCR	C10-C9	7.71	1.46	1.35
51	r1	622	NEX	C14-C13	-7.69	1.25	1.35
51	s	623	NEX	C30-C29	-7.67	1.25	1.35
51	G	623	NEX	C34-C33	-7.62	1.25	1.35
31	d1	404	BCR	C10-C9	7.62	1.45	1.35
31	B1	618	BCR	C10-C9	7.61	1.45	1.35
51	s1	623	NEX	C14-C13	-7.60	1.25	1.35
31	c1	516	BCR	C10-C9	7.59	1.45	1.35
31	b1	619	BCR	C10-C9	7.57	1.45	1.35
51	Y	623	NEX	C34-C33	-7.56	1.25	1.35
51	Y	623	NEX	C30-C29	-7.55	1.25	1.35
51	r1	622	NEX	C10-C9	-7.54	1.25	1.35
51	s1	623	NEX	C10-C9	-7.54	1.25	1.35
51	y	623	NEX	C30-C29	-7.52	1.25	1.35
51	S	623	NEX	C14-C13	-7.52	1.25	1.35
51	N	623	NEX	C14-C13	-7.52	1.25	1.35
51	y	623	NEX	C10-C9	-7.50	1.25	1.35
51	G1	623	NEX	C14-C13	-7.49	1.25	1.35
51	n1	623	NEX	C14-C13	-7.49	1.25	1.35
51	R	622	NEX	C30-C29	-7.49	1.25	1.35
51	G	623	NEX	C30-C29	-7.47	1.25	1.35
51	N1	623	NEX	C14-C13	-7.47	1.25	1.35
51	g	623	NEX	C30-C29	-7.47	1.25	1.35
51	S	623	NEX	C30-C29	-7.46	1.25	1.35
31	a1	411	BCR	C10-C9	7.46	1.45	1.35
51	G1	623	NEX	C30-C29	-7.46	1.25	1.35
51	r	622	NEX	C14-C13	-7.45	1.25	1.35
51	r1	622	NEX	C30-C29	-7.41	1.26	1.35
51	y1	623	NEX	C10-C9	-7.40	1.26	1.35
51	G	623	NEX	C10-C9	-7.38	1.26	1.35
51	g1	623	NEX	C10-C9	-7.38	1.26	1.35
51	N	623	NEX	C34-C33	-7.37	1.26	1.35
31	C	517	BCR	C10-C9	7.37	1.45	1.35
51	S	623	NEX	C34-C33	-7.36	1.26	1.35
51	R1	622	NEX	C14-C13	-7.34	1.26	1.35
51	Y	623	NEX	C14-C13	-7.34	1.26	1.35
45	h	101	RRX	C27-C28	7.33	1.65	1.52
31	D	404	BCR	C10-C9	7.32	1.45	1.35
51	y1	623	NEX	C14-C13	-7.32	1.26	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	N1	623	NEX	C10-C9	-7.32	1.26	1.35
31	c1	515	BCR	C10-C9	7.30	1.45	1.35
51	n1	623	NEX	C10-C9	-7.29	1.26	1.35
51	r	622	NEX	C30-C29	-7.28	1.26	1.35
31	b	618	BCR	C10-C9	7.24	1.45	1.35
51	r	622	NEX	C34-C33	-7.23	1.26	1.35
51	S1	623	NEX	C30-C29	-7.21	1.26	1.35
31	B	618	BCR	C10-C9	7.21	1.45	1.35
51	Y	623	NEX	C10-C9	-7.21	1.26	1.35
31	d	404	BCR	C10-C9	7.21	1.45	1.35
51	g1	623	NEX	C14-C13	-7.20	1.26	1.35
31	c1	514	BCR	C10-C9	7.19	1.45	1.35
51	g1	623	NEX	C30-C29	-7.19	1.26	1.35
51	N1	623	NEX	C34-C33	-7.18	1.26	1.35
51	r	622	NEX	C10-C9	-7.17	1.26	1.35
51	R1	622	NEX	C34-C33	-7.16	1.26	1.35
41	c	527	LMK	O3-C4	7.15	1.44	1.22
31	C1	517	BCR	C10-C9	7.15	1.45	1.35
31	B1	619	BCR	C10-C9	7.14	1.45	1.35
51	S1	623	NEX	C14-C13	-7.13	1.26	1.35
41	C1	527	LMK	O3-C4	7.13	1.43	1.22
51	S1	623	NEX	C34-C33	-7.12	1.26	1.35
51	r1	622	NEX	C34-C33	-7.11	1.26	1.35
51	N1	623	NEX	C30-C29	-7.10	1.26	1.35
51	S	623	NEX	C10-C9	-7.10	1.26	1.35
31	A1	411	BCR	C10-C9	7.10	1.45	1.35
41	c1	527	LMK	O3-C4	7.07	1.43	1.22
41	C	527	LMK	O3-C4	7.03	1.43	1.22
43	d	405	PL9	C7-C3	-7.00	1.44	1.51
51	g1	623	NEX	C34-C33	-7.00	1.26	1.35
51	R	622	NEX	C10-C9	-7.00	1.26	1.35
51	Y1	623	NEX	C14-C13	-6.99	1.26	1.35
51	n1	623	NEX	C34-C33	-6.99	1.26	1.35
51	R1	622	NEX	C30-C29	-6.98	1.26	1.35
31	C	516	BCR	C10-C9	6.98	1.45	1.35
51	s1	623	NEX	C34-C33	-6.96	1.26	1.35
51	S1	623	NEX	C10-C9	-6.96	1.26	1.35
31	c	516	BCR	C10-C9	6.94	1.45	1.35
51	R	622	NEX	C35-C15	-6.92	1.18	1.36
31	c	517	BCR	C10-C9	6.91	1.44	1.35
51	n	623	NEX	C35-C15	-6.89	1.18	1.36
51	G	623	NEX	C35-C15	-6.86	1.18	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	y1	623	NEX	C30-C29	-6.85	1.26	1.35
51	y	623	NEX	C35-C15	-6.84	1.18	1.36
51	G1	623	NEX	C35-C15	-6.81	1.18	1.36
51	n1	623	NEX	C35-C15	-6.80	1.18	1.36
51	y1	623	NEX	C34-C33	-6.80	1.26	1.35
51	s	623	NEX	C35-C15	-6.80	1.18	1.36
51	Y1	623	NEX	C34-C33	-6.78	1.26	1.35
51	N	623	NEX	C35-C15	-6.76	1.18	1.36
51	S	623	NEX	C35-C15	-6.74	1.18	1.36
51	Y1	623	NEX	C10-C9	-6.73	1.26	1.35
51	Y	623	NEX	C35-C15	-6.72	1.18	1.36
51	r	622	NEX	C35-C15	-6.72	1.18	1.36
51	g	623	NEX	C35-C15	-6.71	1.18	1.36
51	r1	622	NEX	C35-C15	-6.71	1.18	1.36
29	B1	603	CLA	MG-NA	6.70	2.22	2.06
31	a	411	BCR	C10-C9	6.66	1.44	1.35
51	R	622	NEX	C11-C12	-6.65	1.17	1.34
31	c	514	BCR	C10-C9	6.65	1.44	1.35
51	n1	623	NEX	C30-C29	-6.63	1.27	1.35
29	r1	612	CLA	MG-NA	6.60	2.22	2.06
45	H	101	RRX	C2-C3	-6.60	1.36	1.52
31	D1	404	BCR	C10-C9	6.60	1.44	1.35
51	g1	623	NEX	C35-C15	-6.59	1.18	1.36
29	b1	602	CLA	MG-NA	6.58	2.21	2.06
45	H	101	RRX	C1-C6	-6.57	1.44	1.53
51	N1	623	NEX	C35-C15	-6.56	1.18	1.36
31	A	411	BCR	C10-C9	6.56	1.44	1.35
51	s	623	NEX	C11-C12	-6.55	1.17	1.34
51	R1	622	NEX	C35-C15	-6.55	1.18	1.36
51	S	623	NEX	C7-C8	6.55	1.42	1.32
29	R1	612	CLA	MG-NA	6.55	2.21	2.06
51	g	623	NEX	C11-C12	-6.54	1.17	1.34
29	R	612	CLA	MG-NA	6.54	2.21	2.06
51	S1	623	NEX	C35-C15	-6.54	1.19	1.36
51	s	623	NEX	C31-C32	-6.52	1.17	1.34
29	S1	611	CLA	MG-NA	6.52	2.21	2.06
45	h1	101	RRX	C2-C3	-6.51	1.36	1.52
51	Y1	623	NEX	C35-C15	-6.51	1.19	1.36
29	g1	614	CLA	MG-NA	6.51	2.21	2.06
51	n	623	NEX	C11-C12	-6.50	1.17	1.34
29	B1	602	CLA	MG-NA	6.49	2.21	2.06
29	s1	613	CLA	MG-NA	6.48	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	s	603	CLA	MG-NA	6.47	2.21	2.06
45	h	101	RRX	C2-C3	-6.47	1.36	1.52
29	G1	602	CLA	MG-NA	6.47	2.21	2.06
51	n	623	NEX	C31-C32	-6.47	1.17	1.34
29	s1	612	CLA	MG-NA	6.47	2.21	2.06
29	N	612	CLA	MG-NA	6.46	2.21	2.06
29	n	602	CLA	MG-NA	6.46	2.21	2.06
29	R	603	CLA	MG-NA	6.46	2.21	2.06
29	s1	614	CLA	MG-NA	6.46	2.21	2.06
51	s1	623	NEX	C35-C15	-6.46	1.19	1.36
31	C	514	BCR	C10-C9	6.46	1.44	1.35
51	Y1	623	NEX	C30-C29	-6.45	1.27	1.35
29	S	603	CLA	MG-NA	6.45	2.21	2.06
29	b1	616	CLA	MG-NA	6.45	2.21	2.06
29	s1	611	CLA	MG-NA	6.44	2.21	2.06
29	s	617	CLA	MG-NA	6.44	2.21	2.06
51	S	623	NEX	C11-C12	-6.43	1.18	1.34
29	g	614	CLA	MG-NA	6.43	2.21	2.06
45	H1	101	RRX	C2-C3	-6.43	1.36	1.52
29	r	612	CLA	MG-NA	6.43	2.21	2.06
29	C1	503	CLA	MG-NA	6.42	2.21	2.06
29	b1	614	CLA	MG-NA	6.42	2.21	2.06
29	r1	603	CLA	MG-NA	6.42	2.21	2.06
29	g1	612	CLA	MG-NA	6.42	2.21	2.06
29	s1	605	CLA	MG-NA	6.42	2.21	2.06
51	s1	623	NEX	C30-C29	-6.42	1.27	1.35
29	y	602	CLA	MG-NA	6.41	2.21	2.06
29	G	612	CLA	MG-NA	6.41	2.21	2.06
29	N1	614	CLA	MG-NA	6.41	2.21	2.06
29	B	616	CLA	MG-NA	6.41	2.21	2.06
29	g	612	CLA	MG-NA	6.41	2.21	2.06
29	g1	611	CLA	MG-NA	6.40	2.21	2.06
29	S	605	CLA	MG-NA	6.40	2.21	2.06
45	H1	101	RRX	C1-C6	-6.40	1.45	1.53
29	c	512	CLA	MG-NA	6.39	2.21	2.06
29	R1	608	CLA	MG-NA	6.39	2.21	2.06
31	B	619	BCR	C10-C9	6.39	1.44	1.35
51	N	623	NEX	C11-C12	-6.39	1.18	1.34
29	N	611	CLA	MG-NA	6.39	2.21	2.06
51	r1	622	NEX	C31-C32	-6.39	1.18	1.34
31	C1	514	BCR	C10-C9	6.39	1.44	1.35
51	N	623	NEX	C31-C32	-6.38	1.18	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	n	612	CLA	MG-NA	6.38	2.21	2.06
29	r	602	CLA	MG-NA	6.38	2.21	2.06
51	Y	623	NEX	C31-C32	-6.37	1.18	1.34
29	B	603	CLA	MG-NA	6.37	2.21	2.06
29	b	602	CLA	MG-NA	6.37	2.21	2.06
29	Y1	603	CLA	MG-NA	6.37	2.21	2.06
29	y	608	CLA	MG-NA	6.36	2.21	2.06
29	Y1	612	CLA	MG-NA	6.36	2.21	2.06
29	n1	612	CLA	MG-NA	6.36	2.21	2.06
29	S1	605	CLA	MG-NA	6.35	2.21	2.06
29	R	608	CLA	MG-NA	6.35	2.21	2.06
29	c1	512	CLA	MG-NA	6.35	2.21	2.06
29	r1	602	CLA	MG-NA	6.34	2.21	2.06
29	G	614	CLA	MG-NA	6.34	2.21	2.06
29	B1	616	CLA	MG-NA	6.34	2.21	2.06
29	n	611	CLA	MG-NA	6.34	2.21	2.06
45	h	101	RRX	C1-C6	-6.33	1.45	1.53
29	R1	602	CLA	MG-NA	6.33	2.21	2.06
29	g1	603	CLA	MG-NA	6.33	2.21	2.06
51	r1	622	NEX	C7-C8	6.33	1.42	1.32
29	r1	604	CLA	MG-NA	6.32	2.21	2.06
51	g1	623	NEX	C11-C12	-6.32	1.18	1.34
51	N1	623	NEX	C11-C12	-6.32	1.18	1.34
29	R1	603	CLA	MG-NA	6.32	2.21	2.06
29	y1	611	CLA	MG-NA	6.32	2.21	2.06
31	b	619	BCR	C10-C9	6.32	1.44	1.35
29	s	605	CLA	MG-NA	6.31	2.21	2.06
51	y	623	NEX	C31-C32	-6.31	1.18	1.34
29	s1	609	CLA	MG-NA	6.31	2.21	2.06
29	c1	513	CLA	MG-NA	6.31	2.21	2.06
29	b	605	CLA	MG-NA	6.31	2.21	2.06
29	r1	608	CLA	MG-NA	6.30	2.21	2.06
29	G	604	CLA	MG-NA	6.30	2.21	2.06
29	s	612	CLA	MG-NA	6.30	2.21	2.06
29	r	603	CLA	MG-NA	6.30	2.21	2.06
29	G	611	CLA	MG-NA	6.30	2.21	2.06
29	d1	403	CLA	MG-NA	6.30	2.21	2.06
29	y	613	CLA	MG-NA	6.30	2.21	2.06
29	S1	603	CLA	MG-NA	6.29	2.21	2.06
29	S1	617	CLA	MG-NA	6.29	2.21	2.06
29	a1	406	CLA	MG-NA	6.29	2.21	2.06
29	R1	604	CLA	MG-NA	6.29	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S	611	CLA	MG-NA	6.29	2.21	2.06
53	R	626	ERG	C16-C17	-6.28	1.41	1.54
29	B1	608	CLA	MG-NA	6.28	2.21	2.06
29	s1	603	CLA	MG-NA	6.28	2.21	2.06
51	G	623	NEX	C31-C32	-6.28	1.18	1.34
29	Y1	608	CLA	MG-NA	6.28	2.21	2.06
29	d1	402	CLA	MG-NA	6.28	2.21	2.06
29	n	614	CLA	MG-NA	6.28	2.21	2.06
51	g	623	NEX	C31-C32	-6.28	1.18	1.34
29	c1	503	CLA	MG-NA	6.27	2.21	2.06
29	a	407	CLA	MG-NA	6.27	2.21	2.06
29	c1	511	CLA	MG-NA	6.27	2.21	2.06
29	s	610	CLA	MG-NA	6.27	2.21	2.06
29	y	603	CLA	MG-NA	6.27	2.21	2.06
29	C	502	CLA	MG-NA	6.27	2.21	2.06
29	G1	604	CLA	MG-NA	6.27	2.21	2.06
51	G1	623	NEX	C31-C32	-6.27	1.18	1.34
29	B	605	CLA	MG-NA	6.26	2.21	2.06
29	C	503	CLA	MG-NA	6.26	2.21	2.06
29	N	614	CLA	MG-NA	6.26	2.21	2.06
29	c1	510	CLA	MG-NA	6.26	2.21	2.06
29	N1	612	CLA	MG-NA	6.26	2.21	2.06
51	Y	623	NEX	C11-C12	-6.26	1.18	1.34
29	C	513	CLA	MG-NA	6.26	2.21	2.06
29	c1	501	CLA	MG-NA	6.26	2.21	2.06
29	r	608	CLA	MG-NA	6.26	2.21	2.06
29	s1	604	CLA	MG-NA	6.25	2.21	2.06
29	b1	604	CLA	MG-NA	6.25	2.21	2.06
29	S	602	CLA	MG-NA	6.25	2.21	2.06
51	y	623	NEX	C11-C12	-6.25	1.18	1.34
29	B1	615	CLA	MG-NA	6.25	2.21	2.06
29	Y	613	CLA	MG-NA	6.24	2.21	2.06
29	C	510	CLA	MG-NA	6.24	2.21	2.06
29	y1	608	CLA	MG-NA	6.24	2.21	2.06
29	s1	602	CLA	MG-NA	6.24	2.21	2.06
51	R1	622	NEX	C7-C8	6.24	1.42	1.32
29	c1	509	CLA	MG-NA	6.24	2.21	2.06
29	r1	610	CLA	MG-NA	6.24	2.21	2.06
29	S	609	CLA	MG-NA	6.23	2.21	2.06
29	G1	612	CLA	MG-NA	6.23	2.21	2.06
29	B1	605	CLA	MG-NA	6.23	2.21	2.06
29	n	613	CLA	MG-NA	6.23	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	R	622	NEX	C31-C32	-6.23	1.18	1.34
29	b1	608	CLA	MG-NA	6.23	2.21	2.06
29	N	613	CLA	MG-NA	6.23	2.21	2.06
29	y1	610	CLA	MG-NA	6.23	2.21	2.06
29	y	611	CLA	MG-NA	6.23	2.21	2.06
29	Y1	602	CLA	MG-NA	6.23	2.21	2.06
29	g1	613	CLA	MG-NA	6.23	2.21	2.06
51	y1	623	NEX	C35-C15	-6.22	1.19	1.36
29	n1	603	CLA	MG-NA	6.22	2.21	2.06
51	s1	623	NEX	C11-C12	-6.22	1.18	1.34
29	s	609	CLA	MG-NA	6.22	2.21	2.06
29	b1	606	CLA	MG-NA	6.22	2.21	2.06
29	Y	614	CLA	MG-NA	6.22	2.21	2.06
29	Y	612	CLA	MG-NA	6.22	2.21	2.06
29	s	604	CLA	MG-NA	6.22	2.21	2.06
29	n1	614	CLA	MG-NA	6.22	2.21	2.06
29	y1	614	CLA	MG-NA	6.22	2.21	2.06
51	G1	623	NEX	C11-C12	-6.22	1.18	1.34
29	Y1	604	CLA	MG-NA	6.22	2.21	2.06
29	N1	603	CLA	MG-NA	6.21	2.21	2.06
29	B	607	CLA	MG-NA	6.21	2.21	2.06
51	r	622	NEX	C31-C32	-6.21	1.18	1.34
29	C	507	CLA	MG-NA	6.21	2.21	2.06
29	b1	612	CLA	MG-NA	6.21	2.21	2.06
29	d	403	CLA	MG-NA	6.21	2.21	2.06
29	n1	611	CLA	MG-NA	6.21	2.21	2.06
29	s1	617	CLA	MG-NA	6.21	2.21	2.06
29	c	507	CLA	MG-NA	6.21	2.21	2.06
29	D1	403	CLA	MG-NA	6.21	2.21	2.06
51	R1	622	NEX	C11-C12	-6.21	1.18	1.34
29	G	602	CLA	MG-NA	6.21	2.21	2.06
29	c	511	CLA	MG-NA	6.20	2.21	2.06
51	r	622	NEX	C11-C12	-6.20	1.18	1.34
29	C	511	CLA	MG-NA	6.20	2.21	2.06
29	C1	501	CLA	MG-NA	6.20	2.21	2.06
29	s1	610	CLA	MG-NA	6.20	2.21	2.06
29	g	603	CLA	MG-NA	6.20	2.21	2.06
29	a1	407	CLA	MG-NA	6.20	2.21	2.06
29	n	610	CLA	MG-NA	6.19	2.21	2.06
29	g	604	CLA	MG-NA	6.19	2.21	2.06
29	G1	614	CLA	MG-NA	6.19	2.21	2.06
29	c	510	CLA	MG-NA	6.19	2.21	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b1	611	CLA	MG-NA	6.19	2.21	2.06
29	b1	617	CLA	MG-NA	6.19	2.21	2.06
29	n1	604	CLA	MG-NA	6.19	2.21	2.06
29	c1	502	CLA	MG-NA	6.18	2.21	2.06
29	y1	612	CLA	MG-NA	6.18	2.21	2.06
29	S	612	CLA	MG-NA	6.18	2.21	2.06
29	B	602	CLA	MG-NA	6.18	2.20	2.06
29	B	610	CLA	MG-NA	6.18	2.20	2.06
29	s	611	CLA	MG-NA	6.18	2.20	2.06
29	r	610	CLA	MG-NA	6.18	2.20	2.06
29	c	502	CLA	MG-NA	6.18	2.20	2.06
51	n1	623	NEX	C11-C12	-6.18	1.18	1.34
29	N	604	CLA	MG-NA	6.17	2.20	2.06
29	y	604	CLA	MG-NA	6.17	2.20	2.06
29	Y	608	CLA	MG-NA	6.17	2.20	2.06
29	b1	609	CLA	MG-NA	6.17	2.20	2.06
29	G	613	CLA	MG-NA	6.17	2.20	2.06
29	C1	502	CLA	MG-NA	6.17	2.20	2.06
29	R1	609	CLA	MG-NA	6.17	2.20	2.06
29	b1	607	CLA	MG-NA	6.17	2.20	2.06
29	g	613	CLA	MG-NA	6.16	2.20	2.06
29	Y	603	CLA	MG-NA	6.16	2.20	2.06
29	b	611	CLA	MG-NA	6.16	2.20	2.06
29	G	603	CLA	MG-NA	6.16	2.20	2.06
29	c1	507	CLA	MG-NA	6.16	2.20	2.06
51	S	623	NEX	C31-C32	-6.16	1.18	1.34
29	R	602	CLA	MG-NA	6.16	2.20	2.06
29	b1	605	CLA	MG-NA	6.15	2.20	2.06
29	C1	513	CLA	MG-NA	6.15	2.20	2.06
29	C1	512	CLA	MG-NA	6.15	2.20	2.06
29	R	604	CLA	MG-NA	6.15	2.20	2.06
29	Y1	610	CLA	MG-NA	6.15	2.20	2.06
29	B1	604	CLA	MG-NA	6.15	2.20	2.06
29	D1	402	CLA	MG-NA	6.15	2.20	2.06
29	c	506	CLA	MG-NA	6.15	2.20	2.06
29	b	608	CLA	MG-NA	6.15	2.20	2.06
29	b1	603	CLA	MG-NA	6.15	2.20	2.06
29	G1	610	CLA	MG-NA	6.14	2.20	2.06
29	B1	617	CLA	MG-NA	6.14	2.20	2.06
29	n	603	CLA	MG-NA	6.14	2.20	2.06
29	b1	615	CLA	MG-NA	6.14	2.20	2.06
29	G1	603	CLA	MG-NA	6.14	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	501	CLA	MG-NA	6.14	2.20	2.06
29	B1	612	CLA	MG-NA	6.14	2.20	2.06
29	S1	604	CLA	MG-NA	6.14	2.20	2.06
29	b1	610	CLA	MG-NA	6.13	2.20	2.06
29	c	503	CLA	MG-NA	6.13	2.20	2.06
29	G1	613	CLA	MG-NA	6.13	2.20	2.06
29	y1	603	CLA	MG-NA	6.13	2.20	2.06
29	a1	410	CLA	MG-NA	6.13	2.20	2.06
29	b	609	CLA	MG-NA	6.13	2.20	2.06
29	y	612	CLA	MG-NA	6.13	2.20	2.06
51	S1	623	NEX	C31-C32	-6.13	1.18	1.34
29	C	512	CLA	MG-NA	6.12	2.20	2.06
29	c1	508	CLA	MG-NA	6.12	2.20	2.06
29	y1	613	CLA	MG-NA	6.12	2.20	2.06
29	g	602	CLA	MG-NA	6.12	2.20	2.06
29	N1	611	CLA	MG-NA	6.12	2.20	2.06
29	c1	506	CLA	MG-NA	6.12	2.20	2.06
29	N1	613	CLA	MG-NA	6.12	2.20	2.06
29	A1	407	CLA	MG-NA	6.12	2.20	2.06
29	A1	406	CLA	MG-NA	6.11	2.20	2.06
29	S1	612	CLA	MG-NA	6.11	2.20	2.06
31	b1	618	BCR	C24-C23	6.11	1.51	1.33
29	S	613	CLA	MG-NA	6.11	2.20	2.06
29	A	407	CLA	MG-NA	6.11	2.20	2.06
29	g1	602	CLA	MG-NA	6.11	2.20	2.06
29	B	608	CLA	MG-NA	6.11	2.20	2.06
51	G	623	NEX	C11-C12	-6.10	1.18	1.34
29	G1	611	CLA	MG-NA	6.10	2.20	2.06
29	n1	613	CLA	MG-NA	6.10	2.20	2.06
29	c	505	CLA	MG-NA	6.10	2.20	2.06
29	r	604	CLA	MG-NA	6.10	2.20	2.06
29	Y	602	CLA	MG-NA	6.10	2.20	2.06
29	B1	613	CLA	MG-NA	6.10	2.20	2.06
29	B1	610	CLA	MG-NA	6.09	2.20	2.06
29	B1	614	CLA	MG-NA	6.09	2.20	2.06
29	N1	602	CLA	MG-NA	6.09	2.20	2.06
29	D	403	CLA	MG-NA	6.09	2.20	2.06
29	C1	511	CLA	MG-NA	6.09	2.20	2.06
29	s	602	CLA	MG-NA	6.09	2.20	2.06
29	B1	609	CLA	MG-NA	6.08	2.20	2.06
29	Y	611	CLA	MG-NA	6.08	2.20	2.06
29	S	614	CLA	MG-NA	6.07	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	505	CLA	MG-NA	6.07	2.20	2.06
29	B	609	CLA	MG-NA	6.07	2.20	2.06
29	b	603	CLA	MG-NA	6.07	2.20	2.06
29	R1	610	CLA	MG-NA	6.07	2.20	2.06
29	N	610	CLA	MG-NA	6.07	2.20	2.06
29	c	513	CLA	MG-NA	6.06	2.20	2.06
31	c1	516	BCR	C24-C23	6.06	1.51	1.33
29	N	602	CLA	MG-NA	6.06	2.20	2.06
29	C1	506	CLA	MG-NA	6.06	2.20	2.06
29	B	612	CLA	MG-NA	6.06	2.20	2.06
31	C	515	BCR	C10-C9	6.06	1.43	1.35
29	n1	610	CLA	MG-NA	6.05	2.20	2.06
53	r	626	ERG	C16-C17	-6.05	1.41	1.54
29	g1	604	CLA	MG-NA	6.05	2.20	2.06
29	C1	504	CLA	MG-NA	6.05	2.20	2.06
29	c	501	CLA	MG-NA	6.05	2.20	2.06
29	N1	604	CLA	MG-NA	6.05	2.20	2.06
29	Y1	614	CLA	MG-NA	6.05	2.20	2.06
29	b	607	CLA	MG-NA	6.05	2.20	2.06
29	S	617	CLA	MG-NA	6.05	2.20	2.06
29	a	410	CLA	MG-NA	6.05	2.20	2.06
29	b	604	CLA	MG-NA	6.04	2.20	2.06
29	C1	508	CLA	MG-NA	6.04	2.20	2.06
51	S1	623	NEX	C11-C12	-6.04	1.19	1.34
29	B	615	CLA	MG-NA	6.04	2.20	2.06
29	B	606	CLA	MG-NA	6.03	2.20	2.06
29	c1	505	CLA	MG-NA	6.03	2.20	2.06
29	S1	609	CLA	MG-NA	6.03	2.20	2.06
29	c	509	CLA	MG-NA	6.03	2.20	2.06
29	g	611	CLA	MG-NA	6.03	2.20	2.06
29	r1	609	CLA	MG-NA	6.03	2.20	2.06
29	C1	507	CLA	MG-NA	6.02	2.20	2.06
29	r	609	CLA	MG-NA	6.02	2.20	2.06
29	B	614	CLA	MG-NA	6.02	2.20	2.06
29	s	613	CLA	MG-NA	6.02	2.20	2.06
51	n1	623	NEX	C7-C8	6.02	1.42	1.32
29	C	508	CLA	MG-NA	6.02	2.20	2.06
29	Y	604	CLA	MG-NA	6.01	2.20	2.06
29	b	614	CLA	MG-NA	6.01	2.20	2.06
29	B	604	CLA	MG-NA	6.01	2.20	2.06
29	n	604	CLA	MG-NA	6.01	2.20	2.06
29	B1	611	CLA	MG-NA	6.00	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	406	CLA	MG-NA	6.00	2.20	2.06
29	y1	602	CLA	MG-NA	6.00	2.20	2.06
29	b	616	CLA	MG-NA	6.00	2.20	2.06
29	c	508	CLA	MG-NA	5.99	2.20	2.06
51	r1	622	NEX	C11-C12	-5.99	1.19	1.34
29	b	617	CLA	MG-NA	5.99	2.20	2.06
29	b	612	CLA	MG-NA	5.99	2.20	2.06
31	B1	618	BCR	C24-C23	5.99	1.51	1.33
51	N1	623	NEX	C31-C32	-5.99	1.19	1.34
29	b	615	CLA	MG-NA	5.98	2.20	2.06
51	n1	623	NEX	C31-C32	-5.98	1.19	1.34
53	R1	626	ERG	C16-C17	-5.98	1.42	1.54
29	C	506	CLA	MG-NA	5.98	2.20	2.06
29	B	617	CLA	MG-NA	5.97	2.20	2.06
29	R	610	CLA	MG-NA	5.97	2.20	2.06
29	S1	614	CLA	MG-NA	5.97	2.20	2.06
29	S1	613	CLA	MG-NA	5.97	2.20	2.06
29	C	509	CLA	MG-NA	5.97	2.20	2.06
29	y1	604	CLA	MG-NA	5.97	2.20	2.06
29	b	610	CLA	MG-NA	5.97	2.20	2.06
31	b1	619	BCR	C24-C23	5.96	1.51	1.33
53	r1	626	ERG	C13-C14	-5.96	1.46	1.56
29	B	611	CLA	MG-NA	5.96	2.20	2.06
29	C	504	CLA	MG-NA	5.96	2.20	2.06
51	s1	623	NEX	C7-C8	5.96	1.41	1.32
29	y	614	CLA	MG-NA	5.96	2.20	2.06
51	s1	623	NEX	C31-C32	-5.96	1.19	1.34
29	C1	509	CLA	MG-NA	5.95	2.20	2.06
29	A1	410	CLA	MG-NA	5.95	2.20	2.06
31	C1	517	BCR	C24-C23	5.95	1.51	1.33
29	G	610	CLA	MG-NA	5.95	2.20	2.06
51	R1	622	NEX	C31-C32	-5.95	1.19	1.34
29	c1	504	CLA	MG-NA	5.94	2.20	2.06
51	Y1	623	NEX	C31-C32	-5.94	1.19	1.34
29	C1	510	CLA	MG-NA	5.94	2.20	2.06
29	d	402	CLA	MG-NA	5.94	2.20	2.06
29	R	609	CLA	MG-NA	5.94	2.20	2.06
29	N	603	CLA	MG-NA	5.94	2.20	2.06
29	B1	606	CLA	MG-NA	5.93	2.20	2.06
29	y	610	CLA	MG-NA	5.93	2.20	2.06
29	S1	602	CLA	MG-NA	5.93	2.20	2.06
29	A1	405	CLA	MG-NA	5.93	2.20	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	515	BCR	C11-C12	-5.93	1.19	1.34
29	n1	602	CLA	MG-NA	5.92	2.20	2.06
29	A	406	CLA	MG-NA	5.92	2.20	2.06
51	g1	623	NEX	C31-C32	-5.92	1.19	1.34
29	S	610	CLA	MG-NA	5.92	2.20	2.06
29	g1	610	CLA	MG-NA	5.91	2.20	2.06
29	s	614	CLA	MG-NA	5.91	2.20	2.06
29	N1	610	CLA	MG-NA	5.90	2.20	2.06
36	B	620	C7Z	C1-C6	-5.90	1.45	1.53
29	b1	613	CLA	MG-NA	5.90	2.20	2.06
29	Y1	611	CLA	MG-NA	5.90	2.20	2.06
29	Y1	613	CLA	MG-NA	5.89	2.20	2.06
29	c	504	CLA	MG-NA	5.89	2.20	2.06
29	a1	405	CLA	MG-NA	5.88	2.20	2.06
29	C1	505	CLA	MG-NA	5.88	2.20	2.06
53	r1	626	ERG	C16-C17	-5.88	1.42	1.54
29	S	604	CLA	MG-NA	5.87	2.20	2.06
36	B1	620	C7Z	C12-C13	5.87	1.58	1.45
51	y1	623	NEX	C11-C12	-5.86	1.19	1.34
51	y1	623	NEX	C31-C32	-5.86	1.19	1.34
29	A	410	CLA	MG-NA	5.85	2.20	2.06
29	B	613	CLA	MG-NA	5.85	2.20	2.06
51	y1	623	NEX	C7-C8	5.85	1.41	1.32
51	s	623	NEX	C7-C8	5.83	1.41	1.32
29	D	402	CLA	MG-NA	5.83	2.20	2.06
29	b	606	CLA	MG-NA	5.81	2.20	2.06
29	a	405	CLA	MG-NA	5.80	2.20	2.06
29	b	613	CLA	MG-NA	5.80	2.20	2.06
29	B1	607	CLA	MG-NA	5.77	2.20	2.06
29	A	405	CLA	MG-NA	5.77	2.20	2.06
36	b1	620	C7Z	C1-C6	-5.76	1.45	1.53
31	b	619	BCR	C24-C23	5.76	1.50	1.33
43	D	405	PL9	C7-C3	-5.75	1.45	1.51
31	A1	411	BCR	C24-C23	5.74	1.50	1.33
31	D1	404	BCR	C24-C23	5.74	1.50	1.33
31	d1	404	BCR	C24-C23	5.73	1.50	1.33
36	b1	620	C7Z	C12-C13	5.72	1.58	1.45
51	r	622	NEX	C7-C8	5.72	1.41	1.32
31	D	404	BCR	C24-C23	5.71	1.50	1.33
31	c1	515	BCR	C24-C23	5.68	1.50	1.33
31	C1	514	BCR	C24-C23	5.68	1.50	1.33
29	S1	610	CLA	MG-NA	5.67	2.19	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	Y1	623	NEX	C7-C8	5.66	1.41	1.32
31	c	516	BCR	C24-C23	5.66	1.50	1.33
53	R1	626	ERG	C1-C2	5.65	1.65	1.53
51	g	623	NEX	C7-C8	5.64	1.41	1.32
31	b	618	BCR	C24-C23	5.64	1.50	1.33
31	c	515	BCR	C10-C9	5.63	1.43	1.35
31	d	404	BCR	C24-C23	5.63	1.50	1.33
31	C	514	BCR	C11-C12	-5.63	1.20	1.34
51	Y1	623	NEX	C11-C12	-5.63	1.20	1.34
29	g	610	CLA	MG-NA	5.62	2.19	2.06
31	c1	514	BCR	C24-C23	5.62	1.50	1.33
31	B	619	BCR	C24-C23	5.61	1.50	1.33
31	B1	619	BCR	C24-C23	5.60	1.50	1.33
29	Y	610	CLA	MG-NA	5.60	2.19	2.06
31	C1	516	BCR	C24-C23	5.57	1.49	1.33
31	C	516	BCR	C24-C23	5.56	1.49	1.33
36	B	620	C7Z	C12-C13	5.55	1.57	1.45
31	a1	411	BCR	C24-C23	5.54	1.49	1.33
31	a1	411	BCR	C11-C12	-5.54	1.20	1.34
36	b	620	C7Z	C1-C6	-5.53	1.46	1.53
31	c1	515	BCR	C11-C12	-5.51	1.20	1.34
31	c	514	BCR	C24-C23	5.50	1.49	1.33
31	c1	517	BCR	C24-C23	5.49	1.49	1.33
36	B	620	C7Z	C24-C25	-5.49	1.42	1.51
45	H1	101	RRX	C19-C18	5.49	1.57	1.45
31	A	411	BCR	C24-C23	5.48	1.49	1.33
31	C1	514	BCR	C11-C12	-5.48	1.20	1.34
31	a	411	BCR	C24-C23	5.48	1.49	1.33
51	Y	623	NEX	C28-C29	-5.48	1.34	1.45
31	C	514	BCR	C24-C23	5.47	1.49	1.33
31	C	515	BCR	C24-C23	5.46	1.49	1.33
31	A	411	BCR	C11-C12	-5.46	1.20	1.34
31	b	619	BCR	C11-C12	-5.45	1.20	1.34
31	B	619	BCR	C11-C12	-5.45	1.20	1.34
51	g	623	NEX	C28-C29	-5.44	1.34	1.45
31	C	517	BCR	C24-C23	5.42	1.49	1.33
53	R1	626	ERG	C13-C14	-5.41	1.47	1.56
31	B	618	BCR	C24-C23	5.41	1.49	1.33
51	n	623	NEX	C28-C29	-5.41	1.34	1.45
31	c	517	BCR	C24-C23	5.40	1.49	1.33
51	R	622	NEX	C28-C29	-5.39	1.34	1.45
31	c	514	BCR	C11-C12	-5.39	1.20	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	Y	623	NEX	C7-C8	5.38	1.40	1.32
36	B1	620	C7Z	C28-C29	5.38	1.57	1.45
31	D1	404	BCR	C11-C12	-5.37	1.20	1.34
36	b	620	C7Z	C12-C13	5.37	1.57	1.45
36	B1	620	C7Z	C1-C6	-5.36	1.46	1.53
51	s	623	NEX	C28-C29	-5.36	1.34	1.45
31	C1	515	BCR	C24-C23	5.35	1.49	1.33
51	y1	623	NEX	C28-C29	-5.35	1.34	1.45
53	R	626	ERG	C1-C2	5.34	1.64	1.53
51	G1	623	NEX	C7-C8	5.33	1.40	1.32
51	N	623	NEX	C28-C29	-5.33	1.34	1.45
31	a	411	BCR	C11-C12	-5.33	1.20	1.34
51	R	622	NEX	C7-C8	5.32	1.40	1.32
36	b1	620	C7Z	C28-C29	5.31	1.57	1.45
31	C	515	BCR	C11-C12	-5.29	1.20	1.34
36	b	620	C7Z	C24-C25	-5.29	1.42	1.51
31	c	516	BCR	C11-C12	-5.28	1.21	1.34
31	c	515	BCR	C24-C23	5.27	1.49	1.33
31	C	517	BCR	C11-C12	-5.27	1.21	1.34
51	g1	623	NEX	C28-C29	-5.26	1.34	1.45
51	g1	623	NEX	C7-C8	5.26	1.40	1.32
51	S1	623	NEX	C28-C29	-5.26	1.34	1.45
31	B	618	BCR	C11-C12	-5.20	1.21	1.34
31	C1	517	BCR	C11-C12	-5.20	1.21	1.34
31	A1	411	BCR	C11-C12	-5.19	1.21	1.34
51	y	623	NEX	C28-C29	-5.18	1.34	1.45
31	c	517	BCR	C11-C12	-5.18	1.21	1.34
53	r	626	ERG	C13-C14	-5.17	1.47	1.56
51	r	622	NEX	C28-C29	-5.17	1.34	1.45
31	C	516	BCR	C11-C12	-5.16	1.21	1.34
31	b1	619	BCR	C11-C12	-5.16	1.21	1.34
45	h1	101	RRX	C2-C1	5.16	1.66	1.54
53	r1	626	ERG	C1-C2	5.15	1.64	1.53
45	h1	101	RRX	C1-C6	-5.14	1.46	1.53
51	N	623	NEX	C7-C8	5.13	1.40	1.32
31	c1	514	BCR	C11-C12	-5.13	1.21	1.34
51	R1	622	NEX	C28-C29	-5.13	1.34	1.45
51	y	623	NEX	C7-C8	5.12	1.40	1.32
51	G	623	NEX	C28-C29	-5.10	1.35	1.45
45	h1	101	RRX	C30-C25	-5.10	1.46	1.53
51	r1	622	NEX	C28-C29	-5.10	1.35	1.45
31	c1	517	BCR	C11-C12	-5.09	1.21	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	S	623	NEX	C28-C29	-5.08	1.35	1.45
53	R	626	ERG	C13-C14	-5.07	1.47	1.56
53	r	626	ERG	C12-C11	-5.06	1.42	1.53
31	b	618	BCR	C11-C12	-5.06	1.21	1.34
45	H	101	RRX	C2-C1	5.06	1.65	1.54
51	N1	623	NEX	C7-C8	5.04	1.40	1.32
51	N1	623	NEX	C28-C29	-5.04	1.35	1.45
45	h1	101	RRX	C19-C18	5.02	1.56	1.45
45	H1	101	RRX	C30-C25	-5.01	1.46	1.53
31	c1	516	BCR	C11-C12	-5.01	1.21	1.34
31	B1	619	BCR	C11-C12	-5.00	1.21	1.34
51	Y1	623	NEX	C28-C29	-5.00	1.35	1.45
45	H1	101	RRX	C2-C1	4.99	1.65	1.54
31	D	404	BCR	C11-C12	-4.98	1.21	1.34
31	C1	516	BCR	C11-C12	-4.98	1.21	1.34
31	d	404	BCR	C11-C12	-4.97	1.21	1.34
45	h1	101	RRX	C8-C9	4.97	1.56	1.45
51	n	623	NEX	C7-C8	4.97	1.40	1.32
36	B1	620	C7Z	C32-C33	4.96	1.56	1.45
51	G1	623	NEX	C28-C29	-4.96	1.35	1.45
36	b1	620	C7Z	C32-C33	4.96	1.56	1.45
51	s1	623	NEX	C1-C6	-4.92	1.46	1.54
53	r1	626	ERG	C12-C11	-4.91	1.42	1.53
53	r1	626	ERG	C7-C6	-4.89	1.27	1.41
53	R	626	ERG	C7-C6	-4.88	1.27	1.41
53	R1	626	ERG	C7-C6	-4.87	1.27	1.41
45	h	101	RRX	C2-C1	4.86	1.65	1.54
31	c	515	BCR	C16-C17	-4.86	1.28	1.43
31	b1	618	BCR	C11-C12	-4.86	1.22	1.34
31	d1	404	BCR	C11-C12	-4.85	1.22	1.34
45	h	101	RRX	C27-C26	-4.85	1.43	1.51
53	R	626	ERG	C12-C11	-4.84	1.43	1.53
36	B	620	C7Z	C28-C29	4.83	1.56	1.45
45	H1	101	RRX	C8-C9	4.82	1.56	1.45
45	H	101	RRX	C19-C18	4.78	1.56	1.45
45	h	101	RRX	C8-C9	4.75	1.56	1.45
53	r	626	ERG	C7-C6	-4.75	1.27	1.41
36	B	620	C7Z	C4-C5	-4.75	1.43	1.51
51	n1	623	NEX	C28-C29	-4.74	1.35	1.45
43	d	405	PL9	C3-C4	-4.73	1.41	1.49
53	R1	626	ERG	C12-C11	-4.73	1.43	1.53
51	s1	623	NEX	C28-C29	-4.72	1.35	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	H	101	RRX	C30-C25	-4.71	1.47	1.53
53	r	626	ERG	C1-C2	4.71	1.63	1.53
31	A	411	BCR	C16-C17	-4.70	1.28	1.43
31	B	619	BCR	C16-C17	-4.67	1.29	1.43
45	h	101	RRX	C19-C18	4.66	1.56	1.45
31	B1	618	BCR	C11-C12	-4.66	1.22	1.34
36	B1	620	C7Z	C31-C30	4.66	1.57	1.43
36	B	620	C7Z	C32-C33	4.64	1.55	1.45
31	C	515	BCR	C16-C17	-4.62	1.29	1.43
36	B1	620	C7Z	C24-C25	-4.61	1.43	1.51
29	C1	508	CLA	MG-ND	-4.61	1.96	2.05
36	B1	620	C7Z	C4-C5	-4.59	1.43	1.51
31	C1	515	BCR	C11-C12	-4.59	1.22	1.34
29	b	609	CLA	MG-ND	-4.57	1.96	2.05
36	b	620	C7Z	C28-C29	4.56	1.55	1.45
45	H	101	RRX	C8-C9	4.55	1.55	1.45
36	b	620	C7Z	C32-C33	4.53	1.55	1.45
51	S1	623	NEX	C7-C8	4.52	1.39	1.32
29	R	603	CLA	MG-ND	-4.52	1.96	2.05
31	a	411	BCR	C16-C17	-4.51	1.29	1.43
29	S1	611	CLA	MG-ND	-4.51	1.96	2.05
31	C	514	BCR	C16-C17	-4.51	1.29	1.43
31	c1	515	BCR	C16-C17	-4.50	1.29	1.43
43	D	405	PL9	C3-C4	-4.50	1.42	1.49
36	B1	620	C7Z	C8-C9	4.49	1.55	1.45
36	b1	620	C7Z	C4-C5	-4.49	1.44	1.51
45	H1	101	RRX	C23-C22	4.48	1.55	1.45
29	Y	610	CLA	C1C-NC	-4.48	1.31	1.37
29	c	505	CLA	MG-ND	-4.47	1.96	2.05
29	r	603	CLA	MG-ND	-4.47	1.96	2.05
53	r	626	ERG	C13-C17	4.47	1.63	1.55
31	A1	411	BCR	C16-C17	-4.47	1.29	1.43
29	b1	611	CLA	MG-ND	-4.46	1.96	2.05
29	C	508	CLA	MG-ND	-4.44	1.97	2.05
31	b	619	BCR	C16-C17	-4.43	1.29	1.43
45	h	101	RRX	C30-C25	-4.43	1.47	1.53
37	c1	518	DGD	O1G-C1A	4.41	1.46	1.33
37	B	623	DGD	O1G-C1A	4.41	1.46	1.33
29	Y1	608	CLA	MG-ND	-4.41	1.97	2.05
31	a1	411	BCR	C16-C17	-4.40	1.29	1.43
29	B1	609	CLA	MG-ND	-4.40	1.97	2.05
29	B1	611	CLA	C1C-NC	-4.40	1.31	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	514	BCR	C16-C17	-4.40	1.29	1.43
43	D	405	PL9	C6-C1	-4.40	1.40	1.48
53	R1	626	ERG	C13-C17	4.39	1.63	1.55
37	b	623	DGD	O1G-C1A	4.39	1.46	1.33
36	b1	620	C7Z	C24-C25	-4.39	1.44	1.51
36	b1	620	C7Z	C31-C30	4.38	1.57	1.43
29	C1	505	CLA	MG-ND	-4.38	1.97	2.05
53	R	626	ERG	C13-C17	4.37	1.63	1.55
37	b1	623	DGD	O1G-C1A	4.37	1.46	1.33
31	c	517	BCR	C16-C17	-4.37	1.29	1.43
31	C1	516	BCR	C16-C17	-4.36	1.29	1.43
29	C	505	CLA	MG-ND	-4.36	1.97	2.05
37	c1	519	DGD	O1G-C1A	4.36	1.46	1.33
45	h1	101	RRX	C23-C22	4.36	1.55	1.45
29	b1	611	CLA	C1C-NC	-4.35	1.31	1.37
37	c	519	DGD	O1G-C1A	4.35	1.46	1.33
31	c	516	BCR	C16-C17	-4.35	1.30	1.43
29	c1	502	CLA	MG-ND	-4.34	1.97	2.05
29	C	506	CLA	MG-ND	-4.34	1.97	2.05
36	b1	620	C7Z	C8-C9	4.34	1.55	1.45
29	G1	612	CLA	MG-ND	-4.33	1.97	2.05
29	c	513	CLA	MG-ND	-4.33	1.97	2.05
29	C1	507	CLA	MG-ND	-4.33	1.97	2.05
45	H1	101	RRX	C12-C13	4.33	1.55	1.45
29	B	604	CLA	MG-ND	-4.33	1.97	2.05
31	C	516	BCR	C16-C17	-4.32	1.30	1.43
29	c	508	CLA	MG-ND	-4.31	1.97	2.05
29	s1	611	CLA	MG-ND	-4.31	1.97	2.05
29	b	604	CLA	MG-ND	-4.31	1.97	2.05
43	d	405	PL9	C6-C1	-4.31	1.40	1.48
29	A	410	CLA	MG-ND	-4.31	1.97	2.05
45	H	101	RRX	C27-C26	-4.30	1.44	1.51
36	B	620	C7Z	C31-C30	4.30	1.56	1.43
37	B1	623	DGD	O1G-C1A	4.30	1.45	1.33
29	B	609	CLA	MG-ND	-4.30	1.97	2.05
45	H1	101	RRX	C3-C4	4.30	1.66	1.52
36	b	620	C7Z	C4-C5	-4.30	1.44	1.51
29	A1	407	CLA	MG-ND	-4.30	1.97	2.05
29	A1	406	CLA	MG-ND	-4.30	1.97	2.05
29	C	507	CLA	MG-ND	-4.29	1.97	2.05
31	D	404	BCR	C16-C17	-4.29	1.30	1.43
29	C	513	CLA	MG-ND	-4.28	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Y1	612	CLA	MG-ND	-4.28	1.97	2.05
29	S1	614	CLA	MG-ND	-4.28	1.97	2.05
29	R1	603	CLA	MG-ND	-4.28	1.97	2.05
29	B	613	CLA	MG-ND	-4.28	1.97	2.05
29	S	602	CLA	MG-ND	-4.27	1.97	2.05
29	s	603	CLA	MG-ND	-4.27	1.97	2.05
36	b	620	C7Z	C31-C30	4.27	1.56	1.43
29	B	612	CLA	MG-ND	-4.26	1.97	2.05
29	B1	617	CLA	MG-ND	-4.26	1.97	2.05
29	c	506	CLA	MG-ND	-4.26	1.97	2.05
31	B	618	BCR	C16-C17	-4.26	1.30	1.43
29	b1	608	CLA	MG-ND	-4.25	1.97	2.05
29	C1	509	CLA	MG-ND	-4.25	1.97	2.05
29	c	507	CLA	MG-ND	-4.25	1.97	2.05
29	b1	612	CLA	MG-ND	-4.25	1.97	2.05
45	h1	101	RRX	C27-C26	-4.25	1.44	1.51
31	d	404	BCR	C16-C17	-4.24	1.30	1.43
31	D1	404	BCR	C16-C17	-4.23	1.30	1.43
29	B	605	CLA	MG-ND	-4.23	1.97	2.05
29	B	611	CLA	MG-ND	-4.23	1.97	2.05
29	s1	612	CLA	MG-ND	-4.23	1.97	2.05
29	r1	610	CLA	MG-ND	-4.22	1.97	2.05
31	b1	619	BCR	C16-C17	-4.22	1.30	1.43
29	g	614	CLA	MG-ND	-4.22	1.97	2.05
29	a1	410	CLA	MG-ND	-4.22	1.97	2.05
53	r1	626	ERG	C16-C15	4.22	1.65	1.54
37	C1	518	DGD	O1G-C1A	4.21	1.45	1.33
45	H	101	RRX	C3-C4	4.21	1.65	1.52
45	H	101	RRX	C12-C13	4.21	1.55	1.45
37	C	519	DGD	O1G-C1A	4.21	1.45	1.33
31	C1	515	BCR	C16-C17	-4.21	1.30	1.43
51	G	623	NEX	C7-C8	4.21	1.39	1.32
37	c1	520	DGD	O1G-C1A	4.21	1.45	1.33
29	D1	402	CLA	MG-ND	-4.21	1.97	2.05
29	c1	510	CLA	MG-ND	-4.21	1.97	2.05
36	B1	620	C7Z	C11-C10	4.21	1.56	1.43
31	c1	514	BCR	C16-C17	-4.21	1.30	1.43
31	C	517	BCR	C16-C17	-4.20	1.30	1.43
29	c1	513	CLA	MG-ND	-4.20	1.97	2.05
29	y1	614	CLA	MG-ND	-4.20	1.97	2.05
36	b1	620	C7Z	C11-C10	4.20	1.56	1.43
29	b	603	CLA	MG-ND	-4.20	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c1	501	CLA	MG-ND	-4.20	1.97	2.05
43	d1	405	PL9	C7-C3	-4.19	1.47	1.51
37	C	518	DGD	O1G-C1A	4.19	1.45	1.33
45	h1	101	RRX	C3-C4	4.18	1.65	1.52
37	C1	520	DGD	O1G-C1A	4.18	1.45	1.33
29	s1	610	CLA	MG-ND	-4.18	1.97	2.05
29	c	509	CLA	MG-ND	-4.18	1.97	2.05
29	R1	610	CLA	MG-ND	-4.18	1.97	2.05
29	y1	610	CLA	MG-ND	-4.18	1.97	2.05
29	S1	603	CLA	MG-ND	-4.18	1.97	2.05
45	h	101	RRX	C3-C4	4.18	1.65	1.52
29	S1	605	CLA	MG-ND	-4.18	1.97	2.05
29	C1	502	CLA	MG-ND	-4.18	1.97	2.05
29	Y1	613	CLA	MG-ND	-4.18	1.97	2.05
45	H1	101	RRX	C27-C26	-4.17	1.44	1.51
29	B	607	CLA	MG-ND	-4.17	1.97	2.05
29	y1	611	CLA	MG-ND	-4.17	1.97	2.05
31	b	618	BCR	C16-C17	-4.16	1.30	1.43
29	A	406	CLA	MG-ND	-4.16	1.97	2.05
29	g	603	CLA	MG-ND	-4.16	1.97	2.05
29	B1	604	CLA	MG-ND	-4.16	1.97	2.05
29	a1	407	CLA	MG-ND	-4.15	1.97	2.05
45	h1	101	RRX	C12-C13	4.15	1.54	1.45
29	c1	508	CLA	MG-ND	-4.15	1.97	2.05
29	s	604	CLA	MG-ND	-4.14	1.97	2.05
31	B1	619	BCR	C16-C17	-4.14	1.30	1.43
29	b	607	CLA	MG-ND	-4.14	1.97	2.05
29	c	512	CLA	MG-ND	-4.14	1.97	2.05
29	B1	611	CLA	MG-ND	-4.14	1.97	2.05
29	b1	613	CLA	MG-ND	-4.14	1.97	2.05
29	N1	604	CLA	MG-ND	-4.13	1.97	2.05
29	S	603	CLA	MG-ND	-4.13	1.97	2.05
29	d	402	CLA	MG-ND	-4.13	1.97	2.05
29	B1	614	CLA	MG-ND	-4.13	1.97	2.05
29	b1	614	CLA	MG-ND	-4.13	1.97	2.05
29	g1	613	CLA	MG-ND	-4.13	1.97	2.05
29	g	610	CLA	MG-ND	-4.13	1.97	2.05
29	D1	403	CLA	MG-ND	-4.12	1.97	2.05
29	D	402	CLA	MG-ND	-4.12	1.97	2.05
29	C1	501	CLA	MG-ND	-4.12	1.97	2.05
29	G1	604	CLA	MG-ND	-4.12	1.97	2.05
45	H1	101	RRX	C20-C21	4.12	1.56	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	c	520	DGD	O1G-C1A	4.12	1.45	1.33
29	G1	602	CLA	MG-ND	-4.12	1.97	2.05
29	B	617	CLA	C1C-NC	-4.12	1.31	1.37
37	c	518	DGD	O1G-C1A	4.12	1.45	1.33
29	B1	613	CLA	MG-ND	-4.12	1.97	2.05
29	a	405	CLA	MG-ND	-4.12	1.97	2.05
29	c1	512	CLA	MG-ND	-4.12	1.97	2.05
37	C	520	DGD	O1G-C1A	4.12	1.45	1.33
29	C	509	CLA	MG-ND	-4.11	1.97	2.05
29	G1	611	CLA	MG-ND	-4.11	1.97	2.05
29	b	612	CLA	C1C-NC	-4.11	1.31	1.37
29	C	506	CLA	C1C-NC	-4.11	1.31	1.37
29	r	602	CLA	MG-ND	-4.11	1.97	2.05
29	C1	503	CLA	MG-ND	-4.11	1.97	2.05
29	B	603	CLA	MG-ND	-4.10	1.97	2.05
29	B	610	CLA	MG-ND	-4.10	1.97	2.05
53	R1	626	ERG	C16-C15	4.10	1.65	1.54
44	f1	101	HEM	C3C-CAC	4.10	1.56	1.47
29	B1	606	CLA	MG-ND	-4.10	1.97	2.05
29	Y	614	CLA	MG-ND	-4.10	1.97	2.05
29	N	604	CLA	MG-ND	-4.10	1.97	2.05
29	b1	617	CLA	MG-ND	-4.10	1.97	2.05
29	C	512	CLA	MG-ND	-4.10	1.97	2.05
29	d1	402	CLA	MG-ND	-4.10	1.97	2.05
29	S1	604	CLA	MG-ND	-4.10	1.97	2.05
29	G1	610	CLA	MG-ND	-4.09	1.97	2.05
53	r	626	ERG	C16-C15	4.09	1.65	1.54
29	n	602	CLA	MG-ND	-4.09	1.97	2.05
31	C1	517	BCR	C16-C17	-4.09	1.30	1.43
29	s	609	CLA	MG-ND	-4.09	1.97	2.05
31	d1	404	BCR	C16-C17	-4.09	1.30	1.43
29	C1	506	CLA	MG-ND	-4.08	1.97	2.05
29	B1	610	CLA	MG-ND	-4.08	1.97	2.05
29	s	611	CLA	MG-ND	-4.08	1.97	2.05
29	g1	603	CLA	MG-ND	-4.08	1.97	2.05
36	B	620	C7Z	C11-C10	4.08	1.56	1.43
29	S	611	CLA	MG-ND	-4.08	1.97	2.05
29	N1	613	CLA	MG-ND	-4.08	1.97	2.05
29	C	510	CLA	MG-ND	-4.08	1.97	2.05
29	Y1	602	CLA	MG-ND	-4.07	1.97	2.05
29	R1	602	CLA	MG-ND	-4.07	1.97	2.05
29	s	602	CLA	MG-ND	-4.07	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	N	613	CLA	MG-ND	-4.06	1.97	2.05
29	R	610	CLA	MG-ND	-4.06	1.97	2.05
29	y	608	CLA	MG-ND	-4.06	1.97	2.05
31	C1	514	BCR	C16-C17	-4.06	1.30	1.43
29	R	609	CLA	MG-ND	-4.06	1.97	2.05
29	B	606	CLA	MG-ND	-4.05	1.97	2.05
29	G	604	CLA	MG-ND	-4.05	1.97	2.05
29	n	613	CLA	MG-ND	-4.05	1.97	2.05
29	B1	615	CLA	MG-ND	-4.05	1.97	2.05
29	b1	615	CLA	MG-ND	-4.05	1.97	2.05
29	s1	617	CLA	MG-ND	-4.05	1.97	2.05
29	y	613	CLA	MG-ND	-4.05	1.97	2.05
29	C	508	CLA	C1C-NC	-4.05	1.31	1.37
29	Y	608	CLA	MG-ND	-4.04	1.97	2.05
37	C1	519	DGD	O1G-C1A	4.04	1.45	1.33
29	N	614	CLA	MG-ND	-4.04	1.97	2.05
45	h	101	RRX	C23-C22	4.03	1.54	1.45
29	g1	602	CLA	MG-ND	-4.03	1.97	2.05
29	c	502	CLA	MG-ND	-4.03	1.97	2.05
29	R	602	CLA	MG-ND	-4.03	1.97	2.05
29	B1	608	CLA	MG-ND	-4.03	1.97	2.05
41	c1	527	LMK	O2-C4	4.03	1.43	1.30
29	y1	603	CLA	MG-ND	-4.03	1.97	2.05
29	B	615	CLA	MG-ND	-4.03	1.97	2.05
29	S	610	CLA	MG-ND	-4.03	1.97	2.05
36	b1	620	C7Z	C15-C14	4.03	1.55	1.43
29	N1	614	CLA	MG-ND	-4.02	1.97	2.05
29	n	604	CLA	MG-ND	-4.02	1.97	2.05
29	r1	609	CLA	MG-ND	-4.02	1.97	2.05
29	a	410	CLA	MG-ND	-4.02	1.97	2.05
29	C1	512	CLA	MG-ND	-4.02	1.97	2.05
29	y	611	CLA	MG-ND	-4.02	1.97	2.05
29	n1	611	CLA	MG-ND	-4.02	1.97	2.05
29	g	612	CLA	MG-ND	-4.02	1.97	2.05
29	G	610	CLA	MG-ND	-4.02	1.97	2.05
29	g1	614	CLA	MG-ND	-4.02	1.97	2.05
41	C	527	LMK	O2-C4	4.02	1.43	1.30
48	G	606	CHL	C3B-C2B	-4.01	1.34	1.40
29	d	403	CLA	MG-ND	-4.01	1.97	2.05
29	b1	607	CLA	MG-ND	-4.01	1.97	2.05
29	a	406	CLA	MG-ND	-4.01	1.97	2.05
29	c	503	CLA	MG-ND	-4.01	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	H1	101	RRX	C15-C14	4.01	1.55	1.43
29	b	617	CLA	MG-ND	-4.01	1.97	2.05
29	C	502	CLA	MG-ND	-4.01	1.97	2.05
29	b1	609	CLA	MG-ND	-4.01	1.97	2.05
29	Y	612	CLA	MG-ND	-4.01	1.97	2.05
29	C1	510	CLA	MG-ND	-4.00	1.97	2.05
29	b	611	CLA	C1C-NC	-4.00	1.31	1.37
41	C1	527	LMK	O2-C4	4.00	1.43	1.30
29	c	510	CLA	MG-ND	-4.00	1.97	2.05
29	N1	612	CLA	MG-ND	-4.00	1.97	2.05
29	S	614	CLA	MG-ND	-4.00	1.97	2.05
29	B1	612	CLA	MG-ND	-4.00	1.97	2.05
29	a1	406	CLA	MG-ND	-4.00	1.97	2.05
29	y1	612	CLA	MG-ND	-4.00	1.97	2.05
29	S	612	CLA	MG-ND	-3.99	1.97	2.05
29	s	610	CLA	MG-ND	-3.99	1.97	2.05
29	S1	617	CLA	MG-ND	-3.99	1.97	2.05
29	b1	606	CLA	MG-ND	-3.99	1.97	2.05
29	c1	509	CLA	MG-ND	-3.99	1.97	2.05
29	b	606	CLA	C1C-NC	-3.99	1.31	1.37
29	r	612	CLA	MG-ND	-3.99	1.97	2.05
29	A	405	CLA	MG-ND	-3.99	1.97	2.05
29	b	612	CLA	MG-ND	-3.99	1.97	2.05
29	C1	504	CLA	MG-ND	-3.99	1.97	2.05
29	Y1	610	CLA	MG-ND	-3.99	1.97	2.05
29	b	611	CLA	MG-ND	-3.99	1.97	2.05
29	c	511	CLA	MG-ND	-3.99	1.97	2.05
29	s	612	CLA	MG-ND	-3.98	1.97	2.05
29	Y	613	CLA	MG-ND	-3.98	1.97	2.05
53	r1	626	ERG	C13-C17	3.98	1.62	1.55
36	b	620	C7Z	C8-C9	3.97	1.54	1.45
29	G1	603	CLA	MG-ND	-3.97	1.97	2.05
29	R1	604	CLA	MG-ND	-3.97	1.97	2.05
29	b1	603	CLA	MG-ND	-3.97	1.97	2.05
29	b1	616	CLA	MG-ND	-3.97	1.97	2.05
29	A1	410	CLA	MG-ND	-3.97	1.97	2.05
29	B	617	CLA	MG-ND	-3.97	1.97	2.05
29	y	612	CLA	MG-ND	-3.96	1.97	2.05
29	g	602	CLA	MG-ND	-3.96	1.97	2.05
29	r	610	CLA	MG-ND	-3.96	1.97	2.05
29	S1	602	CLA	MG-ND	-3.96	1.97	2.05
29	b1	604	CLA	MG-ND	-3.96	1.97	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	505	CLA	C1C-NC	-3.96	1.31	1.37
29	Y1	604	CLA	MG-ND	-3.96	1.97	2.05
29	R	604	CLA	MG-ND	-3.96	1.97	2.05
29	B1	602	CLA	MG-ND	-3.96	1.97	2.05
29	N1	602	CLA	MG-ND	-3.96	1.97	2.05
29	S	613	CLA	MG-ND	-3.95	1.98	2.05
29	Y1	614	CLA	MG-ND	-3.95	1.98	2.05
29	b	616	CLA	MG-ND	-3.95	1.98	2.05
41	c	527	LMK	O2-C4	3.95	1.43	1.30
29	S1	612	CLA	MG-ND	-3.95	1.98	2.05
29	r1	604	CLA	MG-ND	-3.95	1.98	2.05
29	B	612	CLA	C1C-NC	-3.95	1.31	1.37
45	H	101	RRX	C23-C22	3.94	1.54	1.45
29	S	605	CLA	MG-ND	-3.94	1.98	2.05
29	b	606	CLA	MG-ND	-3.94	1.98	2.05
36	b1	620	C7Z	C22-C21	3.94	1.67	1.54
31	c1	517	BCR	C16-C17	-3.94	1.31	1.43
44	F1	101	HEM	C3C-CAC	3.93	1.55	1.47
31	b1	618	BCR	C16-C17	-3.93	1.31	1.43
29	G	613	CLA	MG-ND	-3.93	1.98	2.05
29	Y1	611	CLA	MG-ND	-3.93	1.98	2.05
29	b	613	CLA	MG-ND	-3.93	1.98	2.05
29	c1	504	CLA	MG-ND	-3.93	1.98	2.05
29	A1	405	CLA	MG-ND	-3.93	1.98	2.05
29	y	602	CLA	MG-ND	-3.93	1.98	2.05
29	C1	513	CLA	MG-ND	-3.93	1.98	2.05
29	a	407	CLA	MG-ND	-3.93	1.98	2.05
29	R	608	CLA	MG-ND	-3.93	1.98	2.05
29	S1	610	CLA	MG-ND	-3.92	1.98	2.05
29	c	502	CLA	C1C-NC	-3.92	1.31	1.37
29	s	617	CLA	MG-ND	-3.92	1.98	2.05
29	A	410	CLA	C1C-NC	-3.92	1.31	1.37
29	b1	610	CLA	MG-ND	-3.92	1.98	2.05
29	y	604	CLA	MG-ND	-3.92	1.98	2.05
29	B	611	CLA	C1C-NC	-3.92	1.32	1.37
29	B1	603	CLA	MG-ND	-3.92	1.98	2.05
29	s1	614	CLA	MG-ND	-3.92	1.98	2.05
29	N	602	CLA	MG-ND	-3.92	1.98	2.05
29	Y	602	CLA	MG-ND	-3.92	1.98	2.05
29	n1	603	CLA	MG-ND	-3.92	1.98	2.05
29	n1	614	CLA	MG-ND	-3.91	1.98	2.05
29	s1	605	CLA	MG-ND	-3.91	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	N1	603	CLA	MG-ND	-3.91	1.98	2.05
29	N	612	CLA	MG-ND	-3.91	1.98	2.05
29	s	605	CLA	MG-ND	-3.91	1.98	2.05
29	c	508	CLA	C1C-NC	-3.91	1.32	1.37
53	R	626	ERG	C16-C15	3.91	1.64	1.54
29	S	609	CLA	MG-ND	-3.91	1.98	2.05
29	n1	610	CLA	MG-ND	-3.91	1.98	2.05
29	r1	602	CLA	MG-ND	-3.91	1.98	2.05
36	B1	620	C7Z	C15-C14	3.90	1.55	1.43
29	G1	602	CLA	C1C-NC	-3.90	1.32	1.37
29	y	614	CLA	MG-ND	-3.90	1.98	2.05
29	G1	613	CLA	MG-ND	-3.90	1.98	2.05
29	c1	506	CLA	MG-ND	-3.90	1.98	2.05
29	n1	604	CLA	MG-ND	-3.90	1.98	2.05
29	b	605	CLA	MG-ND	-3.90	1.98	2.05
29	c1	507	CLA	MG-ND	-3.90	1.98	2.05
29	Y1	603	CLA	MG-ND	-3.90	1.98	2.05
29	r	609	CLA	MG-ND	-3.90	1.98	2.05
29	R	610	CLA	C1C-NC	-3.89	1.32	1.37
29	B1	605	CLA	MG-ND	-3.89	1.98	2.05
48	N	606	CHL	C3B-C2B	-3.89	1.35	1.40
29	y1	608	CLA	MG-ND	-3.89	1.98	2.05
29	n	612	CLA	MG-ND	-3.89	1.98	2.05
29	Y	610	CLA	MG-ND	-3.89	1.98	2.05
29	B	608	CLA	MG-ND	-3.89	1.98	2.05
29	G	602	CLA	MG-ND	-3.89	1.98	2.05
29	s	614	CLA	MG-ND	-3.89	1.98	2.05
29	a1	405	CLA	MG-ND	-3.88	1.98	2.05
29	c1	503	CLA	MG-ND	-3.88	1.98	2.05
36	b	620	C7Z	C11-C10	3.88	1.55	1.43
29	Y	604	CLA	MG-ND	-3.88	1.98	2.05
29	N1	610	CLA	MG-ND	-3.88	1.98	2.05
29	b	602	CLA	MG-ND	-3.88	1.98	2.05
29	d1	403	CLA	MG-ND	-3.88	1.98	2.05
29	B1	617	CLA	C1C-NC	-3.88	1.32	1.37
29	C	501	CLA	MG-ND	-3.87	1.98	2.05
29	N	611	CLA	MG-ND	-3.87	1.98	2.05
29	n	614	CLA	MG-ND	-3.87	1.98	2.05
29	s1	604	CLA	MG-ND	-3.87	1.98	2.05
36	B1	620	C7Z	C22-C21	3.87	1.66	1.54
45	h1	101	RRX	C20-C21	3.87	1.55	1.43
29	n	610	CLA	MG-ND	-3.87	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	614	CLA	MG-ND	-3.86	1.98	2.05
29	N	610	CLA	MG-ND	-3.86	1.98	2.05
45	h	101	RRX	C12-C13	3.86	1.54	1.45
36	b	620	C7Z	C22-C21	3.86	1.66	1.54
29	C1	502	CLA	C1C-NC	-3.86	1.32	1.37
36	B	620	C7Z	C8-C9	3.86	1.54	1.45
29	y1	602	CLA	MG-ND	-3.85	1.98	2.05
31	c1	516	BCR	C16-C17	-3.85	1.31	1.43
29	y1	604	CLA	MG-ND	-3.85	1.98	2.05
29	b	608	CLA	MG-ND	-3.85	1.98	2.05
29	R1	609	CLA	MG-ND	-3.85	1.98	2.05
29	N1	611	CLA	MG-ND	-3.85	1.98	2.05
29	B	614	CLA	MG-ND	-3.85	1.98	2.05
29	n	603	CLA	MG-ND	-3.84	1.98	2.05
29	C	503	CLA	MG-ND	-3.84	1.98	2.05
29	B	605	CLA	C1C-NC	-3.84	1.32	1.37
29	C1	504	CLA	C1C-NC	-3.84	1.32	1.37
29	g	611	CLA	MG-ND	-3.84	1.98	2.05
29	B1	607	CLA	MG-ND	-3.83	1.98	2.05
29	B1	606	CLA	C1C-NC	-3.83	1.32	1.37
29	b	615	CLA	MG-ND	-3.83	1.98	2.05
29	C	502	CLA	C1C-NC	-3.83	1.32	1.37
48	S	601	CHL	C3B-C2B	-3.83	1.35	1.40
29	n1	612	CLA	MG-ND	-3.83	1.98	2.05
29	R	612	CLA	MG-ND	-3.82	1.98	2.05
29	b	610	CLA	MG-ND	-3.82	1.98	2.05
29	g1	611	CLA	MG-ND	-3.82	1.98	2.05
29	c	501	CLA	MG-ND	-3.82	1.98	2.05
36	B1	620	C7Z	C27-C26	3.82	1.58	1.45
29	b	605	CLA	C1C-NC	-3.82	1.32	1.37
29	Y	603	CLA	MG-ND	-3.81	1.98	2.05
29	b1	616	CLA	C1C-NC	-3.81	1.32	1.37
29	S1	609	CLA	MG-ND	-3.81	1.98	2.05
29	n1	613	CLA	MG-ND	-3.81	1.98	2.05
29	r	604	CLA	MG-ND	-3.80	1.98	2.05
29	A	407	CLA	MG-ND	-3.80	1.98	2.05
29	g1	610	CLA	MG-ND	-3.80	1.98	2.05
29	S	613	CLA	C1C-NC	-3.80	1.32	1.37
29	b1	613	CLA	C1C-NC	-3.80	1.32	1.37
29	n	611	CLA	MG-ND	-3.80	1.98	2.05
29	G	611	CLA	MG-ND	-3.79	1.98	2.05
29	S1	610	CLA	C1C-NC	-3.79	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Y	602	CLA	C1C-NC	-3.79	1.32	1.37
29	S	604	CLA	MG-ND	-3.79	1.98	2.05
29	C	504	CLA	MG-ND	-3.79	1.98	2.05
31	B1	618	BCR	C16-C17	-3.78	1.31	1.43
29	C1	511	CLA	MG-ND	-3.78	1.98	2.05
29	y1	613	CLA	MG-ND	-3.78	1.98	2.05
36	b1	620	C7Z	C35-C34	3.78	1.55	1.43
29	c1	511	CLA	MG-ND	-3.78	1.98	2.05
29	B	602	CLA	MG-ND	-3.78	1.98	2.05
48	s	601	CHL	C3B-C2B	-3.77	1.35	1.40
29	A	406	CLA	C1C-NC	-3.77	1.32	1.37
45	H	101	RRX	C20-C21	3.77	1.55	1.43
29	g	604	CLA	MG-ND	-3.77	1.98	2.05
36	B1	620	C7Z	C35-C34	3.77	1.55	1.43
29	R1	608	CLA	MG-ND	-3.77	1.98	2.05
29	S	617	CLA	MG-ND	-3.77	1.98	2.05
29	S1	613	CLA	MG-ND	-3.77	1.98	2.05
29	s1	603	CLA	MG-ND	-3.77	1.98	2.05
29	A	405	CLA	C1C-NC	-3.77	1.32	1.37
47	i	101	4RF	O18-C16	3.77	1.44	1.33
29	G1	612	CLA	C1C-NC	-3.76	1.32	1.37
29	Y	611	CLA	MG-ND	-3.76	1.98	2.05
29	b1	602	CLA	MG-ND	-3.76	1.98	2.05
29	B	616	CLA	MG-ND	-3.76	1.98	2.05
29	g	611	CLA	C1C-NC	-3.75	1.32	1.37
29	a1	410	CLA	C1C-NC	-3.75	1.32	1.37
44	F	101	HEM	C3C-CAC	3.75	1.55	1.47
29	s1	613	CLA	MG-ND	-3.75	1.98	2.05
29	c1	505	CLA	MG-ND	-3.75	1.98	2.05
29	C	504	CLA	C1C-NC	-3.75	1.32	1.37
29	S1	614	CLA	C1C-NC	-3.75	1.32	1.37
29	C	511	CLA	MG-ND	-3.74	1.98	2.05
29	g1	604	CLA	MG-ND	-3.74	1.98	2.05
29	r1	608	CLA	C1C-NC	-3.74	1.32	1.37
29	r	608	CLA	MG-ND	-3.74	1.98	2.05
29	R1	612	CLA	MG-ND	-3.74	1.98	2.05
44	F	101	HEM	C3C-C2C	-3.74	1.35	1.40
29	D	403	CLA	MG-ND	-3.74	1.98	2.05
29	C	509	CLA	C1C-NC	-3.74	1.32	1.37
39	B1	625	DGA	OG2-CB1	3.74	1.44	1.34
29	C	505	CLA	C1C-NC	-3.74	1.32	1.37
29	C	501	CLA	C1C-NC	-3.74	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	g	610	CLA	C1C-NC	-3.74	1.32	1.37
29	r1	603	CLA	MG-ND	-3.74	1.98	2.05
29	G	614	CLA	MG-ND	-3.73	1.98	2.05
29	B1	616	CLA	MG-ND	-3.73	1.98	2.05
29	d1	402	CLA	C1C-NC	-3.73	1.32	1.37
29	A1	406	CLA	C1C-NC	-3.72	1.32	1.37
39	B	625	DGA	OG2-CB1	3.72	1.44	1.34
29	g	613	CLA	MG-ND	-3.72	1.98	2.05
29	A1	407	CLA	C1C-NC	-3.72	1.32	1.37
29	g	612	CLA	C1C-NC	-3.72	1.32	1.37
29	s	613	CLA	MG-ND	-3.72	1.98	2.05
29	N	603	CLA	MG-ND	-3.72	1.98	2.05
29	s1	602	CLA	MG-ND	-3.71	1.98	2.05
29	C1	501	CLA	C1C-NC	-3.71	1.32	1.37
29	r1	612	CLA	MG-ND	-3.71	1.98	2.05
36	B	620	C7Z	C21-C26	-3.71	1.48	1.53
29	A	407	CLA	C1C-NC	-3.70	1.32	1.37
36	B	620	C7Z	C22-C21	3.70	1.66	1.54
29	R	602	CLA	C1C-NC	-3.70	1.32	1.37
29	B	608	CLA	C1C-NC	-3.70	1.32	1.37
29	c	504	CLA	C1C-NC	-3.70	1.32	1.37
36	B	620	C7Z	C27-C26	3.70	1.58	1.45
36	b	620	C7Z	C15-C14	3.70	1.54	1.43
44	f	101	HEM	C3C-C2C	-3.70	1.35	1.40
39	C1	524	DGA	OG2-CB1	3.69	1.44	1.34
29	y	610	CLA	MG-ND	-3.69	1.98	2.05
39	b	625	DGA	OG2-CB1	3.69	1.44	1.34
44	F1	101	HEM	C3C-C2C	-3.68	1.35	1.40
29	y	602	CLA	C1C-NC	-3.68	1.32	1.37
29	G	612	CLA	MG-ND	-3.68	1.98	2.05
29	c1	502	CLA	C1C-NC	-3.68	1.32	1.37
29	G	610	CLA	C1C-NC	-3.68	1.32	1.37
29	C	512	CLA	C1C-NC	-3.68	1.32	1.37
29	b1	617	CLA	C1C-NC	-3.67	1.32	1.37
29	D	402	CLA	C1C-NC	-3.67	1.32	1.37
29	G1	614	CLA	MG-ND	-3.67	1.98	2.05
29	R	608	CLA	C1C-NC	-3.67	1.32	1.37
29	S	614	CLA	C1C-NC	-3.67	1.32	1.37
29	y	603	CLA	MG-ND	-3.67	1.98	2.05
29	G	603	CLA	MG-ND	-3.66	1.98	2.05
45	H	101	RRX	C15-C14	3.66	1.54	1.43
29	g1	612	CLA	MG-ND	-3.65	1.98	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	504	CLA	MG-ND	-3.65	1.98	2.05
29	b1	604	CLA	C1C-NC	-3.64	1.32	1.37
29	b1	612	CLA	C1C-NC	-3.64	1.32	1.37
29	B	613	CLA	C1C-NC	-3.64	1.32	1.37
29	G1	603	CLA	C1C-NC	-3.64	1.32	1.37
36	B	620	C7Z	C15-C14	3.64	1.54	1.43
45	h1	101	RRX	C15-C14	3.64	1.54	1.43
29	R	609	CLA	C1C-NC	-3.63	1.32	1.37
29	y1	610	CLA	C1C-NC	-3.63	1.32	1.37
29	b	604	CLA	C1C-NC	-3.63	1.32	1.37
44	f	101	HEM	C3C-CAC	3.63	1.55	1.47
29	n1	602	CLA	MG-ND	-3.63	1.98	2.05
29	G1	604	CLA	C1C-NC	-3.63	1.32	1.37
29	B	610	CLA	C1C-NC	-3.63	1.32	1.37
36	b1	620	C7Z	C27-C26	3.63	1.58	1.45
29	a1	407	CLA	C1C-NC	-3.62	1.32	1.37
29	A1	405	CLA	C1C-NC	-3.62	1.32	1.37
39	b1	625	DGA	OG2-CB1	3.62	1.44	1.34
29	S1	609	CLA	C1C-NC	-3.62	1.32	1.37
47	K	101	4RF	O18-C16	3.62	1.43	1.33
29	A1	410	CLA	C1C-NC	-3.62	1.32	1.37
29	b	617	CLA	C1C-NC	-3.62	1.32	1.37
29	r1	608	CLA	MG-ND	-3.62	1.98	2.05
29	n1	611	CLA	C1C-NC	-3.62	1.32	1.37
29	S1	613	CLA	C1C-NC	-3.61	1.32	1.37
29	Y1	604	CLA	C1C-NC	-3.61	1.32	1.37
29	s1	610	CLA	C1C-NC	-3.61	1.32	1.37
39	j1	101	DGA	OG1-CA1	3.61	1.43	1.33
29	R1	610	CLA	C1C-NC	-3.61	1.32	1.37
29	N	610	CLA	C1C-NC	-3.61	1.32	1.37
45	h	101	RRX	C20-C21	3.61	1.54	1.43
29	G1	610	CLA	C1C-NC	-3.61	1.32	1.37
29	b	613	CLA	C1C-NC	-3.61	1.32	1.37
29	y	610	CLA	C1C-NC	-3.61	1.32	1.37
47	I1	102	4RF	O18-C16	3.60	1.43	1.33
29	S	610	CLA	C1C-NC	-3.60	1.32	1.37
29	C1	510	CLA	C1C-NC	-3.60	1.32	1.37
36	b	620	C7Z	C35-C34	3.60	1.54	1.43
29	c	507	CLA	C1C-NC	-3.59	1.32	1.37
29	s1	609	CLA	MG-ND	-3.59	1.98	2.05
29	S	604	CLA	C1C-NC	-3.59	1.32	1.37
29	b	603	CLA	C1C-NC	-3.59	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	H1	101	RRX	C11-C10	3.59	1.54	1.43
29	d	402	CLA	C1C-NC	-3.59	1.32	1.37
29	c1	504	CLA	C1C-NC	-3.58	1.32	1.37
29	a1	405	CLA	C1C-NC	-3.58	1.32	1.37
29	c	506	CLA	C1C-NC	-3.58	1.32	1.37
29	C	507	CLA	C1C-NC	-3.58	1.32	1.37
29	B	604	CLA	C1C-NC	-3.58	1.32	1.37
47	k	101	4RF	O18-C16	3.58	1.43	1.33
29	S	612	CLA	C1C-NC	-3.58	1.32	1.37
29	n1	604	CLA	C1C-NC	-3.58	1.32	1.37
29	y	613	CLA	C1C-NC	-3.57	1.32	1.37
29	B	606	CLA	C1C-NC	-3.57	1.32	1.37
29	S1	612	CLA	C1C-NC	-3.57	1.32	1.37
29	B	615	CLA	C1C-NC	-3.56	1.32	1.37
29	Y1	614	CLA	C1C-NC	-3.56	1.32	1.37
29	C	506	CLA	C3B-C2B	-3.56	1.35	1.40
29	N	613	CLA	C1C-NC	-3.56	1.32	1.37
47	I	102	4RF	O18-C16	3.56	1.43	1.33
39	J	101	DGA	OG2-CB1	3.56	1.44	1.34
29	C	503	CLA	C1C-NC	-3.56	1.32	1.37
29	G	604	CLA	C1C-NC	-3.55	1.32	1.37
29	r	609	CLA	C1C-NC	-3.55	1.32	1.37
29	n1	610	CLA	C1C-NC	-3.55	1.32	1.37
29	s1	612	CLA	C1C-NC	-3.55	1.32	1.37
29	a	407	CLA	C1C-NC	-3.54	1.32	1.37
29	B	616	CLA	C1C-NC	-3.54	1.32	1.37
29	c	503	CLA	C1C-NC	-3.54	1.32	1.37
29	n	604	CLA	C1C-NC	-3.54	1.32	1.37
29	C1	506	CLA	C1C-NC	-3.53	1.32	1.37
29	C1	511	CLA	C1C-NC	-3.53	1.32	1.37
29	N	602	CLA	C1C-NC	-3.53	1.32	1.37
29	Y1	613	CLA	C1C-NC	-3.53	1.32	1.37
29	N1	604	CLA	C1C-NC	-3.53	1.32	1.37
36	b1	620	C7Z	C38-C25	3.52	1.56	1.50
29	s	613	CLA	C1C-NC	-3.52	1.32	1.37
29	B1	614	CLA	C1C-NC	-3.52	1.32	1.37
29	N1	613	CLA	C1C-NC	-3.52	1.32	1.37
29	S	611	CLA	C1C-NC	-3.52	1.32	1.37
29	G	602	CLA	C1C-NC	-3.52	1.32	1.37
29	b	608	CLA	C1C-NC	-3.52	1.32	1.37
29	c1	501	CLA	C1C-NC	-3.52	1.32	1.37
36	B1	620	C7Z	C7-C6	3.52	1.57	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	607	CLA	C1C-NC	-3.52	1.32	1.37
29	G	612	CLA	C1C-NC	-3.51	1.32	1.37
29	b	609	CLA	C1C-NC	-3.51	1.32	1.37
29	y1	603	CLA	C1C-NC	-3.51	1.32	1.37
29	y1	604	CLA	C1C-NC	-3.51	1.32	1.37
29	r	603	CLA	C1C-NC	-3.50	1.32	1.37
36	B	620	C7Z	C2-C1	3.50	1.65	1.54
29	S1	604	CLA	C1C-NC	-3.50	1.32	1.37
29	S1	605	CLA	C1C-NC	-3.50	1.32	1.37
29	S	609	CLA	C1C-NC	-3.50	1.32	1.37
48	N1	608	CHL	CBB-CAB	3.50	1.52	1.29
47	K1	101	4RF	O18-C16	3.50	1.43	1.33
29	Y1	602	CLA	C1C-NC	-3.50	1.32	1.37
29	C1	513	CLA	C1C-NC	-3.49	1.32	1.37
29	D1	402	CLA	C1C-NC	-3.49	1.32	1.37
29	c	511	CLA	C1C-NC	-3.49	1.32	1.37
29	c	513	CLA	C1C-NC	-3.49	1.32	1.37
29	a	406	CLA	C1C-NC	-3.49	1.32	1.37
29	Y1	610	CLA	C1C-NC	-3.49	1.32	1.37
29	d	403	CLA	C1C-NC	-3.49	1.32	1.37
29	n1	603	CLA	C1C-NC	-3.49	1.32	1.37
39	j1	101	DGA	OG2-CB1	3.49	1.44	1.34
45	H1	101	RRX	C16-C17	3.49	1.54	1.43
29	a1	406	CLA	C1C-NC	-3.48	1.32	1.37
29	g1	613	CLA	C1C-NC	-3.48	1.32	1.37
48	Y1	601	CHL	CBB-CAB	3.48	1.52	1.29
29	S	605	CLA	C1C-NC	-3.48	1.32	1.37
29	B1	602	CLA	C1C-NC	-3.48	1.32	1.37
29	R	604	CLA	C1C-NC	-3.47	1.32	1.37
29	y	614	CLA	C1C-NC	-3.47	1.32	1.37
29	Y	603	CLA	C1C-NC	-3.47	1.32	1.37
29	b1	610	CLA	C1C-NC	-3.47	1.32	1.37
48	y1	609	CHL	CBB-CAB	3.47	1.52	1.29
29	y	611	CLA	C1C-NC	-3.47	1.32	1.37
29	c1	505	CLA	C1C-NC	-3.47	1.32	1.37
36	B1	620	C7Z	C2-C1	3.47	1.65	1.54
29	c	510	CLA	C1C-NC	-3.47	1.32	1.37
36	b	620	C7Z	C27-C26	3.46	1.57	1.45
29	N	614	CLA	C1C-NC	-3.46	1.32	1.37
29	s	614	CLA	C1C-NC	-3.46	1.32	1.37
29	b	616	CLA	C1C-NC	-3.46	1.32	1.37
39	b1	625	DGA	OG1-CA1	3.46	1.43	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B1	604	CLA	C1C-NC	-3.46	1.32	1.37
29	c	501	CLA	C1C-NC	-3.46	1.32	1.37
29	n	610	CLA	C1C-NC	-3.46	1.32	1.37
29	b1	605	CLA	C1C-NC	-3.46	1.32	1.37
29	N1	603	CLA	C1C-NC	-3.46	1.32	1.37
29	R1	604	CLA	C1C-NC	-3.45	1.32	1.37
29	n	603	CLA	C1C-NC	-3.45	1.32	1.37
29	c1	510	CLA	C1C-NC	-3.45	1.32	1.37
29	r	610	CLA	C1C-NC	-3.45	1.32	1.37
29	y	603	CLA	C1C-NC	-3.45	1.32	1.37
29	R1	603	CLA	C1C-NC	-3.45	1.32	1.37
48	S	606	CHL	C3B-C2B	-3.45	1.35	1.40
48	N1	601	CHL	CBB-CAB	3.45	1.52	1.29
29	s1	613	CLA	CBB-CAB	3.45	1.52	1.29
29	C1	508	CLA	C1C-NC	-3.45	1.32	1.37
39	j	101	DGA	OG2-CB1	3.44	1.44	1.34
48	S1	608	CHL	CBB-CAB	3.44	1.52	1.29
29	B	609	CLA	C1C-NC	-3.44	1.32	1.37
29	B	602	CLA	C1C-NC	-3.44	1.32	1.37
29	G	611	CLA	C1C-NC	-3.44	1.32	1.37
29	N1	602	CLA	CBB-CAB	3.44	1.52	1.29
29	n	611	CLA	C1C-NC	-3.44	1.32	1.37
39	c1	524	DGA	OG2-CB1	3.44	1.44	1.34
29	y	612	CLA	C1C-NC	-3.44	1.32	1.37
29	b	610	CLA	C1C-NC	-3.44	1.32	1.37
36	b1	620	C7Z	C7-C6	3.44	1.57	1.45
45	h	101	RRX	C15-C14	3.44	1.54	1.43
29	S	602	CLA	C1C-NC	-3.43	1.32	1.37
29	b1	607	CLA	C1C-NC	-3.43	1.32	1.37
29	c1	512	CLA	C1C-NC	-3.43	1.32	1.37
29	s1	602	CLA	CBB-CAB	3.43	1.52	1.29
48	Y1	609	CHL	C4B-NB	3.43	1.38	1.35
29	c1	511	CLA	C1C-NC	-3.43	1.32	1.37
48	G1	606	CHL	CBB-CAB	3.43	1.52	1.29
29	Y	613	CLA	C1C-NC	-3.43	1.32	1.37
48	Y1	607	CHL	CBB-CAB	3.43	1.52	1.29
48	n1	609	CHL	CBB-CAB	3.42	1.52	1.29
48	y1	606	CHL	CBB-CAB	3.42	1.52	1.29
39	J1	101	DGA	OG2-CB1	3.42	1.44	1.34
29	c	509	CLA	C1C-NC	-3.42	1.32	1.37
29	y1	602	CLA	CBB-CAB	3.42	1.52	1.29
29	Y	612	CLA	C1C-NC	-3.42	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B1	604	CLA	CBB-CAB	3.42	1.52	1.29
47	i1	101	4RF	O18-C16	3.42	1.43	1.33
29	b1	615	CLA	C1C-NC	-3.42	1.32	1.37
29	C	510	CLA	C1C-NC	-3.42	1.32	1.37
29	R1	608	CLA	C1C-NC	-3.42	1.32	1.37
29	n1	602	CLA	CBB-CAB	3.41	1.51	1.29
29	s	604	CLA	C1C-NC	-3.41	1.32	1.37
29	a	405	CLA	C1C-NC	-3.41	1.32	1.37
29	n1	613	CLA	C1C-NC	-3.41	1.32	1.37
48	G	605	CHL	CBB-CAB	3.41	1.51	1.29
29	N1	611	CLA	C1C-NC	-3.41	1.32	1.37
36	b1	620	C7Z	C2-C1	3.41	1.65	1.54
29	B	614	CLA	CBB-CAB	3.41	1.51	1.29
29	b1	608	CLA	CBB-CAB	3.41	1.51	1.29
29	C1	509	CLA	C1C-NC	-3.41	1.32	1.37
48	g1	609	CHL	CBB-CAB	3.41	1.51	1.29
29	R1	608	CLA	CBB-CAB	3.41	1.51	1.29
29	y1	602	CLA	C1C-NC	-3.41	1.32	1.37
29	B1	611	CLA	CBB-CAB	3.41	1.51	1.29
29	b1	608	CLA	C1C-NC	-3.41	1.32	1.37
29	B1	605	CLA	C1C-NC	-3.41	1.32	1.37
48	g	609	CHL	CBB-CAB	3.40	1.51	1.29
29	B	606	CLA	CBB-CAB	3.40	1.51	1.29
48	G1	609	CHL	CBB-CAB	3.40	1.51	1.29
29	Y	608	CLA	C1C-NC	-3.40	1.32	1.37
29	n	610	CLA	CBB-CAB	3.40	1.51	1.29
29	b	611	CLA	CBB-CAB	3.40	1.51	1.29
48	y	607	CHL	CBB-CAB	3.40	1.51	1.29
29	B1	612	CLA	C1C-NC	-3.40	1.32	1.37
29	c1	507	CLA	C1C-NC	-3.40	1.32	1.37
29	c1	508	CLA	CBB-CAB	3.40	1.51	1.29
48	N1	605	CHL	CBB-CAB	3.40	1.51	1.29
29	n	613	CLA	C1C-NC	-3.40	1.32	1.37
29	c1	501	CLA	CBB-CAB	3.40	1.51	1.29
29	N1	614	CLA	CBB-CAB	3.40	1.51	1.29
29	s	609	CLA	C1C-NC	-3.40	1.32	1.37
36	B	620	C7Z	C35-C34	3.40	1.54	1.43
29	s1	610	CLA	CBB-CAB	3.40	1.51	1.29
48	S1	606	CHL	CBB-CAB	3.40	1.51	1.29
29	b1	617	CLA	CBB-CAB	3.40	1.51	1.29
29	b1	616	CLA	CBB-CAB	3.40	1.51	1.29
29	g	611	CLA	CBB-CAB	3.40	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	R1	612	CLA	CBB-CAB	3.40	1.51	1.29
29	S1	610	CLA	CBB-CAB	3.40	1.51	1.29
48	N1	607	CHL	CBB-CAB	3.40	1.51	1.29
48	g1	601	CHL	CBB-CAB	3.40	1.51	1.29
44	f1	101	HEM	C3C-C2C	-3.40	1.35	1.40
29	R	608	CLA	CBB-CAB	3.40	1.51	1.29
29	b	606	CLA	CBB-CAB	3.39	1.51	1.29
29	g1	611	CLA	CBB-CAB	3.39	1.51	1.29
29	c1	503	CLA	CBB-CAB	3.39	1.51	1.29
29	s1	612	CLA	CBB-CAB	3.39	1.51	1.29
48	g1	607	CHL	CBB-CAB	3.39	1.51	1.29
48	n	608	CHL	CBB-CAB	3.39	1.51	1.29
29	g	602	CLA	CBB-CAB	3.39	1.51	1.29
48	N	609	CHL	CBB-CAB	3.39	1.51	1.29
29	G1	614	CLA	CBB-CAB	3.39	1.51	1.29
29	G	614	CLA	C1C-NC	-3.39	1.32	1.37
29	g	602	CLA	C1C-NC	-3.39	1.32	1.37
29	C1	512	CLA	C1C-NC	-3.39	1.32	1.37
29	R1	612	CLA	C1C-NC	-3.39	1.32	1.37
29	G	614	CLA	CBB-CAB	3.39	1.51	1.29
29	G1	603	CLA	CBB-CAB	3.39	1.51	1.29
29	c1	507	CLA	CBB-CAB	3.39	1.51	1.29
29	y1	613	CLA	C1C-NC	-3.39	1.32	1.37
48	Y1	609	CHL	CBB-CAB	3.39	1.51	1.29
29	c1	503	CLA	C1C-NC	-3.39	1.32	1.37
29	G1	612	CLA	CBB-CAB	3.39	1.51	1.29
29	d1	403	CLA	CBB-CAB	3.39	1.51	1.29
47	k1	101	4RF	O18-C16	3.39	1.43	1.33
29	C1	512	CLA	CBB-CAB	3.39	1.51	1.29
29	b1	604	CLA	CBB-CAB	3.39	1.51	1.29
29	s1	611	CLA	C1C-NC	-3.39	1.32	1.37
29	N1	610	CLA	CBB-CAB	3.39	1.51	1.29
29	C	513	CLA	C1C-NC	-3.39	1.32	1.37
29	N	611	CLA	C1C-NC	-3.39	1.32	1.37
48	N	608	CHL	CBB-CAB	3.39	1.51	1.29
48	s1	606	CHL	CBB-CAB	3.39	1.51	1.29
48	s	601	CHL	C4B-NB	3.39	1.38	1.35
29	B1	608	CLA	C1C-NC	-3.38	1.32	1.37
48	r1	607	CHL	CBB-CAB	3.38	1.51	1.29
29	y1	613	CLA	CBB-CAB	3.38	1.51	1.29
29	N	604	CLA	C1C-NC	-3.38	1.32	1.37
48	Y1	605	CHL	CBB-CAB	3.38	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	r1	609	CLA	CBB-CAB	3.38	1.51	1.29
29	B1	602	CLA	CBB-CAB	3.38	1.51	1.29
29	c1	506	CLA	CBB-CAB	3.38	1.51	1.29
29	n1	612	CLA	CBB-CAB	3.38	1.51	1.29
29	g1	610	CLA	CBB-CAB	3.38	1.51	1.29
29	r	608	CLA	CBB-CAB	3.38	1.51	1.29
29	D	403	CLA	C1C-NC	-3.38	1.32	1.37
29	b1	611	CLA	CBB-CAB	3.38	1.51	1.29
29	b	610	CLA	CBB-CAB	3.38	1.51	1.29
29	b1	615	CLA	CBB-CAB	3.38	1.51	1.29
29	n1	614	CLA	CBB-CAB	3.38	1.51	1.29
48	g	605	CHL	CBB-CAB	3.38	1.51	1.29
29	G	603	CLA	CBB-CAB	3.38	1.51	1.29
29	S1	612	CLA	CBB-CAB	3.38	1.51	1.29
29	r	609	CLA	CBB-CAB	3.38	1.51	1.29
29	G1	613	CLA	CBB-CAB	3.38	1.51	1.29
45	H	101	RRX	C11-C10	3.38	1.53	1.43
48	n1	605	CHL	CBB-CAB	3.38	1.51	1.29
29	n1	603	CLA	CBB-CAB	3.38	1.51	1.29
29	y1	604	CLA	CBB-CAB	3.38	1.51	1.29
29	C	511	CLA	CBB-CAB	3.38	1.51	1.29
48	Y	601	CHL	CBB-CAB	3.38	1.51	1.29
29	r1	612	CLA	CBB-CAB	3.38	1.51	1.29
29	s1	605	CLA	CBB-CAB	3.38	1.51	1.29
30	A1	408	PHO	CAC-C3C	-3.38	1.46	1.52
29	r1	610	CLA	CBB-CAB	3.37	1.51	1.29
48	G	601	CHL	CBB-CAB	3.37	1.51	1.29
29	n1	613	CLA	CBB-CAB	3.37	1.51	1.29
29	C1	508	CLA	CBB-CAB	3.37	1.51	1.29
29	N	602	CLA	CBB-CAB	3.37	1.51	1.29
29	c	506	CLA	CBB-CAB	3.37	1.51	1.29
29	s	609	CLA	CBB-CAB	3.37	1.51	1.29
29	R1	604	CLA	CBB-CAB	3.37	1.51	1.29
29	N	603	CLA	C1C-NC	-3.37	1.32	1.37
29	g1	603	CLA	CBB-CAB	3.37	1.51	1.29
29	r	610	CLA	CBB-CAB	3.37	1.51	1.29
29	c	512	CLA	C1C-NC	-3.37	1.32	1.37
29	g	604	CLA	C1C-NC	-3.37	1.32	1.37
29	y	608	CLA	C1C-NC	-3.37	1.32	1.37
48	g	601	CHL	CBB-CAB	3.37	1.51	1.29
48	n	601	CHL	CBB-CAB	3.37	1.51	1.29
29	n	613	CLA	CBB-CAB	3.37	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C1	507	CLA	CBB-CAB	3.37	1.51	1.29
29	G1	602	CLA	CBB-CAB	3.37	1.51	1.29
29	g1	612	CLA	CBB-CAB	3.37	1.51	1.29
29	n	602	CLA	C1C-NC	-3.37	1.32	1.37
29	N1	612	CLA	C1C-NC	-3.37	1.32	1.37
29	A	405	CLA	CBB-CAB	3.37	1.51	1.29
29	Y	604	CLA	C1C-NC	-3.37	1.32	1.37
48	g1	605	CHL	CBB-CAB	3.37	1.51	1.29
29	N1	613	CLA	CBB-CAB	3.37	1.51	1.29
48	G	607	CHL	CBB-CAB	3.37	1.51	1.29
39	c	524	DGA	OG2-CB1	3.37	1.43	1.34
29	c1	512	CLA	CBB-CAB	3.37	1.51	1.29
29	d1	402	CLA	CBB-CAB	3.37	1.51	1.29
29	S	605	CLA	CBB-CAB	3.37	1.51	1.29
29	s	603	CLA	CBB-CAB	3.37	1.51	1.29
29	s1	604	CLA	CBB-CAB	3.37	1.51	1.29
29	Y1	610	CLA	CBB-CAB	3.37	1.51	1.29
48	g	607	CHL	CBB-CAB	3.37	1.51	1.29
29	r1	604	CLA	CBB-CAB	3.37	1.51	1.29
29	n1	611	CLA	CBB-CAB	3.36	1.51	1.29
29	n	612	CLA	CBB-CAB	3.36	1.51	1.29
29	r1	602	CLA	CBB-CAB	3.36	1.51	1.29
33	H1	102	LMG	C19-C18	-3.36	1.32	1.51
29	b1	613	CLA	CBB-CAB	3.36	1.51	1.29
29	g1	602	CLA	CBB-CAB	3.36	1.51	1.29
29	N	611	CLA	CBB-CAB	3.36	1.51	1.29
29	C1	501	CLA	CBB-CAB	3.36	1.51	1.29
29	y	604	CLA	CBB-CAB	3.36	1.51	1.29
29	B1	613	CLA	CBB-CAB	3.36	1.51	1.29
29	R1	602	CLA	CBB-CAB	3.36	1.51	1.29
48	s	606	CHL	CBB-CAB	3.36	1.51	1.29
48	y	601	CHL	CBB-CAB	3.36	1.51	1.29
29	B	608	CLA	CBB-CAB	3.36	1.51	1.29
29	g	612	CLA	CBB-CAB	3.36	1.51	1.29
29	C1	510	CLA	CBB-CAB	3.36	1.51	1.29
29	R1	610	CLA	CBB-CAB	3.36	1.51	1.29
29	R	610	CLA	C3B-C2B	-3.36	1.35	1.40
29	A1	405	CLA	CBB-CAB	3.36	1.51	1.29
29	g1	610	CLA	C1C-NC	-3.36	1.32	1.37
29	B	610	CLA	CBB-CAB	3.36	1.51	1.29
29	y1	611	CLA	CBB-CAB	3.36	1.51	1.29
29	G1	610	CLA	CBB-CAB	3.36	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c1	509	CLA	CBB-CAB	3.36	1.51	1.29
29	s	602	CLA	C1C-NC	-3.36	1.32	1.37
29	y1	610	CLA	CBB-CAB	3.36	1.51	1.29
29	y	610	CLA	CBB-CAB	3.36	1.51	1.29
29	S1	603	CLA	CBB-CAB	3.36	1.51	1.29
29	D1	402	CLA	CBB-CAB	3.36	1.51	1.29
29	y	613	CLA	CBB-CAB	3.36	1.51	1.29
29	Y1	613	CLA	CBB-CAB	3.36	1.51	1.29
29	C	510	CLA	CBB-CAB	3.36	1.51	1.29
29	N	612	CLA	CBB-CAB	3.36	1.51	1.29
29	C1	513	CLA	CBB-CAB	3.36	1.51	1.29
29	b1	610	CLA	CBB-CAB	3.36	1.51	1.29
29	r1	604	CLA	C1C-NC	-3.36	1.32	1.37
29	b1	609	CLA	CBB-CAB	3.36	1.51	1.29
29	s	614	CLA	CBB-CAB	3.36	1.51	1.29
29	b1	606	CLA	C1C-NC	-3.36	1.32	1.37
29	g1	614	CLA	CBB-CAB	3.36	1.51	1.29
29	B1	607	CLA	C1C-NC	-3.36	1.32	1.37
29	s1	617	CLA	CBB-CAB	3.36	1.51	1.29
29	r	604	CLA	C1C-NC	-3.35	1.32	1.37
29	s1	605	CLA	C1C-NC	-3.35	1.32	1.37
29	s	604	CLA	CBB-CAB	3.35	1.51	1.29
29	S1	609	CLA	CBB-CAB	3.35	1.51	1.29
37	C	520	DGD	CAA-C9A	-3.35	1.32	1.51
29	S1	602	CLA	CBB-CAB	3.35	1.51	1.29
37	C	519	DGD	CAB-C9B	-3.35	1.32	1.51
29	Y	608	CLA	CBB-CAB	3.35	1.51	1.29
29	B1	612	CLA	CBB-CAB	3.35	1.51	1.29
48	S	608	CHL	CBB-CAB	3.35	1.51	1.29
29	b1	603	CLA	C1C-NC	-3.35	1.32	1.37
29	S	617	CLA	CBB-CAB	3.35	1.51	1.29
29	B1	608	CLA	CBB-CAB	3.35	1.51	1.29
29	b	608	CLA	CBB-CAB	3.35	1.51	1.29
29	B1	605	CLA	CBB-CAB	3.35	1.51	1.29
29	y1	608	CLA	CBB-CAB	3.35	1.51	1.29
29	r	602	CLA	C1C-NC	-3.35	1.32	1.37
29	N1	611	CLA	CBB-CAB	3.35	1.51	1.29
29	y1	612	CLA	CBB-CAB	3.35	1.51	1.29
29	y	608	CLA	CBB-CAB	3.35	1.51	1.29
29	a1	407	CLA	CBB-CAB	3.35	1.51	1.29
29	a1	405	CLA	CBB-CAB	3.35	1.51	1.29
48	R1	606	CHL	CBB-CAB	3.35	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Y	603	CLA	C3B-C2B	-3.35	1.35	1.40
29	G	612	CLA	CBB-CAB	3.35	1.51	1.29
39	c1	524	DGA	OG1-CA1	3.35	1.43	1.33
29	n1	604	CLA	CBB-CAB	3.35	1.51	1.29
29	S	617	CLA	C1C-NC	-3.35	1.32	1.37
29	b	604	CLA	CBB-CAB	3.35	1.51	1.29
29	g	604	CLA	CBB-CAB	3.35	1.51	1.29
29	b	614	CLA	CBB-CAB	3.35	1.51	1.29
29	s1	609	CLA	CBB-CAB	3.35	1.51	1.29
48	y1	601	CHL	CBB-CAB	3.35	1.51	1.29
29	B1	615	CLA	C1C-NC	-3.35	1.32	1.37
29	Y	602	CLA	CBB-CAB	3.35	1.51	1.29
29	N1	602	CLA	C1C-NC	-3.34	1.32	1.37
29	N	614	CLA	CBB-CAB	3.34	1.51	1.29
29	r	612	CLA	CBB-CAB	3.34	1.51	1.29
29	S1	613	CLA	CBB-CAB	3.34	1.51	1.29
48	S1	607	CHL	CBB-CAB	3.34	1.51	1.29
29	n	611	CLA	CBB-CAB	3.34	1.51	1.29
48	S	607	CHL	CBB-CAB	3.34	1.51	1.29
29	n	614	CLA	CBB-CAB	3.34	1.51	1.29
29	S	604	CLA	CBB-CAB	3.34	1.51	1.29
48	n1	607	CHL	CBB-CAB	3.34	1.51	1.29
29	Y1	611	CLA	C1C-NC	-3.34	1.32	1.37
29	y1	603	CLA	CBB-CAB	3.34	1.51	1.29
29	g	603	CLA	CBB-CAB	3.34	1.51	1.29
33	h	102	LMG	C19-C18	-3.34	1.32	1.51
29	g1	602	CLA	C1C-NC	-3.34	1.32	1.37
29	G1	611	CLA	CBB-CAB	3.34	1.51	1.29
29	r	604	CLA	CBB-CAB	3.34	1.51	1.29
29	C1	511	CLA	CBB-CAB	3.34	1.51	1.29
29	S	603	CLA	CBB-CAB	3.34	1.51	1.29
29	b	603	CLA	CBB-CAB	3.34	1.51	1.29
29	C1	502	CLA	CBB-CAB	3.34	1.51	1.29
29	s	617	CLA	CBB-CAB	3.34	1.51	1.29
29	b1	612	CLA	CBB-CAB	3.34	1.51	1.29
48	G	608	CHL	CBB-CAB	3.34	1.51	1.29
29	C	508	CLA	CBB-CAB	3.34	1.51	1.29
29	R	612	CLA	CBB-CAB	3.34	1.51	1.29
48	G1	601	CHL	CBB-CAB	3.34	1.51	1.29
29	g1	604	CLA	CBB-CAB	3.34	1.51	1.29
29	s	605	CLA	CBB-CAB	3.34	1.51	1.29
29	s1	614	CLA	CBB-CAB	3.34	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	G	602	CLA	CBB-CAB	3.34	1.51	1.29
29	B	604	CLA	CBB-CAB	3.34	1.51	1.29
48	y1	607	CHL	CBB-CAB	3.34	1.51	1.29
29	c1	504	CLA	CBB-CAB	3.34	1.51	1.29
29	c	508	CLA	CBB-CAB	3.33	1.51	1.29
29	y	604	CLA	C1C-NC	-3.33	1.32	1.37
29	Y	604	CLA	CBB-CAB	3.33	1.51	1.29
48	G1	605	CHL	CBB-CAB	3.33	1.51	1.29
29	S	612	CLA	CBB-CAB	3.33	1.51	1.29
29	a1	406	CLA	CBB-CAB	3.33	1.51	1.29
29	b	605	CLA	C3B-C2B	-3.33	1.35	1.40
29	C1	504	CLA	C3B-C2B	-3.33	1.35	1.40
29	C1	503	CLA	CBB-CAB	3.33	1.51	1.29
29	N	610	CLA	CBB-CAB	3.33	1.51	1.29
29	n	604	CLA	CBB-CAB	3.33	1.51	1.29
29	b1	607	CLA	CBB-CAB	3.33	1.51	1.29
29	C	502	CLA	CBB-CAB	3.33	1.51	1.29
29	B1	609	CLA	CBB-CAB	3.33	1.51	1.29
29	Y1	603	CLA	CBB-CAB	3.33	1.51	1.29
48	y	609	CHL	CBB-CAB	3.33	1.51	1.29
45	h1	101	RRX	C11-C10	3.33	1.53	1.43
29	Y1	608	CLA	C1C-NC	-3.33	1.32	1.37
29	b	609	CLA	CBB-CAB	3.33	1.51	1.29
29	Y	611	CLA	CBB-CAB	3.33	1.51	1.29
29	r	602	CLA	CBB-CAB	3.33	1.51	1.29
29	c	512	CLA	CBB-CAB	3.33	1.51	1.29
29	R	602	CLA	CBB-CAB	3.33	1.51	1.29
29	N1	603	CLA	CBB-CAB	3.33	1.51	1.29
48	n1	601	CHL	CBB-CAB	3.33	1.51	1.29
29	B	607	CLA	CBB-CAB	3.33	1.51	1.29
29	S1	617	CLA	CBB-CAB	3.33	1.51	1.29
29	S	609	CLA	CBB-CAB	3.33	1.51	1.29
29	C	507	CLA	CBB-CAB	3.33	1.51	1.29
29	g	614	CLA	CBB-CAB	3.33	1.51	1.29
29	B	602	CLA	CBB-CAB	3.33	1.51	1.29
29	r1	608	CLA	CBB-CAB	3.33	1.51	1.29
29	n1	612	CLA	C1C-NC	-3.33	1.32	1.37
29	r1	609	CLA	C1C-NC	-3.33	1.32	1.37
29	Y	610	CLA	CBB-CAB	3.33	1.51	1.29
29	R1	603	CLA	CBB-CAB	3.33	1.51	1.29
29	B	609	CLA	CBB-CAB	3.32	1.51	1.29
29	B1	610	CLA	CBB-CAB	3.32	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	G	610	CLA	CBB-CAB	3.32	1.51	1.29
29	B	615	CLA	CBB-CAB	3.32	1.51	1.29
29	N	604	CLA	CBB-CAB	3.32	1.51	1.29
29	C1	506	CLA	CBB-CAB	3.32	1.51	1.29
29	s	610	CLA	C3B-C2B	-3.32	1.35	1.40
29	G1	611	CLA	C1C-NC	-3.32	1.32	1.37
29	B1	603	CLA	CBB-CAB	3.32	1.51	1.29
29	B1	606	CLA	CBB-CAB	3.32	1.51	1.29
29	s1	603	CLA	CBB-CAB	3.32	1.51	1.29
29	C	503	CLA	CBB-CAB	3.32	1.51	1.29
29	n1	610	CLA	CBB-CAB	3.32	1.51	1.29
29	Y1	611	CLA	CBB-CAB	3.32	1.51	1.29
48	g1	608	CHL	CBB-CAB	3.32	1.51	1.29
29	Y	612	CLA	CBB-CAB	3.32	1.51	1.29
29	R	603	CLA	C1C-NC	-3.32	1.32	1.37
29	b	614	CLA	C1C-NC	-3.32	1.32	1.37
29	g	610	CLA	CBB-CAB	3.32	1.51	1.29
29	B	607	CLA	C1C-NC	-3.32	1.32	1.37
29	R	610	CLA	CBB-CAB	3.32	1.51	1.29
29	c	507	CLA	CBB-CAB	3.32	1.51	1.29
29	R1	609	CLA	CBB-CAB	3.32	1.51	1.29
29	S1	614	CLA	CBB-CAB	3.32	1.51	1.29
29	s	613	CLA	CBB-CAB	3.32	1.51	1.29
29	c	511	CLA	CBB-CAB	3.32	1.51	1.29
48	n1	608	CHL	CBB-CAB	3.32	1.51	1.29
29	S	613	CLA	CBB-CAB	3.32	1.51	1.29
29	b	612	CLA	CBB-CAB	3.32	1.51	1.29
29	C	512	CLA	CBB-CAB	3.31	1.51	1.29
29	Y1	608	CLA	CBB-CAB	3.31	1.51	1.29
37	c1	519	DGD	CAB-C9B	-3.31	1.33	1.51
39	C	524	DGA	OG2-CB1	3.31	1.43	1.34
29	A	407	CLA	CBB-CAB	3.31	1.51	1.29
29	C1	509	CLA	CBB-CAB	3.31	1.51	1.29
29	c	509	CLA	CBB-CAB	3.31	1.51	1.29
29	B1	607	CLA	CBB-CAB	3.31	1.51	1.29
29	B1	615	CLA	CBB-CAB	3.31	1.51	1.29
33	h	102	LMG	C37-C36	-3.31	1.33	1.51
29	C1	507	CLA	C1C-NC	-3.31	1.32	1.37
29	G	611	CLA	CBB-CAB	3.31	1.51	1.29
29	b1	614	CLA	CBB-CAB	3.31	1.51	1.29
48	g1	606	CHL	CBB-CAB	3.31	1.51	1.29
29	c1	513	CLA	C1C-NC	-3.31	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b1	603	CLA	CBB-CAB	3.31	1.51	1.29
29	B	614	CLA	C1C-NC	-3.31	1.32	1.37
29	Y1	604	CLA	CBB-CAB	3.31	1.51	1.29
33	c	523	LMG	C37-C36	-3.31	1.33	1.51
29	a	405	CLA	CBB-CAB	3.31	1.51	1.29
29	R	604	CLA	CBB-CAB	3.31	1.51	1.29
29	n	602	CLA	CBB-CAB	3.31	1.51	1.29
29	S	610	CLA	CBB-CAB	3.31	1.51	1.29
29	b1	602	CLA	CBB-CAB	3.31	1.51	1.29
29	c1	502	CLA	CBB-CAB	3.31	1.51	1.29
29	b	615	CLA	CBB-CAB	3.31	1.51	1.29
29	A1	407	CLA	CBB-CAB	3.31	1.51	1.29
29	S1	605	CLA	CBB-CAB	3.31	1.51	1.29
48	y1	605	CHL	CBB-CAB	3.31	1.51	1.29
29	C1	505	CLA	CBB-CAB	3.31	1.51	1.29
29	s1	604	CLA	C1C-NC	-3.31	1.32	1.37
29	S	614	CLA	CBB-CAB	3.31	1.51	1.29
29	c1	505	CLA	CBB-CAB	3.31	1.51	1.29
29	c1	513	CLA	CBB-CAB	3.31	1.51	1.29
29	b	607	CLA	CBB-CAB	3.31	1.51	1.29
33	B	622	LMG	C22-C21	-3.30	1.33	1.51
48	r	607	CHL	CBB-CAB	3.30	1.51	1.29
29	G	613	CLA	C1C-NC	-3.30	1.32	1.37
29	N1	612	CLA	CBB-CAB	3.30	1.51	1.29
36	b	620	C7Z	C7-C6	3.30	1.56	1.45
29	B	611	CLA	CBB-CAB	3.30	1.51	1.29
37	c	518	DGD	CAB-C9B	-3.30	1.33	1.51
29	N	603	CLA	CBB-CAB	3.30	1.51	1.29
48	s1	607	CHL	CBB-CAB	3.30	1.51	1.29
48	s1	601	CHL	CBB-CAB	3.30	1.51	1.29
45	H	101	RRX	C4-C5	-3.30	1.44	1.51
29	Y	613	CLA	CBB-CAB	3.30	1.51	1.29
29	g	613	CLA	C1C-NC	-3.30	1.32	1.37
29	g1	603	CLA	C1C-NC	-3.30	1.32	1.37
29	S1	604	CLA	CBB-CAB	3.30	1.51	1.29
29	N1	604	CLA	CBB-CAB	3.30	1.51	1.29
29	C	509	CLA	CBB-CAB	3.30	1.51	1.29
29	c	513	CLA	CBB-CAB	3.30	1.51	1.29
48	Y1	606	CHL	CBB-CAB	3.30	1.51	1.29
29	S	602	CLA	CBB-CAB	3.30	1.51	1.29
33	C1	521	LMG	C40-C39	-3.30	1.33	1.51
29	B1	609	CLA	C1C-NC	-3.30	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	s	612	CLA	CBB-CAB	3.30	1.51	1.29
37	c1	520	DGD	CAA-C9A	-3.30	1.33	1.51
29	c1	510	CLA	CBB-CAB	3.30	1.51	1.29
29	S1	617	CLA	C1C-NC	-3.30	1.32	1.37
33	b	622	LMG	C22-C21	-3.30	1.33	1.51
29	b1	606	CLA	CBB-CAB	3.30	1.51	1.29
48	R	607	CHL	C3B-C2B	-3.30	1.35	1.40
29	c	510	CLA	CBB-CAB	3.29	1.51	1.29
48	g	606	CHL	CBB-CAB	3.29	1.51	1.29
29	r1	603	CLA	CBB-CAB	3.29	1.51	1.29
29	a	407	CLA	CBB-CAB	3.29	1.51	1.29
39	b	625	DGA	OG1-CA1	3.29	1.43	1.33
48	n	605	CHL	CBB-CAB	3.29	1.51	1.29
29	b	613	CLA	CBB-CAB	3.29	1.51	1.29
29	C	504	CLA	CBB-CAB	3.29	1.51	1.29
29	c	504	CLA	CBB-CAB	3.29	1.51	1.29
39	J1	101	DGA	OG1-CA1	3.29	1.42	1.33
29	y	602	CLA	CBB-CAB	3.29	1.51	1.29
29	B1	610	CLA	C1C-NC	-3.29	1.32	1.37
48	s1	608	CHL	C4B-NB	3.29	1.38	1.35
37	C1	520	DGD	CAB-C9B	-3.29	1.33	1.51
29	N	613	CLA	CBB-CAB	3.29	1.51	1.29
29	g1	612	CLA	C1C-NC	-3.29	1.32	1.37
48	S	601	CHL	C4B-NB	3.29	1.38	1.35
33	c1	523	LMG	C22-C21	-3.29	1.33	1.51
33	h1	102	LMG	C19-C18	-3.28	1.33	1.51
29	b1	605	CLA	CBB-CAB	3.28	1.51	1.29
37	c	520	DGD	CAB-C9B	-3.28	1.33	1.51
29	y	611	CLA	CBB-CAB	3.28	1.51	1.29
37	C	519	DGD	CDB-CCB	-3.28	1.33	1.51
29	S1	611	CLA	CBB-CAB	3.28	1.51	1.29
29	Y1	614	CLA	CBB-CAB	3.28	1.51	1.29
29	c	503	CLA	CBB-CAB	3.28	1.51	1.29
29	C	506	CLA	CBB-CAB	3.28	1.51	1.29
29	B	612	CLA	CBB-CAB	3.28	1.51	1.29
29	y1	614	CLA	CBB-CAB	3.28	1.51	1.29
48	R1	607	CHL	CBB-CAB	3.28	1.51	1.29
29	Y	603	CLA	CBB-CAB	3.28	1.51	1.29
29	G	604	CLA	CBB-CAB	3.28	1.51	1.29
29	R	603	CLA	CBB-CAB	3.28	1.51	1.29
29	d	403	CLA	CBB-CAB	3.28	1.51	1.29
29	C1	504	CLA	CBB-CAB	3.28	1.51	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	C1	518	DGD	CAB-C9B	-3.28	1.33	1.51
48	y	605	CHL	CBB-CAB	3.28	1.51	1.29
33	c	521	LMG	C40-C39	-3.28	1.33	1.51
29	G1	604	CLA	CBB-CAB	3.28	1.51	1.29
29	D	403	CLA	CBB-CAB	3.28	1.51	1.29
48	N1	609	CHL	CBB-CAB	3.28	1.51	1.29
33	C1	523	LMG	C25-C24	-3.28	1.33	1.51
29	c	505	CLA	CBB-CAB	3.28	1.51	1.29
29	B1	614	CLA	CBB-CAB	3.28	1.51	1.29
48	G	609	CHL	CBB-CAB	3.28	1.51	1.29
29	c1	511	CLA	CBB-CAB	3.28	1.51	1.29
48	g	606	CHL	C4B-NB	3.28	1.38	1.35
29	b1	609	CLA	C1C-NC	-3.28	1.32	1.37
48	Y	605	CHL	CBB-CAB	3.28	1.51	1.29
29	N	612	CLA	C1C-NC	-3.28	1.32	1.37
37	C	520	DGD	CAB-C9B	-3.28	1.33	1.51
48	N	605	CHL	CBB-CAB	3.27	1.51	1.29
29	B1	616	CLA	CBB-CAB	3.27	1.51	1.29
29	R	609	CLA	CBB-CAB	3.27	1.51	1.29
29	R1	602	CLA	C1C-NC	-3.27	1.32	1.37
29	b1	605	CLA	MG-ND	-3.27	1.99	2.05
37	C	518	DGD	CDB-CCB	-3.27	1.33	1.51
29	n	603	CLA	CBB-CAB	3.27	1.51	1.29
29	y	612	CLA	CBB-CAB	3.27	1.51	1.29
29	y	614	CLA	CBB-CAB	3.27	1.51	1.29
33	C1	523	LMG	C37-C36	-3.27	1.33	1.51
48	S1	601	CHL	C4B-NB	3.27	1.38	1.35
33	B	622	LMG	C19-C18	-3.27	1.33	1.51
48	G1	607	CHL	CBB-CAB	3.27	1.51	1.29
29	A1	410	CLA	CBB-CAB	3.27	1.51	1.29
29	g1	613	CLA	CBB-CAB	3.27	1.51	1.29
29	g	603	CLA	C1C-NC	-3.27	1.32	1.37
29	d	402	CLA	CBB-CAB	3.27	1.50	1.29
37	C1	518	DGD	CDB-CCB	-3.27	1.33	1.51
29	B	605	CLA	CBB-CAB	3.27	1.50	1.29
29	s	602	CLA	CBB-CAB	3.26	1.50	1.29
29	c1	508	CLA	C1C-NC	-3.26	1.32	1.37
29	b	615	CLA	C1C-NC	-3.26	1.32	1.37
33	H1	102	LMG	C40-C39	-3.26	1.33	1.51
29	c	501	CLA	C3B-C2B	-3.26	1.35	1.40
48	G1	608	CHL	CBB-CAB	3.26	1.50	1.29
37	c	519	DGD	CAB-C9B	-3.26	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	b	602	CLA	CBB-CAB	3.26	1.50	1.29
29	s	605	CLA	C1C-NC	-3.26	1.32	1.37
48	Y	609	CHL	CBB-CAB	3.26	1.50	1.29
33	c	523	LMG	C40-C39	-3.26	1.33	1.51
33	c1	521	LMG	C40-C39	-3.26	1.33	1.51
48	N	601	CHL	CBB-CAB	3.26	1.50	1.29
29	s1	603	CLA	C1C-NC	-3.26	1.32	1.37
48	r	606	CHL	CBB-CAB	3.26	1.50	1.29
29	N1	610	CLA	C1C-NC	-3.26	1.32	1.37
29	A	406	CLA	CBB-CAB	3.26	1.50	1.29
29	s	611	CLA	CBB-CAB	3.26	1.50	1.29
33	H	102	LMG	C19-C18	-3.26	1.33	1.51
29	Y1	602	CLA	CBB-CAB	3.26	1.50	1.29
39	j	101	DGA	OG1-CA1	3.26	1.42	1.33
29	s1	609	CLA	C1C-NC	-3.26	1.32	1.37
48	n	609	CHL	CBB-CAB	3.26	1.50	1.29
33	C	523	LMG	C25-C24	-3.26	1.33	1.51
39	C	524	DGA	OG1-CA1	3.26	1.42	1.33
29	g	613	CLA	CBB-CAB	3.26	1.50	1.29
29	s	610	CLA	CBB-CAB	3.26	1.50	1.29
29	B	613	CLA	CBB-CAB	3.26	1.50	1.29
29	G1	614	CLA	C1C-NC	-3.26	1.32	1.37
29	b	616	CLA	CBB-CAB	3.25	1.50	1.29
48	R	607	CHL	CBB-CAB	3.25	1.50	1.29
45	H1	101	RRX	C24-C25	3.25	1.56	1.45
29	C1	505	CLA	C1C-NC	-3.25	1.32	1.37
33	C	523	LMG	C22-C21	-3.25	1.33	1.51
33	A	413	LMG	C19-C18	-3.25	1.33	1.51
29	Y	614	CLA	C1C-NC	-3.25	1.33	1.37
33	c1	523	LMG	C25-C24	-3.25	1.33	1.51
29	c	502	CLA	CBB-CAB	3.25	1.50	1.29
29	C1	503	CLA	C1C-NC	-3.25	1.33	1.37
29	G	613	CLA	CBB-CAB	3.25	1.50	1.29
48	r1	606	CHL	CBB-CAB	3.25	1.50	1.29
29	B	616	CLA	CBB-CAB	3.25	1.50	1.29
37	c	519	DGD	CAA-C9A	-3.25	1.33	1.51
29	s	603	CLA	C1C-NC	-3.25	1.33	1.37
37	c1	519	DGD	CDB-CCB	-3.25	1.33	1.51
29	C	513	CLA	CBB-CAB	3.25	1.50	1.29
33	c1	521	LMG	C22-C21	-3.25	1.33	1.51
29	D	402	CLA	CBB-CAB	3.25	1.50	1.29
37	C1	519	DGD	CAA-C9A	-3.25	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	S	603	CLA	C1C-NC	-3.25	1.33	1.37
33	D1	411	LMG	C19-C18	-3.24	1.33	1.51
48	S	606	CHL	C4B-NB	3.24	1.38	1.35
33	c1	523	LMG	C40-C39	-3.24	1.33	1.51
29	S	611	CLA	CBB-CAB	3.24	1.50	1.29
29	B	603	CLA	CBB-CAB	3.24	1.50	1.29
29	B	603	CLA	C1C-NC	-3.24	1.33	1.37
37	C1	519	DGD	CAB-C9B	-3.24	1.33	1.51
37	c1	520	DGD	CAB-C9B	-3.24	1.33	1.51
33	A1	413	LMG	C19-C18	-3.24	1.33	1.51
33	h1	102	LMG	C37-C36	-3.24	1.33	1.51
29	B	617	CLA	CBB-CAB	3.24	1.50	1.29
47	K	101	4RF	O40-C41	3.24	1.42	1.33
33	C	521	LMG	C40-C39	-3.24	1.33	1.51
39	B	625	DGA	OG1-CA1	3.24	1.42	1.33
33	C	523	LMG	C37-C36	-3.24	1.33	1.51
29	Y	611	CLA	C1C-NC	-3.24	1.33	1.37
29	s1	614	CLA	C1C-NC	-3.24	1.33	1.37
48	N1	606	CHL	C4B-NB	3.24	1.38	1.35
29	b	602	CLA	C1C-NC	-3.24	1.33	1.37
29	c	501	CLA	CBB-CAB	3.24	1.50	1.29
48	n	607	CHL	CBB-CAB	3.24	1.50	1.29
29	n1	614	CLA	C1C-NC	-3.24	1.33	1.37
29	C	501	CLA	CBB-CAB	3.24	1.50	1.29
29	Y	614	CLA	CBB-CAB	3.24	1.50	1.29
37	C	519	DGD	CDA-CCA	-3.24	1.33	1.51
29	n1	602	CLA	C1C-NC	-3.24	1.33	1.37
36	B1	620	C7Z	C38-C25	3.23	1.56	1.50
37	c1	518	DGD	CAB-C9B	-3.23	1.33	1.51
33	c	523	LMG	C43-C42	-3.23	1.33	1.51
29	S1	611	CLA	C1C-NC	-3.23	1.33	1.37
37	c	520	DGD	CAA-C9A	-3.23	1.33	1.51
33	A	413	LMG	C37-C36	-3.23	1.33	1.51
33	c1	523	LMG	C37-C36	-3.23	1.33	1.51
33	C	521	LMG	C22-C21	-3.23	1.33	1.51
48	s1	608	CHL	CBB-CAB	3.23	1.50	1.29
33	H1	102	LMG	C37-C36	-3.23	1.33	1.51
29	c1	506	CLA	C1C-NC	-3.23	1.33	1.37
33	C1	521	LMG	C37-C36	-3.23	1.33	1.51
33	a1	413	LMG	C37-C36	-3.23	1.33	1.51
29	b	605	CLA	CBB-CAB	3.23	1.50	1.29
48	g1	605	CHL	C4B-NB	3.23	1.38	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	y1	614	CLA	C1C-NC	-3.23	1.33	1.37
29	Y1	612	CLA	CBB-CAB	3.23	1.50	1.29
29	D1	403	CLA	CBB-CAB	3.23	1.50	1.29
29	B1	617	CLA	CBB-CAB	3.23	1.50	1.29
36	B1	620	C7Z	C21-C26	-3.23	1.49	1.53
37	c	519	DGD	CDB-CCB	-3.23	1.33	1.51
29	s1	611	CLA	CBB-CAB	3.23	1.50	1.29
29	n	614	CLA	C1C-NC	-3.23	1.33	1.37
37	C	518	DGD	CAB-C9B	-3.23	1.33	1.51
29	G	603	CLA	C1C-NC	-3.23	1.33	1.37
29	g1	611	CLA	C1C-NC	-3.23	1.33	1.37
33	d1	411	LMG	C22-C21	-3.23	1.33	1.51
29	b1	614	CLA	C1C-NC	-3.22	1.33	1.37
33	h	102	LMG	C40-C39	-3.22	1.33	1.51
33	H	102	LMG	C37-C36	-3.22	1.33	1.51
37	c	519	DGD	CDA-CCA	-3.22	1.33	1.51
43	D1	405	PL9	C31-C29	-3.22	1.44	1.51
33	D	411	LMG	C22-C21	-3.22	1.33	1.51
33	c	523	LMG	C25-C24	-3.22	1.33	1.51
33	C	523	LMG	C40-C39	-3.22	1.33	1.51
37	C1	520	DGD	CDB-CCB	-3.22	1.33	1.51
48	S	608	CHL	C4B-NB	3.22	1.38	1.35
39	J	101	DGA	OG1-CA1	3.22	1.42	1.33
29	b	617	CLA	CBB-CAB	3.22	1.50	1.29
48	g	601	CHL	C4B-NB	3.22	1.38	1.35
48	g1	601	CHL	C4B-NB	3.22	1.38	1.35
29	c1	502	CLA	C3B-C2B	-3.22	1.35	1.40
29	a	410	CLA	C1C-NC	-3.22	1.33	1.37
33	b	622	LMG	C19-C18	-3.22	1.33	1.51
37	C1	519	DGD	CDA-CCA	-3.22	1.33	1.51
33	w	201	LMG	C37-C36	-3.22	1.33	1.51
48	n	606	CHL	CBB-CAB	3.22	1.50	1.29
37	c	518	DGD	CDB-CCB	-3.22	1.33	1.51
39	C1	524	DGA	OG1-CA1	3.21	1.42	1.33
36	b	620	C7Z	C21-C26	-3.21	1.49	1.53
33	a1	413	LMG	C19-C18	-3.21	1.33	1.51
29	a1	410	CLA	CBB-CAB	3.21	1.50	1.29
48	g	608	CHL	CBB-CAB	3.21	1.50	1.29
29	y	603	CLA	CBB-CAB	3.21	1.50	1.29
33	H	102	LMG	C40-C39	-3.21	1.33	1.51
33	A	413	LMG	C40-C39	-3.21	1.33	1.51
45	h1	101	RRX	C29-C30	3.21	1.64	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	C1	520	DGD	CAA-C9A	-3.20	1.33	1.51
29	y	603	CLA	C3B-C2B	-3.20	1.35	1.40
29	r	603	CLA	CBB-CAB	3.20	1.50	1.29
29	s	610	CLA	C1C-NC	-3.20	1.33	1.37
29	s	611	CLA	C1C-NC	-3.20	1.33	1.37
29	A1	406	CLA	CBB-CAB	3.20	1.50	1.29
37	C	519	DGD	CAA-C9A	-3.20	1.33	1.51
39	c	524	DGA	OG1-CA1	3.20	1.42	1.33
33	b1	622	LMG	C22-C21	-3.20	1.33	1.51
37	c1	520	DGD	CDB-CCB	-3.20	1.33	1.51
33	w1	201	LMG	C40-C39	-3.20	1.33	1.51
48	N	607	CHL	CBB-CAB	3.20	1.50	1.29
33	c	523	LMG	C22-C21	-3.20	1.33	1.51
48	S	606	CHL	CBB-CAB	3.20	1.50	1.29
29	r1	602	CLA	C1C-NC	-3.20	1.33	1.37
33	a1	413	LMG	C40-C39	-3.20	1.33	1.51
37	C1	519	DGD	CDB-CCB	-3.20	1.33	1.51
29	C	505	CLA	CBB-CAB	3.20	1.50	1.29
29	a	406	CLA	CBB-CAB	3.20	1.50	1.29
33	C	521	LMG	C37-C36	-3.20	1.33	1.51
33	c1	523	LMG	C43-C42	-3.20	1.33	1.51
29	B1	613	CLA	C1C-NC	-3.19	1.33	1.37
33	A1	413	LMG	C40-C39	-3.19	1.33	1.51
48	R	606	CHL	C3A-C2A	-3.19	1.45	1.54
33	a	413	LMG	C37-C36	-3.19	1.33	1.51
33	a	413	LMG	C40-C39	-3.19	1.33	1.51
36	b	620	C7Z	C2-C1	3.19	1.64	1.54
48	N	605	CHL	C4B-NB	3.19	1.38	1.35
48	n	601	CHL	C4B-NB	3.19	1.38	1.35
33	C1	521	LMG	C22-C21	-3.19	1.33	1.51
33	b1	622	LMG	C19-C18	-3.19	1.33	1.51
33	c	521	LMG	C37-C36	-3.19	1.33	1.51
29	A	410	CLA	CBB-CAB	3.19	1.50	1.29
33	d	411	LMG	C22-C21	-3.19	1.33	1.51
36	B	620	C7Z	C7-C6	3.19	1.56	1.45
33	d	411	LMG	C19-C18	-3.19	1.33	1.51
33	c	521	LMG	C22-C21	-3.19	1.33	1.51
33	D	411	LMG	C19-C18	-3.19	1.33	1.51
48	s1	601	CHL	C4B-NB	3.18	1.38	1.35
33	a	413	LMG	C19-C18	-3.18	1.33	1.51
48	Y	606	CHL	CBB-CAB	3.18	1.50	1.29
33	c1	523	LMG	C19-C18	-3.18	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	C1	523	LMG	C40-C39	-3.18	1.33	1.51
48	r	606	CHL	C4B-NB	3.18	1.38	1.35
48	s	608	CHL	C4B-NB	3.18	1.38	1.35
29	g1	614	CLA	C1C-NC	-3.18	1.33	1.37
29	y1	611	CLA	C1C-NC	-3.18	1.33	1.37
29	c1	509	CLA	C1C-NC	-3.18	1.33	1.37
29	r	612	CLA	C1C-NC	-3.18	1.33	1.37
29	s1	613	CLA	C1C-NC	-3.18	1.33	1.37
48	n1	601	CHL	C4B-NB	3.18	1.38	1.35
33	w1	201	LMG	C37-C36	-3.18	1.33	1.51
51	s	623	NEX	C1-C6	-3.18	1.49	1.54
37	c1	518	DGD	CDB-CCB	-3.18	1.33	1.51
33	C	523	LMG	C19-C18	-3.18	1.33	1.51
29	C	511	CLA	C1C-NC	-3.17	1.33	1.37
48	y	606	CHL	C4B-NB	3.17	1.38	1.35
33	W	201	LMG	C40-C39	-3.17	1.33	1.51
37	c1	519	DGD	CDA-CCA	-3.17	1.33	1.51
48	N1	606	CHL	CBB-CAB	3.17	1.50	1.29
29	s1	602	CLA	C1C-NC	-3.17	1.33	1.37
33	W1	201	LMG	C40-C39	-3.17	1.33	1.51
36	b	620	C7Z	C38-C25	3.17	1.56	1.50
48	g	608	CHL	C4B-NB	3.17	1.38	1.35
33	B1	622	LMG	C22-C21	-3.17	1.33	1.51
45	h	101	RRX	C29-C30	3.17	1.64	1.54
33	C	523	LMG	C43-C42	-3.17	1.33	1.51
37	c	520	DGD	CDB-CCB	-3.17	1.33	1.51
33	d1	411	LMG	C19-C18	-3.16	1.33	1.51
33	c	521	LMG	C19-C18	-3.16	1.33	1.51
48	R	606	CHL	C4B-NB	3.16	1.38	1.35
33	W	201	LMG	C37-C36	-3.16	1.33	1.51
33	c1	521	LMG	C37-C36	-3.16	1.33	1.51
33	c1	521	LMG	C19-C18	-3.16	1.33	1.51
37	c1	519	DGD	CAA-C9A	-3.16	1.33	1.51
48	S1	607	CHL	C4B-NB	3.16	1.38	1.35
48	y	606	CHL	CBB-CAB	3.16	1.50	1.29
29	s	612	CLA	C1C-NC	-3.16	1.33	1.37
48	s1	607	CHL	C4B-NB	3.16	1.38	1.35
29	S1	603	CLA	C1C-NC	-3.16	1.33	1.37
48	R1	606	CHL	C4B-NB	3.15	1.38	1.35
33	C	521	LMG	C19-C18	-3.15	1.33	1.51
33	C1	521	LMG	C19-C18	-3.15	1.33	1.51
33	h1	102	LMG	C40-C39	-3.15	1.33	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	Y	607	CHL	CBB-CAB	3.15	1.50	1.29
33	A1	413	LMG	C37-C36	-3.15	1.33	1.51
33	D1	411	LMG	C22-C21	-3.15	1.33	1.51
29	R1	609	CLA	C1C-NC	-3.15	1.33	1.37
29	s	611	CLA	C3B-C2B	-3.14	1.36	1.40
33	c	523	LMG	C19-C18	-3.14	1.33	1.51
29	B1	616	CLA	C1C-NC	-3.14	1.33	1.37
33	w	201	LMG	C40-C39	-3.14	1.34	1.51
48	G	609	CHL	C4B-NB	3.14	1.38	1.35
45	h1	101	RRX	C4-C5	-3.14	1.44	1.51
44	F1	101	HEM	CAB-C3B	3.14	1.56	1.47
29	s	617	CLA	C1C-NC	-3.14	1.33	1.37
29	r1	603	CLA	C1C-NC	-3.14	1.33	1.37
48	s	608	CHL	CBB-CAB	3.14	1.50	1.29
33	B1	622	LMG	C19-C18	-3.14	1.34	1.51
48	N	601	CHL	C4B-NB	3.14	1.38	1.35
29	n	612	CLA	C1C-NC	-3.14	1.33	1.37
29	G1	613	CLA	C1C-NC	-3.14	1.33	1.37
45	h1	101	RRX	C16-C17	3.13	1.53	1.43
29	b1	602	CLA	C1C-NC	-3.13	1.33	1.37
29	S1	602	CLA	C1C-NC	-3.13	1.33	1.37
33	W1	201	LMG	C37-C36	-3.13	1.34	1.51
33	C1	523	LMG	C19-C18	-3.13	1.34	1.51
29	g1	604	CLA	C1C-NC	-3.13	1.33	1.37
29	a	410	CLA	CBB-CAB	3.13	1.50	1.29
48	s	607	CHL	CBB-CAB	3.13	1.50	1.29
48	R1	607	CHL	C4B-NB	3.12	1.38	1.35
29	r1	610	CLA	C1C-NC	-3.12	1.33	1.37
45	H	101	RRX	C16-C17	3.12	1.53	1.43
37	C	520	DGD	CDB-CCB	-3.12	1.34	1.51
47	i1	101	4RF	O40-C41	3.12	1.42	1.33
29	B1	603	CLA	C1C-NC	-3.12	1.33	1.37
33	C1	523	LMG	C43-C42	-3.12	1.34	1.51
29	y1	608	CLA	C1C-NC	-3.12	1.33	1.37
48	G	606	CHL	C4B-NB	3.12	1.38	1.35
29	r	608	CLA	C1C-NC	-3.11	1.33	1.37
29	S	611	CLA	C3B-C2B	-3.11	1.36	1.40
29	s1	617	CLA	C1C-NC	-3.11	1.33	1.37
33	C1	523	LMG	C22-C21	-3.11	1.34	1.51
29	N1	614	CLA	C1C-NC	-3.11	1.33	1.37
48	n	605	CHL	C4B-NB	3.11	1.38	1.35
48	n1	606	CHL	CBB-CAB	3.10	1.49	1.29

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	H1	101	RRX	C29-C30	3.10	1.64	1.54
45	h1	101	RRX	C24-C25	3.10	1.56	1.45
48	s	607	CHL	C3B-C2B	-3.10	1.36	1.40
48	N	606	CHL	CBB-CAB	3.10	1.49	1.29
48	n1	605	CHL	C4B-NB	3.10	1.38	1.35
48	G	606	CHL	CBB-CAB	3.09	1.49	1.29
48	y1	605	CHL	C4B-NB	3.09	1.38	1.35
48	s	601	CHL	CBB-CAB	3.08	1.49	1.29
53	r	626	ERG	C4-C5	3.08	1.58	1.51
29	B	604	CLA	C3B-C2B	-3.08	1.36	1.40
48	g	605	CHL	C4B-NB	3.08	1.38	1.35
48	R	606	CHL	CBB-CAB	3.08	1.49	1.29
29	y1	612	CLA	C1C-NC	-3.07	1.33	1.37
48	S1	601	CHL	CBB-CAB	3.07	1.49	1.29
44	f	101	HEM	CAB-C3B	3.07	1.55	1.47
29	b1	611	CLA	C3B-C2B	-3.06	1.36	1.40
48	G	608	CHL	C4B-NB	3.06	1.37	1.35
47	K1	101	4RF	O40-C41	3.06	1.42	1.33
51	R	622	NEX	C1-C6	-3.06	1.49	1.54
29	R	609	CLA	C3B-C2B	-3.06	1.36	1.40
45	H1	101	RRX	C4-C5	-3.05	1.45	1.51
29	d1	403	CLA	C1C-NC	-3.05	1.33	1.37
48	G1	605	CHL	C4B-NB	3.05	1.37	1.35
48	G1	601	CHL	C3B-C2B	-3.05	1.36	1.40
48	g	609	CHL	C3B-C2B	-3.05	1.36	1.40
45	H	101	RRX	C24-C25	3.04	1.55	1.45
29	Y1	603	CLA	C1C-NC	-3.04	1.33	1.37
29	Y1	612	CLA	C1C-NC	-3.04	1.33	1.37
48	G1	601	CHL	C4B-NB	3.04	1.37	1.35
43	d	405	PL9	C53-C6	-3.04	1.44	1.50
48	Y	605	CHL	C4B-NB	3.03	1.37	1.35
48	y1	601	CHL	C4B-NB	3.03	1.37	1.35
47	I	102	4RF	O40-C41	3.03	1.42	1.33
45	h	101	RRX	C4-C5	-3.03	1.45	1.51
29	n1	612	CLA	C3B-C2B	-3.03	1.36	1.40
29	y	612	CLA	C3B-C2B	-3.03	1.36	1.40
29	N	610	CLA	C3B-C2B	-3.03	1.36	1.40
45	h	101	RRX	C11-C10	3.02	1.52	1.43
47	i	101	4RF	O40-C41	3.02	1.42	1.33
48	g1	609	CHL	C4B-NB	3.02	1.37	1.35
29	g	614	CLA	C1C-NC	-3.02	1.33	1.37
48	Y1	606	CHL	C4B-NB	3.02	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	g1	606	CHL	C4B-NB	3.02	1.37	1.35
48	r1	607	CHL	C4B-NB	3.02	1.37	1.35
39	B1	625	DGA	OG1-CA1	3.02	1.42	1.33
48	G	601	CHL	C4B-NB	3.01	1.37	1.35
48	y1	606	CHL	C4B-NB	3.01	1.37	1.35
29	b	602	CLA	C3B-C2B	-3.01	1.36	1.40
29	D1	403	CLA	C1C-NC	-3.00	1.33	1.37
44	f1	101	HEM	CAB-C3B	3.00	1.55	1.47
48	s1	608	CHL	CHC-C1C	3.00	1.42	1.35
48	r1	606	CHL	C4B-NB	3.00	1.37	1.35
29	S1	613	CLA	C3B-C2B	-3.00	1.36	1.40
48	Y1	601	CHL	C3A-C2A	-3.00	1.46	1.54
29	r1	612	CLA	C1C-NC	-3.00	1.33	1.37
47	k1	101	4RF	O40-C41	3.00	1.42	1.33
29	D	402	CLA	C3B-C2B	-3.00	1.36	1.40
47	k	101	4RF	O40-C41	2.99	1.42	1.33
29	C1	511	CLA	C3B-C2B	-2.99	1.36	1.40
48	n1	608	CHL	C4B-NB	2.99	1.37	1.35
47	I1	102	4RF	O40-C41	2.99	1.42	1.33
51	G	623	NEX	C1-C6	-2.99	1.49	1.54
48	g1	608	CHL	C4B-NB	2.99	1.37	1.35
45	h	101	RRX	C24-C25	2.98	1.55	1.45
48	n1	606	CHL	C4B-NB	2.98	1.37	1.35
29	s1	610	CLA	C3B-C2B	-2.97	1.36	1.40
48	Y1	605	CHL	C4B-NB	2.97	1.37	1.35
29	R	612	CLA	C1C-NC	-2.97	1.33	1.37
44	F	101	HEM	CAB-C3B	2.97	1.55	1.47
48	S	601	CHL	CBB-CAB	2.96	1.48	1.29
29	B1	616	CLA	C3B-C2B	-2.96	1.36	1.40
45	H	101	RRX	C29-C30	2.96	1.64	1.54
29	N1	602	CLA	CHC-C1C	2.96	1.42	1.35
29	n1	602	CLA	CHC-C1C	2.96	1.42	1.35
43	D1	405	PL9	C7-C3	-2.96	1.48	1.51
48	s1	608	CHL	C3B-C2B	-2.95	1.36	1.40
29	b	616	CLA	C3B-C2B	-2.95	1.36	1.40
30	A1	409	PHO	CAC-C3C	-2.95	1.47	1.52
48	N	606	CHL	C4B-NB	2.95	1.37	1.35
29	B1	609	CLA	C3B-C2B	-2.94	1.36	1.40
48	s	607	CHL	C4B-NB	2.94	1.37	1.35
48	G1	608	CHL	C4B-NB	2.94	1.37	1.35
53	R1	626	ERG	C4-C5	2.94	1.58	1.51
45	H1	101	RRX	C7-C6	2.94	1.55	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	s1	608	CHL	C3A-C2A	-2.94	1.46	1.54
48	S	607	CHL	C4B-NB	2.93	1.37	1.35
36	B	620	C7Z	C38-C25	2.93	1.55	1.50
29	n	603	CLA	C3B-C2B	-2.93	1.36	1.40
29	N1	603	CLA	C3B-C2B	-2.93	1.36	1.40
29	B	616	CLA	C3B-C2B	-2.93	1.36	1.40
48	S1	608	CHL	C4B-NB	2.93	1.37	1.35
45	h	101	RRX	C16-C17	2.93	1.52	1.43
29	s1	603	CLA	C3B-C2B	-2.93	1.36	1.40
36	b1	620	C7Z	C21-C26	-2.92	1.49	1.53
29	Y1	614	CLA	C3B-C2B	-2.92	1.36	1.40
29	b	613	CLA	C3B-C2B	-2.92	1.36	1.40
29	s1	613	CLA	CHC-C1C	2.92	1.42	1.35
54	S	625	LPX	P1-O1	2.92	1.71	1.59
48	G	605	CHL	C4B-NB	2.91	1.37	1.35
29	y	614	CLA	C3B-C2B	-2.91	1.36	1.40
48	R	606	CHL	C3B-C2B	-2.91	1.36	1.40
30	a1	408	PHO	CAC-C3C	-2.91	1.47	1.52
48	Y	606	CHL	C4B-NB	2.90	1.37	1.35
48	G1	607	CHL	C4B-NB	2.90	1.37	1.35
48	Y	609	CHL	C4B-NB	2.90	1.37	1.35
54	s	625	LPX	P1-O1	2.90	1.71	1.59
47	i1	101	4RF	O21-C22	2.89	1.42	1.34
48	r	607	CHL	C3B-C2B	-2.89	1.36	1.40
48	n1	605	CHL	C3A-C2A	-2.89	1.46	1.54
29	c1	501	CLA	C3B-C2B	-2.89	1.36	1.40
29	b1	607	CLA	C3B-C2B	-2.89	1.36	1.40
54	S1	625	LPX	P1-O1	2.89	1.71	1.59
52	r1	625	LMT	O3'-C3'	-2.89	1.36	1.43
48	Y	605	CHL	C3B-C2B	-2.88	1.36	1.40
48	g	609	CHL	C4B-NB	2.88	1.37	1.35
45	h1	101	RRX	C7-C6	2.88	1.55	1.45
48	g	608	CHL	C3B-C2B	-2.88	1.36	1.40
54	s1	625	LPX	P1-O1	2.88	1.71	1.59
48	r	607	CHL	C4B-NB	2.88	1.37	1.35
29	Y	613	CLA	C3B-C2B	-2.88	1.36	1.40
48	s1	601	CHL	C3A-C2A	-2.87	1.46	1.54
48	y	605	CHL	C4B-NB	2.87	1.37	1.35
29	r1	612	CLA	CHC-C1C	2.86	1.42	1.35
29	d1	403	CLA	CHC-C1C	2.86	1.42	1.35
29	y1	602	CLA	CHC-C1C	2.86	1.42	1.35
48	n1	607	CHL	C4B-NB	2.86	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	n	606	CHL	C3B-C2B	-2.86	1.36	1.40
48	Y1	601	CHL	C4B-NB	2.86	1.37	1.35
29	C1	503	CLA	CHC-C1C	2.85	1.42	1.35
52	R	625	LMT	O3'-C3'	-2.85	1.36	1.43
30	a1	409	PHO	CAC-C3C	-2.85	1.47	1.52
29	C	501	CLA	C3B-C2B	-2.85	1.36	1.40
29	G	613	CLA	C3B-C2B	-2.85	1.36	1.40
29	N1	604	CLA	C3B-C2B	-2.85	1.36	1.40
29	s1	602	CLA	CHC-C1C	2.85	1.42	1.35
48	Y	606	CHL	C3B-C2B	-2.85	1.36	1.40
48	n	606	CHL	C4B-NB	2.85	1.37	1.35
29	g1	611	CLA	CHC-C1C	2.85	1.42	1.35
29	c1	503	CLA	C3B-C2B	-2.85	1.36	1.40
48	n	601	CHL	C3A-C2A	-2.84	1.46	1.54
29	c	504	CLA	C3B-C2B	-2.84	1.36	1.40
53	r	626	ERG	C9-C8	2.84	1.59	1.51
29	C1	513	CLA	CHC-C1C	2.84	1.42	1.35
29	C1	512	CLA	CHC-C1C	2.84	1.42	1.35
29	G	611	CLA	C3B-C2B	-2.83	1.36	1.40
48	G1	608	CHL	C3B-C2B	-2.83	1.36	1.40
48	g	607	CHL	C4B-NB	2.83	1.37	1.35
48	Y1	606	CHL	C3B-C2B	-2.83	1.36	1.40
29	C	504	CLA	C3B-C2B	-2.83	1.36	1.40
29	g	604	CLA	CHC-C1C	2.83	1.42	1.35
29	r1	610	CLA	CHC-C1C	2.83	1.42	1.35
29	c	510	CLA	C3B-C2B	-2.83	1.36	1.40
48	N1	601	CHL	C4B-NB	2.82	1.37	1.35
29	n	602	CLA	C3B-C2B	-2.82	1.36	1.40
52	r	625	LMT	O3'-C3'	-2.82	1.36	1.43
29	s1	611	CLA	C3B-C2B	-2.81	1.36	1.40
48	s1	606	CHL	C4B-NB	2.81	1.37	1.35
29	B1	608	CLA	C3B-C2B	-2.81	1.36	1.40
29	B	605	CLA	C3B-C2B	-2.81	1.36	1.40
29	S1	602	CLA	CHC-C1C	2.80	1.42	1.35
48	Y1	607	CHL	C3A-C2A	-2.80	1.46	1.54
29	Y	604	CLA	CHC-C1C	2.80	1.42	1.35
29	N	612	CLA	CHC-C1C	2.79	1.42	1.35
29	n	610	CLA	CHC-C1C	2.79	1.42	1.35
29	B1	606	CLA	C3B-C2B	-2.79	1.36	1.40
48	N1	605	CHL	C4B-NB	2.79	1.37	1.35
47	K	101	4RF	O21-C22	2.79	1.42	1.34
48	N1	607	CHL	C4B-NB	2.79	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	D	402	CLA	CHC-C1C	2.79	1.42	1.35
48	G	609	CHL	C3B-C2B	-2.79	1.36	1.40
43	d1	405	PL9	C3-C4	-2.78	1.45	1.49
29	R	610	CLA	CHC-C1C	2.78	1.42	1.35
29	C1	506	CLA	C3B-C2B	-2.78	1.36	1.40
51	g	623	NEX	C1-C6	-2.78	1.49	1.54
29	b	604	CLA	C3B-C2B	-2.78	1.36	1.40
29	Y1	604	CLA	C3B-C2B	-2.78	1.36	1.40
48	R	607	CHL	C4B-NB	2.78	1.37	1.35
48	S1	606	CHL	C3B-C2B	-2.78	1.36	1.40
29	G	604	CLA	C3B-C2B	-2.77	1.36	1.40
29	R	608	CLA	C3B-C2B	-2.77	1.36	1.40
29	g1	604	CLA	CHC-C1C	2.77	1.42	1.35
48	y	609	CHL	C4B-NB	2.77	1.37	1.35
29	R	603	CLA	CHC-C1C	2.77	1.42	1.35
53	R1	626	ERG	C9-C8	2.77	1.58	1.51
53	r1	626	ERG	C9-C8	2.76	1.58	1.51
29	d	402	CLA	CHC-C1C	2.76	1.42	1.35
29	g1	603	CLA	CHC-C1C	2.76	1.42	1.35
29	S1	614	CLA	C3B-C2B	-2.76	1.36	1.40
29	b	615	CLA	CHC-C1C	2.76	1.42	1.35
29	b1	603	CLA	C3B-C2B	-2.76	1.36	1.40
29	y1	614	CLA	C3B-C2B	-2.76	1.36	1.40
29	d	402	CLA	C3B-C2B	-2.76	1.36	1.40
48	G1	606	CHL	C4B-NB	2.76	1.37	1.35
51	s1	623	NEX	C17-C1	-2.75	1.48	1.53
29	b	610	CLA	CHC-C1C	2.75	1.42	1.35
48	Y1	607	CHL	C4B-NB	2.75	1.37	1.35
48	G1	609	CHL	C4B-NB	2.75	1.37	1.35
29	N	602	CLA	CHC-C1C	2.75	1.42	1.35
29	S	609	CLA	C3B-C2B	-2.75	1.36	1.40
29	r	608	CLA	CHC-C1C	2.75	1.42	1.35
29	S	610	CLA	CHC-C1C	2.75	1.42	1.35
29	G1	602	CLA	C3B-C2B	-2.75	1.36	1.40
29	c	507	CLA	C3B-C2B	-2.75	1.36	1.40
29	B1	613	CLA	C3B-C2B	-2.75	1.36	1.40
48	S1	601	CHL	C3B-C2B	-2.75	1.36	1.40
29	N	604	CLA	CHC-C1C	2.74	1.42	1.35
29	b1	604	CLA	CHC-C1C	2.74	1.42	1.35
29	s	610	CLA	CHC-C1C	2.74	1.42	1.35
30	A	409	PHO	CAC-C3C	-2.74	1.47	1.52
29	s	602	CLA	CHC-C1C	2.74	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	n	612	CLA	C3B-C2B	-2.74	1.36	1.40
48	S1	606	CHL	C4B-NB	2.74	1.37	1.35
29	N	612	CLA	C3B-C2B	-2.74	1.36	1.40
53	R	626	ERG	C4-C5	2.73	1.57	1.51
45	h1	101	RRX	C32-C1	2.73	1.59	1.53
29	c	502	CLA	C3B-C2B	-2.73	1.36	1.40
29	r1	603	CLA	CHC-C1C	2.72	1.42	1.35
55	Y1	627	PTY	O7-C6	-2.72	1.39	1.46
45	H	101	RRX	C7-C6	2.72	1.54	1.45
48	n	607	CHL	C4B-NB	2.72	1.37	1.35
29	R	612	CLA	CHC-C1C	2.72	1.41	1.35
29	N1	611	CLA	C3B-C2B	-2.72	1.36	1.40
29	r1	608	CLA	C3B-C2B	-2.72	1.36	1.40
29	N1	612	CLA	C3B-C2B	-2.72	1.36	1.40
29	N	611	CLA	C3B-C2B	-2.72	1.36	1.40
48	g1	606	CHL	C3A-C2A	-2.72	1.46	1.54
29	r	603	CLA	C3B-C2B	-2.72	1.36	1.40
47	i	101	4RF	O21-C22	2.72	1.42	1.34
48	y	607	CHL	C4B-NB	2.72	1.37	1.35
29	n1	612	CLA	CHC-C1C	2.72	1.41	1.35
29	y1	608	CLA	CHC-C1C	2.72	1.41	1.35
29	B	602	CLA	C3B-C2B	-2.71	1.36	1.40
48	n	608	CHL	C4B-NB	2.71	1.37	1.35
29	B	614	CLA	CHC-C1C	2.71	1.41	1.35
47	k1	101	4RF	O21-C22	2.71	1.42	1.34
48	y1	607	CHL	C4B-NB	2.71	1.37	1.35
29	r1	603	CLA	C3B-C2B	-2.71	1.36	1.40
29	Y	614	CLA	C3B-C2B	-2.71	1.36	1.40
29	B	616	CLA	CHC-C1C	2.70	1.41	1.35
29	s	604	CLA	C3B-C2B	-2.70	1.36	1.40
29	S1	603	CLA	CHC-C1C	2.70	1.41	1.35
29	Y1	611	CLA	CHC-C1C	2.70	1.41	1.35
29	S	603	CLA	C3B-C2B	-2.70	1.36	1.40
29	n	611	CLA	C3B-C2B	-2.70	1.36	1.40
45	h	101	RRX	C32-C1	2.70	1.59	1.53
29	g1	610	CLA	CHC-C1C	2.70	1.41	1.35
29	b1	602	CLA	CHC-C1C	2.70	1.41	1.35
48	S	607	CHL	C3B-C2B	-2.70	1.36	1.40
52	R1	625	LMT	O3'-C3'	-2.69	1.36	1.43
29	g	603	CLA	C3B-C2B	-2.69	1.36	1.40
29	b1	603	CLA	CHC-C1C	2.69	1.41	1.35
29	c	504	CLA	CHC-C1C	2.69	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C1	505	CLA	CHC-C1C	2.69	1.41	1.35
52	R	625	LMT	O2'-C2'	-2.69	1.36	1.43
29	Y1	612	CLA	C3B-C2B	-2.69	1.36	1.40
50	G1	622	XAT	O24-C25	-2.68	1.42	1.46
38	S	626	3PH	O31-C31	2.68	1.41	1.33
47	k	101	4RF	O21-C22	2.68	1.41	1.34
29	c1	511	CLA	C3B-C2B	-2.68	1.36	1.40
48	N	608	CHL	C4B-NB	2.68	1.37	1.35
47	K1	101	4RF	O21-C22	2.68	1.41	1.34
29	c1	508	CLA	CHC-C1C	2.68	1.41	1.35
29	s	612	CLA	CHC-C1C	2.68	1.41	1.35
29	c	511	CLA	CHC-C1C	2.68	1.41	1.35
53	r1	626	ERG	C4-C5	2.68	1.57	1.51
29	n	612	CLA	CHC-C1C	2.68	1.41	1.35
29	r	610	CLA	CHC-C1C	2.68	1.41	1.35
29	B1	607	CLA	CHC-C1C	2.67	1.41	1.35
29	b1	602	CLA	C3B-C2B	-2.67	1.36	1.40
29	Y	614	CLA	CHC-C1C	2.67	1.41	1.35
29	S	610	CLA	C3B-C2B	-2.67	1.36	1.40
48	N1	606	CHL	C3B-C2B	-2.67	1.36	1.40
29	b1	610	CLA	CHC-C1C	2.67	1.41	1.35
29	s	614	CLA	CHC-C1C	2.67	1.41	1.35
29	B	617	CLA	C3B-C2B	-2.67	1.36	1.40
29	C	510	CLA	CHC-C1C	2.67	1.41	1.35
29	R1	603	CLA	CHC-C1C	2.67	1.41	1.35
29	r1	602	CLA	CHC-C1C	2.67	1.41	1.35
29	b1	608	CLA	CHC-C1C	2.67	1.41	1.35
29	s1	604	CLA	CHC-C1C	2.67	1.41	1.35
29	s	613	CLA	C3B-C2B	-2.66	1.36	1.40
29	N	603	CLA	CHC-C1C	2.66	1.41	1.35
53	R1	626	ERG	C14-C8	2.66	1.58	1.51
29	G	613	CLA	CHC-C1C	2.66	1.41	1.35
29	D1	403	CLA	CHC-C1C	2.66	1.41	1.35
29	R	610	CLA	C1C-C2C	2.66	1.49	1.44
29	b1	605	CLA	CHC-C1C	2.66	1.41	1.35
29	r1	604	CLA	CHC-C1C	2.66	1.41	1.35
38	s	626	3PH	O31-C31	2.66	1.41	1.33
29	n	614	CLA	CHC-C1C	2.66	1.41	1.35
29	g	604	CLA	C3B-C2B	-2.66	1.36	1.40
29	c1	513	CLA	CHC-C1C	2.66	1.41	1.35
29	c1	505	CLA	CHC-C1C	2.66	1.41	1.35
48	s	606	CHL	C4B-NB	2.66	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	y1	614	CLA	CHC-C1C	2.65	1.41	1.35
29	c1	512	CLA	CHC-C1C	2.65	1.41	1.35
29	D1	402	CLA	CHC-C1C	2.65	1.41	1.35
29	g	602	CLA	CHC-C1C	2.65	1.41	1.35
29	G1	613	CLA	CHC-C1C	2.65	1.41	1.35
29	y	602	CLA	C3B-C2B	-2.65	1.36	1.40
29	r1	610	CLA	C1C-C2C	2.65	1.49	1.44
29	R1	603	CLA	C3B-C2B	-2.65	1.36	1.40
29	n1	610	CLA	CHC-C1C	2.65	1.41	1.35
29	c	512	CLA	CHC-C1C	2.64	1.41	1.35
29	Y1	611	CLA	C3B-C2B	-2.64	1.36	1.40
29	n	604	CLA	C3B-C2B	-2.64	1.36	1.40
29	g	613	CLA	CHC-C1C	2.64	1.41	1.35
29	B1	607	CLA	C3B-C2B	-2.64	1.36	1.40
48	g1	607	CHL	C4B-NB	2.64	1.37	1.35
29	a1	406	CLA	CHC-C1C	2.64	1.41	1.35
29	n1	614	CLA	CHC-C1C	2.64	1.41	1.35
29	S1	609	CLA	C3B-C2B	-2.64	1.36	1.40
29	r	609	CLA	CHC-C1C	2.64	1.41	1.35
29	B1	604	CLA	CHC-C1C	2.64	1.41	1.35
29	S1	610	CLA	CHC-C1C	2.63	1.41	1.35
29	r	612	CLA	C3B-C2B	-2.63	1.36	1.40
29	y1	612	CLA	CHC-C1C	2.63	1.41	1.35
29	N	613	CLA	C3B-C2B	-2.63	1.36	1.40
29	S	602	CLA	C3B-C2B	-2.63	1.36	1.40
29	S	609	CLA	CHC-C1C	2.63	1.41	1.35
29	S1	609	CLA	CHC-C1C	2.63	1.41	1.35
29	r	602	CLA	CHC-C1C	2.63	1.41	1.35
29	G	603	CLA	CHC-C1C	2.62	1.41	1.35
29	n1	610	CLA	C3B-C2B	-2.62	1.36	1.40
29	n	603	CLA	CHC-C1C	2.62	1.41	1.35
29	B1	603	CLA	CHC-C1C	2.62	1.41	1.35
48	y1	609	CHL	C4B-NB	2.62	1.37	1.35
29	g1	602	CLA	CHC-C1C	2.62	1.41	1.35
29	s1	617	CLA	CHC-C1C	2.62	1.41	1.35
48	n1	609	CHL	C4B-NB	2.62	1.37	1.35
29	n	604	CLA	CHC-C1C	2.62	1.41	1.35
29	c1	504	CLA	C3B-C2B	-2.62	1.36	1.40
29	S1	617	CLA	CHC-C1C	2.62	1.41	1.35
29	b1	614	CLA	CHC-C1C	2.62	1.41	1.35
29	y1	603	CLA	C3B-C2B	-2.62	1.36	1.40
29	y1	613	CLA	CHC-C1C	2.62	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	G	607	CHL	C4B-NB	2.62	1.37	1.35
29	S1	612	CLA	CHC-C1C	2.61	1.41	1.35
29	s	605	CLA	CHC-C1C	2.61	1.41	1.35
29	C	511	CLA	CHC-C1C	2.61	1.41	1.35
29	y	614	CLA	CHC-C1C	2.61	1.41	1.35
29	b	602	CLA	CHC-C1C	2.61	1.41	1.35
48	n	609	CHL	C4B-NB	2.61	1.37	1.35
29	B1	602	CLA	C3B-C2B	-2.61	1.36	1.40
52	r	625	LMT	O2'-C2'	-2.61	1.36	1.43
48	Y	609	CHL	C3B-C2B	-2.61	1.36	1.40
29	R	602	CLA	CHC-C1C	2.60	1.41	1.35
48	N1	608	CHL	C4B-NB	2.60	1.37	1.35
29	c1	509	CLA	CHC-C1C	2.60	1.41	1.35
29	Y1	612	CLA	CHC-C1C	2.60	1.41	1.35
29	B	607	CLA	CHC-C1C	2.60	1.41	1.35
29	y	611	CLA	CHC-C1C	2.60	1.41	1.35
29	r1	609	CLA	CHC-C1C	2.60	1.41	1.35
29	C	513	CLA	CHC-C1C	2.60	1.41	1.35
30	A	408	PHO	CAC-C3C	-2.60	1.47	1.52
29	C	505	CLA	C3B-C2B	-2.60	1.36	1.40
55	y1	627	PTY	O7-C6	-2.60	1.40	1.46
29	a	405	CLA	CHC-C1C	2.60	1.41	1.35
55	Y	627	PTY	O7-C8	2.60	1.41	1.35
45	H1	101	RRX	C32-C1	2.60	1.58	1.53
29	c1	513	CLA	C1C-C2C	2.59	1.49	1.44
29	S	603	CLA	CHC-C1C	2.59	1.41	1.35
29	r	603	CLA	CHC-C1C	2.59	1.41	1.35
29	c	501	CLA	CHC-C1C	2.59	1.41	1.35
33	D1	411	LMG	C37-C36	-2.59	1.33	1.51
29	b1	609	CLA	C3B-C2B	-2.59	1.36	1.40
29	b	609	CLA	CHC-C1C	2.59	1.41	1.35
29	B	615	CLA	CHC-C1C	2.59	1.41	1.35
29	c1	507	CLA	CHC-C1C	2.59	1.41	1.35
45	h	101	RRX	C7-C6	2.59	1.54	1.45
30	a	408	PHO	CAC-C3C	-2.59	1.47	1.52
29	C	508	CLA	CHC-C1C	2.59	1.41	1.35
50	g1	622	XAT	O24-C25	-2.59	1.42	1.46
29	d1	402	CLA	CHC-C1C	2.59	1.41	1.35
29	B1	610	CLA	CHC-C1C	2.59	1.41	1.35
29	c	513	CLA	CHC-C1C	2.58	1.41	1.35
29	D	403	CLA	CHC-C1C	2.58	1.41	1.35
29	r1	608	CLA	CHC-C1C	2.58	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
55	Y	626	PTY	O7-C6	-2.58	1.40	1.46
29	R1	609	CLA	CHC-C1C	2.58	1.41	1.35
30	a	409	PHO	CAC-C3C	-2.58	1.47	1.52
29	S1	605	CLA	CHC-C1C	2.58	1.41	1.35
29	R	612	CLA	C3B-C2B	-2.58	1.36	1.40
29	g1	614	CLA	CHC-C1C	2.58	1.41	1.35
48	S	601	CHL	CHC-C1C	2.58	1.41	1.35
29	s1	609	CLA	CHC-C1C	2.58	1.41	1.35
29	C1	501	CLA	C3B-C2B	-2.58	1.36	1.40
43	D	405	PL9	C7-C8	-2.58	1.46	1.50
53	R	626	ERG	C14-C8	2.58	1.58	1.51
29	N	603	CLA	C3B-C2B	-2.57	1.36	1.40
43	D1	405	PL9	C53-C6	-2.57	1.45	1.50
29	G1	610	CLA	CHC-C1C	2.57	1.41	1.35
55	y	626	PTY	O4-C30	2.57	1.40	1.33
29	s	611	CLA	CHC-C1C	2.57	1.41	1.35
29	g1	613	CLA	C3B-C2B	-2.57	1.36	1.40
29	G	602	CLA	CHC-C1C	2.57	1.41	1.35
29	c1	503	CLA	CHC-C1C	2.57	1.41	1.35
29	b	603	CLA	CHC-C1C	2.57	1.41	1.35
29	B1	616	CLA	CHC-C1C	2.57	1.41	1.35
29	B	603	CLA	CHC-C1C	2.57	1.41	1.35
29	B1	605	CLA	C3B-C2B	-2.56	1.36	1.40
29	S	604	CLA	CHC-C1C	2.56	1.41	1.35
29	N1	610	CLA	CHC-C1C	2.56	1.41	1.35
29	Y	603	CLA	CHC-C1C	2.56	1.41	1.35
29	S	612	CLA	CHC-C1C	2.56	1.41	1.35
29	n	613	CLA	CHC-C1C	2.56	1.41	1.35
29	G	614	CLA	CHC-C1C	2.56	1.41	1.35
29	b	613	CLA	CHC-C1C	2.56	1.41	1.35
29	d	403	CLA	CHC-C1C	2.56	1.41	1.35
29	g	612	CLA	CHC-C1C	2.55	1.41	1.35
29	s	605	CLA	C3B-C2B	-2.55	1.36	1.40
29	s1	614	CLA	CHC-C1C	2.55	1.41	1.35
29	b1	609	CLA	CHC-C1C	2.55	1.41	1.35
29	b	611	CLA	C3B-C2B	-2.55	1.36	1.40
29	b1	602	CLA	C1C-C2C	2.55	1.49	1.44
52	R	625	LMT	O2B-C2B	-2.55	1.37	1.43
29	C1	510	CLA	CHC-C1C	2.55	1.41	1.35
29	b1	612	CLA	CHC-C1C	2.55	1.41	1.35
29	C1	507	CLA	C3B-C2B	-2.55	1.36	1.40
29	r	604	CLA	C3B-C2B	-2.55	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
50	r	621	XAT	O24-C25	-2.54	1.42	1.46
29	G	610	CLA	CHC-C1C	2.54	1.41	1.35
29	s1	614	CLA	C3B-C2B	-2.54	1.36	1.40
38	b1	624	3PH	O31-C31	2.54	1.40	1.33
33	D	411	LMG	C37-C36	-2.54	1.33	1.51
29	b	616	CLA	CHC-C1C	2.54	1.41	1.35
29	b	607	CLA	CHC-C1C	2.54	1.41	1.35
48	N	607	CHL	C4B-NB	2.54	1.37	1.35
29	Y	612	CLA	C3B-C2B	-2.54	1.36	1.40
29	g	610	CLA	C3B-C2B	-2.54	1.36	1.40
29	y1	611	CLA	CHC-C1C	2.54	1.41	1.35
29	y	613	CLA	CHC-C1C	2.54	1.41	1.35
44	f1	101	HEM	FE-ND	2.54	2.09	1.96
29	R1	610	CLA	CHC-C1C	2.54	1.41	1.35
29	Y1	603	CLA	CHC-C1C	2.54	1.41	1.35
29	S	604	CLA	C3B-C2B	-2.54	1.36	1.40
33	d	411	LMG	C37-C36	-2.54	1.33	1.51
29	G	612	CLA	CHC-C1C	2.53	1.41	1.35
29	c1	510	CLA	CHC-C1C	2.53	1.41	1.35
48	G	601	CHL	C3B-C2B	-2.53	1.36	1.40
29	Y1	604	CLA	CHC-C1C	2.53	1.41	1.35
29	n	611	CLA	CHC-C1C	2.53	1.41	1.35
29	N	614	CLA	C3B-C2B	-2.53	1.36	1.40
48	G	608	CHL	C3B-C2B	-2.53	1.36	1.40
38	t1	101	3PH	O31-C31	2.53	1.40	1.33
48	y	609	CHL	C3B-C2B	-2.53	1.36	1.40
29	S	614	CLA	CHC-C1C	2.53	1.41	1.35
48	R1	606	CHL	C3B-C2B	-2.53	1.36	1.40
29	C	504	CLA	CHC-C1C	2.53	1.41	1.35
29	b	617	CLA	CHC-C1C	2.53	1.41	1.35
29	D1	402	CLA	C3B-C2B	-2.53	1.36	1.40
29	A	410	CLA	CHC-C1C	2.52	1.41	1.35
29	B1	604	CLA	C3B-C2B	-2.52	1.36	1.40
29	B1	608	CLA	CHC-C1C	2.52	1.41	1.35
47	I1	102	4RF	O21-C22	2.52	1.41	1.34
29	S1	611	CLA	C3B-C2B	-2.52	1.36	1.40
29	S1	613	CLA	CHC-C1C	2.52	1.41	1.35
53	R	626	ERG	C9-C8	2.52	1.58	1.51
54	S1	625	LPX	P1-O2	2.52	1.69	1.59
29	B1	613	CLA	CHC-C1C	2.52	1.41	1.35
29	C1	507	CLA	CHC-C1C	2.52	1.41	1.35
29	b1	607	CLA	CHC-C1C	2.52	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Y	612	CLA	CHC-C1C	2.52	1.41	1.35
29	S	617	CLA	CHC-C1C	2.51	1.41	1.35
55	Y	626	PTY	O4-C30	2.51	1.40	1.33
29	Y1	608	CLA	CHC-C1C	2.51	1.41	1.35
29	s1	612	CLA	CHC-C1C	2.51	1.41	1.35
33	d1	411	LMG	C37-C36	-2.51	1.33	1.51
29	n1	613	CLA	CHC-C1C	2.51	1.41	1.35
29	A	407	CLA	C3B-C2B	-2.51	1.36	1.40
29	B1	612	CLA	CHC-C1C	2.51	1.41	1.35
29	g1	612	CLA	CHC-C1C	2.51	1.41	1.35
29	y	602	CLA	CHC-C1C	2.51	1.41	1.35
29	N1	613	CLA	CHC-C1C	2.51	1.41	1.35
29	S	611	CLA	CHC-C1C	2.51	1.41	1.35
50	g	622	XAT	O24-C25	-2.51	1.42	1.46
29	B	612	CLA	CHC-C1C	2.51	1.41	1.35
29	R1	602	CLA	CHC-C1C	2.51	1.41	1.35
29	g	603	CLA	CHC-C1C	2.50	1.41	1.35
29	A	405	CLA	CHC-C1C	2.50	1.41	1.35
29	C1	502	CLA	CHC-C1C	2.50	1.41	1.35
29	y	604	CLA	CHC-C1C	2.50	1.41	1.35
29	y	610	CLA	CHC-C1C	2.50	1.41	1.35
29	B	604	CLA	CHC-C1C	2.50	1.41	1.35
48	n	605	CHL	C3B-C2B	-2.50	1.36	1.40
38	B1	624	3PH	O31-C31	2.50	1.40	1.33
29	s	613	CLA	CHC-C1C	2.50	1.41	1.35
29	g1	613	CLA	CHC-C1C	2.50	1.41	1.35
29	C1	508	CLA	CHC-C1C	2.50	1.41	1.35
55	Y1	626	PTY	O7-C8	2.50	1.41	1.34
29	C	503	CLA	C3B-C2B	-2.50	1.36	1.40
29	C	502	CLA	CHC-C1C	2.50	1.41	1.35
29	B1	614	CLA	C3B-C2B	-2.50	1.36	1.40
38	b	624	3PH	O21-C2	-2.49	1.40	1.46
29	B	613	CLA	C3D-C4D	-2.49	1.38	1.44
29	G1	612	CLA	CHC-C1C	2.49	1.41	1.35
48	G1	609	CHL	C3B-C2B	-2.49	1.36	1.40
48	Y	601	CHL	C4B-NB	2.49	1.37	1.35
29	A1	405	CLA	CHC-C1C	2.49	1.41	1.35
29	s1	603	CLA	CHC-C1C	2.49	1.41	1.35
45	H	101	RRX	C32-C1	2.49	1.58	1.53
29	s	609	CLA	CHC-C1C	2.49	1.41	1.35
29	c1	502	CLA	CHC-C1C	2.49	1.41	1.35
29	c	509	CLA	CHC-C1C	2.49	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c	508	CLA	CHC-C1C	2.48	1.41	1.35
55	y	627	PTY	O7-C8	2.48	1.40	1.35
29	g	614	CLA	CHC-C1C	2.48	1.41	1.35
49	N1	621	LUT	C1-C6	-2.48	1.50	1.53
29	B1	615	CLA	CHC-C1C	2.48	1.41	1.35
31	B	618	BCR	C1-C6	-2.48	1.50	1.53
55	y	626	PTY	O7-C6	-2.48	1.40	1.46
38	T	101	3PH	O21-C21	2.48	1.41	1.34
29	a1	410	CLA	CHC-C1C	2.48	1.41	1.35
29	N	604	CLA	C3B-C2B	-2.48	1.36	1.40
29	Y	602	CLA	C3B-C2B	-2.48	1.36	1.40
29	Y1	610	CLA	CHC-C1C	2.48	1.41	1.35
29	y1	604	CLA	C3B-C2B	-2.48	1.36	1.40
29	N1	614	CLA	CHC-C1C	2.48	1.41	1.35
29	A1	406	CLA	C4B-NB	-2.48	1.33	1.35
29	C1	502	CLA	C3B-C2B	-2.48	1.36	1.40
29	B	610	CLA	CHC-C1C	2.48	1.41	1.35
29	C	505	CLA	CHC-C1C	2.48	1.41	1.35
38	S1	626	3PH	O21-C2	-2.48	1.40	1.46
29	s1	610	CLA	CHC-C1C	2.47	1.41	1.35
29	r1	609	CLA	C3B-C2B	-2.47	1.36	1.40
29	N	611	CLA	CHC-C1C	2.47	1.41	1.35
29	r	612	CLA	CHC-C1C	2.47	1.41	1.35
29	N	610	CLA	CHC-C1C	2.47	1.41	1.35
52	R	625	LMT	O3B-C3B	-2.47	1.37	1.43
29	b1	608	CLA	C1C-C2C	2.47	1.49	1.44
29	n	602	CLA	CHC-C1C	2.47	1.41	1.35
29	y	603	CLA	CHC-C1C	2.47	1.41	1.35
48	s1	607	CHL	C3B-C2B	-2.46	1.36	1.40
29	s1	613	CLA	C1C-C2C	2.46	1.49	1.44
29	N	614	CLA	CHC-C1C	2.46	1.41	1.35
29	b	609	CLA	C3B-C2B	-2.46	1.37	1.40
31	C1	514	BCR	C12-C13	-2.46	1.40	1.45
29	B	608	CLA	CHC-C1C	2.46	1.41	1.35
43	d	405	PL9	C26-C24	-2.46	1.46	1.51
38	s1	626	3PH	O21-C2	-2.46	1.40	1.46
29	Y	611	CLA	CHC-C1C	2.46	1.41	1.35
29	Y1	614	CLA	CHC-C1C	2.46	1.41	1.35
43	D	405	PL9	C53-C6	-2.46	1.45	1.50
29	y1	610	CLA	CHC-C1C	2.46	1.41	1.35
37	b1	623	DGD	O5D-C1E	2.46	1.44	1.40
29	y	612	CLA	CHC-C1C	2.46	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	508	CLA	C3B-C2B	-2.45	1.37	1.40
29	c1	505	CLA	C3B-C2B	-2.45	1.37	1.40
29	G1	604	CLA	CHC-C1C	2.45	1.41	1.35
48	Y	607	CHL	C4B-NB	2.45	1.37	1.35
29	R	603	CLA	C3B-C2B	-2.45	1.37	1.40
29	B	602	CLA	CHC-C1C	2.45	1.41	1.35
29	C	503	CLA	CHC-C1C	2.45	1.41	1.35
29	y	608	CLA	CHC-C1C	2.45	1.41	1.35
29	C	508	CLA	C3D-C4D	-2.45	1.38	1.44
29	R1	608	CLA	C3B-C2B	-2.45	1.37	1.40
29	s	604	CLA	CHC-C1C	2.45	1.41	1.35
29	b	604	CLA	CHC-C1C	2.45	1.41	1.35
29	G1	614	CLA	CHC-C1C	2.45	1.41	1.35
29	n1	611	CLA	CHC-C1C	2.44	1.41	1.35
29	G1	604	CLA	C3B-C2B	-2.44	1.37	1.40
29	R1	612	CLA	C3B-C2B	-2.44	1.37	1.40
29	s1	611	CLA	CHC-C1C	2.44	1.41	1.35
29	B1	611	CLA	C3B-C2B	-2.44	1.37	1.40
29	B	611	CLA	C3B-C2B	-2.44	1.37	1.40
29	s	603	CLA	CHC-C1C	2.44	1.41	1.35
29	a	407	CLA	C3B-C2B	-2.44	1.37	1.40
29	b1	616	CLA	C3B-C2B	-2.44	1.37	1.40
29	n1	603	CLA	C3B-C2B	-2.44	1.37	1.40
29	R1	608	CLA	CHC-C1C	2.44	1.41	1.35
29	N1	611	CLA	CHC-C1C	2.44	1.41	1.35
29	Y1	602	CLA	CHC-C1C	2.44	1.41	1.35
29	c1	506	CLA	CHC-C1C	2.44	1.41	1.35
31	c	515	BCR	C12-C13	-2.44	1.40	1.45
29	s	617	CLA	CHC-C1C	2.44	1.41	1.35
29	S1	614	CLA	CHC-C1C	2.44	1.41	1.35
29	y1	614	CLA	C1C-C2C	2.44	1.49	1.44
29	S1	603	CLA	C1C-C2C	2.44	1.49	1.44
29	S1	602	CLA	C3B-C2B	-2.44	1.37	1.40
29	G	611	CLA	CHC-C1C	2.44	1.41	1.35
29	n1	613	CLA	C3B-C2B	-2.43	1.37	1.40
48	r1	607	CHL	C3B-C2B	-2.43	1.37	1.40
48	N	609	CHL	C4B-NB	2.43	1.37	1.35
29	B1	609	CLA	CHC-C1C	2.43	1.41	1.35
29	C	501	CLA	CHC-C1C	2.43	1.41	1.35
29	s	602	CLA	C3B-C2B	-2.43	1.37	1.40
29	d	402	CLA	C3D-C4D	-2.43	1.38	1.44
38	t	101	3PH	O31-C31	2.43	1.40	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
43	d	405	PL9	C46-C44	-2.43	1.46	1.51
29	Y1	613	CLA	CHC-C1C	2.43	1.41	1.35
29	g1	614	CLA	C1B-NB	2.43	1.37	1.35
29	s1	605	CLA	CHC-C1C	2.43	1.41	1.35
29	b	608	CLA	CHC-C1C	2.43	1.41	1.35
29	C	502	CLA	C3B-C2B	-2.42	1.37	1.40
29	D	403	CLA	C3B-C2B	-2.42	1.37	1.40
29	d1	402	CLA	C3B-C2B	-2.42	1.37	1.40
50	y	622	XAT	O24-C25	-2.42	1.42	1.46
50	Y1	622	XAT	O24-C25	-2.42	1.42	1.46
29	Y1	603	CLA	C3B-C2B	-2.42	1.37	1.40
29	c	503	CLA	CHC-C1C	2.42	1.41	1.35
29	c	508	CLA	C3B-C2B	-2.42	1.37	1.40
29	S	605	CLA	CHC-C1C	2.42	1.41	1.35
29	G	612	CLA	C3B-C2B	-2.42	1.37	1.40
38	T	101	3PH	O31-C31	2.42	1.40	1.33
29	b	607	CLA	C3B-C2B	-2.42	1.37	1.40
50	n	622	XAT	O24-C25	-2.42	1.42	1.46
29	S1	604	CLA	CHC-C1C	2.41	1.41	1.35
29	s1	605	CLA	C1B-NB	2.41	1.37	1.35
29	g	610	CLA	CHC-C1C	2.41	1.41	1.35
29	R1	610	CLA	C1C-C2C	2.41	1.49	1.44
29	c1	504	CLA	CHC-C1C	2.41	1.41	1.35
48	N	601	CHL	C3B-C2B	-2.41	1.37	1.40
29	a1	407	CLA	CHC-C1C	2.41	1.41	1.35
52	R1	625	LMT	O3B-C3B	-2.41	1.37	1.43
29	N	613	CLA	CHC-C1C	2.41	1.41	1.35
29	G1	603	CLA	CHC-C1C	2.41	1.41	1.35
29	r	604	CLA	CHC-C1C	2.41	1.41	1.35
29	c	505	CLA	C3B-C2B	-2.41	1.37	1.40
29	b1	613	CLA	C3B-C2B	-2.41	1.37	1.40
52	r	625	LMT	O3B-C3B	-2.41	1.37	1.43
29	C1	511	CLA	CHC-C1C	2.40	1.41	1.35
29	R	602	CLA	C3B-C2B	-2.40	1.37	1.40
29	r	609	CLA	C3B-C2B	-2.40	1.37	1.40
29	B1	602	CLA	CHC-C1C	2.40	1.41	1.35
29	a	405	CLA	C3D-C4D	-2.40	1.38	1.44
29	B	617	CLA	CHC-C1C	2.40	1.41	1.35
50	G	622	XAT	O24-C25	-2.40	1.42	1.46
29	g	612	CLA	C3B-C2B	-2.40	1.37	1.40
44	f1	101	HEM	CAA-C2A	2.40	1.55	1.52
30	a	408	PHO	CBD-CGD	-2.39	1.49	1.52

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	g	611	CLA	C3B-C2B	-2.39	1.37	1.40
29	R1	604	CLA	CHC-C1C	2.39	1.41	1.35
29	a	410	CLA	CHC-C1C	2.39	1.41	1.35
38	S1	626	3PH	O31-C31	2.39	1.40	1.33
29	B	609	CLA	CHC-C1C	2.39	1.41	1.35
38	B	624	3PH	O31-C31	2.39	1.40	1.33
29	g1	603	CLA	C3B-C2B	-2.39	1.37	1.40
29	B	611	CLA	CHC-C1C	2.39	1.41	1.35
29	Y	608	CLA	C3B-C2B	-2.39	1.37	1.40
29	S1	605	CLA	C3B-C2B	-2.39	1.37	1.40
29	S1	610	CLA	C3B-C2B	-2.39	1.37	1.40
29	b	613	CLA	C3D-C4D	-2.39	1.38	1.44
29	R	604	CLA	CHC-C1C	2.39	1.41	1.35
38	T1	101	3PH	O31-C31	2.39	1.40	1.33
29	r1	612	CLA	C1C-C2C	2.39	1.49	1.44
29	C	507	CLA	C3B-C2B	-2.39	1.37	1.40
48	y	606	CHL	C3B-C2B	-2.39	1.37	1.40
29	A	407	CLA	CHC-C1C	2.38	1.41	1.35
29	G1	611	CLA	CHC-C1C	2.38	1.41	1.35
29	b1	615	CLA	CHC-C1C	2.38	1.41	1.35
29	s1	609	CLA	C3B-C2B	-2.38	1.37	1.40
29	c1	511	CLA	CHC-C1C	2.38	1.41	1.35
52	r	625	LMT	O2B-C2B	-2.38	1.37	1.43
29	g1	604	CLA	C1C-C2C	2.38	1.49	1.44
39	C	524	DGA	OG2-CG2	-2.38	1.40	1.46
48	r1	606	CHL	C3A-C2A	-2.38	1.47	1.54
38	s1	626	3PH	O31-C31	2.38	1.40	1.33
29	S	602	CLA	CHC-C1C	2.38	1.41	1.35
29	C	512	CLA	CHC-C1C	2.38	1.41	1.35
29	c1	501	CLA	CHC-C1C	2.38	1.41	1.35
29	N1	612	CLA	CHC-C1C	2.38	1.41	1.35
45	h	101	RRX	C35-C13	2.38	1.55	1.50
55	y1	626	PTY	O7-C6	-2.38	1.40	1.46
29	a	407	CLA	CHC-C1C	2.38	1.41	1.35
53	r1	626	ERG	C14-C8	2.37	1.57	1.51
52	r1	625	LMT	O2'-C2'	-2.37	1.37	1.43
45	h1	101	RRX	C35-C13	2.37	1.55	1.50
29	R1	609	CLA	C1B-NB	2.37	1.37	1.35
29	R	612	CLA	C1C-C2C	2.37	1.49	1.44
29	D	402	CLA	C3D-C4D	-2.37	1.38	1.44
29	g1	612	CLA	C3B-C2B	-2.37	1.37	1.40
29	y1	604	CLA	C1B-NB	2.37	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	B	620	C7Z	C20-C13	2.37	1.55	1.50
29	C1	501	CLA	CHC-C1C	2.37	1.41	1.35
29	S	614	CLA	C3B-C2B	-2.36	1.37	1.40
29	R	609	CLA	CHC-C1C	2.36	1.41	1.35
29	s1	605	CLA	C1A-CHA	2.36	1.52	1.43
29	Y	608	CLA	CHC-C1C	2.36	1.41	1.35
44	f1	101	HEM	FE-NB	2.36	2.08	1.96
29	c	510	CLA	CHC-C1C	2.36	1.41	1.35
29	b	614	CLA	CHC-C1C	2.36	1.41	1.35
29	b	605	CLA	C1A-CHA	2.36	1.52	1.43
29	A1	410	CLA	CHC-C1C	2.36	1.41	1.35
29	G1	611	CLA	C3B-C2B	-2.36	1.37	1.40
29	g1	603	CLA	C1C-C2C	2.36	1.49	1.44
29	y	608	CLA	C3B-C2B	-2.36	1.37	1.40
29	S1	604	CLA	C3B-C2B	-2.36	1.37	1.40
48	N1	609	CHL	C4B-NB	2.36	1.37	1.35
29	B	613	CLA	CHC-C1C	2.36	1.41	1.35
29	b	604	CLA	C3D-C4D	-2.36	1.38	1.44
29	r	602	CLA	C3B-C2B	-2.36	1.37	1.40
29	A1	406	CLA	CHC-C1C	2.35	1.41	1.35
29	s1	611	CLA	C1A-CHA	2.35	1.52	1.43
29	R1	612	CLA	C1A-CHA	2.35	1.52	1.43
29	B	612	CLA	C3B-C2B	-2.35	1.37	1.40
29	S	613	CLA	CHC-C1C	2.35	1.41	1.35
29	b	606	CLA	CHC-C1C	2.35	1.41	1.35
29	n1	614	CLA	C3B-C2B	-2.35	1.37	1.40
55	Y1	626	PTY	O7-C6	-2.35	1.40	1.46
44	f	101	HEM	FE-NB	2.35	2.08	1.96
38	b1	624	3PH	O21-C2	-2.35	1.40	1.46
36	B1	620	C7Z	C20-C13	2.35	1.55	1.50
55	Y1	626	PTY	O4-C30	2.35	1.40	1.33
29	g1	602	CLA	C1C-C2C	2.35	1.49	1.44
47	I	102	4RF	O21-C22	2.35	1.40	1.34
36	b	620	C7Z	C20-C13	2.35	1.55	1.50
48	y	601	CHL	C4B-NB	2.35	1.37	1.35
29	C1	503	CLA	C1C-C2C	2.35	1.49	1.44
36	b1	620	C7Z	C20-C13	2.35	1.55	1.50
29	G	604	CLA	CHC-C1C	2.35	1.41	1.35
29	G1	602	CLA	C4B-NB	-2.35	1.33	1.35
29	N1	603	CLA	CHC-C1C	2.35	1.41	1.35
38	B	624	3PH	O21-C2	-2.35	1.40	1.46
29	S1	611	CLA	CHC-C1C	2.34	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
45	H1	101	RRX	C35-C13	2.34	1.55	1.50
38	b	624	3PH	O31-C31	2.34	1.40	1.33
48	S	601	CHL	C3A-C2A	-2.34	1.47	1.54
29	B	606	CLA	CHC-C1C	2.34	1.41	1.35
29	N	604	CLA	C3D-C4D	-2.34	1.38	1.44
29	n1	604	CLA	CHC-C1C	2.34	1.41	1.35
54	s1	625	LPX	P1-O2	2.34	1.68	1.59
29	b1	606	CLA	CHC-C1C	2.34	1.41	1.35
30	a	409	PHO	CMD-C2D	-2.34	1.46	1.51
29	G	604	CLA	C3D-C4D	-2.34	1.38	1.44
29	a	406	CLA	CHC-C1C	2.34	1.41	1.35
29	B1	617	CLA	C3B-C2B	-2.34	1.37	1.40
29	B1	603	CLA	C3B-C2B	-2.33	1.37	1.40
29	Y1	612	CLA	C1C-C2C	2.33	1.49	1.44
29	B	605	CLA	CHC-C1C	2.33	1.40	1.35
29	c	512	CLA	C1C-C2C	2.33	1.49	1.44
29	r1	602	CLA	C3B-C2B	-2.33	1.37	1.40
29	B1	603	CLA	C1A-CHA	2.33	1.52	1.43
29	n	602	CLA	C1C-C2C	2.33	1.49	1.44
30	A	409	PHO	CMD-C2D	-2.33	1.46	1.51
29	g	614	CLA	C3B-C2B	-2.33	1.37	1.40
29	c1	511	CLA	C1A-CHA	2.33	1.52	1.43
29	B1	606	CLA	CHC-C1C	2.33	1.40	1.35
38	B1	624	3PH	O21-C2	-2.33	1.40	1.46
29	b1	614	CLA	C3B-C2B	-2.33	1.37	1.40
29	B1	617	CLA	CHC-C1C	2.33	1.40	1.35
29	C	510	CLA	C3D-C4D	-2.33	1.38	1.44
55	y1	626	PTY	O4-C1	-2.32	1.39	1.45
48	n	605	CHL	C3A-C2A	-2.32	1.48	1.54
48	N	605	CHL	C3B-C2B	-2.32	1.37	1.40
29	Y1	614	CLA	C3D-C4D	-2.32	1.38	1.44
29	B1	614	CLA	CHC-C1C	2.32	1.40	1.35
29	g1	611	CLA	C1C-C2C	2.32	1.49	1.44
29	b	603	CLA	C3B-C2B	-2.32	1.37	1.40
29	b	617	CLA	C3B-C2B	-2.32	1.37	1.40
50	r1	621	XAT	O24-C25	-2.32	1.42	1.46
29	R1	609	CLA	C3B-C2B	-2.32	1.37	1.40
48	y1	605	CHL	C3B-C2B	-2.32	1.37	1.40
36	b1	620	C7Z	C40-C33	2.32	1.55	1.50
29	S1	603	CLA	C3B-C2B	-2.32	1.37	1.40
38	S	626	3PH	O21-C21	2.32	1.40	1.34
29	A1	405	CLA	C3B-C2B	-2.31	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C1	507	CLA	C3D-C4D	-2.31	1.39	1.44
29	c1	505	CLA	C1A-CHA	2.31	1.52	1.43
29	C1	509	CLA	C3B-C2B	-2.31	1.37	1.40
48	r	606	CHL	C3B-C2B	-2.31	1.37	1.40
29	B1	615	CLA	C1C-C2C	2.31	1.49	1.44
29	y1	603	CLA	CHC-C1C	2.31	1.40	1.35
29	n1	603	CLA	CHC-C1C	2.31	1.40	1.35
29	y1	614	CLA	C3D-C4D	-2.31	1.39	1.44
29	B1	607	CLA	C3D-C4D	-2.31	1.39	1.44
29	r1	608	CLA	C1A-CHA	2.31	1.52	1.43
29	s	609	CLA	C1A-CHA	2.31	1.52	1.43
29	c	506	CLA	C3B-C2B	-2.31	1.37	1.40
29	C	509	CLA	C3B-C2B	-2.30	1.37	1.40
29	B1	605	CLA	CHC-C1C	2.30	1.40	1.35
29	Y1	608	CLA	C1C-C2C	2.30	1.49	1.44
29	n	614	CLA	C1C-C2C	2.30	1.49	1.44
29	C1	508	CLA	C3B-C2B	-2.30	1.37	1.40
50	R1	621	XAT	O24-C25	-2.30	1.42	1.46
30	a	408	PHO	CMC-C2C	-2.30	1.46	1.51
29	Y	613	CLA	CHC-C1C	2.30	1.40	1.35
29	C	509	CLA	CHC-C1C	2.30	1.40	1.35
29	R	602	CLA	C1C-C2C	2.30	1.49	1.44
29	s	603	CLA	C1A-CHA	2.30	1.52	1.43
29	r	603	CLA	C1C-C2C	2.30	1.49	1.44
55	y1	626	PTY	O4-C30	2.30	1.40	1.33
29	y1	603	CLA	C3D-C4D	-2.30	1.39	1.44
29	C	509	CLA	C3D-C4D	-2.30	1.39	1.44
36	b	620	C7Z	C18-C5	2.30	1.54	1.50
55	y	627	PTY	O7-C6	-2.30	1.40	1.46
29	C	513	CLA	C3B-C2B	-2.30	1.37	1.40
29	r	612	CLA	C1A-CHA	2.30	1.52	1.43
29	N	613	CLA	C1A-CHA	2.29	1.52	1.43
29	B1	608	CLA	C1A-CHA	2.29	1.52	1.43
29	S	614	CLA	C3D-C4D	-2.29	1.39	1.44
29	n1	611	CLA	C3B-C2B	-2.29	1.37	1.40
29	y1	608	CLA	C3B-C2B	-2.29	1.37	1.40
29	Y	610	CLA	CHC-C1C	2.29	1.40	1.35
55	y1	626	PTY	O7-C8	2.29	1.40	1.34
29	c	502	CLA	CHC-C1C	2.29	1.40	1.35
29	S	605	CLA	C1A-CHA	2.29	1.52	1.43
29	n	611	CLA	C1A-CHA	2.29	1.52	1.43
29	c1	509	CLA	C1C-C2C	2.29	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
48	N	605	CHL	C3A-C2A	-2.29	1.48	1.54
48	n	605	CHL	CHC-C1C	2.29	1.40	1.35
29	c	507	CLA	CHC-C1C	2.29	1.40	1.35
29	R1	612	CLA	CHC-C1C	2.29	1.40	1.35
53	R1	626	ERG	C11-C9	2.28	1.57	1.53
29	s1	613	CLA	C3B-C2B	-2.28	1.37	1.40
31	C	515	BCR	C1-C6	-2.28	1.50	1.53
29	C1	509	CLA	CHC-C1C	2.28	1.40	1.35
30	A	409	PHO	CMC-C2C	-2.28	1.46	1.51
29	y1	604	CLA	CHC-C1C	2.28	1.40	1.35
29	R	612	CLA	C1A-CHA	2.28	1.52	1.43
55	Y	627	PTY	O7-C6	-2.28	1.40	1.46
34	a1	414	SPH	C3-C4	2.28	1.53	1.50
48	g	605	CHL	C3B-C2B	-2.28	1.37	1.40
29	y1	602	CLA	C1C-C2C	2.28	1.49	1.44
38	s	626	3PH	O21-C21	2.28	1.40	1.34
29	C1	513	CLA	C1C-C2C	2.28	1.49	1.44
29	S1	611	CLA	C1A-CHA	2.28	1.52	1.43
29	c	505	CLA	CHC-C1C	2.28	1.40	1.35
29	a1	405	CLA	CHC-C1C	2.28	1.40	1.35
29	g	613	CLA	C1A-CHA	2.28	1.52	1.43
29	Y1	610	CLA	C1A-CHA	2.28	1.52	1.43
29	G1	602	CLA	C1A-CHA	2.27	1.52	1.43
29	c	510	CLA	C3D-C4D	-2.27	1.39	1.44
29	B	603	CLA	C3B-C2B	-2.27	1.37	1.40
48	N1	605	CHL	C3B-C2B	-2.27	1.37	1.40
29	c	506	CLA	C3D-C4D	-2.27	1.39	1.44
29	c1	510	CLA	C3D-C4D	-2.27	1.39	1.44
29	g	613	CLA	C3B-C2B	-2.27	1.37	1.40
54	S	625	LPX	P1-O2	2.27	1.68	1.59
29	C1	512	CLA	C1C-C2C	2.27	1.49	1.44
29	A1	407	CLA	CHC-C1C	2.27	1.40	1.35
29	C	507	CLA	CHC-C1C	2.27	1.40	1.35
29	B	607	CLA	C3D-C4D	-2.27	1.39	1.44
29	b	612	CLA	CHC-C1C	2.27	1.40	1.35
29	N1	604	CLA	CHC-C1C	2.27	1.40	1.35
29	Y	613	CLA	C1A-CHA	2.27	1.52	1.43
29	B1	610	CLA	C3B-C2B	-2.27	1.37	1.40
29	y1	613	CLA	C3B-C2B	-2.27	1.37	1.40
29	r1	602	CLA	C1C-C2C	2.27	1.49	1.44
29	d1	403	CLA	C1C-C2C	2.27	1.49	1.44
29	g1	614	CLA	C1C-C2C	2.27	1.49	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	g1	610	CLA	C3D-C4D	-2.27	1.39	1.44
29	c1	513	CLA	C3B-C2B	-2.27	1.37	1.40
29	N1	610	CLA	C3B-C2B	-2.27	1.37	1.40
29	C	507	CLA	C1A-CHA	2.27	1.52	1.43
29	B	604	CLA	C3D-C4D	-2.26	1.39	1.44
29	s1	612	CLA	C1A-CHA	2.26	1.52	1.43
30	a	408	PHO	CMB-C2B	-2.26	1.46	1.51
29	s1	612	CLA	C1C-C2C	2.26	1.48	1.44
38	b	624	3PH	O21-C21	2.26	1.40	1.34
29	Y1	608	CLA	C3B-C2B	-2.26	1.37	1.40
29	y1	602	CLA	C3B-C2B	-2.26	1.37	1.40
29	c1	510	CLA	C3B-C2B	-2.26	1.37	1.40
29	b	602	CLA	C1C-C2C	2.26	1.48	1.44
38	b	624	3PH	O31-C3	-2.26	1.40	1.45
52	R1	625	LMT	O2B-C2B	-2.26	1.37	1.43
38	T1	101	3PH	O21-C21	2.26	1.40	1.34
29	c	511	CLA	C3B-C2B	-2.26	1.37	1.40
29	a1	407	CLA	C1A-CHA	2.26	1.52	1.43
43	d	405	PL9	C52-C5	-2.26	1.46	1.50
29	R	603	CLA	C1C-C2C	2.26	1.48	1.44
29	B	608	CLA	C3B-C2B	-2.26	1.37	1.40
29	c	509	CLA	C3D-C4D	-2.26	1.39	1.44
29	B1	614	CLA	CHD-C1D	2.26	1.42	1.38
29	G1	613	CLA	C1C-C2C	2.26	1.48	1.44
29	C1	506	CLA	CHC-C1C	2.26	1.40	1.35
29	b1	613	CLA	CHC-C1C	2.26	1.40	1.35
52	r1	625	LMT	O3B-C3B	-2.26	1.37	1.43
29	G	614	CLA	C1A-CHA	2.26	1.52	1.43
29	c	513	CLA	C1C-C2C	2.26	1.48	1.44
29	G1	612	CLA	C1B-NB	2.26	1.37	1.35
29	B1	605	CLA	C1A-CHA	2.26	1.52	1.43
29	Y1	603	CLA	C1C-C2C	2.26	1.48	1.44
29	s1	612	CLA	C3B-C2B	-2.26	1.37	1.40
48	S	608	CHL	C3B-C2B	-2.25	1.37	1.40
29	b1	605	CLA	C1A-CHA	2.25	1.52	1.43
29	R	610	CLA	C4B-NB	-2.25	1.33	1.35
48	n	608	CHL	C3A-C2A	-2.25	1.48	1.54
29	N	602	CLA	C1C-C2C	2.25	1.48	1.44
29	A	405	CLA	C3D-C4D	-2.25	1.39	1.44
29	C	506	CLA	C3D-C4D	-2.25	1.39	1.44
29	S	611	CLA	C1A-CHA	2.25	1.52	1.43
29	D1	403	CLA	C1C-C2C	2.25	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
51	g1	623	NEX	O24-C25	-2.25	1.43	1.46
29	b1	608	CLA	C1A-CHA	2.25	1.52	1.43
38	t1	101	3PH	O21-C2	-2.24	1.41	1.46
29	Y	602	CLA	CHC-C1C	2.24	1.40	1.35
38	T	101	3PH	O31-C3	-2.24	1.40	1.45
29	B	616	CLA	C1A-CHA	2.24	1.52	1.43
29	G	603	CLA	C3B-C2B	-2.24	1.37	1.40
38	b1	624	3PH	O21-C21	2.24	1.40	1.34
29	g1	611	CLA	C1A-CHA	2.24	1.52	1.43
29	B	615	CLA	C3D-C4D	-2.24	1.39	1.44
29	B1	602	CLA	C1A-CHA	2.24	1.52	1.43
29	N	610	CLA	C1A-CHA	2.24	1.52	1.43
29	a	406	CLA	C3D-C4D	-2.24	1.39	1.44
29	C1	502	CLA	C3D-C4D	-2.24	1.39	1.44
29	c	505	CLA	C3D-C4D	-2.24	1.39	1.44
29	b	615	CLA	C3D-C4D	-2.24	1.39	1.44
29	b1	603	CLA	C1C-C2C	2.24	1.48	1.44
29	c1	508	CLA	C1C-C2C	2.24	1.48	1.44
29	R1	604	CLA	C3B-C2B	-2.24	1.37	1.40
29	s	614	CLA	C3D-C4D	-2.24	1.39	1.44
29	y	613	CLA	C1A-CHA	2.24	1.52	1.43
29	C1	504	CLA	CHC-C1C	2.24	1.40	1.35
30	a1	408	PHO	CMB-C2B	-2.23	1.46	1.51
29	n	613	CLA	C1A-CHA	2.23	1.52	1.43
29	y	608	CLA	C3D-C4D	-2.23	1.39	1.44
29	a	407	CLA	C1A-CHA	2.23	1.52	1.43
51	n	623	NEX	C1-C6	-2.23	1.50	1.54
29	B	611	CLA	C3D-C4D	-2.23	1.39	1.44
29	B1	610	CLA	C1A-CHA	2.23	1.52	1.43
30	A	408	PHO	CMD-C2D	-2.23	1.46	1.51
29	n1	603	CLA	C1A-CHA	2.23	1.52	1.43
29	s	605	CLA	C1A-CHA	2.23	1.52	1.43
43	d	405	PL9	C7-C8	-2.23	1.47	1.50
29	r	602	CLA	C3D-C4D	-2.23	1.39	1.44
34	a	414	SPH	C3-C4	2.23	1.53	1.50
29	B	608	CLA	C1A-CHA	2.23	1.52	1.43
29	r	610	CLA	C3B-C2B	-2.23	1.37	1.40
29	s	611	CLA	C1A-CHA	2.23	1.52	1.43
29	r1	612	CLA	C1A-CHA	2.23	1.52	1.43
53	r1	626	ERG	C11-C9	2.23	1.57	1.53
29	R1	603	CLA	C1A-CHA	2.23	1.52	1.43
29	Y1	608	CLA	C3D-C4D	-2.23	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a1	406	CLA	C3D-C4D	-2.23	1.39	1.44
39	c	524	DGA	OG2-CG2	-2.23	1.41	1.46
29	c	507	CLA	C3D-C4D	-2.22	1.39	1.44
29	S1	605	CLA	C1A-CHA	2.22	1.52	1.43
29	y1	610	CLA	C1A-CHA	2.22	1.52	1.43
29	A	410	CLA	C4B-NB	-2.22	1.33	1.35
29	b	616	CLA	C3D-C4D	-2.22	1.39	1.44
29	c1	501	CLA	C1A-CHA	2.22	1.52	1.43
29	G1	603	CLA	C3B-C2B	-2.22	1.37	1.40
29	C	503	CLA	C1A-CHA	2.22	1.52	1.43
29	Y	611	CLA	C3B-C2B	-2.22	1.37	1.40
48	s	608	CHL	C3B-C2B	-2.22	1.37	1.40
29	c	512	CLA	C1A-CHA	2.22	1.52	1.43
52	R	625	LMT	O4'-C4B	-2.22	1.37	1.43
29	G1	614	CLA	C1A-CHA	2.22	1.52	1.43
29	y	604	CLA	C1A-CHA	2.22	1.52	1.43
29	y1	612	CLA	C1C-C2C	2.22	1.48	1.44
29	b	614	CLA	C1A-CHA	2.22	1.52	1.43
48	s	601	CHL	CHC-C1C	2.22	1.40	1.35
29	b1	605	CLA	C3B-C2B	-2.22	1.37	1.40
29	s1	609	CLA	C1A-CHA	2.22	1.52	1.43
29	C1	510	CLA	C3B-C2B	-2.22	1.37	1.40
29	s	610	CLA	C1A-CHA	2.22	1.52	1.43
29	b	608	CLA	C1A-CHA	2.22	1.52	1.43
29	C1	501	CLA	C1A-CHA	2.21	1.52	1.43
29	b1	617	CLA	CHC-C1C	2.21	1.40	1.35
29	g1	612	CLA	C1B-NB	2.21	1.37	1.35
29	G1	604	CLA	C1A-CHA	2.21	1.52	1.43
29	Y	614	CLA	C3D-C4D	-2.21	1.39	1.44
29	N	611	CLA	C1A-CHA	2.21	1.52	1.43
51	R	622	NEX	C18-C5	-2.21	1.49	1.52
29	N	614	CLA	C1A-CHA	2.21	1.52	1.43
48	g1	609	CHL	C3B-C2B	-2.21	1.37	1.40
30	A	408	PHO	CMC-C2C	-2.21	1.46	1.51
29	R	608	CLA	C1A-CHA	2.21	1.52	1.43
29	s	603	CLA	C3B-C2B	-2.21	1.37	1.40
29	R1	602	CLA	C1C-C2C	2.21	1.48	1.44
29	N1	613	CLA	C3B-C2B	-2.21	1.37	1.40
29	y1	612	CLA	C1A-CHA	2.21	1.52	1.43
29	R	603	CLA	C3D-C4D	-2.21	1.39	1.44
30	a	409	PHO	CMC-C2C	-2.21	1.46	1.51
29	g	611	CLA	CHC-C1C	2.21	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	a1	409	PHO	CMC-C2C	-2.21	1.46	1.51
29	b1	609	CLA	C1A-CHA	2.21	1.52	1.43
29	s1	613	CLA	C1A-CHA	2.21	1.52	1.43
31	C	517	BCR	C12-C13	-2.21	1.41	1.45
29	A	410	CLA	C3D-C4D	-2.21	1.39	1.44
29	n	610	CLA	C3B-C2B	-2.21	1.37	1.40
29	b	603	CLA	C3D-C4D	-2.20	1.39	1.44
50	N	622	XAT	O24-C25	-2.20	1.43	1.46
29	s1	610	CLA	C1A-CHA	2.20	1.52	1.43
29	Y1	613	CLA	C3D-C4D	-2.20	1.39	1.44
29	G1	612	CLA	C3B-C2B	-2.20	1.37	1.40
29	R1	602	CLA	C3B-C2B	-2.20	1.37	1.40
29	n	612	CLA	C1A-CHA	2.20	1.52	1.43
29	C	505	CLA	C3D-C4D	-2.20	1.39	1.44
29	g1	614	CLA	C1A-CHA	2.20	1.52	1.43
29	n	610	CLA	C1C-C2C	2.20	1.48	1.44
55	Y	626	PTY	O7-C8	2.20	1.40	1.34
29	B1	603	CLA	C1C-C2C	2.20	1.48	1.44
29	G1	613	CLA	C1A-CHA	2.20	1.52	1.43
29	s	614	CLA	C3B-C2B	-2.20	1.37	1.40
38	S1	626	3PH	O21-C21	2.20	1.40	1.34
29	C	512	CLA	C1A-CHA	2.20	1.52	1.43
29	S	602	CLA	C3D-C4D	-2.20	1.39	1.44
38	t	101	3PH	O21-C21	2.20	1.40	1.34
29	s1	609	CLA	C1B-NB	2.20	1.37	1.35
48	G1	605	CHL	C3B-C2B	-2.20	1.37	1.40
29	g	604	CLA	C3D-C4D	-2.20	1.39	1.44
29	n	603	CLA	C1A-CHA	2.20	1.52	1.43
51	s1	623	NEX	C4-C3	2.20	1.55	1.52
43	d	405	PL9	C21-C19	-2.20	1.46	1.51
29	n1	602	CLA	C1C-C2C	2.20	1.48	1.44
29	r1	604	CLA	C1A-CHA	2.20	1.52	1.43
43	D1	405	PL9	C7-C8	-2.19	1.47	1.50
29	b	606	CLA	C3B-C2B	-2.19	1.37	1.40
48	n1	606	CHL	C3B-C2B	-2.19	1.37	1.40
29	Y1	602	CLA	C3D-C4D	-2.19	1.39	1.44
29	s	613	CLA	C1A-CHA	2.19	1.52	1.43
29	b1	606	CLA	C3D-C4D	-2.19	1.39	1.44
48	Y	601	CHL	C3A-C2A	-2.19	1.48	1.54
29	n	614	CLA	C3B-C2B	-2.19	1.37	1.40
38	B	624	3PH	O21-C21	2.19	1.40	1.34
29	n1	611	CLA	C1A-CHA	2.19	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	N1	602	CLA	C1C-C2C	2.19	1.48	1.44
29	R1	608	CLA	C1A-CHA	2.19	1.52	1.43
29	C	511	CLA	C1A-CHA	2.19	1.52	1.43
51	g	623	NEX	O24-C25	-2.19	1.43	1.46
29	c	511	CLA	C3D-C4D	-2.19	1.39	1.44
29	R	608	CLA	CHC-C1C	2.19	1.40	1.35
29	c	501	CLA	C3D-C4D	-2.19	1.39	1.44
29	G1	610	CLA	C1C-C2C	2.19	1.48	1.44
29	B1	607	CLA	C1C-C2C	2.19	1.48	1.44
52	R1	625	LMT	O1'-C1'	-2.19	1.36	1.40
29	Y1	612	CLA	C1A-CHA	2.19	1.52	1.43
29	s	617	CLA	C1A-CHA	2.18	1.52	1.43
29	c	506	CLA	CHC-C1C	2.18	1.40	1.35
29	R	609	CLA	C3D-C4D	-2.18	1.39	1.44
29	n1	604	CLA	C1A-CHA	2.18	1.52	1.43
48	y	609	CHL	C3A-C2A	-2.18	1.48	1.54
29	y	602	CLA	C3D-C4D	-2.18	1.39	1.44
29	S1	602	CLA	C1C-C2C	2.18	1.48	1.44
29	S1	613	CLA	C1A-CHA	2.18	1.52	1.43
29	c1	503	CLA	C1A-CHA	2.18	1.52	1.43
29	B	609	CLA	C3D-C4D	-2.18	1.39	1.44
29	C	507	CLA	C3D-C4D	-2.18	1.39	1.44
52	r	625	LMT	O4'-C4B	-2.18	1.37	1.43
29	b1	602	CLA	C1A-CHA	2.18	1.52	1.43
53	r	626	ERG	C14-C8	2.18	1.57	1.51
29	N1	614	CLA	C1A-CHA	2.18	1.52	1.43
50	n1	622	XAT	O24-C25	-2.18	1.43	1.46
29	B	605	CLA	C3D-C4D	-2.18	1.39	1.44
29	N1	604	CLA	C3D-C4D	-2.18	1.39	1.44
29	b1	614	CLA	C1A-CHA	2.18	1.52	1.43
48	N	608	CHL	C3A-C2A	-2.18	1.48	1.54
29	b	607	CLA	C3D-C4D	-2.18	1.39	1.44
48	N	609	CHL	C3A-C2A	-2.18	1.48	1.54
29	s	612	CLA	C3D-C4D	-2.18	1.39	1.44
29	B	612	CLA	C3D-C4D	-2.17	1.39	1.44
48	G	605	CHL	C3B-C2B	-2.17	1.37	1.40
29	r1	609	CLA	C1C-C2C	2.17	1.48	1.44
29	c1	508	CLA	C3D-C4D	-2.17	1.39	1.44
29	c	513	CLA	C3D-C4D	-2.17	1.39	1.44
29	S	605	CLA	C3B-C2B	-2.17	1.37	1.40
29	B	614	CLA	C1A-CHA	2.17	1.52	1.43
29	g	614	CLA	C1C-C2C	2.17	1.48	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	R1	603	CLA	C1C-C2C	2.17	1.48	1.44
29	n1	614	CLA	C1C-C2C	2.17	1.48	1.44
29	B	602	CLA	C1A-CHA	2.17	1.52	1.43
38	s	626	3PH	O21-C2	-2.17	1.41	1.46
36	B1	620	C7Z	C40-C33	2.17	1.55	1.50
38	t	101	3PH	O21-C2	-2.17	1.41	1.46
29	Y1	603	CLA	C3D-C4D	-2.17	1.39	1.44
29	g	610	CLA	C1A-CHA	2.17	1.52	1.43
29	c1	512	CLA	C1A-CHA	2.17	1.52	1.43
29	C	510	CLA	C3B-C2B	-2.17	1.37	1.40
55	y	627	PTY	O4-C1	-2.17	1.40	1.45
39	c1	524	DGA	OG2-CG2	-2.17	1.41	1.46
29	g	611	CLA	C1A-CHA	2.17	1.52	1.43
29	g1	612	CLA	C1A-CHA	2.17	1.52	1.43
29	C	501	CLA	C3D-C4D	-2.17	1.39	1.44
29	D	403	CLA	C1A-CHA	2.17	1.52	1.43
29	Y	610	CLA	C1A-CHA	2.17	1.52	1.43
29	S	617	CLA	C3B-C2B	-2.17	1.37	1.40
30	A1	409	PHO	CMC-C2C	-2.17	1.46	1.51
29	Y	602	CLA	C3D-C4D	-2.17	1.39	1.44
29	C1	503	CLA	C3D-C4D	-2.17	1.39	1.44
29	Y	608	CLA	C1A-CHA	2.17	1.52	1.43
29	N1	611	CLA	CHD-C1D	2.17	1.42	1.38
29	S1	610	CLA	C3D-C4D	-2.17	1.39	1.44
31	C	514	BCR	C12-C13	-2.17	1.41	1.45
29	B	603	CLA	C1A-CHA	2.17	1.52	1.43
29	S1	603	CLA	C1A-CHA	2.17	1.52	1.43
55	Y1	626	PTY	O4-C1	-2.17	1.40	1.45
29	d	403	CLA	C3B-C2B	-2.17	1.37	1.40
29	N1	611	CLA	C3D-C4D	-2.17	1.39	1.44
29	G	611	CLA	C1A-CHA	2.17	1.52	1.43
29	s1	605	CLA	C1C-C2C	2.16	1.48	1.44
29	r	610	CLA	C1A-CHA	2.16	1.52	1.43
29	c	507	CLA	C4B-NB	-2.16	1.33	1.35
38	B1	624	3PH	O21-C21	2.16	1.40	1.34
29	y	614	CLA	C3D-C4D	-2.16	1.39	1.44
29	A1	406	CLA	C1A-CHA	2.16	1.52	1.43
29	A1	407	CLA	C3D-C4D	-2.16	1.39	1.44
54	s	625	LPX	P1-O2	2.16	1.68	1.59
29	G	603	CLA	C1C-C2C	2.16	1.48	1.44
29	g	614	CLA	MG-NC	2.16	2.11	2.06
29	B1	606	CLA	C1A-CHA	2.16	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a1	410	CLA	C4B-NB	-2.16	1.33	1.35
29	a1	405	CLA	C1A-CHA	2.16	1.52	1.43
39	j	101	DGA	OG2-CG2	-2.16	1.41	1.46
29	N1	610	CLA	C1A-CHA	2.16	1.52	1.43
29	Y	613	CLA	C3D-C4D	-2.16	1.39	1.44
29	G1	610	CLA	C3D-C4D	-2.16	1.39	1.44
29	S	612	CLA	C1A-CHA	2.16	1.52	1.43
29	R1	609	CLA	C1A-CHA	2.16	1.52	1.43
29	b1	616	CLA	CHC-C1C	2.16	1.40	1.35
29	A	407	CLA	C1A-CHA	2.16	1.52	1.43
29	G1	610	CLA	C3B-C2B	-2.16	1.37	1.40
29	B1	613	CLA	C3D-C4D	-2.16	1.39	1.44
30	A1	408	PHO	CMB-C2B	-2.16	1.46	1.51
29	r1	610	CLA	C3B-C2B	-2.16	1.37	1.40
29	c	505	CLA	C1A-CHA	2.16	1.52	1.43
29	b1	604	CLA	C1B-NB	2.16	1.37	1.35
29	y1	610	CLA	C3D-C4D	-2.16	1.39	1.44
29	A1	410	CLA	C1A-CHA	2.16	1.52	1.43
50	R	621	XAT	O24-C25	-2.16	1.43	1.46
29	n	614	CLA	C1A-CHA	2.15	1.52	1.43
38	T1	101	3PH	O31-C3	-2.15	1.40	1.45
50	y1	622	XAT	O24-C25	-2.15	1.43	1.46
29	C1	507	CLA	C1C-C2C	2.15	1.48	1.44
29	b1	609	CLA	C1C-C2C	2.15	1.48	1.44
29	g1	612	CLA	C1C-C2C	2.15	1.48	1.44
29	S1	605	CLA	C1C-C2C	2.15	1.48	1.44
29	Y1	602	CLA	C3B-C2B	-2.15	1.37	1.40
29	s	617	CLA	C3D-C4D	-2.15	1.39	1.44
29	Y1	613	CLA	C3B-C2B	-2.15	1.37	1.40
29	B1	609	CLA	C1C-C2C	2.15	1.48	1.44
29	r1	603	CLA	C1A-CHA	2.15	1.52	1.43
29	y1	610	CLA	C3B-C2B	-2.15	1.37	1.40
29	n1	612	CLA	C1A-CHA	2.15	1.52	1.43
29	N1	602	CLA	C3B-C2B	-2.15	1.37	1.40
52	R1	625	LMT	O5B-C5B	-2.15	1.39	1.44
30	A1	408	PHO	CMC-C2C	-2.15	1.46	1.51
29	r	608	CLA	C1A-CHA	2.15	1.52	1.43
30	a1	409	PHO	CMB-C2B	-2.15	1.46	1.51
29	r	608	CLA	CHD-C1D	2.15	1.42	1.38
29	d1	402	CLA	C3D-C4D	-2.15	1.39	1.44
48	n	606	CHL	C3A-C2A	-2.15	1.48	1.54
29	B1	615	CLA	C1A-CHA	2.14	1.52	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a	406	CLA	C3B-C2B	-2.14	1.37	1.40
29	R	612	CLA	C1B-NB	2.14	1.37	1.35
29	y	612	CLA	C1A-CHA	2.14	1.52	1.43
29	s1	603	CLA	C1A-CHA	2.14	1.52	1.43
29	b1	615	CLA	C3D-C4D	-2.14	1.39	1.44
29	b	612	CLA	C3B-C2B	-2.14	1.37	1.40
29	Y1	611	CLA	C1A-CHA	2.14	1.52	1.43
29	b	611	CLA	C3D-C4D	-2.14	1.39	1.44
29	R	604	CLA	C3B-C2B	-2.14	1.37	1.40
29	b	606	CLA	C3D-C4D	-2.14	1.39	1.44
29	n	604	CLA	C3D-C4D	-2.14	1.39	1.44
50	N1	622	XAT	O24-C25	-2.14	1.43	1.46
29	s	604	CLA	C3D-C4D	-2.14	1.39	1.44
29	y	603	CLA	C1A-CHA	2.14	1.52	1.43
29	S	609	CLA	C1A-CHA	2.14	1.52	1.43
29	b	610	CLA	C1A-CHA	2.14	1.52	1.43
29	A1	406	CLA	C3B-C2B	-2.14	1.37	1.40
29	C1	510	CLA	C1C-C2C	2.14	1.48	1.44
29	R1	609	CLA	C1C-C2C	2.14	1.48	1.44
29	y1	608	CLA	C1B-NB	2.14	1.37	1.35
29	c	507	CLA	C1A-CHA	2.14	1.52	1.43
29	g	610	CLA	C3D-C4D	-2.14	1.39	1.44
29	a1	410	CLA	C1A-CHA	2.14	1.52	1.43
29	Y	612	CLA	C3D-C4D	-2.14	1.39	1.44
29	b	609	CLA	C3D-C4D	-2.14	1.39	1.44
29	S1	617	CLA	C1C-C2C	2.14	1.48	1.44
43	d1	405	PL9	C53-C6	-2.14	1.46	1.50
29	n	602	CLA	C3D-C4D	-2.14	1.39	1.44
29	y1	608	CLA	C3D-C4D	-2.14	1.39	1.44
45	H	101	RRX	C35-C13	2.14	1.55	1.50
29	d1	402	CLA	C1A-CHA	2.13	1.52	1.43
29	n1	612	CLA	C1C-C2C	2.13	1.48	1.44
29	s	603	CLA	C1C-C2C	2.13	1.48	1.44
29	c	503	CLA	C3D-C4D	-2.13	1.39	1.44
29	C	501	CLA	C1A-CHA	2.13	1.52	1.43
29	S	613	CLA	C3D-C4D	-2.13	1.39	1.44
29	S1	604	CLA	C1A-CHA	2.13	1.52	1.43
29	S	603	CLA	C1A-CHA	2.13	1.52	1.43
29	n1	613	CLA	C1A-CHA	2.13	1.51	1.43
29	b	617	CLA	C1A-CHA	2.13	1.51	1.43
29	R1	602	CLA	C1A-CHA	2.13	1.51	1.43
29	c	513	CLA	C1A-CHA	2.13	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c1	513	CLA	C1A-CHA	2.13	1.51	1.43
29	b	609	CLA	C1C-C2C	2.13	1.48	1.44
29	C1	513	CLA	C3D-C4D	-2.13	1.39	1.44
29	b	614	CLA	C3B-C2B	-2.13	1.37	1.40
29	b1	608	CLA	C3B-C2B	-2.13	1.37	1.40
29	B1	614	CLA	C3D-C4D	-2.13	1.39	1.44
29	B	610	CLA	C3B-C2B	-2.13	1.37	1.40
29	C	505	CLA	C1A-CHA	2.13	1.51	1.43
29	y1	604	CLA	C1A-CHA	2.13	1.51	1.43
29	g	603	CLA	C3D-C4D	-2.13	1.39	1.44
29	y	608	CLA	C1A-CHA	2.13	1.51	1.43
29	b	602	CLA	C1A-CHA	2.13	1.51	1.43
29	R	610	CLA	C3D-C4D	-2.13	1.39	1.44
29	B1	617	CLA	C3D-C4D	-2.13	1.39	1.44
30	A	409	PHO	CMB-C2B	-2.13	1.46	1.51
31	b	618	BCR	C1-C6	-2.13	1.50	1.53
29	B	605	CLA	C1A-CHA	2.13	1.51	1.43
29	g	614	CLA	C1A-CHA	2.13	1.51	1.43
29	y	611	CLA	C3D-C4D	-2.13	1.39	1.44
29	C1	509	CLA	C3D-C4D	-2.13	1.39	1.44
29	S	604	CLA	C1A-CHA	2.13	1.51	1.43
51	G1	623	NEX	O24-C25	-2.12	1.43	1.46
29	Y	612	CLA	C1A-CHA	2.12	1.51	1.43
50	Y	622	XAT	O24-C25	-2.12	1.43	1.46
30	a	408	PHO	CMD-C2D	-2.12	1.46	1.51
29	g	612	CLA	C1A-CHA	2.12	1.51	1.43
29	S	603	CLA	MG-NC	2.12	2.11	2.06
29	b	607	CLA	C1A-CHA	2.12	1.51	1.43
29	g1	613	CLA	C1C-C2C	2.12	1.48	1.44
29	r1	604	CLA	C1C-C2C	2.12	1.48	1.44
29	c1	501	CLA	C3D-C4D	-2.12	1.39	1.44
29	g	602	CLA	C3B-C2B	-2.12	1.37	1.40
29	y1	611	CLA	C3B-C2B	-2.12	1.37	1.40
51	n	623	NEX	O24-C25	-2.12	1.43	1.46
29	c1	505	CLA	C1C-C2C	2.12	1.48	1.44
29	G1	612	CLA	C3D-C4D	-2.12	1.39	1.44
29	G	613	CLA	C1A-CHA	2.12	1.51	1.43
29	b	612	CLA	C1A-CHA	2.12	1.51	1.43
29	s1	611	CLA	C1B-NB	2.12	1.37	1.35
29	b1	612	CLA	C3D-C4D	-2.12	1.39	1.44
29	R1	604	CLA	C1A-CHA	2.12	1.51	1.43
29	r	603	CLA	C1A-CHA	2.12	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	s1	605	CLA	C3D-C4D	-2.12	1.39	1.44
29	b1	612	CLA	C1A-CHA	2.12	1.51	1.43
29	y1	613	CLA	C1A-CHA	2.12	1.51	1.43
39	C1	524	DGA	CB2-CB1	2.12	1.56	1.50
29	b1	604	CLA	C1C-C2C	2.12	1.48	1.44
29	N	612	CLA	C1A-CHA	2.12	1.51	1.43
29	G1	612	CLA	C1C-C2C	2.12	1.48	1.44
29	S1	609	CLA	C1A-CHA	2.12	1.51	1.43
29	A	406	CLA	CHC-C1C	2.12	1.40	1.35
29	C	503	CLA	C3D-C4D	-2.12	1.39	1.44
29	B1	606	CLA	C3D-C4D	-2.12	1.39	1.44
29	Y	610	CLA	C3D-C4D	-2.12	1.39	1.44
29	B	614	CLA	C1C-C2C	2.12	1.48	1.44
29	a	406	CLA	C1A-CHA	2.12	1.51	1.43
43	D1	405	PL9	C3-C4	-2.12	1.46	1.49
29	N	603	CLA	C1A-CHA	2.12	1.51	1.43
29	n1	614	CLA	C1A-CHA	2.12	1.51	1.43
29	b1	613	CLA	C1A-CHA	2.12	1.51	1.43
29	B	617	CLA	C1A-CHA	2.12	1.51	1.43
52	r1	625	LMT	O2B-C2B	-2.12	1.38	1.43
38	t1	101	3PH	O21-C21	2.11	1.40	1.34
29	B	606	CLA	C1A-CHA	2.11	1.51	1.43
29	S1	611	CLA	MG-NC	2.11	2.11	2.06
29	c1	509	CLA	C3D-C4D	-2.11	1.39	1.44
29	g1	614	CLA	MG-NC	2.11	2.11	2.06
29	C1	508	CLA	C1D-ND	-2.11	1.35	1.37
29	b	612	CLA	C3D-C4D	-2.11	1.39	1.44
29	C	506	CLA	C1A-CHA	2.11	1.51	1.43
29	s1	613	CLA	C1B-NB	2.11	1.37	1.35
29	B1	609	CLA	C1A-CHA	2.11	1.51	1.43
29	s1	603	CLA	C1C-C2C	2.11	1.48	1.44
30	A1	408	PHO	CMD-C2D	-2.11	1.46	1.51
29	c	508	CLA	C3D-C4D	-2.11	1.39	1.44
29	c	512	CLA	C3D-C4D	-2.11	1.39	1.44
29	C	513	CLA	C3D-C4D	-2.11	1.39	1.44
36	B	620	C7Z	C40-C33	2.11	1.55	1.50
29	y1	603	CLA	C1C-C2C	2.11	1.48	1.44
29	b	610	CLA	C3D-C4D	-2.11	1.39	1.44
29	b	611	CLA	CHC-C1C	2.11	1.40	1.35
29	G	610	CLA	C1A-CHA	2.11	1.51	1.43
29	d	403	CLA	C3D-C4D	-2.11	1.39	1.44
29	s	609	CLA	C3B-C2B	-2.11	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	B1	602	CLA	C1C-C2C	2.11	1.48	1.44
29	Y1	603	CLA	C1A-CHA	2.11	1.51	1.43
29	S	612	CLA	C3D-C4D	-2.11	1.39	1.44
29	s1	614	CLA	C1A-CHA	2.11	1.51	1.43
29	r1	610	CLA	C1A-CHA	2.11	1.51	1.43
29	N1	614	CLA	C3D-C4D	-2.11	1.39	1.44
29	b1	617	CLA	C3B-C2B	-2.11	1.37	1.40
29	C1	501	CLA	C3D-C4D	-2.11	1.39	1.44
29	N	612	CLA	C3D-C4D	-2.11	1.39	1.44
29	g1	602	CLA	C1A-CHA	2.11	1.51	1.43
29	d	402	CLA	C1C-C2C	2.11	1.48	1.44
48	g	601	CHL	C3A-C2A	-2.10	1.48	1.54
55	y	626	PTY	O7-C8	2.10	1.40	1.34
52	R1	625	LMT	O4'-C4B	-2.10	1.38	1.43
29	s1	605	CLA	MG-NC	2.10	2.11	2.06
36	b	620	C7Z	C10-C9	-2.10	1.33	1.35
29	Y	603	CLA	C3D-C4D	-2.10	1.39	1.44
29	r	604	CLA	C1A-CHA	2.10	1.51	1.43
30	a1	408	PHO	CMD-C2D	-2.10	1.46	1.51
29	y	602	CLA	C1B-NB	2.10	1.37	1.35
29	r	609	CLA	C3D-C4D	-2.10	1.39	1.44
29	C1	511	CLA	C1A-CHA	2.10	1.51	1.43
29	B	606	CLA	C3B-C2B	-2.10	1.37	1.40
51	y1	623	NEX	O24-C25	-2.10	1.43	1.46
30	a1	408	PHO	CMC-C2C	-2.10	1.46	1.51
29	A	406	CLA	C1A-CHA	2.10	1.51	1.43
29	b1	607	CLA	C1A-CHA	2.10	1.51	1.43
29	R	608	CLA	C3D-C4D	-2.10	1.39	1.44
55	y1	627	PTY	O7-C8	2.10	1.39	1.35
29	b1	614	CLA	MG-NC	2.10	2.11	2.06
29	b1	614	CLA	C1C-C2C	2.10	1.48	1.44
36	B1	620	C7Z	C18-C5	2.10	1.54	1.50
29	r	608	CLA	C3D-C4D	-2.10	1.39	1.44
29	B	615	CLA	C1A-CHA	2.10	1.51	1.43
29	c1	504	CLA	C1A-CHA	2.10	1.51	1.43
29	G	604	CLA	C1A-CHA	2.10	1.51	1.43
29	N1	612	CLA	C1A-CHA	2.10	1.51	1.43
29	s	602	CLA	C3D-C4D	-2.10	1.39	1.44
29	D	403	CLA	C1B-NB	2.10	1.37	1.35
29	G	602	CLA	C1A-CHA	2.10	1.51	1.43
29	S1	617	CLA	C1A-CHA	2.10	1.51	1.43
29	b	605	CLA	C3D-C4D	-2.10	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	R	603	CLA	C1A-CHA	2.10	1.51	1.43
29	R1	610	CLA	C3B-C2B	-2.10	1.37	1.40
29	c	504	CLA	C3D-C4D	-2.10	1.39	1.44
29	R1	608	CLA	C1C-C2C	2.09	1.48	1.44
29	y1	611	CLA	C1A-CHA	2.09	1.51	1.43
48	Y	609	CHL	C3D-C2D	-2.09	1.33	1.39
29	n	614	CLA	C1B-NB	2.09	1.37	1.35
47	k	101	4RF	O21-C20	-2.09	1.41	1.46
29	a	410	CLA	C1A-CHA	2.09	1.51	1.43
29	S	609	CLA	C3D-C4D	-2.09	1.39	1.44
29	g	603	CLA	C1A-CHA	2.09	1.51	1.43
29	s1	609	CLA	C1C-C2C	2.09	1.48	1.44
29	y1	610	CLA	C1C-C2C	2.09	1.48	1.44
29	D1	402	CLA	C3D-C4D	-2.09	1.39	1.44
29	B	607	CLA	C1A-CHA	2.09	1.51	1.43
29	N	602	CLA	C3B-C2B	-2.09	1.37	1.40
29	C1	506	CLA	C3D-C4D	-2.09	1.39	1.44
29	C1	510	CLA	C3D-C4D	-2.09	1.39	1.44
29	y	610	CLA	C1A-CHA	2.09	1.51	1.43
52	R1	625	LMT	O5'-C5'	-2.09	1.39	1.44
29	y	603	CLA	C3D-C4D	-2.09	1.39	1.44
29	S	617	CLA	C1A-CHA	2.09	1.51	1.43
29	s	609	CLA	C3D-C4D	-2.09	1.39	1.44
29	D1	403	CLA	C1A-CHA	2.09	1.51	1.43
29	R1	610	CLA	C1A-CHA	2.09	1.51	1.43
29	C	504	CLA	C3D-C4D	-2.09	1.39	1.44
29	s	611	CLA	C1C-C2C	2.09	1.48	1.44
29	S1	612	CLA	C1A-CHA	2.09	1.51	1.43
29	b1	604	CLA	C3B-C2B	-2.09	1.37	1.40
29	A1	405	CLA	C3D-C4D	-2.09	1.39	1.44
29	r1	609	CLA	C1A-CHA	2.09	1.51	1.43
31	C	515	BCR	C12-C13	-2.09	1.41	1.45
29	N1	603	CLA	C1A-CHA	2.09	1.51	1.43
29	g1	603	CLA	C3D-C4D	-2.09	1.39	1.44
29	b1	612	CLA	C3B-C2B	-2.09	1.37	1.40
51	G	623	NEX	O24-C25	-2.09	1.43	1.46
29	s1	605	CLA	C3B-C2B	-2.09	1.37	1.40
29	S	613	CLA	C1A-CHA	2.09	1.51	1.43
48	N1	601	CHL	C3B-C2B	-2.09	1.37	1.40
29	B	617	CLA	C3D-C4D	-2.09	1.39	1.44
29	G1	611	CLA	C1A-CHA	2.09	1.51	1.43
29	g	602	CLA	C3D-C4D	-2.08	1.39	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	Y	611	CLA	C1A-CHA	2.08	1.51	1.43
29	C1	510	CLA	C1A-CHA	2.08	1.51	1.43
29	n1	602	CLA	C3B-C2B	-2.08	1.37	1.40
29	n1	613	CLA	C3D-C4D	-2.08	1.39	1.44
29	G1	603	CLA	C1A-CHA	2.08	1.51	1.43
29	c	503	CLA	C3B-C2B	-2.08	1.37	1.40
29	d	403	CLA	C1A-CHA	2.08	1.51	1.43
29	N	603	CLA	C3D-C4D	-2.08	1.39	1.44
29	n1	612	CLA	CHD-C1D	2.08	1.42	1.38
29	B	616	CLA	C1C-C2C	2.08	1.48	1.44
29	A1	407	CLA	C3B-C2B	-2.08	1.37	1.40
29	y	603	CLA	C1B-NB	2.08	1.37	1.35
29	b1	606	CLA	C1A-CHA	2.08	1.51	1.43
29	B	603	CLA	C1C-C2C	2.08	1.48	1.44
29	g	602	CLA	C1C-C2C	2.08	1.48	1.44
29	y	608	CLA	C1C-C2C	2.08	1.48	1.44
37	b	623	DGD	O5D-C1E	2.08	1.43	1.40
38	s1	626	3PH	O21-C21	2.08	1.40	1.34
29	B1	617	CLA	C1A-CHA	2.08	1.51	1.43
55	Y	627	PTY	O4-C1	-2.08	1.40	1.45
33	h	102	LMG	C22-C21	-2.08	1.32	1.49
29	g1	613	CLA	C1A-CHA	2.08	1.51	1.43
29	s1	614	CLA	C1C-C2C	2.08	1.48	1.44
47	I	102	4RF	O21-C20	-2.08	1.41	1.46
29	G	610	CLA	C3B-C2B	-2.08	1.37	1.40
29	C	511	CLA	C3D-C4D	-2.08	1.39	1.44
29	S	610	CLA	C3D-C4D	-2.08	1.39	1.44
29	S	617	CLA	C3D-C4D	-2.08	1.39	1.44
29	s1	602	CLA	C3D-C4D	-2.08	1.39	1.44
29	g1	604	CLA	C1A-CHA	2.08	1.51	1.43
29	Y	608	CLA	C3D-C4D	-2.08	1.39	1.44
29	A1	410	CLA	C3D-C4D	-2.08	1.39	1.44
29	s	605	CLA	C3D-C4D	-2.08	1.39	1.44
29	D1	403	CLA	CHD-C1D	2.08	1.42	1.38
29	B	615	CLA	C1C-C2C	2.08	1.48	1.44
29	S1	604	CLA	C3D-C4D	-2.08	1.39	1.44
37	c1	518	DGD	O3G-C1D	2.08	1.43	1.40
29	N	612	CLA	MG-NC	2.08	2.11	2.06
29	A	406	CLA	C3D-C4D	-2.08	1.39	1.44
29	s1	617	CLA	C1C-C2C	2.07	1.48	1.44
51	s	623	NEX	O24-C25	-2.07	1.43	1.46
29	c	501	CLA	C1A-CHA	2.07	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	C	502	CLA	C1A-CHA	2.07	1.51	1.43
29	C	502	CLA	C3D-C4D	-2.07	1.39	1.44
29	g1	614	CLA	C3D-C4D	-2.07	1.39	1.44
29	Y	611	CLA	CHD-C1D	2.07	1.42	1.38
31	a1	411	BCR	C12-C13	-2.07	1.41	1.45
48	N1	606	CHL	CHC-C1C	2.07	1.40	1.35
29	A	410	CLA	C1C-C2C	2.07	1.48	1.44
29	b	617	CLA	C3D-C4D	-2.07	1.39	1.44
29	c1	505	CLA	C1B-NB	2.07	1.37	1.35
29	B	614	CLA	C3B-C2B	-2.07	1.37	1.40
29	c1	506	CLA	C1A-CHA	2.07	1.51	1.43
33	H	102	LMG	C22-C21	-2.07	1.32	1.49
51	Y1	623	NEX	C11-C10	2.07	1.49	1.43
29	Y1	602	CLA	C1A-CHA	2.07	1.51	1.43
29	C	511	CLA	C3B-C2B	-2.07	1.37	1.40
29	C1	503	CLA	C3B-C2B	-2.07	1.37	1.40
29	C1	508	CLA	C3D-C4D	-2.07	1.39	1.44
29	B1	611	CLA	CHC-C1C	2.07	1.40	1.35
29	G	613	CLA	C1C-C2C	2.07	1.48	1.44
29	n	610	CLA	C1A-CHA	2.07	1.51	1.43
29	S	605	CLA	C3D-C4D	-2.07	1.39	1.44
44	F	101	HEM	CMB-C2B	2.07	1.55	1.50
29	r1	603	CLA	C1C-C2C	2.07	1.48	1.44
29	y	613	CLA	C3D-C4D	-2.07	1.39	1.44
48	S1	601	CHL	CHC-C1C	2.07	1.40	1.35
29	c	504	CLA	C1A-CHA	2.07	1.51	1.43
29	r	608	CLA	C1C-C2C	2.07	1.48	1.44
29	d1	402	CLA	C1C-C2C	2.07	1.48	1.44
29	b1	615	CLA	C1A-CHA	2.07	1.51	1.43
29	a1	406	CLA	C1A-CHA	2.07	1.51	1.43
51	S	623	NEX	O24-C25	-2.07	1.43	1.46
29	n	610	CLA	C3D-C4D	-2.07	1.39	1.44
49	S1	621	LUT	C1-C6	-2.07	1.50	1.53
29	A	407	CLA	CHD-C1D	2.07	1.42	1.38
29	A	407	CLA	C3D-C4D	-2.06	1.39	1.44
37	c	518	DGD	CGB-CFB	-2.06	1.32	1.49
29	y1	612	CLA	C3B-C2B	-2.06	1.37	1.40
29	s	610	CLA	C1C-C2C	2.06	1.48	1.44
29	s	610	CLA	C3D-C4D	-2.06	1.39	1.44
29	c1	503	CLA	C3D-C4D	-2.06	1.39	1.44
29	g	604	CLA	C1C-C2C	2.06	1.48	1.44
29	c1	507	CLA	CHD-C1D	2.06	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	a1	406	CLA	C1C-C2C	2.06	1.48	1.44
29	A1	407	CLA	CHD-C1D	2.06	1.42	1.38
44	f1	101	HEM	CMB-C2B	2.06	1.55	1.50
29	b	609	CLA	C1A-CHA	2.06	1.51	1.43
29	B1	611	CLA	C1A-CHA	2.06	1.51	1.43
29	s	602	CLA	C1C-C2C	2.06	1.48	1.44
48	n1	606	CHL	CHC-C1C	2.06	1.40	1.35
29	B	616	CLA	C3D-C4D	-2.06	1.39	1.44
29	b1	616	CLA	C3D-C4D	-2.06	1.39	1.44
29	y1	608	CLA	C1C-C2C	2.06	1.48	1.44
29	b	606	CLA	C1A-CHA	2.06	1.51	1.43
37	c1	519	DGD	CGA-CFA	-2.06	1.33	1.49
29	G1	602	CLA	CHC-C1C	2.06	1.40	1.35
29	Y	610	CLA	C3B-C2B	-2.06	1.37	1.40
37	c1	520	DGD	CDA-CCA	-2.06	1.33	1.49
38	B	624	3PH	O31-C3	-2.06	1.40	1.45
29	B	603	CLA	C3D-C4D	-2.06	1.39	1.44
29	B1	608	CLA	C1C-C2C	2.06	1.48	1.44
29	C1	508	CLA	C1C-C2C	2.06	1.48	1.44
29	S1	611	CLA	C1C-C2C	2.06	1.48	1.44
29	S1	609	CLA	C3D-C4D	-2.06	1.39	1.44
29	Y	604	CLA	C3B-C2B	-2.06	1.37	1.40
29	s1	612	CLA	MG-NC	2.06	2.11	2.06
29	D	403	CLA	C1C-C2C	2.06	1.48	1.44
29	c1	510	CLA	C1C-C2C	2.06	1.48	1.44
29	B	609	CLA	C1A-CHA	2.06	1.51	1.43
29	s1	614	CLA	C1B-NB	2.05	1.37	1.35
29	G	602	CLA	C3D-C4D	-2.05	1.39	1.44
29	b1	607	CLA	C3D-C4D	-2.05	1.39	1.44
29	g	603	CLA	C1C-C2C	2.05	1.48	1.44
29	c	502	CLA	C1A-CHA	2.05	1.51	1.43
37	C	519	DGD	CGB-CFB	-2.05	1.33	1.49
29	B1	605	CLA	C3D-C4D	-2.05	1.39	1.44
29	g1	602	CLA	C3D-C4D	-2.05	1.39	1.44
29	g1	612	CLA	MG-NC	2.05	2.11	2.06
29	a	410	CLA	C3D-C4D	-2.05	1.39	1.44
48	y	606	CHL	C3A-C2A	-2.05	1.48	1.54
29	r	604	CLA	C3D-C4D	-2.05	1.39	1.44
39	J	101	DGA	OG2-CG2	-2.05	1.41	1.46
29	B1	616	CLA	C3D-C4D	-2.05	1.39	1.44
29	G1	610	CLA	C1A-CHA	2.05	1.51	1.43
48	y	601	CHL	C3A-C2A	-2.05	1.48	1.54

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
33	h	102	LMG	C43-C42	-2.05	1.33	1.49
29	R	602	CLA	C3D-C4D	-2.05	1.39	1.44
29	c1	513	CLA	C3D-C4D	-2.05	1.39	1.44
29	y1	611	CLA	C3D-C4D	-2.05	1.39	1.44
29	B	609	CLA	C3B-C2B	-2.05	1.37	1.40
29	G	603	CLA	C1A-CHA	2.05	1.51	1.43
29	Y1	603	CLA	C1B-NB	2.05	1.37	1.35
29	b1	611	CLA	C1A-CHA	2.05	1.51	1.43
29	n	604	CLA	C1A-CHA	2.05	1.51	1.43
29	N1	613	CLA	C1C-C2C	2.05	1.48	1.44
29	R1	604	CLA	C3D-C4D	-2.05	1.39	1.44
29	b1	602	CLA	MG-NC	2.05	2.11	2.06
36	B	620	C7Z	C18-C5	2.05	1.54	1.50
48	Y	606	CHL	CHC-C1C	2.05	1.40	1.35
29	S	604	CLA	C3D-C4D	-2.05	1.39	1.44
29	Y1	611	CLA	C3D-C4D	-2.05	1.39	1.44
29	s1	612	CLA	C3D-C4D	-2.05	1.39	1.44
29	C1	509	CLA	C1A-CHA	2.05	1.51	1.43
29	y	604	CLA	C3D-C4D	-2.05	1.39	1.44
43	d	405	PL9	C16-C14	-2.05	1.47	1.51
29	n	603	CLA	C1C-C2C	2.05	1.48	1.44
29	y1	602	CLA	C3D-C4D	-2.05	1.39	1.44
29	Y	610	CLA	C4B-NB	-2.05	1.33	1.35
29	Y	608	CLA	C1C-C2C	2.05	1.48	1.44
52	R1	625	LMT	O2'-C2'	-2.05	1.38	1.43
29	a1	410	CLA	C3D-C4D	-2.05	1.39	1.44
29	a	410	CLA	C4B-NB	-2.04	1.33	1.35
29	C	504	CLA	C1A-CHA	2.04	1.51	1.43
29	R	604	CLA	C3D-C4D	-2.04	1.39	1.44
29	c	503	CLA	C1A-CHA	2.04	1.51	1.43
29	S1	602	CLA	C3D-C4D	-2.04	1.39	1.44
29	d1	403	CLA	C1A-CHA	2.04	1.51	1.43
39	B1	625	DGA	CB2-CB1	2.04	1.56	1.50
29	S	603	CLA	C1C-C2C	2.04	1.48	1.44
29	s1	617	CLA	C3D-C4D	-2.04	1.39	1.44
29	C	506	CLA	C4B-NB	-2.04	1.33	1.35
29	A1	405	CLA	C1A-CHA	2.04	1.51	1.43
37	C1	520	DGD	CGB-CFB	-2.04	1.33	1.49
29	S1	605	CLA	C3D-C4D	-2.04	1.39	1.44
34	A1	414	SPH	C3-C4	2.04	1.53	1.50
29	c1	512	CLA	C1C-C2C	2.04	1.48	1.44
29	n1	613	CLA	C1B-NB	2.04	1.37	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
49	r1	620	LUT	C1-C6	-2.04	1.51	1.53
33	A1	413	LMG	C22-C21	-2.04	1.33	1.49
29	Y	614	CLA	C1B-NB	2.04	1.37	1.35
29	D1	403	CLA	C3D-C4D	-2.04	1.39	1.44
29	C1	505	CLA	C1A-CHA	2.04	1.51	1.43
33	C	521	LMG	C43-C42	-2.04	1.33	1.49
29	s	609	CLA	C1C-C2C	2.04	1.48	1.44
29	b1	610	CLA	C1B-NB	2.04	1.37	1.35
37	C1	519	DGD	CGB-CFB	-2.04	1.33	1.49
29	s1	602	CLA	C1A-CHA	2.04	1.51	1.43
37	C	520	DGD	CDA-CCA	-2.04	1.33	1.49
29	G	610	CLA	C3D-C4D	-2.04	1.39	1.44
49	g	621	LUT	C22-C21	-2.04	1.52	1.54
29	R	604	CLA	C1A-CHA	2.04	1.51	1.43
48	y	607	CHL	CHC-C1C	2.04	1.40	1.35
29	c1	507	CLA	C3D-C4D	-2.04	1.39	1.44
29	b	613	CLA	C1A-CHA	2.04	1.51	1.43
31	c1	517	BCR	C12-C13	-2.04	1.41	1.45
48	g	601	CHL	C3B-C2B	-2.04	1.37	1.40
29	b	616	CLA	C1A-CHA	2.04	1.51	1.43
38	T1	101	3PH	O21-C2	-2.04	1.41	1.46
48	Y1	606	CHL	C3A-C2A	-2.04	1.48	1.54
29	g1	611	CLA	MG-NC	2.03	2.11	2.06
29	R	608	CLA	CHD-C1D	2.03	1.42	1.38
29	b	615	CLA	C1C-C2C	2.03	1.48	1.44
33	A1	413	LMG	C43-C42	-2.03	1.33	1.49
29	B1	616	CLA	C1A-CHA	2.03	1.51	1.43
29	Y1	610	CLA	C3D-C4D	-2.03	1.39	1.44
29	Y	603	CLA	C1A-CHA	2.03	1.51	1.43
33	a1	413	LMG	C43-C42	-2.03	1.33	1.49
37	C	519	DGD	CGA-CFA	-2.03	1.33	1.49
29	b1	610	CLA	C3D-C4D	-2.03	1.39	1.44
33	H1	102	LMG	C22-C21	-2.03	1.33	1.49
29	a1	410	CLA	CHD-C1D	2.03	1.42	1.38
29	Y	602	CLA	CHD-C1D	2.03	1.42	1.38
33	c	521	LMG	C43-C42	-2.03	1.33	1.49
29	S	610	CLA	C1A-CHA	2.03	1.51	1.43
29	b1	610	CLA	C1A-CHA	2.03	1.51	1.43
29	B	606	CLA	C3D-C4D	-2.03	1.39	1.44
29	S1	614	CLA	C3D-C4D	-2.03	1.39	1.44
29	b1	610	CLA	C1C-C2C	2.03	1.48	1.44
29	R	610	CLA	C1A-CHA	2.03	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	y1	602	CLA	C1A-CHA	2.03	1.51	1.43
29	B	611	CLA	C1A-CHA	2.03	1.51	1.43
48	g1	608	CHL	C3B-C2B	-2.03	1.37	1.40
29	S	610	CLA	C1C-C2C	2.03	1.48	1.44
29	s	612	CLA	C1C-C2C	2.03	1.48	1.44
29	B1	610	CLA	C1C-C2C	2.03	1.48	1.44
48	S1	601	CHL	C3A-C2A	-2.03	1.48	1.54
29	N1	613	CLA	C1A-CHA	2.03	1.51	1.43
37	c1	518	DGD	CGB-CFB	-2.03	1.33	1.49
29	A1	406	CLA	C3D-C4D	-2.03	1.39	1.44
29	y	611	CLA	C1A-CHA	2.03	1.51	1.43
33	D	411	LMG	C25-C24	-2.03	1.33	1.49
29	r	610	CLA	C1C-C2C	2.03	1.48	1.44
29	C1	505	CLA	C1C-C2C	2.03	1.48	1.44
29	c1	503	CLA	C1C-C2C	2.03	1.48	1.44
29	B	610	CLA	C1A-CHA	2.03	1.51	1.43
29	c	508	CLA	C1A-CHA	2.03	1.51	1.43
29	R1	602	CLA	C3D-C4D	-2.03	1.39	1.44
29	Y	614	CLA	C1C-C2C	2.03	1.48	1.44
51	N1	623	NEX	C1-C6	-2.03	1.51	1.54
29	y	603	CLA	MG-NC	2.03	2.11	2.06
29	b	608	CLA	C3B-C2B	-2.03	1.37	1.40
48	s	606	CHL	CHC-C1C	2.02	1.40	1.35
33	A	413	LMG	C43-C42	-2.02	1.33	1.49
30	a	408	PHO	C3B-C2B	-2.02	1.37	1.40
29	S1	617	CLA	C3D-C4D	-2.02	1.39	1.44
29	c1	502	CLA	C3D-C4D	-2.02	1.39	1.44
32	C	526	SQD	O47-C45	-2.02	1.41	1.46
29	c1	505	CLA	C3D-C4D	-2.02	1.39	1.44
29	b	609	CLA	C1D-ND	-2.02	1.35	1.37
38	b1	624	3PH	O31-C3	-2.02	1.40	1.45
29	a1	407	CLA	C1C-C2C	2.02	1.48	1.44
29	r	610	CLA	C3D-C4D	-2.02	1.39	1.44
29	b1	614	CLA	C3D-C4D	-2.02	1.39	1.44
29	R	612	CLA	MG-NC	2.02	2.11	2.06
33	A	413	LMG	C22-C21	-2.02	1.33	1.49
33	H	102	LMG	C43-C42	-2.02	1.33	1.49
39	j1	101	DGA	OG2-CG2	-2.02	1.41	1.46
36	b	620	C7Z	C40-C33	2.02	1.55	1.50
41	c1	527	LMK	O8-C28	2.02	1.43	1.40
30	A	408	PHO	CMB-C2B	-2.02	1.46	1.51
33	b	622	LMG	C25-C24	-2.02	1.33	1.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	c1	504	CLA	C3D-C4D	-2.02	1.39	1.44
29	s1	614	CLA	MG-NC	2.02	2.11	2.06
29	C1	512	CLA	C3D-C4D	-2.02	1.39	1.44
29	n1	604	CLA	C3D-C4D	-2.02	1.39	1.44
29	R1	610	CLA	C3D-C4D	-2.02	1.39	1.44
29	s	612	CLA	C1A-CHA	2.02	1.51	1.43
29	b1	615	CLA	C3B-C2B	-2.02	1.37	1.40
29	B1	612	CLA	C1A-CHA	2.02	1.51	1.43
29	B1	614	CLA	C1A-CHA	2.02	1.51	1.43
29	Y1	602	CLA	MG-NC	2.02	2.11	2.06
55	Y1	627	PTY	O7-C8	2.02	1.39	1.35
33	h1	102	LMG	C22-C21	-2.02	1.33	1.49
29	y	610	CLA	C3D-C4D	-2.02	1.39	1.44
29	b	614	CLA	C3D-C4D	-2.02	1.39	1.44
33	a1	413	LMG	C22-C21	-2.02	1.33	1.49
29	c	511	CLA	C1A-CHA	2.02	1.51	1.43
33	C1	521	LMG	C43-C42	-2.02	1.33	1.49
29	B1	613	CLA	C1A-CHA	2.02	1.51	1.43
29	B	607	CLA	CHD-C1D	2.02	1.42	1.38
47	k	101	4RF	C19-C20	2.02	1.56	1.50
29	b1	602	CLA	C1B-NB	2.02	1.37	1.35
29	D	402	CLA	C1C-C2C	2.02	1.48	1.44
29	c1	509	CLA	CHD-C1D	2.02	1.42	1.38
29	Y1	613	CLA	C1A-CHA	2.02	1.51	1.43
29	G	614	CLA	MG-NC	2.02	2.11	2.06
33	a	413	LMG	C22-C21	-2.02	1.33	1.49
29	n1	602	CLA	C1A-CHA	2.01	1.51	1.43
38	S1	626	3PH	O31-C3	-2.01	1.40	1.45
29	y1	614	CLA	C1A-CHA	2.01	1.51	1.43
29	C	509	CLA	C1A-CHA	2.01	1.51	1.43
29	s1	613	CLA	MG-NC	2.01	2.11	2.06
29	r	612	CLA	C1C-C2C	2.01	1.48	1.44
37	C1	518	DGD	CGB-CFB	-2.01	1.33	1.49
29	C1	504	CLA	C1A-CHA	2.01	1.51	1.43
29	N1	612	CLA	C3D-C4D	-2.01	1.39	1.44
29	b1	604	CLA	C3D-C4D	-2.01	1.39	1.44
29	b1	613	CLA	C3D-C4D	-2.01	1.39	1.44
29	A	410	CLA	C1A-CHA	2.01	1.51	1.43
29	r	602	CLA	C1A-CHA	2.01	1.51	1.43
29	N1	604	CLA	C1A-CHA	2.01	1.51	1.43
33	D1	411	LMG	C25-C24	-2.01	1.33	1.49
29	R	602	CLA	C1A-CHA	2.01	1.51	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	t	101	3PH	O31-C3	-2.01	1.40	1.45
33	c1	521	LMG	C25-C24	-2.01	1.33	1.49
29	g	604	CLA	C1A-CHA	2.01	1.51	1.43
33	B1	622	LMG	C25-C24	-2.01	1.33	1.49
29	C1	511	CLA	C3D-C4D	-2.01	1.39	1.44
37	C1	519	DGD	CGA-CFA	-2.01	1.33	1.49
37	c1	520	DGD	CGB-CFB	-2.01	1.33	1.49
31	b	619	BCR	C12-C13	-2.01	1.41	1.45
29	B	613	CLA	C4B-NB	-2.01	1.33	1.35
29	Y	611	CLA	C3D-C4D	-2.01	1.39	1.44
52	R	625	LMT	O1'-C1'	-2.01	1.36	1.40
37	C	518	DGD	CGB-CFB	-2.01	1.33	1.49
29	B	613	CLA	C1A-CHA	2.01	1.51	1.43
29	c	506	CLA	C1A-CHA	2.01	1.51	1.43
29	C1	503	CLA	C1A-CHA	2.01	1.51	1.43
29	S1	602	CLA	C1A-CHA	2.01	1.51	1.43
33	B	622	LMG	C25-C24	-2.01	1.33	1.49
29	Y	614	CLA	C1A-CHA	2.01	1.51	1.43
29	a	410	CLA	C1C-C2C	2.01	1.48	1.44
33	a	413	LMG	C43-C42	-2.01	1.33	1.49
29	R	609	CLA	C1A-CHA	2.01	1.51	1.43
29	B1	602	CLA	C1B-NB	2.01	1.37	1.35
29	S	605	CLA	CHD-C1D	2.01	1.42	1.38
29	c	512	CLA	MG-NC	2.01	2.11	2.06
30	A1	409	PHO	CMB-C2B	-2.01	1.46	1.51
29	b	604	CLA	C1A-CHA	2.01	1.51	1.43
29	y	612	CLA	C3D-C4D	-2.01	1.39	1.44
47	I1	102	4RF	C15-C16	2.01	1.56	1.50
29	S1	604	CLA	C1B-NB	2.00	1.37	1.35
29	B	610	CLA	C3D-C4D	-2.00	1.39	1.44
29	N	602	CLA	C1A-CHA	2.00	1.51	1.43
36	b1	620	C7Z	C18-C5	2.00	1.54	1.50
33	H1	102	LMG	C43-C42	-2.00	1.33	1.49
29	B1	606	CLA	CHD-C1D	2.00	1.42	1.38
29	Y	602	CLA	C4B-NB	-2.00	1.33	1.35
29	B1	604	CLA	C3D-C4D	-2.00	1.39	1.44
29	R	608	CLA	MG-NC	2.00	2.11	2.06
29	c	506	CLA	CHD-C1D	2.00	1.42	1.38
29	S	612	CLA	C4B-NB	-2.00	1.33	1.35
29	S	602	CLA	C1A-CHA	2.00	1.51	1.43
29	s1	617	CLA	C1A-CHA	2.00	1.51	1.43
29	c1	502	CLA	CHD-C1D	2.00	1.42	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	G1	614	CLA	C1B-NB	2.00	1.37	1.35
29	b	603	CLA	C1A-CHA	2.00	1.51	1.43
29	y1	608	CLA	C1A-CHA	2.00	1.51	1.43
29	B1	603	CLA	MG-NC	2.00	2.11	2.06
48	g1	606	CHL	C1A-CHA	-2.00	1.34	1.43
37	C	520	DGD	CGB-CFB	-2.00	1.33	1.49

All (8657) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	L	101	LHG	O7-C7-C8	22.97	161.00	111.50
40	l	101	LHG	O7-C7-C8	22.96	160.99	111.50
29	R	609	CLA	C4-C3-C5	-22.39	77.60	115.27
38	S	626	3PH	O21-C21-C22	22.18	159.31	111.50
38	S1	626	3PH	O21-C21-C22	22.13	159.19	111.50
38	s	626	3PH	O21-C21-C22	22.09	159.10	111.50
29	R1	609	CLA	C4-C3-C5	-22.08	78.13	115.27
38	s1	626	3PH	O21-C21-C22	21.57	157.99	111.50
29	R1	609	CLA	C5-C3-C2	18.90	159.36	121.12
29	R	609	CLA	C5-C3-C2	18.45	158.44	121.12
38	s1	626	3PH	O21-C21-O22	-18.36	79.33	123.70
38	S	626	3PH	O21-C21-O22	-18.24	79.63	123.70
38	S1	626	3PH	O21-C21-O22	-18.23	79.65	123.70
38	s	626	3PH	O21-C21-O22	-18.22	79.68	123.70
40	L	101	LHG	O7-C7-O9	-17.95	80.33	123.70
40	l	101	LHG	O7-C7-O9	-17.94	80.35	123.70
50	y1	622	XAT	C37-C21-C36	-17.87	81.02	107.37
31	C	516	BCR	C10-C11-C12	17.78	178.70	123.22
31	C1	516	BCR	C10-C11-C12	17.69	178.43	123.22
31	C	515	BCR	C10-C11-C12	17.65	178.29	123.22
31	D	404	BCR	C10-C11-C12	17.60	178.14	123.22
31	b	618	BCR	C10-C11-C12	17.52	177.90	123.22
31	c	515	BCR	C10-C11-C12	17.51	177.85	123.22
50	Y1	622	XAT	C37-C21-C36	-17.50	81.55	107.37
31	B	618	BCR	C10-C11-C12	17.46	177.69	123.22
31	d	404	BCR	C10-C11-C12	17.43	177.60	123.22
31	c1	514	BCR	C10-C11-C12	17.37	177.44	123.22
31	A1	411	BCR	C10-C11-C12	17.37	177.41	123.22
31	c	514	BCR	C10-C11-C12	17.36	177.38	123.22
31	c	517	BCR	C10-C11-C12	17.26	177.08	123.22
31	C	514	BCR	C10-C11-C12	17.25	177.04	123.22
31	c	516	BCR	C10-C11-C12	17.24	177.03	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	517	BCR	C10-C11-C12	17.18	176.82	123.22
31	c1	516	BCR	C10-C11-C12	17.13	176.68	123.22
31	A	411	BCR	C10-C11-C12	16.95	176.10	123.22
31	a	411	BCR	C10-C11-C12	16.90	175.97	123.22
50	Y	622	XAT	C37-C21-C36	-16.76	82.65	107.37
29	R	609	CLA	C4-C3-C2	-16.69	80.87	123.68
31	b	619	BCR	C10-C11-C12	16.65	175.17	123.22
31	b1	619	BCR	C10-C11-C12	16.63	175.11	123.22
29	R1	609	CLA	C4-C3-C2	-16.54	81.25	123.68
31	B1	619	BCR	C10-C11-C12	16.39	174.36	123.22
31	B1	618	BCR	C10-C11-C12	16.33	174.17	123.22
31	C1	517	BCR	C10-C11-C12	16.27	173.98	123.22
31	c1	515	BCR	C10-C11-C12	16.22	173.83	123.22
31	c1	517	BCR	C10-C11-C12	16.18	173.72	123.22
31	B1	619	BCR	C16-C15-C14	16.04	156.32	123.47
31	C1	514	BCR	C10-C11-C12	15.99	173.10	123.22
31	a1	411	BCR	C10-C11-C12	15.98	173.09	123.22
50	y	622	XAT	C37-C21-C36	-15.95	83.85	107.37
31	d1	404	BCR	C10-C11-C12	15.74	172.34	123.22
31	B	619	BCR	C10-C11-C12	15.44	171.40	123.22
31	c1	514	BCR	C16-C15-C14	15.33	154.87	123.47
31	C1	516	BCR	C16-C15-C14	15.30	154.82	123.47
31	C1	515	BCR	C16-C15-C14	15.29	154.80	123.47
31	D1	404	BCR	C11-C10-C9	15.23	149.05	127.31
31	c1	517	BCR	C16-C15-C14	15.14	154.48	123.47
31	b1	618	BCR	C10-C11-C12	14.89	169.68	123.22
31	b1	619	BCR	C11-C10-C9	14.85	148.50	127.31
31	D1	404	BCR	C10-C11-C12	14.78	169.36	123.22
31	C1	516	BCR	C11-C10-C9	14.69	148.28	127.31
31	c1	516	BCR	C11-C10-C9	14.64	148.21	127.31
31	c1	514	BCR	C11-C10-C9	14.52	148.04	127.31
31	c1	515	BCR	C16-C15-C14	14.46	153.09	123.47
31	C1	517	BCR	C11-C10-C9	14.46	147.94	127.31
31	b1	618	BCR	C16-C15-C14	14.45	153.07	123.47
31	B1	618	BCR	C11-C10-C9	14.41	147.87	127.31
31	B1	618	BCR	C16-C15-C14	14.34	152.84	123.47
31	c1	515	BCR	C11-C10-C9	14.29	147.70	127.31
31	b	618	BCR	C16-C15-C14	13.84	151.83	123.47
31	c1	516	BCR	C16-C15-C14	13.82	151.78	123.47
31	C	514	BCR	C16-C15-C14	13.76	151.65	123.47
31	a	411	BCR	C11-C10-C9	13.69	146.85	127.31
31	d1	404	BCR	C21-C20-C19	13.69	165.93	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	517	BCR	C21-C20-C19	13.67	165.88	123.22
31	c	516	BCR	C11-C10-C9	13.65	146.80	127.31
31	c	514	BCR	C11-C10-C9	13.63	146.77	127.31
31	B1	619	BCR	C21-C20-C19	13.52	165.40	123.22
31	c	514	BCR	C16-C15-C14	13.46	151.06	123.47
31	c1	517	BCR	C21-C20-C19	13.46	165.23	123.22
31	C1	514	BCR	C21-C20-C19	13.46	165.23	123.22
31	d1	404	BCR	C16-C15-C14	13.39	150.90	123.47
50	y1	622	XAT	C37-C21-C22	-13.39	85.72	108.98
31	C1	516	BCR	C21-C20-C19	13.36	164.91	123.22
31	C1	517	BCR	C16-C15-C14	13.28	150.68	123.47
31	D1	404	BCR	C16-C15-C14	13.22	150.55	123.47
53	r	626	ERG	C15-C14-C8	-13.20	100.44	120.44
31	c	517	BCR	C21-C20-C19	13.10	164.09	123.22
31	C1	515	BCR	C10-C11-C12	12.91	163.50	123.22
50	Y	622	XAT	C37-C21-C22	-12.79	86.76	108.98
31	A	411	BCR	C11-C10-C9	12.77	145.53	127.31
31	C1	514	BCR	C16-C15-C14	12.70	149.50	123.47
50	y	622	XAT	C37-C21-C22	-12.69	86.94	108.98
31	d	404	BCR	C21-C20-C19	12.66	162.71	123.22
31	a1	411	BCR	C21-C20-C19	12.61	162.57	123.22
31	B	618	BCR	C16-C15-C14	12.60	149.29	123.47
31	C	516	BCR	C11-C10-C9	12.56	145.23	127.31
31	D	404	BCR	C21-C20-C19	12.52	162.29	123.22
31	b1	619	BCR	C16-C15-C14	12.50	149.09	123.47
31	c	517	BCR	C11-C10-C9	12.42	145.03	127.31
31	C1	517	BCR	C21-C20-C19	12.40	161.90	123.22
31	b	618	BCR	C11-C10-C9	12.38	144.97	127.31
31	A	411	BCR	C21-C20-C19	12.36	161.78	123.22
31	C	515	BCR	C16-C15-C14	12.35	148.77	123.47
31	D1	404	BCR	C21-C20-C19	12.35	161.75	123.22
53	R	626	ERG	C15-C14-C8	-12.23	101.90	120.44
31	C	517	BCR	C11-C10-C9	12.15	144.65	127.31
31	b	619	BCR	C11-C10-C9	12.04	144.49	127.31
31	a	411	BCR	C21-C20-C19	12.00	160.68	123.22
31	B	618	BCR	C11-C10-C9	11.99	144.42	127.31
31	c	515	BCR	C11-C12-C13	11.94	159.94	126.42
31	a	411	BCR	C16-C15-C14	11.92	147.88	123.47
31	C1	517	BCR	C11-C12-C13	11.84	159.68	126.42
31	d	404	BCR	C11-C12-C13	11.78	159.52	126.42
31	c	515	BCR	C16-C15-C14	11.77	147.59	123.47
31	B	619	BCR	C21-C20-C19	11.70	159.72	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	514	BCR	C21-C20-C19	11.69	159.71	123.22
31	A	411	BCR	C11-C12-C13	11.64	159.11	126.42
31	C	514	BCR	C11-C10-C9	11.63	143.91	127.31
31	B1	618	BCR	C21-C20-C19	11.61	159.44	123.22
38	s1	626	3PH	O22-C21-C22	-11.54	78.69	123.73
31	b1	619	BCR	C21-C20-C19	11.54	159.22	123.22
31	c1	515	BCR	C21-C20-C19	11.49	159.07	123.22
31	b	619	BCR	C11-C12-C13	11.46	158.61	126.42
31	D	404	BCR	C11-C10-C9	11.45	143.66	127.31
31	A1	411	BCR	C21-C20-C19	11.43	158.89	123.22
31	b1	618	BCR	C21-C20-C19	11.38	158.72	123.22
31	c	517	BCR	C11-C12-C13	11.37	158.35	126.42
31	c1	516	BCR	C21-C20-C19	11.36	158.68	123.22
31	d	404	BCR	C16-C15-C14	11.35	146.72	123.47
31	c	516	BCR	C21-C20-C19	11.32	158.54	123.22
31	A1	411	BCR	C11-C12-C13	11.32	158.21	126.42
38	S1	626	3PH	O22-C21-C22	-11.32	79.59	123.73
38	s	626	3PH	O22-C21-C22	-11.31	79.62	123.73
31	C	517	BCR	C11-C12-C13	11.28	158.10	126.42
38	S	626	3PH	O22-C21-C22	-11.27	79.75	123.73
31	b	619	BCR	C16-C15-C14	11.26	146.55	123.47
31	c	516	BCR	C16-C15-C14	11.26	146.53	123.47
50	Y1	622	XAT	C37-C21-C22	-11.21	89.51	108.98
31	c	517	BCR	C16-C15-C14	11.20	146.42	123.47
31	B1	619	BCR	C11-C10-C9	11.19	143.28	127.31
53	R1	626	ERG	C15-C14-C8	-11.16	103.52	120.44
31	a1	411	BCR	C16-C15-C14	11.14	146.30	123.47
31	C	515	BCR	C11-C10-C9	11.06	143.09	127.31
40	l	101	LHG	O9-C7-C8	-11.05	80.64	123.73
31	C	516	BCR	C21-C20-C19	11.03	157.65	123.22
31	C	516	BCR	C11-C12-C13	11.02	157.36	126.42
40	L	101	LHG	O9-C7-C8	-11.00	80.81	123.73
31	b	619	BCR	C21-C20-C19	11.00	157.54	123.22
31	d	404	BCR	C11-C10-C9	10.97	142.97	127.31
31	C	517	BCR	C16-C15-C14	10.92	145.84	123.47
31	b1	619	BCR	C11-C12-C13	10.91	157.07	126.42
31	A1	411	BCR	C11-C10-C9	10.85	142.79	127.31
29	Y	610	CLA	C4A-NA-C1A	10.80	111.56	106.71
31	D	404	BCR	C11-C12-C13	10.77	156.68	126.42
31	c1	514	BCR	C21-C20-C19	10.77	156.81	123.22
31	a1	411	BCR	C11-C12-C13	10.74	156.59	126.42
31	c1	517	BCR	C11-C10-C9	10.74	142.63	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C1	515	BCR	C21-C20-C19	10.73	156.70	123.22
31	c	516	BCR	C11-C12-C13	10.71	156.51	126.42
31	b	618	BCR	C21-C20-C19	10.65	156.47	123.22
31	D	404	BCR	C16-C15-C14	10.64	145.26	123.47
31	C	516	BCR	C16-C15-C14	10.56	145.12	123.47
31	a	411	BCR	C11-C12-C13	10.56	156.09	126.42
31	C	514	BCR	C11-C12-C13	10.53	156.01	126.42
31	C	514	BCR	C21-C20-C19	10.52	156.03	123.22
29	b	605	CLA	C4A-NA-C1A	10.45	111.40	106.71
31	A	411	BCR	C16-C15-C14	10.41	144.80	123.47
29	b	606	CLA	C4A-NA-C1A	10.41	111.39	106.71
31	b	618	BCR	C11-C12-C13	10.38	155.59	126.42
31	B	618	BCR	C21-C20-C19	10.38	155.60	123.22
31	C	515	BCR	C11-C12-C13	10.33	155.43	126.42
31	B	618	BCR	C11-C12-C13	10.29	155.32	126.42
31	B1	619	BCR	C11-C12-C13	10.29	155.32	126.42
31	b1	618	BCR	C11-C12-C13	10.26	155.24	126.42
29	y1	613	CLA	C4A-NA-C1A	10.25	111.31	106.71
29	R1	610	CLA	C4A-NA-C1A	10.24	111.31	106.71
29	A	406	CLA	C4A-NA-C1A	10.23	111.31	106.71
29	g1	610	CLA	C4A-NA-C1A	10.23	111.31	106.71
29	a1	407	CLA	C4A-NA-C1A	10.22	111.30	106.71
29	s1	609	CLA	C4A-NA-C1A	10.21	111.30	106.71
29	Y1	613	CLA	C4A-NA-C1A	10.19	111.29	106.71
31	d1	404	BCR	C11-C10-C9	10.19	141.85	127.31
29	b	612	CLA	C4A-NA-C1A	10.17	111.28	106.71
29	s	613	CLA	C4A-NA-C1A	10.17	111.28	106.71
31	d1	404	BCR	C11-C12-C13	10.15	154.94	126.42
31	A1	411	BCR	C16-C15-C14	10.15	144.27	123.47
53	r1	626	ERG	C15-C14-C8	-10.14	105.07	120.44
29	y1	604	CLA	C4A-NA-C1A	10.11	111.25	106.71
29	a1	405	CLA	C4A-NA-C1A	10.08	111.24	106.71
29	B	617	CLA	C4A-NA-C1A	10.08	111.24	106.71
29	n	613	CLA	C4A-NA-C1A	10.07	111.23	106.71
31	B	619	BCR	C11-C12-C13	10.05	154.66	126.42
29	b	614	CLA	C4A-NA-C1A	10.04	111.22	106.71
29	N	610	CLA	C4A-NA-C1A	10.04	111.22	106.71
29	N	613	CLA	C4A-NA-C1A	10.04	111.22	106.71
29	b	610	CLA	C4A-NA-C1A	10.02	111.21	106.71
29	g	610	CLA	C4A-NA-C1A	10.00	111.20	106.71
29	c	513	CLA	C4A-NA-C1A	9.97	111.19	106.71
29	C1	511	CLA	C4A-NA-C1A	9.96	111.19	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	509	CLA	C4A-NA-C1A	9.96	111.18	106.71
29	y	603	CLA	C4A-NA-C1A	9.96	111.18	106.71
29	Y	613	CLA	C4A-NA-C1A	9.94	111.17	106.71
29	y	604	CLA	C4A-NA-C1A	9.93	111.17	106.71
29	G1	613	CLA	C4A-NA-C1A	9.93	111.17	106.71
29	S	613	CLA	C4A-NA-C1A	9.92	111.17	106.71
29	c	505	CLA	C4A-NA-C1A	9.92	111.17	106.71
29	N1	604	CLA	C4A-NA-C1A	9.92	111.17	106.71
29	b	617	CLA	C4A-NA-C1A	9.91	111.16	106.71
29	b	608	CLA	C4A-NA-C1A	9.91	111.16	106.71
29	C1	509	CLA	C4A-NA-C1A	9.91	111.16	106.71
29	b1	609	CLA	C4A-NA-C1A	9.90	111.16	106.71
29	S	605	CLA	C4A-NA-C1A	9.90	111.16	106.71
29	B	606	CLA	C4A-NA-C1A	9.89	111.15	106.71
29	A1	410	CLA	C4A-NA-C1A	9.86	111.14	106.71
29	N	614	CLA	C4A-NA-C1A	9.86	111.14	106.71
31	C1	514	BCR	C11-C10-C9	9.85	141.37	127.31
29	n	603	CLA	C4A-NA-C1A	9.81	111.12	106.71
29	B	608	CLA	C4A-NA-C1A	9.78	111.10	106.71
29	B	609	CLA	C4A-NA-C1A	9.77	111.10	106.71
31	a1	411	BCR	C11-C10-C9	9.76	141.24	127.31
29	G1	614	CLA	C4A-NA-C1A	9.75	111.09	106.71
29	B	613	CLA	C4A-NA-C1A	9.75	111.09	106.71
29	g1	604	CLA	C4A-NA-C1A	9.73	111.08	106.71
29	b1	613	CLA	C4A-NA-C1A	9.73	111.08	106.71
29	C	501	CLA	C4A-NA-C1A	9.71	111.07	106.71
31	c	515	BCR	C20-C19-C18	9.70	153.67	126.42
29	C1	501	CLA	C4A-NA-C1A	9.68	111.06	106.71
29	g	613	CLA	C4A-NA-C1A	9.67	111.05	106.71
29	C	512	CLA	C4A-NA-C1A	9.64	111.04	106.71
29	N1	610	CLA	C4A-NA-C1A	9.64	111.04	106.71
29	B1	605	CLA	C4A-NA-C1A	9.64	111.04	106.71
29	N	603	CLA	C4A-NA-C1A	9.61	111.03	106.71
29	B1	617	CLA	C4A-NA-C1A	9.61	111.03	106.71
29	S1	613	CLA	C4A-NA-C1A	9.61	111.03	106.71
29	Y	603	CLA	C4A-NA-C1A	9.60	111.02	106.71
31	B	619	BCR	C16-C15-C14	9.59	143.12	123.47
29	b	613	CLA	C4A-NA-C1A	9.59	111.02	106.71
29	r	604	CLA	C4A-NA-C1A	9.59	111.02	106.71
29	g	611	CLA	C4A-NA-C1A	9.58	111.01	106.71
29	B	614	CLA	C4A-NA-C1A	9.58	111.01	106.71
29	B1	612	CLA	C4A-NA-C1A	9.58	111.01	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	N1	614	CLA	C4A-NA-C1A	9.57	111.01	106.71
29	c1	504	CLA	C4A-NA-C1A	9.57	111.01	106.71
29	n1	613	CLA	C4A-NA-C1A	9.55	111.00	106.71
29	c1	505	CLA	C4A-NA-C1A	9.54	110.99	106.71
29	y	613	CLA	C4A-NA-C1A	9.53	110.99	106.71
29	n1	610	CLA	C4A-NA-C1A	9.53	110.99	106.71
29	S	604	CLA	C4A-NA-C1A	9.52	110.99	106.71
29	a	407	CLA	C4A-NA-C1A	9.51	110.98	106.71
29	G1	604	CLA	C4A-NA-C1A	9.51	110.98	106.71
29	n1	614	CLA	C4A-NA-C1A	9.51	110.98	106.71
31	c1	514	BCR	C11-C12-C13	9.50	153.12	126.42
31	c1	516	BCR	C11-C12-C13	9.50	153.10	126.42
31	C1	516	BCR	C11-C12-C13	9.50	153.09	126.42
29	r	610	CLA	C4A-NA-C1A	9.49	110.97	106.71
29	s1	611	CLA	C4A-NA-C1A	9.49	110.97	106.71
29	G1	603	CLA	C4A-NA-C1A	9.49	110.97	106.71
29	n	604	CLA	C4A-NA-C1A	9.48	110.97	106.71
29	n1	603	CLA	C4A-NA-C1A	9.48	110.97	106.71
29	G1	611	CLA	C4A-NA-C1A	9.47	110.96	106.71
31	C	515	BCR	C21-C20-C19	9.47	152.77	123.22
29	N1	603	CLA	C4A-NA-C1A	9.46	110.96	106.71
29	B	610	CLA	C4A-NA-C1A	9.44	110.95	106.71
29	A	405	CLA	C4A-NA-C1A	9.44	110.95	106.71
51	s1	623	NEX	C2-C1-C6	9.43	118.38	109.21
29	c1	511	CLA	C4A-NA-C1A	9.43	110.95	106.71
29	C	506	CLA	C4A-NA-C1A	9.43	110.94	106.71
29	N1	613	CLA	C4A-NA-C1A	9.42	110.94	106.71
29	S1	609	CLA	C4A-NA-C1A	9.39	110.93	106.71
29	B1	611	CLA	C4A-NA-C1A	9.37	110.92	106.71
29	n	611	CLA	C4A-NA-C1A	9.37	110.92	106.71
29	Y	604	CLA	C4A-NA-C1A	9.37	110.92	106.71
29	C	507	CLA	C4A-NA-C1A	9.36	110.92	106.71
29	B1	602	CLA	C4A-NA-C1A	9.36	110.91	106.71
29	c1	512	CLA	C4A-NA-C1A	9.36	110.91	106.71
29	s	611	CLA	C4A-NA-C1A	9.35	110.91	106.71
29	a	406	CLA	C4A-NA-C1A	9.35	110.91	106.71
29	c1	501	CLA	C4A-NA-C1A	9.33	110.90	106.71
29	G	611	CLA	C4A-NA-C1A	9.33	110.90	106.71
29	Y	612	CLA	C4A-NA-C1A	9.33	110.90	106.71
29	c	507	CLA	C4A-NA-C1A	9.32	110.90	106.71
29	S	617	CLA	C4A-NA-C1A	9.32	110.89	106.71
29	b1	607	CLA	C4A-NA-C1A	9.32	110.89	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S	611	CLA	C4A-NA-C1A	9.31	110.89	106.71
29	C	513	CLA	C4A-NA-C1A	9.30	110.89	106.71
29	s	617	CLA	C4A-NA-C1A	9.29	110.88	106.71
29	b1	608	CLA	C4A-NA-C1A	9.28	110.88	106.71
29	c1	507	CLA	C4A-NA-C1A	9.27	110.87	106.71
29	c1	513	CLA	C4A-NA-C1A	9.26	110.87	106.71
29	G	603	CLA	C4A-NA-C1A	9.26	110.87	106.71
29	s	609	CLA	C4A-NA-C1A	9.26	110.87	106.71
29	g1	611	CLA	C4A-NA-C1A	9.26	110.87	106.71
29	B	602	CLA	C4A-NA-C1A	9.25	110.86	106.71
29	R1	609	CLA	C4A-NA-C1A	9.24	110.86	106.71
29	B	605	CLA	C4A-NA-C1A	9.24	110.86	106.71
29	b1	612	CLA	C4A-NA-C1A	9.23	110.86	106.71
31	c1	516	BCR	C20-C19-C18	9.23	152.35	126.42
29	A	410	CLA	C4A-NA-C1A	9.23	110.86	106.71
29	B	615	CLA	C4A-NA-C1A	9.23	110.86	106.71
29	G	602	CLA	C4A-NA-C1A	9.23	110.86	106.71
29	y	612	CLA	C4A-NA-C1A	9.23	110.86	106.71
29	B1	610	CLA	C4A-NA-C1A	9.23	110.86	106.71
29	b	615	CLA	C4A-NA-C1A	9.23	110.85	106.71
31	b1	618	BCR	C11-C10-C9	9.22	140.47	127.31
29	b1	615	CLA	C4A-NA-C1A	9.22	110.85	106.71
29	c1	506	CLA	C4A-NA-C1A	9.22	110.85	106.71
29	S	612	CLA	C4A-NA-C1A	9.20	110.84	106.71
29	y	610	CLA	C4A-NA-C1A	9.20	110.84	106.71
29	B1	615	CLA	C4A-NA-C1A	9.20	110.84	106.71
29	a	410	CLA	C4A-NA-C1A	9.20	110.84	106.71
29	G1	602	CLA	C4A-NA-C1A	9.19	110.84	106.71
29	S1	604	CLA	C4A-NA-C1A	9.19	110.84	106.71
29	G1	610	CLA	C4A-NA-C1A	9.18	110.83	106.71
29	Y	608	CLA	C4A-NA-C1A	9.18	110.83	106.71
29	S1	611	CLA	C4A-NA-C1A	9.17	110.83	106.71
29	c1	503	CLA	C4A-NA-C1A	9.17	110.83	106.71
29	n1	604	CLA	C4A-NA-C1A	9.16	110.83	106.71
29	B1	608	CLA	C4A-NA-C1A	9.16	110.82	106.71
29	B1	609	CLA	C4A-NA-C1A	9.16	110.82	106.71
29	c	502	CLA	C4A-NA-C1A	9.16	110.82	106.71
29	D	403	CLA	C4A-NA-C1A	9.15	110.82	106.71
29	C	505	CLA	C4A-NA-C1A	9.15	110.82	106.71
29	y1	612	CLA	C4A-NA-C1A	9.15	110.82	106.71
29	A1	406	CLA	C4A-NA-C1A	9.14	110.81	106.71
29	C1	502	CLA	C4A-NA-C1A	9.13	110.81	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Y	602	CLA	C4A-NA-C1A	9.12	110.81	106.71
51	s1	623	NEX	C17-C1-C6	-9.12	102.31	110.47
31	C	515	BCR	C20-C19-C18	9.11	152.02	126.42
29	C	502	CLA	C4A-NA-C1A	9.11	110.80	106.71
29	b	602	CLA	C4A-NA-C1A	9.10	110.80	106.71
29	n	610	CLA	C4A-NA-C1A	9.10	110.80	106.71
29	s	605	CLA	C4A-NA-C1A	9.10	110.80	106.71
29	s1	605	CLA	C4A-NA-C1A	9.09	110.79	106.71
29	B1	603	CLA	C4A-NA-C1A	9.09	110.79	106.71
29	r1	609	CLA	C4A-NA-C1A	9.08	110.79	106.71
29	G	613	CLA	C4A-NA-C1A	9.08	110.79	106.71
29	b1	605	CLA	C4A-NA-C1A	9.06	110.78	106.71
29	Y1	602	CLA	C4A-NA-C1A	9.06	110.78	106.71
31	c	515	BCR	C11-C10-C9	9.05	140.22	127.31
29	S1	605	CLA	C4A-NA-C1A	9.04	110.77	106.71
29	B1	606	CLA	C4A-NA-C1A	9.04	110.77	106.71
29	G	610	CLA	C4A-NA-C1A	9.02	110.76	106.71
29	C	503	CLA	C4A-NA-C1A	9.01	110.76	106.71
29	y	608	CLA	C4A-NA-C1A	9.01	110.75	106.71
29	C1	510	CLA	C4A-NA-C1A	9.00	110.75	106.71
29	s1	614	CLA	C4A-NA-C1A	9.00	110.75	106.71
29	s1	613	CLA	C4A-NA-C1A	9.00	110.75	106.71
29	s	603	CLA	C4A-NA-C1A	8.99	110.75	106.71
29	s1	603	CLA	C4A-NA-C1A	8.99	110.75	106.71
29	g	612	CLA	C4A-NA-C1A	8.98	110.75	106.71
29	R1	608	CLA	C4A-NA-C1A	8.98	110.74	106.71
31	c1	517	BCR	C11-C12-C13	8.97	151.62	126.42
29	Y1	608	CLA	C4A-NA-C1A	8.97	110.74	106.71
29	b1	606	CLA	C4A-NA-C1A	8.97	110.74	106.71
29	G1	612	CLA	C4A-NA-C1A	8.96	110.74	106.71
29	c	504	CLA	C4A-NA-C1A	8.96	110.73	106.71
31	c	515	BCR	C21-C20-C19	8.95	151.16	123.22
29	S1	612	CLA	C4A-NA-C1A	8.95	110.73	106.71
31	A1	411	BCR	C20-C19-C18	8.95	151.56	126.42
29	R1	612	CLA	C4A-NA-C1A	8.95	110.73	106.71
29	a1	410	CLA	C4A-NA-C1A	8.95	110.73	106.71
29	A1	405	CLA	C4A-NA-C1A	8.94	110.72	106.71
31	c1	514	BCR	C20-C19-C18	8.94	151.53	126.42
29	g1	612	CLA	C4A-NA-C1A	8.94	110.72	106.71
29	Y1	612	CLA	C4A-NA-C1A	8.93	110.72	106.71
29	N1	612	CLA	C4A-NA-C1A	8.92	110.72	106.71
29	S1	617	CLA	C4A-NA-C1A	8.92	110.72	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	607	CLA	C4A-NA-C1A	8.91	110.71	106.71
31	B1	618	BCR	C20-C19-C18	8.91	151.44	126.42
29	n1	611	CLA	C4A-NA-C1A	8.91	110.71	106.71
31	C1	515	BCR	C20-C19-C18	8.91	151.44	126.42
29	c	512	CLA	C4A-NA-C1A	8.90	110.71	106.71
29	R	609	CLA	C4A-NA-C1A	8.90	110.71	106.71
29	R1	604	CLA	C4A-NA-C1A	8.87	110.70	106.71
31	C	514	BCR	C20-C19-C18	8.87	151.33	126.42
29	S1	610	CLA	C4A-NA-C1A	8.87	110.69	106.71
31	C1	514	BCR	C11-C12-C13	8.86	151.32	126.42
29	S1	614	CLA	C4A-NA-C1A	8.86	110.69	106.71
29	a	405	CLA	C4A-NA-C1A	8.85	110.69	106.71
29	c	511	CLA	C4A-NA-C1A	8.85	110.69	106.71
29	A	407	CLA	C4A-NA-C1A	8.85	110.68	106.71
29	R	610	CLA	C4A-NA-C1A	8.85	110.68	106.71
29	b1	603	CLA	C4A-NA-C1A	8.84	110.68	106.71
29	r1	608	CLA	C4A-NA-C1A	8.83	110.68	106.71
29	g1	614	CLA	C4A-NA-C1A	8.83	110.68	106.71
29	r1	604	CLA	C4A-NA-C1A	8.83	110.68	106.71
29	b	609	CLA	C4A-NA-C1A	8.83	110.67	106.71
31	B1	618	BCR	C11-C12-C13	8.83	151.21	126.42
31	D1	404	BCR	C11-C12-C13	8.82	151.20	126.42
29	y	614	CLA	C4A-NA-C1A	8.82	110.67	106.71
29	Y1	610	CLA	C4A-NA-C1A	8.81	110.67	106.71
29	R	612	CLA	C4A-NA-C1A	8.79	110.66	106.71
29	c	509	CLA	C4A-NA-C1A	8.79	110.66	106.71
31	b	618	BCR	C20-C19-C18	8.79	151.12	126.42
29	C	511	CLA	C4A-NA-C1A	8.79	110.66	106.71
29	y1	611	CLA	C4A-NA-C1A	8.79	110.66	106.71
29	b1	604	CLA	C4A-NA-C1A	8.77	110.65	106.71
29	N1	602	CLA	C4A-NA-C1A	8.76	110.65	106.71
29	N	602	CLA	C4A-NA-C1A	8.76	110.64	106.71
29	s1	617	CLA	C4A-NA-C1A	8.76	110.64	106.71
29	C1	505	CLA	C4A-NA-C1A	8.75	110.64	106.71
29	c	503	CLA	C4A-NA-C1A	8.75	110.64	106.71
29	g1	613	CLA	C4A-NA-C1A	8.75	110.64	106.71
29	N	604	CLA	C4A-NA-C1A	8.74	110.63	106.71
29	C1	506	CLA	C4A-NA-C1A	8.73	110.63	106.71
29	B	603	CLA	C4A-NA-C1A	8.72	110.63	106.71
29	C	504	CLA	C4A-NA-C1A	8.72	110.62	106.71
29	B	612	CLA	C4A-NA-C1A	8.71	110.62	106.71
29	B1	607	CLA	C4A-NA-C1A	8.70	110.62	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	501	CLA	C4A-NA-C1A	8.70	110.62	106.71
29	b	603	CLA	C4A-NA-C1A	8.69	110.61	106.71
29	c	510	CLA	C4A-NA-C1A	8.68	110.61	106.71
29	R1	602	CLA	C4A-NA-C1A	8.68	110.61	106.71
29	y1	610	CLA	C4A-NA-C1A	8.68	110.61	106.71
29	G	614	CLA	C4A-NA-C1A	8.66	110.60	106.71
29	r	603	CLA	C4A-NA-C1A	8.66	110.60	106.71
29	Y	611	CLA	C4A-NA-C1A	8.61	110.58	106.71
29	b	611	CLA	C4A-NA-C1A	8.61	110.58	106.71
29	r	612	CLA	C4A-NA-C1A	8.61	110.58	106.71
29	S	614	CLA	C4A-NA-C1A	8.60	110.57	106.71
29	S	602	CLA	C4A-NA-C1A	8.60	110.57	106.71
29	c	506	CLA	C4A-NA-C1A	8.59	110.57	106.71
29	R	604	CLA	C4A-NA-C1A	8.58	110.56	106.71
29	b1	617	CLA	C4A-NA-C1A	8.57	110.56	106.71
29	n	614	CLA	C4A-NA-C1A	8.57	110.56	106.71
29	B	604	CLA	C4A-NA-C1A	8.55	110.55	106.71
29	Y	614	CLA	C4A-NA-C1A	8.54	110.55	106.71
29	D1	402	CLA	C4A-NA-C1A	8.54	110.55	106.71
31	b1	618	BCR	C20-C19-C18	8.54	150.40	126.42
29	s	604	CLA	C4A-NA-C1A	8.53	110.54	106.71
29	B	616	CLA	C4A-NA-C1A	8.52	110.54	106.71
29	G	612	CLA	C4A-NA-C1A	8.51	110.53	106.71
29	d1	402	CLA	C4A-NA-C1A	8.51	110.53	106.71
29	R	608	CLA	C4A-NA-C1A	8.51	110.53	106.71
29	s	612	CLA	C4A-NA-C1A	8.50	110.53	106.71
29	C1	504	CLA	C4A-NA-C1A	8.49	110.52	106.71
29	S1	602	CLA	C4A-NA-C1A	8.48	110.52	106.71
29	S1	603	CLA	C4A-NA-C1A	8.48	110.52	106.71
29	R1	603	CLA	C4A-NA-C1A	8.47	110.52	106.71
29	b1	610	CLA	C4A-NA-C1A	8.47	110.52	106.71
29	N	611	CLA	C4A-NA-C1A	8.46	110.51	106.71
29	B1	616	CLA	C4A-NA-C1A	8.45	110.51	106.71
29	R	603	CLA	C4A-NA-C1A	8.43	110.50	106.71
29	Y1	604	CLA	C4A-NA-C1A	8.43	110.50	106.71
29	r1	603	CLA	C4A-NA-C1A	8.43	110.50	106.71
29	s1	610	CLA	C4A-NA-C1A	8.42	110.49	106.71
29	b	604	CLA	C4A-NA-C1A	8.42	110.49	106.71
29	s	602	CLA	C4A-NA-C1A	8.39	110.48	106.71
31	c1	515	BCR	C20-C19-C18	8.38	149.95	126.42
29	G	604	CLA	C4A-NA-C1A	8.37	110.47	106.71
31	B	618	BCR	C20-C19-C18	8.36	149.90	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	r	609	CLA	C4A-NA-C1A	8.36	110.46	106.71
29	g1	602	CLA	C4A-NA-C1A	8.35	110.46	106.71
29	s1	604	CLA	C4A-NA-C1A	8.34	110.46	106.71
29	N1	611	CLA	C4A-NA-C1A	8.31	110.44	106.71
29	s1	612	CLA	C4A-NA-C1A	8.31	110.44	106.71
29	g	603	CLA	C4A-NA-C1A	8.30	110.44	106.71
31	c1	515	BCR	C11-C12-C13	8.30	149.72	126.42
29	c	508	CLA	C4A-NA-C1A	8.29	110.43	106.71
29	S	609	CLA	C4A-NA-C1A	8.29	110.43	106.71
29	d	402	CLA	C4A-NA-C1A	8.29	110.43	106.71
29	D	402	CLA	C4A-NA-C1A	8.29	110.43	106.71
29	S	610	CLA	C4A-NA-C1A	8.28	110.43	106.71
29	g	614	CLA	C4A-NA-C1A	8.28	110.43	106.71
29	y1	603	CLA	C4A-NA-C1A	8.27	110.42	106.71
31	b1	619	BCR	C20-C19-C18	8.26	149.63	126.42
29	b	616	CLA	C4A-NA-C1A	8.25	110.42	106.71
29	B	611	CLA	C4A-NA-C1A	8.25	110.42	106.71
29	Y1	603	CLA	C4A-NA-C1A	8.25	110.41	106.71
29	y1	602	CLA	C4A-NA-C1A	8.24	110.41	106.71
31	C	516	BCR	C20-C19-C18	8.24	149.57	126.42
29	B	607	CLA	C4A-NA-C1A	8.24	110.41	106.71
29	B1	613	CLA	C4A-NA-C1A	8.23	110.41	106.71
29	b1	616	CLA	C4A-NA-C1A	8.23	110.41	106.71
29	s	614	CLA	C4A-NA-C1A	8.23	110.40	106.71
29	C1	512	CLA	C4A-NA-C1A	8.23	110.40	106.71
29	n1	602	CLA	C4A-NA-C1A	8.20	110.39	106.71
29	y1	608	CLA	C4A-NA-C1A	8.19	110.39	106.71
29	r1	602	CLA	C4A-NA-C1A	8.19	110.39	106.71
29	g	602	CLA	C4A-NA-C1A	8.18	110.39	106.71
29	a1	406	CLA	C4A-NA-C1A	8.16	110.37	106.71
31	b	619	BCR	C20-C19-C18	8.16	149.33	126.42
29	Y1	611	CLA	C4A-NA-C1A	8.14	110.37	106.71
29	r1	610	CLA	C4A-NA-C1A	8.14	110.37	106.71
29	r	608	CLA	C4A-NA-C1A	8.14	110.36	106.71
31	c	514	BCR	C11-C12-C13	8.13	149.25	126.42
29	s1	602	CLA	C4A-NA-C1A	8.12	110.36	106.71
29	d1	403	CLA	C4A-NA-C1A	8.11	110.35	106.71
29	y	611	CLA	C4A-NA-C1A	8.10	110.35	106.71
29	B1	614	CLA	C4A-NA-C1A	8.05	110.33	106.71
29	b1	602	CLA	C4A-NA-C1A	8.05	110.33	106.71
29	y1	614	CLA	C4A-NA-C1A	8.05	110.32	106.71
29	r1	612	CLA	C4A-NA-C1A	8.04	110.32	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c1	509	CLA	C4A-NA-C1A	8.01	110.31	106.71
29	C1	508	CLA	C4A-NA-C1A	8.00	110.30	106.71
29	c1	502	CLA	C4A-NA-C1A	8.00	110.30	106.71
29	b1	611	CLA	C4A-NA-C1A	7.98	110.29	106.71
31	c	516	BCR	C20-C19-C18	7.97	148.80	126.42
41	C	527	LMK	O2-C4-O3	-7.94	106.07	124.09
29	b1	614	CLA	C4A-NA-C1A	7.94	110.27	106.71
29	C1	503	CLA	C4A-NA-C1A	7.93	110.27	106.71
29	g1	603	CLA	C4A-NA-C1A	7.93	110.27	106.71
29	S	603	CLA	C4A-NA-C1A	7.92	110.27	106.71
29	N	612	CLA	C4A-NA-C1A	7.85	110.23	106.71
29	n	612	CLA	C4A-NA-C1A	7.85	110.23	106.71
29	R	602	CLA	C4A-NA-C1A	7.82	110.22	106.71
29	A1	407	CLA	C4A-NA-C1A	7.82	110.22	106.71
41	C1	527	LMK	O2-C4-O3	-7.82	106.33	124.09
29	n1	612	CLA	C4A-NA-C1A	7.82	110.22	106.71
29	C	510	CLA	C4A-NA-C1A	7.81	110.22	106.71
29	D1	403	CLA	C4A-NA-C1A	7.77	110.20	106.71
29	d	403	CLA	C4A-NA-C1A	7.75	110.19	106.71
29	y	602	CLA	C4A-NA-C1A	7.70	110.17	106.71
29	g	604	CLA	C4A-NA-C1A	7.69	110.16	106.71
29	Y1	614	CLA	C4A-NA-C1A	7.69	110.16	106.71
31	c	514	BCR	C20-C19-C18	7.67	147.97	126.42
29	C1	513	CLA	C4A-NA-C1A	7.65	110.15	106.71
31	a	411	BCR	C20-C19-C18	7.63	147.85	126.42
31	C1	517	BCR	C20-C19-C18	7.58	147.71	126.42
50	Y	622	XAT	C36-C21-C22	7.57	122.14	108.98
29	B	609	CLA	O2D-CGD-CBD	7.56	124.70	111.27
50	Y1	622	XAT	C37-C21-C26	-7.53	89.71	110.05
43	D1	405	PL9	C7-C3-C4	7.53	123.00	116.88
45	h	101	RRX	C33-C5-C6	-7.50	116.10	124.53
50	y	622	XAT	C37-C21-C26	-7.44	89.96	110.05
29	s1	602	CLA	O2D-CGD-CBD	7.41	124.43	111.27
31	B	619	BCR	C11-C10-C9	7.40	137.87	127.31
29	r	602	CLA	C4A-NA-C1A	7.40	110.03	106.71
29	n	602	CLA	C4A-NA-C1A	7.38	110.03	106.71
29	c1	508	CLA	C4A-NA-C1A	7.37	110.02	106.71
49	s1	621	LUT	C21-C26-C27	7.36	122.00	112.70
29	c1	510	CLA	C4A-NA-C1A	7.36	110.01	106.71
29	C	508	CLA	C4A-NA-C1A	7.35	110.01	106.71
31	B	619	BCR	C20-C19-C18	7.33	146.99	126.42
29	C1	507	CLA	C4A-NA-C1A	7.32	110.00	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	s	610	CLA	C4A-NA-C1A	7.32	110.00	106.71
31	A	411	BCR	C20-C19-C18	7.30	146.93	126.42
45	h1	101	RRX	C33-C5-C6	-7.30	116.33	124.53
29	a	407	CLA	O2D-CGD-CBD	7.26	124.17	111.27
50	Y	622	XAT	C37-C21-C26	-7.25	90.47	110.05
45	H	101	RRX	C38-C26-C25	-7.24	116.40	124.53
53	R	626	ERG	C14-C13-C17	7.22	107.42	99.72
29	B1	604	CLA	C4A-NA-C1A	7.21	109.95	106.71
31	D1	404	BCR	C20-C19-C18	7.19	146.61	126.42
45	h	101	RRX	C38-C26-C25	-7.17	116.47	124.53
31	a1	411	BCR	C20-C19-C18	7.16	146.53	126.42
29	g1	610	CLA	CMD-C2D-C1D	7.15	137.31	124.71
29	r	604	CLA	O2A-C1-C2	7.14	125.68	108.97
29	R1	604	CLA	O2A-C1-C2	7.12	125.61	108.97
29	R	604	CLA	O2A-C1-C2	7.10	125.57	108.97
50	y1	622	XAT	C36-C21-C22	7.07	121.26	108.98
36	b	620	C7Z	C15-C14-C13	-7.05	117.25	127.31
36	b1	620	C7Z	C2-C3-C4	7.05	119.95	110.30
49	Y1	621	LUT	C21-C26-C27	7.04	121.60	112.70
50	Y1	622	XAT	C36-C21-C22	7.02	121.18	108.98
45	H1	101	RRX	C38-C26-C25	-7.00	116.67	124.53
31	D	404	BCR	C20-C19-C18	6.96	145.96	126.42
39	c	524	DGA	CDB-CCB-CBB	-6.94	79.17	114.42
29	Y1	614	CLA	CMD-C2D-C1D	6.90	136.87	124.71
49	s1	621	LUT	C35-C34-C33	-6.84	117.55	127.31
31	C1	514	BCR	C20-C19-C18	6.79	145.50	126.42
45	h1	101	RRX	C38-C26-C25	-6.75	116.94	124.53
29	a1	407	CLA	O2D-CGD-CBD	6.74	123.25	111.27
29	S	602	CLA	O2D-CGD-CBD	6.69	123.16	111.27
29	S1	610	CLA	CMD-C2D-C1D	6.69	136.50	124.71
29	R1	609	CLA	O2A-C1-C2	6.68	126.20	108.64
39	B	625	DGA	CDB-CCB-CBB	-6.68	80.54	114.42
53	r	626	ERG	C14-C13-C17	6.65	106.82	99.72
29	n1	614	CLA	O2A-C1-C2	6.64	124.50	108.97
29	B1	603	CLA	O2A-C1-C2	6.64	126.08	108.64
39	C	524	DGA	CDB-CCB-CBB	-6.63	80.78	114.42
31	C	517	BCR	C20-C19-C18	6.62	145.02	126.42
39	C1	524	DGA	CDB-CCB-CBB	-6.62	80.84	114.42
51	s1	623	NEX	C19-C9-C10	-6.61	113.66	122.92
50	y1	622	XAT	C37-C21-C26	-6.60	92.22	110.05
39	b	625	DGA	CDB-CCB-CBB	-6.59	80.95	114.42
29	a	406	CLA	CMD-C2D-C1D	6.59	136.32	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	g1	621	LUT	C35-C34-C33	-6.58	117.91	127.31
31	d	404	BCR	C20-C19-C18	6.58	144.90	126.42
51	G	623	NEX	C2-C1-C6	6.57	115.60	109.21
31	c	517	BCR	C20-C19-C18	6.56	144.84	126.42
29	Y1	602	CLA	O2D-CGD-CBD	6.55	122.91	111.27
29	R	612	CLA	O2A-C1-C2	6.54	125.84	108.64
29	a	405	CLA	O2A-C1-C2	6.54	125.83	108.64
51	s	623	NEX	C2-C1-C6	6.54	115.56	109.21
50	y	622	XAT	C36-C21-C22	6.53	120.32	108.98
31	B1	619	BCR	C20-C19-C18	6.51	144.70	126.42
29	g1	614	CLA	CMD-C2D-C1D	6.49	136.16	124.71
31	c1	515	BCR	C15-C14-C13	-6.45	118.11	127.31
41	c	527	LMK	O2-C4-O3	-6.43	109.49	124.09
29	B1	614	CLA	CMD-C2D-C1D	6.42	136.03	124.71
41	c1	527	LMK	O2-C4-O3	-6.42	109.51	124.09
39	b1	625	DGA	CDB-CCB-CBB	-6.42	81.86	114.42
29	s1	603	CLA	O2D-CGD-CBD	6.40	122.64	111.27
31	c1	517	BCR	C20-C19-C18	6.40	144.38	126.42
29	Y	604	CLA	O2D-CGD-CBD	6.39	122.63	111.27
29	b1	612	CLA	O2D-CGD-CBD	6.39	122.63	111.27
29	b	609	CLA	O2D-CGD-CBD	6.39	122.62	111.27
29	R1	602	CLA	O2A-C1-C2	6.36	125.34	108.64
29	a1	406	CLA	CMD-C2D-C1D	6.35	135.91	124.71
53	r1	626	ERG	C12-C13-C14	6.35	117.34	107.27
39	B1	625	DGA	CDB-CCB-CBB	-6.35	82.20	114.42
39	c1	524	DGA	CDB-CCB-CBB	-6.32	82.34	114.42
29	B1	612	CLA	O2A-C1-C2	6.32	125.23	108.64
49	g1	621	LUT	C21-C26-C27	6.31	120.68	112.70
49	R1	620	LUT	C21-C26-C27	6.31	120.68	112.70
50	Y	622	XAT	C31-C30-C29	-6.31	118.31	127.31
51	R	622	NEX	C2-C1-C6	6.31	115.34	109.21
53	R1	626	ERG	C1-C2-C3	6.29	118.54	110.47
49	r1	620	LUT	C21-C26-C27	6.29	120.65	112.70
29	N1	604	CLA	CMD-C2D-C1D	6.26	135.74	124.71
29	s1	604	CLA	CMD-C2D-C1D	6.25	135.73	124.71
29	N1	604	CLA	O2A-C1-C2	6.25	125.06	108.64
50	n	622	XAT	C31-C30-C29	-6.24	118.41	127.31
45	h	101	RRX	C24-C25-C26	-6.23	106.37	121.46
29	B1	607	CLA	CMD-C2D-C1D	6.23	135.69	124.71
49	S1	620	LUT	C21-C26-C27	6.21	120.56	112.70
49	N1	621	LUT	C21-C26-C27	6.21	120.55	112.70
29	c1	504	CLA	O2A-C1-C2	6.18	124.89	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C1	511	CLA	CMD-C2D-C1D	6.18	135.61	124.71
29	a1	405	CLA	CMD-C2D-C1D	6.18	135.60	124.71
29	G1	614	CLA	O2A-C1-C2	6.16	123.37	108.97
53	R1	626	ERG	C14-C13-C17	6.15	106.28	99.72
29	b	614	CLA	CMD-C2D-C1D	6.15	135.54	124.71
29	C1	501	CLA	O2A-C1-C2	6.14	124.78	108.64
29	r1	603	CLA	O2A-C1-C2	6.14	124.77	108.64
31	d1	404	BCR	C20-C19-C18	6.14	143.66	126.42
45	H	101	RRX	C23-C22-C21	-6.13	109.53	118.94
49	r1	620	LUT	C35-C34-C33	-6.13	118.56	127.31
29	N	604	CLA	O2D-CGD-CBD	6.10	122.11	111.27
53	r1	626	ERG	C14-C13-C17	6.10	106.23	99.72
36	b1	620	C7Z	C38-C25-C26	-6.10	117.68	124.53
29	Y	614	CLA	CMD-C2D-C1D	6.09	135.45	124.71
29	c	513	CLA	O2A-C1-C2	6.09	124.64	108.64
29	S	605	CLA	O2D-CGD-CBD	6.09	122.09	111.27
29	s	602	CLA	O2D-CGD-CBD	6.09	122.08	111.27
49	y1	620	LUT	C7-C8-C9	-6.08	117.04	126.23
29	A	407	CLA	O2A-C1-C2	6.08	124.60	108.64
29	B1	613	CLA	CMD-C2D-C1D	6.08	135.42	124.71
53	R	626	ERG	C1-C2-C3	6.07	118.26	110.47
51	y	623	NEX	C17-C1-C6	-6.07	105.04	110.47
29	A1	405	CLA	O2A-C1-C2	6.07	124.58	108.64
29	R1	610	CLA	O2D-CGD-CBD	6.06	122.04	111.27
29	B1	609	CLA	O2D-CGD-CBD	6.06	122.04	111.27
29	y	603	CLA	O2D-CGD-CBD	6.06	122.03	111.27
49	y1	621	LUT	C7-C8-C9	-6.06	117.08	126.23
49	y1	621	LUT	C11-C10-C9	-6.05	118.68	127.31
29	S1	609	CLA	CMD-C2D-C1D	6.05	135.37	124.71
29	S1	603	CLA	O2D-CGD-CBD	6.05	122.01	111.27
50	R	621	XAT	C31-C30-C29	-6.05	118.68	127.31
31	c1	517	BCR	C15-C14-C13	-6.05	118.68	127.31
29	B1	607	CLA	O2D-CGD-CBD	6.04	122.00	111.27
29	N1	603	CLA	O2A-C1-C2	6.04	124.50	108.64
29	N	604	CLA	CMD-C2D-C1D	6.03	135.35	124.71
29	r	610	CLA	CMD-C2D-C1D	6.03	135.34	124.71
50	N	622	XAT	O4-C5-C4	-6.03	108.85	113.38
45	H	101	RRX	C24-C23-C22	6.02	135.34	126.23
49	R	620	LUT	C21-C26-C27	6.02	120.31	112.70
29	N1	611	CLA	CMD-C2D-C1D	6.01	135.31	124.71
29	S	614	CLA	CMD-C2D-C1D	6.01	135.30	124.71
29	C	504	CLA	O2A-C1-C2	6.01	124.42	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	505	CLA	O2D-CGD-CBD	6.00	121.93	111.27
31	C1	515	BCR	C11-C12-C13	6.00	143.27	126.42
29	r	608	CLA	CMD-C2D-C1D	6.00	135.28	124.71
29	S1	604	CLA	O2A-C1-C2	6.00	124.39	108.64
51	S1	623	NEX	C17-C1-C6	-5.99	105.11	110.47
29	n1	613	CLA	O2A-C1-C2	5.99	124.37	108.64
29	A	410	CLA	O2D-CGD-CBD	5.99	121.91	111.27
29	B1	606	CLA	CMD-C2D-C1D	5.98	135.25	124.71
29	r1	612	CLA	CMD-C2D-C1D	5.98	135.25	124.71
29	B1	611	CLA	O2D-CGD-CBD	5.98	121.89	111.27
29	y1	608	CLA	CMD-C2D-C1D	5.97	135.23	124.71
29	B1	616	CLA	CMD-C2D-C1D	5.96	135.22	124.71
45	h	101	RRX	C23-C22-C21	-5.96	109.79	118.94
29	S1	602	CLA	O2D-CGD-CBD	5.95	121.85	111.27
29	B	605	CLA	O2D-CGD-CBD	5.95	121.84	111.27
29	b1	609	CLA	O2D-CGD-CBD	5.95	121.84	111.27
29	c	501	CLA	CMD-C2D-C1D	5.94	135.19	124.71
29	a	407	CLA	O2A-C1-C2	5.94	122.86	108.97
29	c	504	CLA	O2A-C1-C2	5.94	124.25	108.64
29	c	506	CLA	CMD-C2D-C1D	5.94	135.18	124.71
29	D	403	CLA	O2D-CGD-CBD	5.94	121.82	111.27
45	h	101	RRX	C24-C23-C22	5.94	135.21	126.23
29	s	610	CLA	O2A-C1-C2	5.93	124.23	108.64
29	A	405	CLA	CMD-C2D-C1D	5.93	135.16	124.71
53	r	626	ERG	C12-C13-C14	5.93	116.67	107.27
29	g	602	CLA	O2A-C1-C2	5.92	124.21	108.64
29	n	614	CLA	O2A-C1-C2	5.92	122.81	108.97
29	C	509	CLA	CMD-C2D-C1D	5.92	135.15	124.71
45	H	101	RRX	C24-C25-C26	-5.92	107.12	121.46
29	N1	614	CLA	O2A-C1-C2	5.92	122.81	108.97
29	C1	512	CLA	CMD-C2D-C1D	5.92	135.14	124.71
29	g1	610	CLA	O2A-C1-C2	5.92	124.18	108.64
29	a1	406	CLA	O2A-C1-C2	5.92	124.18	108.64
29	C1	513	CLA	CMD-C2D-C1D	5.92	135.14	124.71
36	B	620	C7Z	C18-C5-C6	-5.91	117.89	124.53
29	s1	609	CLA	O2A-C1-C2	5.91	124.18	108.64
29	b	611	CLA	CMD-C2D-C1D	5.91	135.13	124.71
50	n1	622	XAT	C31-C30-C29	-5.91	118.88	127.31
29	g	603	CLA	O2A-C1-C2	5.90	124.15	108.64
29	R	608	CLA	O2A-C1-C2	5.90	124.14	108.64
29	c1	503	CLA	CMD-C2D-C1D	5.90	135.11	124.71
29	c1	511	CLA	CMD-C2D-C1D	5.90	135.11	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	g1	620	LUT	C35-C34-C33	-5.90	118.89	127.31
29	c	505	CLA	O2D-CGD-CBD	5.90	121.75	111.27
29	b	603	CLA	O2A-C1-C2	5.90	124.13	108.64
29	n	610	CLA	O2A-C1-C2	5.90	124.13	108.64
29	G	613	CLA	CMD-C2D-C1D	5.89	135.10	124.71
29	A	405	CLA	O2A-C1-C2	5.89	124.12	108.64
29	G	614	CLA	CMD-C2D-C1D	5.89	135.10	124.71
29	y	604	CLA	O2D-CGD-CBD	5.89	121.74	111.27
29	C	509	CLA	O2D-CGD-CBD	5.89	121.73	111.27
29	B	606	CLA	CMD-C2D-C1D	5.89	135.09	124.71
29	c1	510	CLA	CMD-C2D-C1D	5.89	135.09	124.71
45	H	101	RRX	C11-C10-C9	-5.89	118.91	127.31
50	r1	621	XAT	O4-C5-C4	-5.88	108.97	113.38
29	r1	604	CLA	O2A-C1-C2	5.87	122.71	108.97
29	b1	615	CLA	CMD-C2D-C1D	5.87	135.06	124.71
49	y1	620	LUT	C21-C26-C27	5.87	120.12	112.70
29	c	502	CLA	O2D-CGD-CBD	5.87	121.70	111.27
29	c1	501	CLA	O2A-C1-C2	5.86	124.04	108.64
29	S1	602	CLA	O2A-C1-C2	5.86	124.03	108.64
29	n1	602	CLA	CMD-C2D-C1D	5.86	135.03	124.71
29	c1	507	CLA	O2A-C1-C2	5.85	124.01	108.64
29	C	502	CLA	O2A-C1-C2	5.85	124.00	108.64
29	R1	608	CLA	CMD-C2D-C1D	5.84	135.01	124.71
29	G	602	CLA	CMD-C2D-C1D	5.84	135.00	124.71
29	b1	608	CLA	O2A-C1-C2	5.84	123.97	108.64
29	G1	613	CLA	O2A-C1-C2	5.84	123.97	108.64
36	b1	620	C7Z	C15-C14-C13	-5.84	118.98	127.31
50	g	622	XAT	C31-C30-C29	-5.84	118.98	127.31
29	b1	605	CLA	O2D-CGD-CBD	5.84	121.64	111.27
29	S1	612	CLA	O2D-CGD-CBD	5.83	121.63	111.27
29	c	502	CLA	O2A-C1-C2	5.83	123.96	108.64
36	B1	620	C7Z	C35-C34-C33	-5.83	118.99	127.31
29	s1	610	CLA	O2A-C1-C2	5.83	123.95	108.64
29	C1	505	CLA	O2D-CGD-CBD	5.83	121.62	111.27
29	n	604	CLA	O2A-C1-C2	5.82	123.93	108.64
29	c1	508	CLA	O2A-C1-C2	5.82	123.93	108.64
49	N	621	LUT	C21-C26-C27	5.82	120.05	112.70
29	r	610	CLA	O2A-C1-C2	5.81	123.91	108.64
29	B1	605	CLA	CMD-C2D-C1D	5.81	134.95	124.71
29	G	611	CLA	O2D-CGD-CBD	5.81	121.59	111.27
29	g	611	CLA	O2A-C1-C2	5.81	123.89	108.64
29	S	604	CLA	O2A-C1-C2	5.80	123.89	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	n	614	CLA	CMD-C2D-C1D	5.80	134.94	124.71
29	s	602	CLA	O2A-C1-C2	5.80	123.88	108.64
50	n	622	XAT	C15-C14-C13	-5.80	119.04	127.31
29	D1	402	CLA	O2D-CGD-CBD	5.79	121.56	111.27
29	c1	506	CLA	O2D-CGD-CBD	5.79	121.56	111.27
29	g	604	CLA	O2A-C1-C2	5.79	122.50	108.97
29	a1	410	CLA	O2D-CGD-CBD	5.79	121.55	111.27
29	s1	604	CLA	O2A-C1-C2	5.79	123.85	108.64
36	B	620	C7Z	C11-C10-C9	-5.78	119.05	127.31
29	s	603	CLA	O2D-CGD-CBD	5.78	121.54	111.27
50	g	622	XAT	O4-C5-C4	-5.78	109.04	113.38
29	n	610	CLA	O2D-CGD-CBD	5.78	121.54	111.27
29	G	614	CLA	O2A-C1-C2	5.78	122.49	108.97
29	c1	504	CLA	CMD-C2D-C1D	5.78	134.90	124.71
29	b	613	CLA	O2D-CGD-CBD	5.78	121.54	111.27
49	S	620	LUT	C21-C26-C25	5.78	121.77	111.42
29	C1	506	CLA	CMD-C2D-C1D	5.78	134.89	124.71
49	r	620	LUT	C21-C26-C25	5.77	121.76	111.42
29	c	501	CLA	O2D-CGD-CBD	5.77	121.52	111.27
29	b	607	CLA	O2D-CGD-CBD	5.77	121.52	111.27
29	c1	507	CLA	CMD-C2D-C1D	5.77	134.88	124.71
29	C	510	CLA	CMD-C2D-C1D	5.77	134.88	124.71
29	y1	614	CLA	CMD-C2D-C1D	5.77	134.88	124.71
29	d	403	CLA	CMD-C2D-C1D	5.77	134.88	124.71
29	B	607	CLA	CMD-C2D-C1D	5.76	134.87	124.71
29	G	602	CLA	O2D-CGD-CBD	5.76	121.51	111.27
29	r1	602	CLA	O2D-CGD-CBD	5.76	121.51	111.27
29	g	604	CLA	CMD-C2D-C1D	5.76	134.87	124.71
29	C	512	CLA	O2D-CGD-CBD	5.76	121.50	111.27
29	c	510	CLA	CMD-C2D-C1D	5.76	134.86	124.71
29	c	509	CLA	CMD-C2D-C1D	5.76	134.86	124.71
49	G1	621	LUT	C21-C26-C27	5.75	119.97	112.70
29	G	604	CLA	O2A-C1-C2	5.75	122.42	108.97
29	b1	613	CLA	CMD-C2D-C1D	5.75	134.85	124.71
29	N	614	CLA	O2A-C1-C2	5.75	122.41	108.97
29	N	612	CLA	O2D-CGD-CBD	5.75	121.48	111.27
29	c1	505	CLA	O2D-CGD-CBD	5.74	121.48	111.27
36	b	620	C7Z	C11-C10-C9	-5.74	119.12	127.31
29	b1	607	CLA	O2D-CGD-CBD	5.74	121.47	111.27
50	R	621	XAT	C15-C14-C13	-5.74	119.12	127.31
31	C1	515	BCR	C11-C10-C9	5.74	135.50	127.31
29	Y1	604	CLA	O2D-CGD-CBD	5.73	121.46	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B1	615	CLA	CMD-C2D-C1D	5.73	134.81	124.71
29	D	403	CLA	O2A-C1-C2	5.73	123.70	108.64
29	R1	610	CLA	O2A-C1-C2	5.73	123.70	108.64
29	d	402	CLA	O2A-C1-C2	5.73	123.70	108.64
45	h	101	RRX	C21-C20-C19	-5.73	105.33	123.22
29	b	612	CLA	O2D-CGD-CBD	5.73	121.45	111.27
29	Y	613	CLA	CMD-C2D-C1D	5.73	134.81	124.71
29	n1	611	CLA	O2A-C1-C2	5.73	122.36	108.97
29	S	612	CLA	O2D-CGD-CBD	5.72	121.43	111.27
29	R	608	CLA	CMD-C2D-C1D	5.72	134.79	124.71
29	b	603	CLA	CMD-C2D-C1D	5.72	134.79	124.71
53	R	626	ERG	C12-C13-C14	5.70	116.32	107.27
31	C1	516	BCR	C20-C19-C18	5.70	142.44	126.42
29	S	604	CLA	CMD-C2D-C1D	5.70	134.76	124.71
29	c1	513	CLA	O2A-C1-C2	5.70	123.62	108.64
50	G	622	XAT	C15-C14-C13	-5.69	119.19	127.31
29	s	614	CLA	CMD-C2D-C1D	5.69	134.75	124.71
29	s1	610	CLA	CMD-C2D-C1D	5.69	134.74	124.71
29	Y	613	CLA	O2D-CGD-CBD	5.69	121.37	111.27
29	b	613	CLA	CMD-C2D-C1D	5.68	134.73	124.71
29	G1	613	CLA	CMD-C2D-C1D	5.68	134.73	124.71
29	c	506	CLA	O2A-C1-C2	5.68	123.57	108.64
29	C1	502	CLA	O2A-C1-C2	5.68	123.56	108.64
29	Y1	613	CLA	CMD-C2D-C1D	5.68	134.72	124.71
29	R	602	CLA	O2D-CGD-CBD	5.67	121.35	111.27
29	B	613	CLA	O2D-CGD-CBD	5.67	121.34	111.27
29	D1	403	CLA	O2D-CGD-CBD	5.67	121.34	111.27
29	b	615	CLA	O2A-C1-C2	5.67	123.54	108.64
29	r	604	CLA	CMD-C2D-C1D	5.67	134.70	124.71
29	R	612	CLA	CMD-C2D-C1D	5.67	134.70	124.71
29	G1	604	CLA	CMD-C2D-C1D	5.66	134.69	124.71
29	G1	602	CLA	O2A-C1-C2	5.66	123.51	108.64
29	B1	614	CLA	O2A-C1-C2	5.66	123.51	108.64
29	S1	614	CLA	O2D-CGD-CBD	5.66	121.32	111.27
29	B1	602	CLA	CMD-C2D-C1D	5.66	134.68	124.71
29	b1	602	CLA	CMD-C2D-C1D	5.66	134.68	124.71
29	B1	606	CLA	O2A-C1-C2	5.65	123.49	108.64
29	d1	402	CLA	O2D-CGD-CBD	5.65	121.31	111.27
29	b	602	CLA	CMD-C2D-C1D	5.65	134.67	124.71
29	y1	612	CLA	O2D-CGD-CBD	5.65	121.31	111.27
29	D1	402	CLA	O2A-C1-C2	5.65	123.49	108.64
29	Y1	602	CLA	CMD-C2D-C1D	5.65	134.67	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C1	503	CLA	CMD-C2D-C1D	5.65	134.67	124.71
29	G1	610	CLA	CMD-C2D-C1D	5.64	134.66	124.71
29	g	613	CLA	O2A-C1-C2	5.64	123.46	108.64
29	B	606	CLA	O2D-CGD-CBD	5.63	121.28	111.27
29	g	614	CLA	O2A-C1-C2	5.63	122.14	108.97
29	a	410	CLA	O2D-CGD-CBD	5.63	121.27	111.27
29	G	610	CLA	CMD-C2D-C1D	5.63	134.63	124.71
29	y1	613	CLA	CMD-C2D-C1D	5.63	134.63	124.71
29	r	609	CLA	O2A-C1-C2	5.63	123.42	108.64
29	N1	602	CLA	O2A-C1-C2	5.63	123.42	108.64
29	d1	403	CLA	CMD-C2D-C1D	5.63	134.63	124.71
51	N1	623	NEX	C5-C4-C3	5.62	118.40	111.75
29	G1	602	CLA	CMD-C2D-C1D	5.62	134.61	124.71
29	s1	602	CLA	O2A-C1-C2	5.61	123.39	108.64
45	H	101	RRX	C21-C20-C19	-5.61	105.71	123.22
29	a	410	CLA	O2A-C1-C2	5.61	123.38	108.64
29	B1	603	CLA	CMD-C2D-C1D	5.61	134.59	124.71
29	y1	603	CLA	CMD-C2D-C1D	5.61	134.59	124.71
29	y	608	CLA	CMD-C2D-C1D	5.60	134.59	124.71
29	S1	613	CLA	CMD-C2D-C1D	5.60	134.59	124.71
29	B1	613	CLA	O2A-C1-C2	5.60	123.36	108.64
29	c1	503	CLA	O2D-CGD-CBD	5.60	121.22	111.27
29	a	406	CLA	O2A-C1-C2	5.60	123.36	108.64
29	y	610	CLA	CMD-C2D-C1D	5.60	134.58	124.71
29	R	610	CLA	O2D-CGD-CBD	5.60	121.22	111.27
29	y1	602	CLA	CMD-C2D-C1D	5.60	134.58	124.71
29	B	615	CLA	CMD-C2D-C1D	5.60	134.58	124.71
49	S	621	LUT	C21-C26-C27	5.60	119.78	112.70
29	Y1	610	CLA	CMD-C2D-C1D	5.60	134.58	124.71
29	C1	509	CLA	CMD-C2D-C1D	5.60	134.57	124.71
29	N	603	CLA	CMD-C2D-C1D	5.59	134.57	124.71
29	G1	603	CLA	CMD-C2D-C1D	5.59	134.57	124.71
29	C1	504	CLA	O2A-C1-C2	5.59	123.33	108.64
29	Y1	603	CLA	CMD-C2D-C1D	5.59	134.57	124.71
29	C	507	CLA	O2D-CGD-CBD	5.59	121.20	111.27
29	g	610	CLA	CMD-C2D-C1D	5.59	134.56	124.71
29	S1	602	CLA	CMD-C2D-C1D	5.59	134.56	124.71
29	b	615	CLA	O2D-CGD-CBD	5.59	121.20	111.27
49	y1	621	LUT	C35-C34-C33	-5.59	119.34	127.31
29	B	611	CLA	O2A-C1-C2	5.59	123.32	108.64
29	y	614	CLA	CMD-C2D-C1D	5.58	134.55	124.71
37	B	623	DGD	O2G-C1B-C2B	5.58	123.53	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	s	614	CLA	O2D-CGD-CBD	5.58	121.18	111.27
49	N	620	LUT	C21-C26-C25	5.58	121.41	111.42
29	y	602	CLA	O2D-CGD-CBD	5.58	121.18	111.27
29	N1	603	CLA	CMD-C2D-C1D	5.58	134.54	124.71
29	C1	508	CLA	O2A-C1-C2	5.57	123.28	108.64
49	n1	621	LUT	C21-C26-C27	5.57	119.74	112.70
29	R	604	CLA	CMD-C2D-C1D	5.57	134.53	124.71
29	b	605	CLA	CMD-C2D-C1D	5.57	134.53	124.71
29	B	612	CLA	O2A-C1-C2	5.57	123.26	108.64
29	d	402	CLA	CMD-C2D-C1D	5.56	134.52	124.71
29	Y1	610	CLA	O2A-C1-C2	5.56	123.25	108.64
29	N	610	CLA	CMD-C2D-C1D	5.56	134.50	124.71
29	n	611	CLA	CMD-C2D-C1D	5.56	134.50	124.71
29	N	603	CLA	O2A-C1-C2	5.55	123.22	108.64
29	c1	512	CLA	O2A-C1-C2	5.55	123.22	108.64
29	a	407	CLA	CMD-C2D-C1D	5.55	134.50	124.71
29	b1	605	CLA	CMD-C2D-C1D	5.55	134.50	124.71
50	g1	622	XAT	C15-C14-C13	-5.55	119.39	127.31
29	B1	607	CLA	O2A-C1-C2	5.55	123.22	108.64
29	g1	612	CLA	CMD-C2D-C1D	5.55	134.49	124.71
50	g1	622	XAT	C31-C30-C29	-5.55	119.39	127.31
29	n1	613	CLA	CMD-C2D-C1D	5.55	134.49	124.71
29	s1	602	CLA	CMD-C2D-C1D	5.55	134.49	124.71
29	Y	611	CLA	CMD-C2D-C1D	5.54	134.49	124.71
29	g1	614	CLA	O2A-C1-C2	5.54	121.93	108.97
29	s	605	CLA	CMD-C2D-C1D	5.54	134.48	124.71
50	g	622	XAT	C15-C14-C13	-5.54	119.40	127.31
29	b	606	CLA	CMD-C2D-C1D	5.54	134.48	124.71
29	b	610	CLA	O2D-CGD-CBD	5.54	121.11	111.27
29	g1	602	CLA	CMD-C2D-C1D	5.54	134.47	124.71
29	G1	610	CLA	O2D-CGD-CBD	5.54	121.11	111.27
29	Y1	611	CLA	CMD-C2D-C1D	5.54	134.47	124.71
29	C	501	CLA	CMD-C2D-C1D	5.54	134.47	124.71
29	y	611	CLA	O2A-C1-C2	5.54	123.19	108.64
29	Y1	611	CLA	O2D-CGD-CBD	5.53	121.10	111.27
29	C1	505	CLA	O2A-C1-C2	5.53	123.17	108.64
29	r1	603	CLA	CMD-C2D-C1D	5.53	134.46	124.71
49	n	620	LUT	C21-C26-C25	5.53	121.32	111.42
29	N	604	CLA	O2A-C1-C2	5.52	123.16	108.64
29	r	604	CLA	O2D-CGD-CBD	5.52	121.08	111.27
29	G	612	CLA	CMD-C2D-C1D	5.52	134.45	124.71
50	N1	622	XAT	C31-C30-C29	-5.52	119.43	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	513	CLA	O2D-CGD-CBD	5.52	121.08	111.27
29	r	609	CLA	CMD-C2D-C1D	5.52	134.44	124.71
29	D1	403	CLA	CMD-C2D-C1D	5.52	134.44	124.71
29	d1	402	CLA	CMD-C2D-C1D	5.52	134.44	124.71
29	b	617	CLA	O2D-CGD-CBD	5.52	121.07	111.27
29	s1	613	CLA	CMD-C2D-C1D	5.52	134.43	124.71
29	r	612	CLA	O2D-CGD-CBD	5.51	121.06	111.27
29	b	615	CLA	CMD-C2D-C1D	5.51	134.43	124.71
29	g1	613	CLA	O2A-C1-C2	5.51	123.12	108.64
29	G	604	CLA	CMD-C2D-C1D	5.51	134.42	124.71
50	N	622	XAT	C31-C30-C29	-5.51	119.45	127.31
29	B	602	CLA	CMD-C2D-C1D	5.51	134.42	124.71
29	G1	604	CLA	O2D-CGD-CBD	5.50	121.05	111.27
29	r	612	CLA	O2A-C1-C2	5.50	123.09	108.64
29	n	604	CLA	O2D-CGD-CBD	5.50	121.04	111.27
49	g	621	LUT	C21-C26-C27	5.50	119.65	112.70
29	b1	610	CLA	CMD-C2D-C1D	5.50	134.40	124.71
50	Y1	622	XAT	C15-C14-C13	-5.50	119.47	127.31
29	Y	610	CLA	CMD-C2D-C1D	5.50	134.40	124.71
29	D	402	CLA	O2A-C1-C2	5.49	123.07	108.64
29	G	610	CLA	O2A-C1-C2	5.49	123.07	108.64
29	n1	604	CLA	CMD-C2D-C1D	5.49	134.39	124.71
29	S	605	CLA	CMD-C2D-C1D	5.49	134.39	124.71
29	c	507	CLA	O2D-CGD-CBD	5.49	121.03	111.27
29	y1	610	CLA	O2A-C1-C2	5.49	123.06	108.64
29	g	603	CLA	CMD-C2D-C1D	5.49	134.39	124.71
49	r	620	LUT	C11-C10-C9	-5.49	119.48	127.31
29	D	402	CLA	CMD-C2D-C1D	5.49	134.38	124.71
29	Y1	604	CLA	CMD-C2D-C1D	5.49	134.38	124.71
29	s	604	CLA	CMD-C2D-C1D	5.48	134.38	124.71
29	c	510	CLA	O2A-C1-C2	5.48	123.04	108.64
29	c	513	CLA	O2D-CGD-CBD	5.48	121.00	111.27
49	n1	621	LUT	C35-C34-C33	-5.48	119.49	127.31
29	b1	613	CLA	O2D-CGD-CBD	5.48	121.00	111.27
29	C	508	CLA	CMD-C2D-C1D	5.48	134.37	124.71
29	C1	501	CLA	CMD-C2D-C1D	5.48	134.37	124.71
42	d1	401	BCT	O2-C-O1	5.47	133.74	119.55
29	s	604	CLA	O2D-CGD-CBD	5.47	120.99	111.27
29	c1	508	CLA	CMD-C2D-C1D	5.47	134.35	124.71
51	Y1	623	NEX	C38-C25-C24	5.47	120.43	114.28
29	n1	603	CLA	CMD-C2D-C1D	5.47	134.35	124.71
36	B1	620	C7Z	C38-C25-C26	-5.47	118.39	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C1	502	CLA	O2D-CGD-CBD	5.47	120.98	111.27
45	H	101	RRX	C37-C22-C23	5.47	126.69	118.08
29	c1	509	CLA	CMD-C2D-C1D	5.47	134.35	124.71
29	N	602	CLA	O2D-CGD-CBD	5.46	120.97	111.27
29	C	506	CLA	CMD-C2D-C1D	5.46	134.33	124.71
29	S	609	CLA	CMD-C2D-C1D	5.46	134.33	124.71
29	S	617	CLA	O2A-C1-C2	5.46	122.97	108.64
29	r1	608	CLA	CMD-C2D-C1D	5.45	134.32	124.71
49	Y1	621	LUT	C21-C26-C25	5.45	121.18	111.42
29	C	503	CLA	O2D-CGD-CBD	5.45	120.95	111.27
29	s	617	CLA	O2D-CGD-CBD	5.45	120.95	111.27
29	y1	604	CLA	O2D-CGD-CBD	5.45	120.95	111.27
29	b	605	CLA	O2D-CGD-CBD	5.45	120.95	111.27
29	C1	512	CLA	O2A-C1-C2	5.45	122.95	108.64
29	y1	610	CLA	CMD-C2D-C1D	5.45	134.31	124.71
29	b1	606	CLA	CMD-C2D-C1D	5.45	134.31	124.71
29	y	613	CLA	O2D-CGD-CBD	5.44	120.94	111.27
29	s	613	CLA	O2A-C1-C2	5.44	122.93	108.64
29	G1	611	CLA	O2A-C1-C2	5.44	122.93	108.64
29	B	608	CLA	CMD-C2D-C1D	5.44	134.29	124.71
29	b1	613	CLA	O2A-C1-C2	5.43	122.92	108.64
29	Y	603	CLA	CMD-C2D-C1D	5.43	134.29	124.71
29	s	613	CLA	CMD-C2D-C1D	5.43	134.29	124.71
29	n1	612	CLA	CMD-C2D-C1D	5.43	134.28	124.71
29	R	610	CLA	CMD-C2D-C1D	5.43	134.28	124.71
49	g	620	LUT	C21-C26-C27	5.43	119.56	112.70
29	D	403	CLA	CMD-C2D-C1D	5.43	134.28	124.71
29	b1	612	CLA	CMD-C2D-C1D	5.43	134.28	124.71
29	A1	407	CLA	O2D-CGD-CBD	5.42	120.91	111.27
29	g1	612	CLA	O2D-CGD-CBD	5.42	120.90	111.27
29	A1	410	CLA	O2D-CGD-CBD	5.42	120.90	111.27
29	d	403	CLA	O2D-CGD-CBD	5.42	120.90	111.27
29	n1	602	CLA	O2D-CGD-CBD	5.42	120.90	111.27
29	a1	410	CLA	O2A-C1-C2	5.42	122.87	108.64
29	c	504	CLA	CMD-C2D-C1D	5.41	134.25	124.71
29	g	603	CLA	O2D-CGD-CBD	5.41	120.89	111.27
29	B1	612	CLA	CMD-C2D-C1D	5.41	134.25	124.71
29	S1	604	CLA	CMD-C2D-C1D	5.41	134.25	124.71
29	C1	507	CLA	CMD-C2D-C1D	5.41	134.25	124.71
29	S	605	CLA	O2A-C1-C2	5.41	122.85	108.64
50	N	622	XAT	C15-C14-C13	-5.41	119.59	127.31
29	N	612	CLA	CMD-C2D-C1D	5.41	134.24	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	617	CLA	O2D-CGD-CBD	5.41	120.88	111.27
29	y1	611	CLA	O2A-C1-C2	5.40	122.84	108.64
49	y	621	LUT	C21-C26-C27	5.40	119.53	112.70
29	C1	509	CLA	O2D-CGD-CBD	5.40	120.87	111.27
29	N1	604	CLA	O2D-CGD-CBD	5.40	120.86	111.27
29	n1	603	CLA	O2D-CGD-CBD	5.40	120.86	111.27
36	B1	620	C7Z	C11-C10-C9	-5.40	119.61	127.31
29	y1	611	CLA	O2D-CGD-CBD	5.40	120.86	111.27
29	c	507	CLA	CMD-C2D-C1D	5.40	134.23	124.71
29	C	506	CLA	O2D-CGD-CBD	5.40	120.86	111.27
29	G	602	CLA	O2A-C1-C2	5.40	122.81	108.64
29	c1	501	CLA	CMD-C2D-C1D	5.39	134.22	124.71
29	C	502	CLA	O2D-CGD-CBD	5.39	120.85	111.27
29	Y	603	CLA	O2D-CGD-CBD	5.39	120.85	111.27
29	r1	612	CLA	O2A-C1-C2	5.39	122.81	108.64
31	D1	404	BCR	C35-C13-C12	5.39	126.58	118.08
29	y1	613	CLA	O2D-CGD-CBD	5.39	120.85	111.27
29	R1	612	CLA	O2A-C1-C2	5.39	122.80	108.64
51	s1	623	NEX	C4-C3-C2	5.39	121.18	110.77
29	D1	402	CLA	CMD-C2D-C1D	5.39	134.21	124.71
29	B	613	CLA	CMD-C2D-C1D	5.39	134.21	124.71
29	R1	604	CLA	CMD-C2D-C1D	5.39	134.21	124.71
29	y1	612	CLA	CMD-C2D-C1D	5.39	134.21	124.71
29	b1	610	CLA	O2A-C1-C2	5.39	122.79	108.64
29	g1	610	CLA	O2D-CGD-CBD	5.39	120.84	111.27
49	g	620	LUT	C15-C14-C13	-5.38	119.62	127.31
29	n1	611	CLA	CMD-C2D-C1D	5.38	134.20	124.71
29	s1	614	CLA	O2D-CGD-CBD	5.38	120.83	111.27
29	n1	614	CLA	O2D-CGD-CBD	5.38	120.83	111.27
29	Y1	612	CLA	O2D-CGD-CBD	5.38	120.83	111.27
29	s	605	CLA	O2A-C1-C2	5.38	122.77	108.64
29	C	507	CLA	O2A-C1-C2	5.38	122.77	108.64
29	c1	506	CLA	O2A-C1-C2	5.38	122.77	108.64
29	s	605	CLA	O2D-CGD-CBD	5.38	120.82	111.27
49	y	620	LUT	C21-C26-C25	5.38	121.05	111.42
29	A	407	CLA	CMD-C2D-C1D	5.38	134.19	124.71
29	g	611	CLA	O2D-CGD-CBD	5.37	120.82	111.27
29	Y	612	CLA	O2D-CGD-CBD	5.37	120.82	111.27
29	Y	608	CLA	O2A-C1-C2	5.37	122.76	108.64
29	c	511	CLA	CMD-C2D-C1D	5.37	134.18	124.71
45	h	101	RRX	C34-C9-C8	5.37	126.54	118.08
29	s	610	CLA	CMD-C2D-C1D	5.37	134.18	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b1	604	CLA	CMD-C2D-C1D	5.37	134.18	124.71
36	b	620	C7Z	C38-C25-C26	-5.37	118.50	124.53
29	r1	609	CLA	O2A-C1-C2	5.37	122.74	108.64
29	b1	606	CLA	O2A-C1-C2	5.37	122.74	108.64
49	Y	621	LUT	C21-C26-C25	5.36	121.03	111.42
29	N	613	CLA	O2A-C1-C2	5.36	122.73	108.64
29	d	402	CLA	O2D-CGD-CBD	5.36	120.80	111.27
49	g1	621	LUT	C11-C10-C9	-5.36	119.66	127.31
29	c1	508	CLA	O2D-CGD-CBD	5.36	120.79	111.27
29	N	603	CLA	O2D-CGD-CBD	5.36	120.79	111.27
29	c1	504	CLA	O2D-CGD-CBD	5.36	120.78	111.27
29	c1	511	CLA	O2A-C1-C2	5.35	122.71	108.64
29	n	614	CLA	O2D-CGD-CBD	5.35	120.78	111.27
29	y	612	CLA	O2D-CGD-CBD	5.35	120.77	111.27
29	c1	513	CLA	O2D-CGD-CBD	5.35	120.77	111.27
29	s	617	CLA	CMD-C2D-C1D	5.35	134.14	124.71
29	Y1	603	CLA	O2A-C1-C2	5.35	122.69	108.64
29	s1	605	CLA	O2A-C1-C2	5.35	122.69	108.64
29	B	604	CLA	O2A-C1-C2	5.35	122.68	108.64
29	N1	610	CLA	O2A-C1-C2	5.35	122.68	108.64
29	B	606	CLA	O2A-C1-C2	5.34	122.68	108.64
29	n	612	CLA	CMD-C2D-C1D	5.34	134.13	124.71
29	S1	617	CLA	O2A-C1-C2	5.34	122.68	108.64
29	B	605	CLA	CMD-C2D-C1D	5.34	134.13	124.71
29	y1	604	CLA	CMD-C2D-C1D	5.34	134.13	124.71
29	g1	611	CLA	O2D-CGD-CBD	5.34	120.76	111.27
29	g1	604	CLA	CMD-C2D-C1D	5.34	134.13	124.71
29	n	611	CLA	O2A-C1-C2	5.34	121.45	108.97
29	r1	608	CLA	O2A-C1-C2	5.34	122.66	108.64
29	b1	604	CLA	O2A-C1-C2	5.33	122.65	108.64
29	s	612	CLA	O2D-CGD-CBD	5.33	120.75	111.27
29	b1	614	CLA	CMD-C2D-C1D	5.33	134.11	124.71
29	s1	614	CLA	CMD-C2D-C1D	5.33	134.11	124.71
29	G	603	CLA	O2A-C1-C2	5.33	122.64	108.64
29	n	602	CLA	CMD-C2D-C1D	5.33	134.10	124.71
29	B1	602	CLA	O2D-CGD-CBD	5.33	120.73	111.27
49	n	621	LUT	C21-C26-C25	5.33	120.96	111.42
29	N	610	CLA	O2A-C1-C2	5.32	122.63	108.64
29	c	509	CLA	O2D-CGD-CBD	5.32	120.72	111.27
29	S1	609	CLA	O2D-CGD-CBD	5.32	120.72	111.27
49	y	621	LUT	C22-C23-C24	-5.32	105.69	111.74
29	C	503	CLA	CMD-C2D-C1D	5.32	134.09	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
45	h1	101	RRX	C21-C20-C19	-5.32	106.62	123.22
29	c	503	CLA	CMD-C2D-C1D	5.32	134.08	124.71
29	y1	610	CLA	O2D-CGD-CBD	5.32	120.71	111.27
29	B	614	CLA	CMD-C2D-C1D	5.31	134.07	124.71
29	C1	501	CLA	O2D-CGD-CBD	5.31	120.71	111.27
49	s	621	LUT	C21-C26-C27	5.31	119.42	112.70
51	G1	623	NEX	C2-C1-C6	5.31	114.37	109.21
50	n1	622	XAT	C15-C14-C13	-5.31	119.73	127.31
29	S1	617	CLA	O2D-CGD-CBD	5.31	120.70	111.27
49	n1	621	LUT	C21-C26-C25	5.31	120.93	111.42
29	s1	603	CLA	O2A-C1-C2	5.31	122.58	108.64
49	s	621	LUT	C21-C26-C25	5.31	120.92	111.42
29	r	612	CLA	CMD-C2D-C1D	5.31	134.06	124.71
29	C	510	CLA	O2D-CGD-CBD	5.31	120.70	111.27
29	b1	603	CLA	O2D-CGD-CBD	5.30	120.69	111.27
29	G	603	CLA	CMD-C2D-C1D	5.30	134.06	124.71
29	b1	611	CLA	O2D-CGD-CBD	5.30	120.69	111.27
29	S	602	CLA	O2A-C1-C2	5.30	122.57	108.64
49	g	621	LUT	C22-C23-C24	-5.30	105.71	111.74
29	c	510	CLA	O2D-CGD-CBD	5.30	120.69	111.27
49	G1	620	LUT	C21-C26-C25	5.30	120.91	111.42
29	r1	603	CLA	O2D-CGD-CBD	5.30	120.68	111.27
29	B	608	CLA	O2A-C1-C2	5.30	122.56	108.64
29	B	610	CLA	O2D-CGD-CBD	5.29	120.68	111.27
29	A1	410	CLA	CMD-C2D-C1D	5.29	134.04	124.71
29	b1	610	CLA	O2D-CGD-CBD	5.29	120.67	111.27
29	d	403	CLA	O2A-C1-C2	5.29	122.55	108.64
29	s1	603	CLA	CMD-C2D-C1D	5.29	134.04	124.71
29	N1	611	CLA	O2D-CGD-CBD	5.29	120.67	111.27
29	G1	602	CLA	O2D-CGD-CBD	5.29	120.67	111.27
49	s1	620	LUT	C21-C26-C27	5.29	119.39	112.70
29	s1	613	CLA	O2A-C1-C2	5.29	122.53	108.64
29	S1	617	CLA	CMD-C2D-C1D	5.29	134.03	124.71
29	b	608	CLA	CMD-C2D-C1D	5.28	134.02	124.71
29	a	405	CLA	CMD-C2D-C1D	5.28	134.02	124.71
29	G	603	CLA	O2D-CGD-CBD	5.28	120.65	111.27
29	b	608	CLA	O2A-C1-C2	5.28	122.51	108.64
29	g1	603	CLA	O2A-C1-C2	5.28	122.51	108.64
29	B	604	CLA	O2D-CGD-CBD	5.28	120.65	111.27
29	b	610	CLA	CMD-C2D-C1D	5.28	134.01	124.71
29	S	609	CLA	O2D-CGD-CBD	5.28	120.64	111.27
29	b	612	CLA	CMD-C2D-C1D	5.27	134.01	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	g	620	LUT	C31-C30-C29	-5.27	119.78	127.31
29	c	508	CLA	O2A-C1-C2	5.27	122.49	108.64
49	r1	620	LUT	C11-C10-C9	-5.27	119.79	127.31
29	n	610	CLA	CMD-C2D-C1D	5.27	134.00	124.71
49	G	621	LUT	C21-C26-C27	5.27	119.36	112.70
29	r1	610	CLA	O2A-C1-C2	5.27	122.48	108.64
29	s1	609	CLA	CMD-C2D-C1D	5.27	134.00	124.71
29	n1	602	CLA	O2A-C1-C2	5.27	122.47	108.64
37	b	623	DGD	O2G-C1B-C2B	5.26	122.85	111.50
49	g	621	LUT	C21-C26-C25	5.26	120.85	111.42
29	g1	613	CLA	O2D-CGD-CBD	5.26	120.62	111.27
29	S1	605	CLA	O2A-C1-C2	5.26	122.47	108.64
29	s1	605	CLA	O2D-CGD-CBD	5.26	120.62	111.27
29	g	611	CLA	CMD-C2D-C1D	5.26	133.98	124.71
29	b1	617	CLA	CMD-C2D-C1D	5.26	133.98	124.71
29	s1	617	CLA	CMD-C2D-C1D	5.25	133.97	124.71
29	r	602	CLA	CMD-C2D-C1D	5.25	133.97	124.71
29	N	614	CLA	O2D-CGD-CBD	5.25	120.59	111.27
29	b1	609	CLA	O2A-C1-C2	5.25	122.43	108.64
29	C	511	CLA	CMD-C2D-C1D	5.25	133.96	124.71
29	N	611	CLA	CMD-C2D-C1D	5.25	133.96	124.71
49	y1	621	LUT	C22-C23-C24	-5.25	105.77	111.74
29	N1	613	CLA	CMD-C2D-C1D	5.24	133.95	124.71
29	G	611	CLA	O2A-C1-C2	5.24	122.41	108.64
49	G	621	LUT	C21-C26-C25	5.24	120.81	111.42
49	N1	621	LUT	C21-C26-C25	5.24	120.80	111.42
29	B1	616	CLA	O2A-C1-C2	5.24	122.40	108.64
29	g1	602	CLA	O2D-CGD-CBD	5.24	120.57	111.27
49	r	620	LUT	C7-C8-C9	-5.23	118.33	126.23
49	y1	621	LUT	C21-C26-C27	5.23	119.31	112.70
29	b	606	CLA	O2A-C1-C2	5.23	122.38	108.64
29	b1	603	CLA	O2A-C1-C2	5.23	122.38	108.64
29	A	406	CLA	CMD-C2D-C1D	5.23	133.93	124.71
29	c	512	CLA	O2D-CGD-CBD	5.23	120.56	111.27
29	g	610	CLA	O2D-CGD-CBD	5.23	120.56	111.27
29	S	617	CLA	O2D-CGD-CBD	5.23	120.56	111.27
29	S1	610	CLA	O2A-C1-C2	5.23	122.37	108.64
29	Y	604	CLA	CMD-C2D-C1D	5.23	133.93	124.71
29	B	607	CLA	O2D-CGD-CBD	5.22	120.55	111.27
49	g1	621	LUT	C21-C26-C25	5.22	120.78	111.42
29	S1	603	CLA	O2A-C1-C2	5.22	122.36	108.64
29	y1	608	CLA	O2D-CGD-CBD	5.22	120.55	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C1	507	CLA	O2A-C1-C2	5.22	122.36	108.64
29	Y	602	CLA	O2A-C1-C2	5.22	122.34	108.64
29	R1	612	CLA	CMD-C2D-C1D	5.22	133.91	124.71
29	N1	614	CLA	O2D-CGD-CBD	5.21	120.53	111.27
49	N	621	LUT	C21-C26-C25	5.21	120.76	111.42
29	b	607	CLA	CMD-C2D-C1D	5.21	133.90	124.71
29	N1	612	CLA	CMD-C2D-C1D	5.21	133.90	124.71
50	N1	622	XAT	C15-C14-C13	-5.21	119.88	127.31
29	G	604	CLA	O2D-CGD-CBD	5.21	120.53	111.27
29	C	505	CLA	CMD-C2D-C1D	5.21	133.89	124.71
29	B	613	CLA	O2A-C1-C2	5.21	122.32	108.64
29	b1	605	CLA	O2A-C1-C2	5.20	122.31	108.64
29	B1	611	CLA	O2A-C1-C2	5.20	122.31	108.64
29	A1	406	CLA	CMD-C2D-C1D	5.20	133.88	124.71
49	S	620	LUT	C15-C14-C13	-5.20	119.89	127.31
50	y1	622	XAT	C31-C30-C29	-5.20	119.89	127.31
29	s1	605	CLA	CMD-C2D-C1D	5.20	133.87	124.71
29	G1	610	CLA	O2A-C1-C2	5.20	122.29	108.64
29	y	610	CLA	O2D-CGD-CBD	5.20	120.50	111.27
29	y	614	CLA	O2D-CGD-CBD	5.20	120.50	111.27
29	b	604	CLA	O2D-CGD-CBD	5.20	120.50	111.27
29	C1	506	CLA	O2A-C1-C2	5.19	122.28	108.64
29	b1	604	CLA	O2D-CGD-CBD	5.19	120.50	111.27
29	S1	613	CLA	O2A-C1-C2	5.19	122.28	108.64
29	b1	611	CLA	CMD-C2D-C1D	5.19	133.86	124.71
29	C	504	CLA	CMD-C2D-C1D	5.19	133.86	124.71
29	G1	614	CLA	CMD-C2D-C1D	5.19	133.86	124.71
29	n	612	CLA	O2D-CGD-CBD	5.19	120.49	111.27
29	G1	612	CLA	O2D-CGD-CBD	5.19	120.49	111.27
29	B1	616	CLA	O2D-CGD-CBD	5.19	120.48	111.27
29	C1	502	CLA	CMD-C2D-C1D	5.19	133.85	124.71
29	y1	612	CLA	O2A-C1-C2	5.18	122.26	108.64
29	n1	614	CLA	CMD-C2D-C1D	5.18	133.85	124.71
29	s1	611	CLA	CMD-C2D-C1D	5.18	133.85	124.71
29	B	605	CLA	O2A-C1-C2	5.18	122.25	108.64
29	b	616	CLA	O2D-CGD-CBD	5.18	120.47	111.27
29	Y1	610	CLA	O2D-CGD-CBD	5.18	120.47	111.27
29	R1	602	CLA	CMD-C2D-C1D	5.18	133.84	124.71
29	C1	504	CLA	O2D-CGD-CBD	5.18	120.47	111.27
29	A1	405	CLA	CMD-C2D-C1D	5.18	133.84	124.71
29	y1	602	CLA	O2A-C1-C2	5.18	122.24	108.64
29	r1	604	CLA	CMD-C2D-C1D	5.17	133.83	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	G	610	CLA	O2D-CGD-CBD	5.17	120.45	111.27
29	s	612	CLA	CMD-C2D-C1D	5.17	133.82	124.71
29	N	611	CLA	O2D-CGD-CBD	5.17	120.45	111.27
29	b	614	CLA	O2A-C1-C2	5.17	122.22	108.64
49	s1	620	LUT	C21-C26-C25	5.16	120.67	111.42
29	r	608	CLA	O2D-CGD-CBD	5.16	120.44	111.27
29	s	602	CLA	CMD-C2D-C1D	5.16	133.81	124.71
29	Y	613	CLA	O2A-C1-C2	5.16	122.20	108.64
29	C1	510	CLA	CMD-C2D-C1D	5.16	133.81	124.71
29	Y	610	CLA	O2D-CGD-CBD	5.16	120.44	111.27
29	b1	609	CLA	CMD-C2D-C1D	5.16	133.81	124.71
29	S1	603	CLA	CMD-C2D-C1D	5.16	133.81	124.71
49	r1	620	LUT	C7-C8-C9	-5.16	118.44	126.23
29	b	607	CLA	O2A-C1-C2	5.15	122.18	108.64
29	n1	612	CLA	O2D-CGD-CBD	5.15	120.42	111.27
45	h	101	RRX	C8-C9-C10	-5.15	111.03	118.94
29	G1	603	CLA	O2A-C1-C2	5.15	122.17	108.64
29	B1	608	CLA	O2A-C1-C2	5.15	122.17	108.64
29	b1	611	CLA	O2A-C1-C2	5.15	122.17	108.64
29	b1	616	CLA	O2D-CGD-CBD	5.15	120.42	111.27
29	s	603	CLA	O2A-C1-C2	5.15	122.17	108.64
29	c	504	CLA	O2D-CGD-CBD	5.15	120.41	111.27
29	c1	511	CLA	O2D-CGD-CBD	5.15	120.41	111.27
29	b	604	CLA	CMD-C2D-C1D	5.14	133.78	124.71
29	R1	609	CLA	C1-C2-C3	-5.14	117.15	126.04
29	b	612	CLA	O2A-C1-C2	5.14	122.15	108.64
29	D1	403	CLA	O2A-C1-C2	5.14	122.15	108.64
49	G	620	LUT	C21-C26-C25	5.14	120.62	111.42
31	b1	618	BCR	C30-C25-C26	-5.14	115.38	122.61
29	R	609	CLA	O2D-CGD-CBD	5.14	120.39	111.27
50	y	622	XAT	C7-C8-C9	-5.13	117.56	125.53
50	Y	622	XAT	C15-C14-C13	-5.13	119.98	127.31
29	y1	611	CLA	CMD-C2D-C1D	5.13	133.76	124.71
29	r	602	CLA	O2D-CGD-CBD	5.13	120.38	111.27
29	B	611	CLA	CMD-C2D-C1D	5.13	133.75	124.71
29	N	611	CLA	O2A-C1-C2	5.13	120.96	108.97
29	r	603	CLA	O2D-CGD-CBD	5.12	120.37	111.27
29	C	504	CLA	O2D-CGD-CBD	5.12	120.37	111.27
29	S	603	CLA	CMD-C2D-C1D	5.12	133.74	124.71
29	c1	501	CLA	O2D-CGD-CBD	5.12	120.37	111.27
36	b1	620	C7Z	C35-C34-C33	-5.12	120.00	127.31
29	B	611	CLA	O2D-CGD-CBD	5.12	120.36	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	506	CLA	O2D-CGD-CBD	5.12	120.36	111.27
29	n	603	CLA	O2D-CGD-CBD	5.12	120.36	111.27
29	B	616	CLA	O2D-CGD-CBD	5.11	120.36	111.27
29	s1	614	CLA	O2A-C1-C2	5.11	122.07	108.64
29	C	502	CLA	CMD-C2D-C1D	5.11	133.72	124.71
29	N1	611	CLA	O2A-C1-C2	5.11	120.92	108.97
29	r1	609	CLA	CMD-C2D-C1D	5.11	133.72	124.71
29	B1	603	CLA	O2D-CGD-CBD	5.11	120.34	111.27
29	n1	610	CLA	O2D-CGD-CBD	5.11	120.34	111.27
50	y1	622	XAT	C15-C14-C13	-5.10	120.03	127.31
29	b1	611	CLA	C2C-C1C-NC	5.10	114.75	109.97
29	Y	602	CLA	CMD-C2D-C1D	5.10	133.71	124.71
29	y	603	CLA	CMD-C2D-C1D	5.10	133.71	124.71
36	b	620	C7Z	C18-C5-C6	-5.10	118.80	124.53
29	c	501	CLA	O2A-C1-C2	5.10	122.04	108.64
29	s	609	CLA	CMD-C2D-C1D	5.10	133.70	124.71
29	C	505	CLA	O2A-C1-C2	5.10	122.04	108.64
29	B1	604	CLA	CMD-C2D-C1D	5.10	133.70	124.71
29	B	615	CLA	O2D-CGD-CBD	5.10	120.33	111.27
29	b	608	CLA	O2D-CGD-CBD	5.10	120.33	111.27
49	n1	620	LUT	C21-C26-C25	5.10	120.55	111.42
29	g	612	CLA	CMD-C2D-C1D	5.10	133.69	124.71
50	y	622	XAT	C31-C30-C29	-5.09	120.04	127.31
29	C1	511	CLA	O2A-C1-C2	5.09	122.02	108.64
29	B1	605	CLA	O2A-C1-C2	5.09	122.02	108.64
29	G1	611	CLA	CMD-C2D-C1D	5.09	133.69	124.71
29	s	610	CLA	O2D-CGD-CBD	5.09	120.32	111.27
29	b1	617	CLA	O2D-CGD-CBD	5.09	120.31	111.27
29	c1	506	CLA	CMD-C2D-C1D	5.09	133.69	124.71
29	S1	613	CLA	O2D-CGD-CBD	5.09	120.31	111.27
29	C1	506	CLA	O2D-CGD-CBD	5.09	120.31	111.27
29	B	616	CLA	CMD-C2D-C1D	5.09	133.68	124.71
45	H1	101	RRX	C24-C23-C22	5.09	133.92	126.23
49	Y1	621	LUT	C7-C8-C9	-5.09	118.55	126.23
51	g1	623	NEX	C2-C1-C6	5.08	114.15	109.21
49	s	620	LUT	C21-C26-C25	5.08	120.53	111.42
49	r	620	LUT	C21-C26-C27	5.08	119.13	112.70
29	g	614	CLA	O2D-CGD-CBD	5.08	120.30	111.27
29	B	602	CLA	O2D-CGD-CBD	5.08	120.29	111.27
29	C	507	CLA	CMD-C2D-C1D	5.08	133.66	124.71
55	y	627	PTY	O7-C8-C11	5.08	120.43	111.09
29	G1	613	CLA	O2D-CGD-CBD	5.07	120.29	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	G	613	CLA	O2A-C1-C2	5.07	121.97	108.64
29	R1	602	CLA	O2D-CGD-CBD	5.07	120.28	111.27
29	c1	505	CLA	CMD-C2D-C1D	5.07	133.66	124.71
29	R1	608	CLA	O2A-C1-C2	5.07	121.97	108.64
29	C	508	CLA	CMB-C2B-C1B	-5.07	120.67	128.46
29	b	606	CLA	O2D-CGD-CBD	5.07	120.28	111.27
29	B	609	CLA	O2A-C1-C2	5.07	121.97	108.64
49	N	621	LUT	C22-C23-C24	-5.07	105.97	111.74
29	y	602	CLA	CMD-C2D-C1D	5.07	133.65	124.71
53	r	626	ERG	C18-C13-C12	-5.07	102.58	110.59
29	Y1	608	CLA	CMD-C2D-C1D	5.07	133.65	124.71
29	b1	612	CLA	O2A-C1-C2	5.07	121.96	108.64
29	c	508	CLA	CMD-C2D-C1D	5.07	133.64	124.71
29	g	602	CLA	CMD-C2D-C1D	5.07	133.64	124.71
29	Y	608	CLA	CMD-C2D-C1D	5.06	133.64	124.71
29	G1	614	CLA	O2D-CGD-CBD	5.06	120.27	111.27
29	S1	605	CLA	CMD-C2D-C1D	5.06	133.63	124.71
29	N	610	CLA	O2D-CGD-CBD	5.06	120.26	111.27
45	h	101	RRX	C37-C22-C23	5.06	126.05	118.08
29	g	602	CLA	O2D-CGD-CBD	5.06	120.26	111.27
29	R	610	CLA	O2A-C1-C2	5.06	121.93	108.64
29	Y	602	CLA	O2D-CGD-CBD	5.06	120.26	111.27
29	c	512	CLA	O2A-C1-C2	5.06	121.93	108.64
29	C1	503	CLA	O2D-CGD-CBD	5.06	120.25	111.27
29	b1	602	CLA	O2A-C1-C2	5.05	121.92	108.64
29	G	611	CLA	CMD-C2D-C1D	5.05	133.62	124.71
29	c1	507	CLA	O2D-CGD-CBD	5.05	120.25	111.27
29	N1	614	CLA	CMD-C2D-C1D	5.05	133.62	124.71
29	Y1	614	CLA	O2A-C1-C2	5.05	121.91	108.64
29	B	604	CLA	CMD-C2D-C1D	5.05	133.61	124.71
29	b1	603	CLA	CMD-C2D-C1D	5.05	133.61	124.71
29	B	603	CLA	O2A-C1-C2	5.05	121.89	108.64
36	B	620	C7Z	C21-C26-C25	-5.04	115.51	122.61
31	b1	618	BCR	C15-C14-C13	-5.04	120.12	127.31
29	R	612	CLA	O2D-CGD-CBD	5.04	120.22	111.27
29	b	616	CLA	CMD-C2D-C1D	5.04	133.59	124.71
29	C1	503	CLA	O2A-C1-C2	5.04	121.88	108.64
49	s1	621	LUT	C21-C26-C25	5.04	120.44	111.42
29	B	610	CLA	CMD-C2D-C1D	5.04	133.59	124.71
29	B	612	CLA	O2D-CGD-CBD	5.04	120.22	111.27
49	N1	620	LUT	C22-C23-C24	-5.04	106.01	111.74
51	y	623	NEX	C38-C25-C24	5.04	119.95	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	Y1	622	XAT	C31-C30-C29	-5.04	120.12	127.31
49	y1	621	LUT	C21-C26-C25	5.03	120.44	111.42
29	b1	616	CLA	CMD-C2D-C1D	5.03	133.59	124.71
29	b1	615	CLA	O2D-CGD-CBD	5.03	120.21	111.27
29	g1	613	CLA	CMD-C2D-C1D	5.03	133.58	124.71
29	c	505	CLA	CMD-C2D-C1D	5.03	133.58	124.71
29	B	609	CLA	CMD-C2D-C1D	5.03	133.58	124.71
29	B	617	CLA	CMD-C2D-C1D	5.03	133.57	124.71
51	Y1	623	NEX	O24-C25-C24	-5.03	109.61	113.38
36	b	620	C7Z	C27-C28-C29	-5.02	118.64	126.23
29	B	603	CLA	O2D-CGD-CBD	5.02	120.20	111.27
43	d1	405	PL9	C7-C3-C4	5.02	120.96	116.88
49	Y1	621	LUT	C35-C34-C33	-5.02	120.14	127.31
29	d1	402	CLA	O2A-C1-C2	5.02	121.83	108.64
29	n	613	CLA	O2A-C1-C2	5.02	121.82	108.64
29	B	607	CLA	O2A-C1-C2	5.02	121.82	108.64
29	Y	614	CLA	O2D-CGD-CBD	5.02	120.18	111.27
51	s	623	NEX	C38-C25-C24	5.02	119.92	114.28
29	c	503	CLA	O2D-CGD-CBD	5.01	120.18	111.27
29	N	614	CLA	CMD-C2D-C1D	5.01	133.55	124.71
29	S	610	CLA	O2A-C1-C2	5.01	121.81	108.64
29	y1	603	CLA	O2A-C1-C2	5.01	121.81	108.64
50	N	622	XAT	O24-C25-C24	5.01	117.14	113.38
29	s	617	CLA	O2A-C1-C2	5.01	121.80	108.64
29	n1	604	CLA	O2A-C1-C2	5.01	121.79	108.64
29	N1	610	CLA	CMD-C2D-C1D	5.01	133.53	124.71
29	S	610	CLA	CMD-C2D-C1D	5.01	133.53	124.71
29	S1	611	CLA	O2D-CGD-CBD	5.00	120.15	111.27
29	C	511	CLA	O2D-CGD-CBD	5.00	120.15	111.27
31	C1	516	BCR	C15-C14-C13	-5.00	120.18	127.31
29	S	614	CLA	O2D-CGD-CBD	5.00	120.15	111.27
29	b1	607	CLA	O2A-C1-C2	5.00	121.76	108.64
29	C	510	CLA	O2A-C1-C2	4.99	121.76	108.64
29	S1	604	CLA	O2D-CGD-CBD	4.99	120.14	111.27
29	B	617	CLA	O2A-C1-C2	4.99	121.75	108.64
29	R1	608	CLA	O2D-CGD-CBD	4.99	120.14	111.27
55	Y	627	PTY	O7-C8-C11	4.99	120.27	111.09
29	S	613	CLA	CMD-C2D-C1D	4.99	133.51	124.71
49	n1	620	LUT	C21-C26-C27	4.99	119.01	112.70
29	a1	407	CLA	O2A-C1-C2	4.99	120.63	108.97
29	B1	604	CLA	O2D-CGD-CBD	4.99	120.13	111.27
29	R1	604	CLA	O2D-CGD-CBD	4.98	120.12	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B1	608	CLA	CMD-C2D-C1D	4.98	133.50	124.71
29	y1	608	CLA	O2A-C1-C2	4.98	121.73	108.64
29	b1	606	CLA	O2D-CGD-CBD	4.98	120.12	111.27
29	b1	608	CLA	CMD-C2D-C1D	4.98	133.50	124.71
29	C	508	CLA	O2A-C1-C2	4.98	121.73	108.64
29	s1	610	CLA	O2D-CGD-CBD	4.98	120.12	111.27
29	c1	503	CLA	O2A-C1-C2	4.98	121.72	108.64
50	r	621	XAT	O4-C5-C4	-4.98	109.64	113.38
29	b1	617	CLA	O2A-C1-C2	4.98	121.71	108.64
29	y1	602	CLA	O2D-CGD-CBD	4.97	120.11	111.27
29	R	608	CLA	O2D-CGD-CBD	4.97	120.11	111.27
50	N	622	XAT	C18-C5-C4	4.97	119.87	114.28
29	C1	513	CLA	O2D-CGD-CBD	4.97	120.10	111.27
50	G	622	XAT	C31-C30-C29	-4.97	120.22	127.31
29	g	614	CLA	CMD-C2D-C1D	4.97	133.47	124.71
29	Y	612	CLA	CMD-C2D-C1D	4.97	133.47	124.71
48	s1	608	CHL	CHD-C1D-ND	-4.97	119.89	124.45
29	S	617	CLA	CMD-C2D-C1D	4.97	133.47	124.71
45	H1	101	RRX	C15-C14-C13	-4.97	120.22	127.31
29	Y	611	CLA	O2D-CGD-CBD	4.97	120.09	111.27
29	d1	403	CLA	O2A-C1-C2	4.97	121.69	108.64
29	y	604	CLA	CMD-C2D-C1D	4.97	133.46	124.71
29	b1	608	CLA	O2D-CGD-CBD	4.96	120.09	111.27
29	d1	403	CLA	O2D-CGD-CBD	4.96	120.08	111.27
29	s1	609	CLA	O2D-CGD-CBD	4.96	120.08	111.27
29	Y1	613	CLA	O2D-CGD-CBD	4.96	120.08	111.27
29	c1	502	CLA	O2D-CGD-CBD	4.95	120.07	111.27
49	s1	621	LUT	C31-C30-C29	-4.95	120.24	127.31
29	y	611	CLA	O2D-CGD-CBD	4.95	120.06	111.27
29	Y1	613	CLA	O2A-C1-C2	4.95	121.64	108.64
51	g1	623	NEX	C38-C25-C24	4.95	119.84	114.28
29	S	611	CLA	CMD-C2D-C1D	4.94	133.43	124.71
29	n1	610	CLA	O2A-C1-C2	4.94	121.63	108.64
29	B	603	CLA	CMD-C2D-C1D	4.94	133.42	124.71
29	y1	614	CLA	O2D-CGD-CBD	4.94	120.04	111.27
29	b	614	CLA	O2D-CGD-CBD	4.94	120.04	111.27
29	Y	614	CLA	O2A-C1-C2	4.94	121.61	108.64
29	N1	603	CLA	O2D-CGD-CBD	4.93	120.03	111.27
29	C1	504	CLA	CMD-C2D-C1D	4.93	133.41	124.71
29	R	602	CLA	O2A-C1-C2	4.93	121.60	108.64
29	c	507	CLA	O2A-C1-C2	4.93	121.60	108.64
29	s	609	CLA	O2D-CGD-CBD	4.93	120.03	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	s1	604	CLA	O2D-CGD-CBD	4.93	120.03	111.27
29	R	603	CLA	O2A-C1-C2	4.93	121.59	108.64
49	y	621	LUT	C21-C26-C25	4.93	120.25	111.42
29	y	604	CLA	O2A-C1-C2	4.93	121.59	108.64
29	b	603	CLA	O2D-CGD-CBD	4.93	120.02	111.27
29	A1	407	CLA	O2A-C1-C2	4.93	121.58	108.64
29	r1	610	CLA	O2D-CGD-CBD	4.92	120.01	111.27
29	y1	604	CLA	O2A-C1-C2	4.92	121.57	108.64
29	r1	612	CLA	O2D-CGD-CBD	4.92	120.01	111.27
29	y1	603	CLA	O2D-CGD-CBD	4.92	120.01	111.27
29	c1	512	CLA	CMD-C2D-C1D	4.92	133.38	124.71
29	Y1	614	CLA	O2D-CGD-CBD	4.92	120.00	111.27
29	n	603	CLA	CMD-C2D-C1D	4.91	133.37	124.71
29	n	613	CLA	O2D-CGD-CBD	4.91	119.99	111.27
29	S	613	CLA	O2A-C1-C2	4.91	121.54	108.64
29	n	604	CLA	CMD-C2D-C1D	4.91	133.37	124.71
29	a	410	CLA	CMD-C2D-C1D	4.91	133.36	124.71
29	r1	602	CLA	O2A-C1-C2	4.91	121.53	108.64
51	g1	623	NEX	C31-C30-C29	4.91	134.31	127.31
29	R	603	CLA	O2D-CGD-CBD	4.90	119.98	111.27
39	C1	524	DGA	OG2-CB1-CB2	4.90	122.07	111.50
29	B1	617	CLA	O2A-C1-C2	4.90	121.52	108.64
29	B1	610	CLA	CMD-C2D-C1D	4.90	133.35	124.71
53	R1	626	ERG	C12-C13-C14	4.90	115.04	107.27
29	y1	614	CLA	O2A-C1-C2	4.90	121.52	108.64
29	y	603	CLA	O2A-C1-C2	4.90	121.51	108.64
29	A1	407	CLA	CMD-C2D-C1D	4.90	133.35	124.71
29	R1	612	CLA	O2D-CGD-CBD	4.90	119.97	111.27
50	G1	622	XAT	C18-C5-C4	4.89	119.78	114.28
29	g	604	CLA	O2D-CGD-CBD	4.89	119.96	111.27
29	C1	512	CLA	O2D-CGD-CBD	4.89	119.96	111.27
49	G1	621	LUT	C11-C10-C9	-4.89	120.33	127.31
29	g1	604	CLA	O2A-C1-C2	4.89	120.41	108.97
29	Y	608	CLA	O2D-CGD-CBD	4.89	119.96	111.27
29	S	614	CLA	O2A-C1-C2	4.89	121.47	108.64
29	n	602	CLA	O2A-C1-C2	4.88	121.47	108.64
29	S	612	CLA	CMD-C2D-C1D	4.88	133.31	124.71
36	b	620	C7Z	C35-C34-C33	-4.88	120.35	127.31
48	Y	605	CHL	CHD-C1D-ND	-4.88	119.97	124.45
29	R	604	CLA	O2D-CGD-CBD	4.88	119.94	111.27
50	n	622	XAT	O24-C25-C24	4.88	117.05	113.38
29	n1	613	CLA	CAA-C2A-C3A	-4.88	99.42	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	g1	603	CLA	CMD-C2D-C1D	4.88	133.31	124.71
36	B1	620	C7Z	C21-C26-C25	-4.88	115.75	122.61
29	g	613	CLA	O2D-CGD-CBD	4.87	119.93	111.27
55	y1	627	PTY	O7-C8-C11	4.87	120.06	111.09
29	Y1	604	CLA	O2A-C1-C2	4.87	121.44	108.64
29	n	613	CLA	CAA-C2A-C3A	-4.87	99.44	112.78
49	g	620	LUT	C21-C26-C25	4.87	120.14	111.42
29	S1	614	CLA	O2A-C1-C2	4.87	121.43	108.64
29	S	604	CLA	O2D-CGD-CBD	4.87	119.92	111.27
29	c	511	CLA	O2D-CGD-CBD	4.86	119.91	111.27
29	A	410	CLA	O2A-C1-C2	4.86	121.41	108.64
29	Y	603	CLA	O2A-C1-C2	4.86	121.40	108.64
29	a1	410	CLA	CMD-C2D-C1D	4.85	133.27	124.71
29	c1	510	CLA	O2D-CGD-CBD	4.85	119.89	111.27
29	N	602	CLA	CMD-C2D-C1D	4.85	133.26	124.71
29	Y1	608	CLA	O2D-CGD-CBD	4.85	119.88	111.27
29	S	613	CLA	O2D-CGD-CBD	4.84	119.88	111.27
49	N1	620	LUT	C21-C26-C25	4.84	120.09	111.42
29	b1	607	CLA	CMD-C2D-C1D	4.84	133.25	124.71
48	N1	601	CHL	C4A-NA-C1A	4.84	108.88	106.71
51	y1	623	NEX	C38-C25-C24	4.84	119.72	114.28
50	n1	622	XAT	C18-C5-C4	4.84	119.72	114.28
29	r1	608	CLA	O2D-CGD-CBD	4.84	119.86	111.27
29	g	610	CLA	O2A-C1-C2	4.84	121.34	108.64
29	S	603	CLA	O2A-C1-C2	4.83	121.34	108.64
29	c1	502	CLA	CMD-C2D-C1D	4.83	133.23	124.71
29	a1	405	CLA	O2D-CGD-CBD	4.83	119.86	111.27
36	b1	620	C7Z	C1-C6-C5	-4.83	115.81	122.61
33	a1	413	LMG	O7-C10-C11	4.83	121.91	111.50
29	s1	611	CLA	O2A-C1-C2	4.83	121.33	108.64
29	B	616	CLA	O2A-C1-C2	4.83	121.33	108.64
29	B1	602	CLA	O2A-C1-C2	4.83	121.32	108.64
29	g1	604	CLA	O2D-CGD-CBD	4.83	119.84	111.27
29	s1	611	CLA	O2D-CGD-CBD	4.82	119.84	111.27
29	c	502	CLA	CMD-C2D-C1D	4.82	133.21	124.71
31	c	515	BCR	C12-C13-C14	-4.82	111.54	118.94
40	g1	624	LHG	O7-C7-C8	4.82	121.89	111.50
29	y	608	CLA	O2A-C1-C2	4.82	121.30	108.64
29	s	609	CLA	O2A-C1-C2	4.82	121.29	108.64
29	s	611	CLA	O2A-C1-C2	4.81	121.28	108.64
29	C1	507	CLA	O2D-CGD-CBD	4.81	119.82	111.27
50	G	622	XAT	C18-C5-C4	4.81	119.69	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	r	603	CLA	O2A-C1-C2	4.80	121.26	108.64
29	r	610	CLA	O2D-CGD-CBD	4.80	119.80	111.27
29	s1	617	CLA	O2D-CGD-CBD	4.80	119.80	111.27
49	N1	620	LUT	C21-C26-C27	4.80	118.77	112.70
50	Y1	622	XAT	C38-C25-C24	4.80	119.68	114.28
29	Y1	612	CLA	CMD-C2D-C1D	4.80	133.16	124.71
29	A	410	CLA	CMD-C2D-C1D	4.79	133.16	124.71
29	r	609	CLA	O2D-CGD-CBD	4.79	119.78	111.27
29	B1	611	CLA	CMD-C2D-C1D	4.79	133.16	124.71
29	Y	612	CLA	O2A-C1-C2	4.79	121.22	108.64
29	c1	502	CLA	O2A-C1-C2	4.79	121.22	108.64
29	s	604	CLA	O2A-C1-C2	4.79	121.21	108.64
49	Y1	621	LUT	C35-C15-C14	-4.79	113.67	123.47
37	b1	623	DGD	O2G-C1B-C2B	4.78	121.81	111.50
29	r1	602	CLA	CMD-C2D-C1D	4.78	133.14	124.71
29	B	610	CLA	O2A-C1-C2	4.78	121.20	108.64
49	Y1	620	LUT	C21-C26-C25	4.78	119.98	111.42
49	Y1	621	LUT	C22-C23-C24	-4.78	106.30	111.74
29	N	602	CLA	O2A-C1-C2	4.78	121.20	108.64
29	B1	617	CLA	CMD-C2D-C1D	4.78	133.14	124.71
49	Y	620	LUT	C21-C26-C25	4.78	119.97	111.42
29	S	611	CLA	O2D-CGD-CBD	4.78	119.75	111.27
36	B1	620	C7Z	C15-C14-C13	-4.77	120.50	127.31
50	r	621	XAT	C18-C5-C4	4.77	119.65	114.28
29	n1	611	CLA	O2D-CGD-CBD	4.77	119.75	111.27
29	C1	505	CLA	CMD-C2D-C1D	4.77	133.12	124.71
29	S1	611	CLA	O2A-C1-C2	4.77	121.17	108.64
49	G1	621	LUT	C21-C26-C25	4.77	119.96	111.42
29	B1	612	CLA	O2D-CGD-CBD	4.77	119.74	111.27
29	C1	510	CLA	O2D-CGD-CBD	4.77	119.74	111.27
49	S1	621	LUT	C21-C26-C25	4.77	119.95	111.42
29	R	603	CLA	CMD-C2D-C1D	4.76	133.11	124.71
29	N1	613	CLA	O2D-CGD-CBD	4.76	119.73	111.27
38	b	624	3PH	O21-C21-C22	4.76	121.77	111.50
29	g	613	CLA	CMD-C2D-C1D	4.76	133.10	124.71
29	S1	611	CLA	CMD-C2D-C1D	4.76	133.10	124.71
50	G	622	XAT	C38-C25-C24	4.76	119.63	114.28
29	B1	617	CLA	O2D-CGD-CBD	4.76	119.72	111.27
50	n1	622	XAT	C7-C8-C9	-4.75	118.15	125.53
50	R	621	XAT	O24-C25-C24	4.75	116.95	113.38
29	C	501	CLA	O2D-CGD-CBD	4.75	119.72	111.27
49	g1	620	LUT	C21-C26-C25	4.75	119.93	111.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	R1	610	CLA	C1-C2-C3	-4.75	117.83	126.04
40	L1	101	LHG	O7-C7-C8	4.75	121.74	111.50
29	y	612	CLA	CMD-C2D-C1D	4.75	133.08	124.71
43	d	405	PL9	C7-C3-C4	4.75	120.74	116.88
29	s	603	CLA	CMD-C2D-C1D	4.75	133.08	124.71
29	y	602	CLA	O2A-C1-C2	4.74	121.09	108.64
29	C	513	CLA	O2A-C1-C2	4.74	121.08	108.64
49	s	620	LUT	C21-C26-C27	4.74	118.69	112.70
29	Y1	611	CLA	O2A-C1-C2	4.74	121.08	108.64
29	G1	604	CLA	O2A-C1-C2	4.73	120.04	108.97
49	N1	621	LUT	C18-C5-C6	-4.73	119.21	124.53
51	g	623	NEX	C38-C25-C24	4.73	119.60	114.28
29	Y	604	CLA	O2A-C1-C2	4.73	121.06	108.64
43	D	405	PL9	C7-C3-C4	4.73	120.72	116.88
29	S1	614	CLA	CMD-C2D-C1D	4.72	133.04	124.71
29	b1	614	CLA	O2D-CGD-CBD	4.72	119.66	111.27
29	s1	612	CLA	O2D-CGD-CBD	4.72	119.66	111.27
29	a1	405	CLA	O2A-C1-C2	4.72	121.05	108.64
50	n	622	XAT	C18-C5-C4	4.71	119.58	114.28
48	Y	609	CHL	CHD-C1D-ND	-4.71	120.12	124.45
29	Y1	602	CLA	O2A-C1-C2	4.71	121.02	108.64
29	N1	612	CLA	O2D-CGD-CBD	4.71	119.64	111.27
29	y	613	CLA	CMD-C2D-C1D	4.71	133.01	124.71
29	a1	406	CLA	O2D-CGD-CBD	4.71	119.64	111.27
45	h1	101	RRX	C24-C25-C26	-4.71	110.06	121.46
50	y	622	XAT	C18-C5-C4	4.71	119.58	114.28
29	N	613	CLA	O2D-CGD-CBD	4.70	119.63	111.27
29	B1	606	CLA	O2D-CGD-CBD	4.70	119.63	111.27
29	D	402	CLA	O2D-CGD-CBD	4.70	119.63	111.27
29	R	609	CLA	CMD-C2D-C1D	4.70	133.00	124.71
51	y1	623	NEX	C31-C30-C29	4.70	134.02	127.31
45	h1	101	RRX	C37-C22-C23	4.70	125.49	118.08
29	b	605	CLA	O2A-C1-C2	4.70	120.99	108.64
29	C	512	CLA	O2A-C1-C2	4.70	120.99	108.64
29	N1	610	CLA	O2D-CGD-CBD	4.70	119.62	111.27
33	b	622	LMG	O7-C10-C11	4.70	121.63	111.50
29	B1	605	CLA	O2D-CGD-CBD	4.70	119.61	111.27
29	g1	602	CLA	O2A-C1-C2	4.70	120.98	108.64
33	B	622	LMG	O7-C10-C11	4.70	121.62	111.50
29	A1	406	CLA	O2D-CGD-CBD	4.70	119.61	111.27
29	y	612	CLA	O2A-C1-C2	4.69	120.97	108.64
50	N	622	XAT	C38-C25-C24	4.69	119.56	114.28

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	y	610	CLA	O2A-C1-C2	4.69	120.97	108.64
29	s	611	CLA	CMD-C2D-C1D	4.69	132.98	124.71
29	B1	604	CLA	O2A-C1-C2	4.69	120.96	108.64
29	a	406	CLA	O2D-CGD-CBD	4.68	119.59	111.27
50	r1	621	XAT	C38-C25-C24	4.68	119.55	114.28
29	B	614	CLA	O2D-CGD-CBD	4.68	119.59	111.27
29	b1	602	CLA	O2D-CGD-CBD	4.68	119.58	111.27
29	s	613	CLA	O2D-CGD-CBD	4.68	119.58	111.27
29	Y1	603	CLA	O2D-CGD-CBD	4.68	119.58	111.27
51	s	623	NEX	C16-C1-C6	-4.67	106.29	110.47
29	A1	405	CLA	O2D-CGD-CBD	4.67	119.57	111.27
29	b1	616	CLA	O2A-C1-C2	4.67	120.91	108.64
49	Y	621	LUT	C22-C23-C24	-4.67	106.43	111.74
29	b	611	CLA	O2A-C1-C2	4.67	120.90	108.64
33	a	413	LMG	O7-C10-C11	4.66	121.55	111.50
49	S	621	LUT	C21-C26-C25	4.66	119.77	111.42
29	c1	505	CLA	O2A-C1-C2	4.66	120.89	108.64
31	b	618	BCR	C33-C5-C4	4.66	122.57	113.62
29	y	611	CLA	CMD-C2D-C1D	4.66	132.93	124.71
31	B1	619	BCR	C15-C14-C13	-4.66	120.66	127.31
43	D1	405	PL9	C7-C3-C2	-4.66	117.18	123.30
49	R	620	LUT	C35-C34-C33	-4.66	120.67	127.31
45	H	101	RRX	C4-C5-C6	-4.65	115.98	122.73
48	n	609	CHL	CMA-C3A-C4A	4.65	124.27	111.77
50	Y1	622	XAT	C7-C8-C9	-4.65	118.32	125.53
29	B	612	CLA	CMD-C2D-C1D	4.65	132.90	124.71
51	r	622	NEX	C27-C28-C29	-4.65	118.32	125.53
29	c	508	CLA	O2D-CGD-CBD	4.64	119.52	111.27
51	N	623	NEX	C38-C25-C24	4.64	119.50	114.28
29	Y1	612	CLA	O2A-C1-C2	4.64	120.84	108.64
29	A	406	CLA	O2D-CGD-CBD	4.64	119.51	111.27
29	C	503	CLA	O2A-C1-C2	4.64	120.83	108.64
29	b	616	CLA	O2A-C1-C2	4.64	120.83	108.64
50	R1	621	XAT	C38-C25-C24	4.64	119.50	114.28
29	b	602	CLA	O2A-C1-C2	4.64	120.82	108.64
29	B1	613	CLA	O2D-CGD-CBD	4.64	119.51	111.27
31	b	618	BCR	C33-C5-C6	-4.64	119.32	124.53
29	S	609	CLA	O2A-C1-C2	4.63	120.81	108.64
29	A	407	CLA	O2D-CGD-CBD	4.63	119.50	111.27
50	g	622	XAT	C38-C25-C24	4.63	119.48	114.28
29	S	602	CLA	CMD-C2D-C1D	4.63	132.87	124.71
29	n1	604	CLA	O2D-CGD-CBD	4.62	119.48	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	609	CLA	O2A-C1-C2	4.62	120.79	108.64
33	A	413	LMG	O7-C10-C11	4.62	121.46	111.50
29	B	608	CLA	O2D-CGD-CBD	4.62	119.47	111.27
29	b	611	CLA	O2D-CGD-CBD	4.61	119.46	111.27
29	r1	609	CLA	O2D-CGD-CBD	4.61	119.46	111.27
29	R	609	CLA	O2A-C1-C2	4.61	120.75	108.64
36	b	620	C7Z	C7-C8-C9	-4.61	119.27	126.23
29	R1	603	CLA	O2A-C1-C2	4.61	120.74	108.64
51	n	623	NEX	C38-C25-C24	4.60	119.46	114.28
29	b	604	CLA	O2A-C1-C2	4.60	120.72	108.64
29	g1	603	CLA	O2D-CGD-CBD	4.60	119.44	111.27
29	N1	602	CLA	CMD-C2D-C1D	4.60	132.81	124.71
50	N1	622	XAT	O4-C5-C4	-4.60	109.93	113.38
29	R1	609	CLA	CMD-C2D-C1D	4.59	132.81	124.71
51	R1	622	NEX	C2-C1-C6	4.59	113.68	109.21
29	B1	614	CLA	O2D-CGD-CBD	4.59	119.42	111.27
51	S	623	NEX	C38-C25-C24	4.59	119.44	114.28
29	b	602	CLA	O2D-CGD-CBD	4.59	119.42	111.27
29	y	608	CLA	O2D-CGD-CBD	4.59	119.42	111.27
50	Y	622	XAT	C38-C25-C24	4.58	119.43	114.28
37	B1	623	DGD	O2G-C1B-C2B	4.58	121.37	111.50
31	C1	515	BCR	C15-C14-C13	-4.58	120.78	127.31
33	w1	201	LMG	O7-C10-C11	4.58	121.37	111.50
31	C1	516	BCR	C33-C5-C6	-4.58	119.39	124.53
29	n	613	CLA	CMD-C2D-C1D	4.57	132.78	124.71
29	b1	615	CLA	O2A-C1-C2	4.57	120.66	108.64
53	r1	626	ERG	C13-C17-C20	-4.57	113.53	119.43
45	H	101	RRX	C33-C5-C6	-4.57	119.39	124.53
49	S1	621	LUT	C35-C34-C33	-4.57	120.78	127.31
29	B	602	CLA	O2A-C1-C2	4.57	120.64	108.64
49	g1	621	LUT	C22-C23-C24	-4.57	106.54	111.74
29	y	613	CLA	O2A-C1-C2	4.57	120.64	108.64
29	N	613	CLA	CMD-C2D-C1D	4.57	132.76	124.71
33	h	102	LMG	O7-C10-C11	4.57	121.34	111.50
29	R	602	CLA	CMD-C2D-C1D	4.57	132.76	124.71
55	Y1	627	PTY	O7-C8-C11	4.57	119.49	111.09
51	Y	623	NEX	C38-C25-C24	4.56	119.42	114.28
45	h1	101	RRX	C24-C23-C22	4.56	133.12	126.23
29	n	602	CLA	O2D-CGD-CBD	4.55	119.36	111.27
29	B1	608	CLA	O2D-CGD-CBD	4.55	119.36	111.27
33	w	201	LMG	O7-C10-C11	4.55	121.31	111.50
29	s1	602	CLA	C1-C2-C3	-4.55	118.18	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	Y1	623	NEX	C38-C25-C26	-4.54	114.65	122.26
29	c1	509	CLA	O2D-CGD-CBD	4.54	119.34	111.27
45	h	101	RRX	C1-C6-C5	-4.54	116.22	122.61
49	y1	621	LUT	C3-C4-C5	-4.54	102.81	111.85
53	R	626	ERG	C18-C13-C12	-4.54	103.42	110.59
29	s	614	CLA	O2A-C1-C2	4.54	120.56	108.64
29	r	602	CLA	O2A-C1-C2	4.53	120.55	108.64
29	n	611	CLA	O2D-CGD-CBD	4.53	119.32	111.27
51	r1	622	NEX	C17-C1-C6	-4.53	106.42	110.47
29	A	405	CLA	O2D-CGD-CBD	4.53	119.31	111.27
29	G	612	CLA	O2D-CGD-CBD	4.52	119.31	111.27
29	N1	613	CLA	O2A-C1-C2	4.52	120.52	108.64
29	r	608	CLA	O2A-C1-C2	4.52	120.52	108.64
45	h	101	RRX	C16-C17-C18	-4.52	120.86	127.31
29	B	614	CLA	O2A-C1-C2	4.52	120.50	108.64
29	r1	610	CLA	CMD-C2D-C1D	4.52	132.67	124.71
29	y	614	CLA	O2A-C1-C2	4.51	120.50	108.64
51	r1	622	NEX	C2-C1-C6	4.51	113.60	109.21
29	g1	611	CLA	O2A-C1-C2	4.51	120.50	108.64
29	b	617	CLA	O2A-C1-C2	4.51	120.49	108.64
33	W	201	LMG	O7-C10-C11	4.51	121.22	111.50
36	B1	620	C7Z	C22-C23-C24	4.51	116.48	110.30
48	y1	601	CHL	CHD-C1D-ND	-4.51	120.31	124.45
29	b1	616	CLA	C2C-C1C-NC	4.51	114.20	109.97
50	g	622	XAT	C18-C5-C4	4.51	119.35	114.28
29	C	508	CLA	CMB-C2B-C3B	4.50	133.11	124.68
29	C	506	CLA	O2A-C1-C2	4.50	120.47	108.64
36	B	620	C7Z	C38-C25-C26	-4.50	119.47	124.53
36	B1	620	C7Z	C2-C3-C4	4.50	116.47	110.30
29	C	513	CLA	CMD-C2D-C1D	4.50	132.64	124.71
29	B1	610	CLA	O2D-CGD-CBD	4.50	119.26	111.27
40	Y1	624	LHG	O7-C7-C8	4.50	121.19	111.50
50	y	622	XAT	C36-C21-C26	4.49	122.18	110.05
29	S	611	CLA	O2A-C1-C2	4.49	120.44	108.64
40	c	525	LHG	O7-C7-C8	4.49	121.18	111.50
29	b1	614	CLA	O2A-C1-C2	4.48	120.42	108.64
29	N1	604	CLA	C1-C2-C3	-4.48	118.29	126.04
38	t	101	3PH	O21-C21-C22	4.48	121.16	111.50
51	R	622	NEX	C16-C1-C6	-4.48	106.46	110.47
50	N1	622	XAT	C18-C5-C4	4.48	119.32	114.28
29	R1	609	CLA	O2D-CGD-CBD	4.47	119.21	111.27
36	b1	620	C7Z	C7-C8-C9	-4.47	119.48	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	r	621	XAT	C38-C25-C24	4.47	119.31	114.28
29	G	614	CLA	O2D-CGD-CBD	4.47	119.20	111.27
49	G1	621	LUT	C15-C14-C13	-4.46	120.94	127.31
29	n1	613	CLA	O2D-CGD-CBD	4.46	119.20	111.27
29	c1	512	CLA	O2D-CGD-CBD	4.46	119.20	111.27
29	Y	610	CLA	O2A-C1-C2	4.46	120.36	108.64
50	g1	622	XAT	C38-C25-C24	4.46	119.30	114.28
29	G1	611	CLA	O2D-CGD-CBD	4.46	119.19	111.27
29	a	406	CLA	C1-C2-C3	-4.45	118.34	126.04
29	s1	617	CLA	O2A-C1-C2	4.45	120.34	108.64
29	R1	610	CLA	CMD-C2D-C1D	4.45	132.56	124.71
29	S1	609	CLA	O2A-C1-C2	4.45	120.33	108.64
29	n1	603	CLA	O2A-C1-C2	4.45	120.32	108.64
31	C	516	BCR	C33-C5-C6	-4.45	119.53	124.53
29	N1	602	CLA	O2D-CGD-CBD	4.45	119.17	111.27
40	s	624	LHG	O7-C7-C8	4.45	121.08	111.50
29	C	508	CLA	O2D-CGD-CBD	4.45	119.17	111.27
29	g	603	CLA	C1-C2-C3	-4.45	118.35	126.04
49	N1	621	LUT	C22-C23-C24	-4.44	106.68	111.74
49	Y	621	LUT	C21-C26-C27	4.44	118.32	112.70
36	b1	620	C7Z	C27-C28-C29	-4.43	119.55	126.23
29	c	511	CLA	O2A-C1-C2	4.43	120.27	108.64
29	C	501	CLA	O2A-C1-C2	4.42	120.25	108.64
49	Y1	620	LUT	C21-C26-C27	4.42	118.28	112.70
51	R	622	NEX	C38-C25-C24	4.41	119.25	114.28
53	R1	626	ERG	C2-C1-C10	4.41	122.30	112.74
29	b	609	CLA	CMB-C2B-C1B	-4.41	121.68	128.46
49	Y	620	LUT	C21-C26-C27	4.41	118.28	112.70
29	r1	604	CLA	O2D-CGD-CBD	4.41	119.10	111.27
29	r1	602	CLA	CMA-C3A-C4A	4.41	123.61	111.77
49	G1	620	LUT	C21-C26-C27	4.40	118.27	112.70
53	R	626	ERG	C2-C1-C10	4.40	122.28	112.74
40	n	624	LHG	O7-C7-C8	4.40	120.99	111.50
45	h	101	RRX	C10-C11-C12	-4.40	109.49	123.22
45	h	101	RRX	C15-C14-C13	-4.39	121.04	127.31
51	r1	622	NEX	C19-C9-C10	-4.39	116.77	122.92
39	J1	101	DGA	OG2-CB1-CB2	4.39	120.96	111.50
49	R	620	LUT	C11-C10-C9	-4.38	121.05	127.31
29	s	611	CLA	O2D-CGD-CBD	4.38	119.06	111.27
29	C1	509	CLA	O2A-C1-C2	4.38	120.15	108.64
50	Y1	622	XAT	C36-C21-C26	4.38	121.87	110.05
36	b	620	C7Z	C31-C30-C29	-4.38	121.06	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	S1	624	LHG	O7-C7-C8	4.37	120.92	111.50
29	C	509	CLA	O2A-C1-C2	4.37	120.11	108.64
51	Y	623	NEX	C2-C1-C6	4.36	113.45	109.21
45	h1	101	RRX	C7-C8-C9	4.36	132.83	126.23
50	Y	622	XAT	C7-C8-C9	-4.36	118.76	125.53
29	c1	513	CLA	CMD-C2D-C1D	4.36	132.40	124.71
29	B1	609	CLA	O2A-C1-C2	4.35	120.08	108.64
38	B1	624	3PH	O21-C21-C22	4.35	120.88	111.50
29	S1	610	CLA	O2D-CGD-CBD	4.35	119.00	111.27
55	y	626	PTY	O7-C8-C11	4.35	120.87	111.50
49	n	620	LUT	C15-C14-C13	-4.35	121.11	127.31
50	n1	622	XAT	C38-C25-C24	4.35	119.17	114.28
40	D	408	LHG	O7-C7-C8	4.34	120.86	111.50
29	S1	612	CLA	CMD-C2D-C1D	4.34	132.36	124.71
40	N1	624	LHG	O7-C7-C8	4.34	120.85	111.50
48	g	605	CHL	C4A-NA-C1A	4.34	108.66	106.71
36	B	620	C7Z	C35-C34-C33	-4.33	121.12	127.31
31	b	618	BCR	C1-C6-C5	-4.33	116.51	122.61
29	G	613	CLA	O2D-CGD-CBD	4.33	118.97	111.27
49	s1	620	LUT	C22-C23-C24	-4.33	106.81	111.74
29	c	503	CLA	O2A-C1-C2	4.33	120.01	108.64
29	b	605	CLA	C2C-C1C-NC	4.32	114.02	109.97
31	b1	618	BCR	C1-C6-C5	-4.32	116.52	122.61
29	g	612	CLA	O2D-CGD-CBD	4.32	118.95	111.27
50	Y1	622	XAT	O4-C5-C4	-4.32	110.14	113.38
29	C1	501	CLA	C1-C2-C3	-4.32	118.57	126.04
31	B	618	BCR	C33-C5-C4	4.32	121.91	113.62
29	a	405	CLA	O2D-CGD-CBD	4.31	118.93	111.27
29	Y	611	CLA	O2A-C1-C2	4.31	119.97	108.64
49	G	620	LUT	C35-C34-C33	-4.31	121.16	127.31
29	C	512	CLA	CMD-C2D-C1D	4.31	132.31	124.71
48	n1	605	CHL	CHD-C1D-ND	-4.31	120.50	124.45
29	B1	615	CLA	O2D-CGD-CBD	4.31	118.92	111.27
29	g1	614	CLA	O2D-CGD-CBD	4.30	118.91	111.27
38	B	624	3PH	O21-C21-C22	4.30	120.77	111.50
51	R	622	NEX	C5-C6-C1	4.30	123.96	119.70
29	B1	611	CLA	C2C-C1C-NC	4.30	114.00	109.97
29	C	511	CLA	O2A-C1-C2	4.30	119.93	108.64
49	R1	620	LUT	C7-C8-C9	-4.29	119.75	126.23
29	n	603	CLA	O2A-C1-C2	4.29	119.92	108.64
29	y1	613	CLA	O2A-C1-C2	4.29	119.91	108.64
29	A	406	CLA	O2A-C1-C2	4.29	119.91	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	d1	408	LHG	O7-C7-C8	4.29	120.75	111.50
51	R1	622	NEX	C38-C25-C24	4.29	119.10	114.28
40	y	624	LHG	O7-C7-C8	4.29	120.74	111.50
49	Y1	620	LUT	C35-C34-C33	-4.29	121.19	127.31
49	N1	620	LUT	C7-C8-C9	-4.28	119.76	126.23
29	R1	603	CLA	CMD-C2D-C1D	4.28	132.26	124.71
33	W1	201	LMG	O7-C10-C11	4.28	120.72	111.50
49	G	621	LUT	C22-C23-C24	-4.28	106.88	111.74
50	R1	621	XAT	C31-C30-C29	-4.27	121.21	127.31
29	a1	407	CLA	CMD-C2D-C1D	4.27	132.25	124.71
50	G	622	XAT	O4-C5-C4	-4.27	110.17	113.38
53	r	626	ERG	C4-C5-C10	4.27	122.09	116.42
29	C1	510	CLA	O2A-C1-C2	4.27	119.85	108.64
29	S1	605	CLA	O2D-CGD-CBD	4.27	118.85	111.27
45	h	101	RRX	C7-C6-C5	-4.26	111.13	121.46
48	g	606	CHL	CHD-C1D-ND	-4.26	120.54	124.45
50	N1	622	XAT	C38-C25-C24	4.26	119.08	114.28
29	S	610	CLA	O2D-CGD-CBD	4.26	118.84	111.27
48	n1	601	CHL	CHD-C1D-ND	-4.26	120.54	124.45
50	N	622	XAT	C7-C8-C9	-4.26	118.92	125.53
29	c1	510	CLA	O2A-C1-C2	4.26	119.82	108.64
29	y1	611	CLA	C1-C2-C3	-4.26	118.68	126.04
29	B	615	CLA	O2A-C1-C2	4.26	119.82	108.64
29	A	410	CLA	CMB-C2B-C3B	4.26	132.64	124.68
53	R1	626	ERG	C2-C3-C4	4.26	116.14	110.31
45	h	101	RRX	C7-C8-C9	4.25	132.66	126.23
29	b	609	CLA	CMD-C2D-C1D	4.25	132.21	124.71
50	y	622	XAT	C15-C14-C13	-4.25	121.24	127.31
48	r1	607	CHL	CHD-C1D-ND	-4.25	120.55	124.45
29	C	506	CLA	C2C-C1C-NC	4.25	113.95	109.97
49	N	621	LUT	C15-C14-C13	-4.24	121.26	127.31
40	C	525	LHG	O7-C7-C8	4.24	120.64	111.50
49	n1	620	LUT	C15-C14-C13	-4.24	121.26	127.31
29	c	513	CLA	CMD-C2D-C1D	4.24	132.18	124.71
40	G	624	LHG	O7-C7-C8	4.24	120.63	111.50
29	S1	617	CLA	C1-C2-C3	-4.24	119.90	126.75
39	B1	625	DGA	OG2-CB1-CB2	4.24	120.63	111.50
29	c	505	CLA	O2A-C1-C2	4.24	119.77	108.64
33	C1	521	LMG	O7-C10-C11	4.23	120.62	111.50
29	C1	508	CLA	CMD-C2D-C1D	4.23	132.17	124.71
40	Y	624	LHG	O7-C7-C8	4.22	120.60	111.50
49	s1	621	LUT	C11-C10-C9	-4.22	121.28	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	n1	624	LHG	O7-C7-C8	4.22	120.59	111.50
33	C	521	LMG	O7-C10-C11	4.21	120.58	111.50
51	s1	623	NEX	C38-C25-C24	4.21	119.02	114.28
29	b1	612	CLA	C1-C2-C3	-4.21	118.76	126.04
29	R1	610	CLA	C2D-C1D-ND	4.21	113.20	110.10
29	B1	614	CLA	C2C-C1C-NC	4.21	113.91	109.97
48	g1	609	CHL	CHD-C1D-ND	-4.20	120.59	124.45
49	g1	621	LUT	C7-C8-C9	-4.20	119.89	126.23
49	G	620	LUT	C7-C8-C9	-4.20	119.89	126.23
45	H1	101	RRX	C24-C25-C26	-4.19	111.30	121.46
33	c	523	LMG	O7-C10-C11	4.19	120.54	111.50
49	G	620	LUT	C21-C26-C27	4.19	118.00	112.70
31	B	618	BCR	C1-C6-C5	-4.19	116.71	122.61
48	n	605	CHL	CHD-C1D-ND	-4.19	120.60	124.45
31	c1	515	BCR	C33-C5-C6	-4.19	119.83	124.53
45	h1	101	RRX	C34-C9-C8	4.18	124.67	118.08
40	D	410	LHG	O7-C7-C8	4.18	120.52	111.50
29	a	406	CLA	CHD-C1D-ND	-4.18	120.61	124.45
51	R1	622	NEX	C31-C30-C29	4.18	133.28	127.31
51	G1	623	NEX	C38-C25-C24	4.18	118.98	114.28
29	R	608	CLA	C2C-C1C-NC	4.18	113.89	109.97
45	H1	101	RRX	C11-C10-C9	-4.18	121.35	127.31
29	b1	604	CLA	CMA-C3A-C4A	4.17	122.99	111.77
29	C1	504	CLA	C1-C2-C3	-4.17	118.83	126.04
47	i1	101	4RF	O21-C22-C24	4.17	120.49	111.50
50	y1	622	XAT	C18-C5-C4	4.17	118.97	114.28
49	Y	621	LUT	C35-C34-C33	-4.17	121.36	127.31
51	S1	623	NEX	C27-C28-C29	-4.17	119.06	125.53
29	B1	603	CLA	C1-C2-C3	-4.17	118.83	126.04
50	y1	622	XAT	C7-C8-C9	-4.17	119.07	125.53
39	j1	101	DGA	OG2-CB1-CB2	4.16	120.47	111.50
48	N	601	CHL	CHD-C1D-ND	-4.16	120.63	124.45
49	r1	620	LUT	C15-C14-C13	-4.16	121.37	127.31
50	r1	621	XAT	C32-C33-C34	4.15	125.31	118.94
51	G	623	NEX	C17-C1-C6	-4.15	106.76	110.47
29	c1	505	CLA	C1-C2-C3	-4.15	118.86	126.04
29	r	610	CLA	C1-C2-C3	-4.15	118.86	126.04
36	B	620	C7Z	C31-C30-C29	-4.15	121.39	127.31
29	C1	508	CLA	O2D-CGD-CBD	4.14	118.63	111.27
29	Y1	608	CLA	C1-C2-C3	-4.14	120.05	126.75
51	y1	623	NEX	O24-C25-C24	-4.14	110.27	113.38
36	B	620	C7Z	C7-C8-C9	-4.14	119.98	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	y1	620	LUT	C21-C26-C25	4.14	118.84	111.42
49	r	620	LUT	C35-C34-C33	-4.14	121.40	127.31
40	d1	409	LHG	O7-C7-C8	4.13	120.41	111.50
29	s1	613	CLA	O2D-CGD-CBD	4.13	118.61	111.27
48	g	609	CHL	CHD-C1D-ND	-4.13	120.66	124.45
49	G1	621	LUT	C35-C34-C33	-4.13	121.42	127.31
48	g	605	CHL	CHD-C1D-ND	-4.12	120.66	124.45
29	R1	603	CLA	O2D-CGD-CBD	4.12	118.59	111.27
29	C1	511	CLA	O2D-CGD-CBD	4.12	118.59	111.27
29	c	507	CLA	C2C-C1C-NC	4.11	113.83	109.97
50	R1	621	XAT	C18-C5-C4	4.11	118.91	114.28
53	R	626	ERG	C2-C3-C4	4.11	115.94	110.31
29	B1	610	CLA	O2A-C1-C2	4.11	119.42	108.64
48	N	605	CHL	CHD-C1D-ND	-4.10	120.68	124.45
50	r1	621	XAT	C18-C5-C4	4.10	118.90	114.28
29	G1	612	CLA	CMD-C2D-C1D	4.10	131.94	124.71
29	C1	513	CLA	O2A-C1-C2	4.10	119.41	108.64
48	N1	605	CHL	CHD-C1D-ND	-4.10	120.69	124.45
51	G1	623	NEX	C39-C29-C30	-4.10	117.19	122.92
48	n1	609	CHL	CHD-C1D-ND	-4.10	120.69	124.45
48	R1	607	CHL	C2C-C3C-C4C	4.09	109.41	106.49
45	h1	101	RRX	C7-C6-C5	-4.09	111.55	121.46
50	r	621	XAT	C15-C14-C13	-4.09	121.47	127.31
31	c	516	BCR	C33-C5-C6	-4.09	119.93	124.53
31	C1	515	BCR	C33-C5-C6	-4.09	119.93	124.53
50	Y	622	XAT	C18-C5-C4	4.08	118.87	114.28
48	g1	605	CHL	CHD-C1D-ND	-4.08	120.70	124.45
29	c	513	CLA	CAA-C2A-C3A	-4.07	101.62	112.78
31	B1	619	BCR	C33-C5-C6	-4.07	119.96	124.53
29	n1	604	CLA	C1-C2-C3	-4.07	119.01	126.04
39	J	101	DGA	OG2-CB1-CB2	4.06	120.26	111.50
50	y1	622	XAT	C19-C9-C10	-4.06	117.23	122.92
33	h1	102	LMG	O7-C10-C11	4.05	120.24	111.50
29	g1	611	CLA	CMD-C2D-C1D	4.05	131.86	124.71
37	c1	518	DGD	O2G-C1B-C2B	4.05	120.23	111.50
29	B	614	CLA	C2D-C1D-ND	4.05	113.09	110.10
50	Y1	622	XAT	C18-C5-C4	4.05	118.84	114.28
49	G1	621	LUT	C31-C30-C29	-4.05	121.53	127.31
29	n	610	CLA	CAA-C2A-C3A	-4.05	101.69	112.78
38	t1	101	3PH	O21-C21-C22	4.05	120.23	111.50
29	a1	406	CLA	C1-C2-C3	-4.05	119.04	126.04
49	n	621	LUT	C21-C26-C27	4.05	117.82	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	b1	624	3PH	O21-C21-C22	4.05	120.23	111.50
53	R	626	ERG	C7-C6-C5	-4.05	116.10	123.20
51	S1	623	NEX	C38-C25-C24	4.05	118.83	114.28
29	a1	405	CLA	CHD-C1D-ND	-4.05	120.73	124.45
29	n1	602	CLA	CHD-C1D-ND	-4.05	120.74	124.45
29	d1	403	CLA	CMB-C2B-C3B	4.05	132.25	124.68
33	c	521	LMG	O7-C10-C11	4.04	120.22	111.50
45	H1	101	RRX	C30-C25-C26	-4.04	116.92	122.61
49	R1	620	LUT	C35-C34-C33	-4.04	121.54	127.31
32	m1	101	SQD	O7-S-C6	-4.04	102.13	106.94
50	r	621	XAT	O24-C25-C24	4.04	116.42	113.38
29	G1	602	CLA	C2C-C1C-NC	4.04	113.76	109.97
33	A1	413	LMG	O7-C10-C11	4.04	120.21	111.50
33	c1	521	LMG	O7-C10-C11	4.04	120.21	111.50
37	C	519	DGD	O2G-C1B-C2B	4.04	120.20	111.50
37	c	518	DGD	O2G-C1B-C2B	4.04	120.20	111.50
49	R	620	LUT	C21-C26-C25	4.04	118.65	111.42
45	H1	101	RRX	C21-C20-C19	-4.04	110.62	123.22
50	R1	621	XAT	C15-C14-C13	-4.04	121.55	127.31
29	C1	508	CLA	CMB-C2B-C1B	-4.03	122.26	128.46
49	R1	620	LUT	C11-C10-C9	-4.03	121.55	127.31
40	s1	624	LHG	O7-C7-C8	4.03	120.19	111.50
29	n1	610	CLA	CMD-C2D-C1D	4.03	131.81	124.71
29	B1	609	CLA	CMD-C2D-C1D	4.03	131.81	124.71
51	G	623	NEX	C38-C25-C24	4.03	118.81	114.28
49	Y1	621	LUT	C11-C10-C9	-4.03	121.56	127.31
51	r	622	NEX	C38-C25-C24	4.03	118.81	114.28
40	d	410	LHG	O7-C7-C8	4.03	120.18	111.50
53	r	626	ERG	C7-C6-C5	-4.02	116.14	123.20
49	g1	621	LUT	C31-C30-C29	-4.02	121.57	127.31
49	S1	620	LUT	C21-C26-C25	4.02	118.62	111.42
49	r1	620	LUT	C31-C30-C29	-4.02	121.57	127.31
45	H1	101	RRX	C7-C8-C9	-4.02	120.17	126.23
49	n	620	LUT	C11-C10-C9	-4.01	121.59	127.31
29	b	610	CLA	O2A-C1-C2	4.01	119.17	108.64
29	A1	407	CLA	C2C-C1C-NC	4.01	113.73	109.97
29	c	509	CLA	O2A-C1-C2	4.01	119.17	108.64
29	B1	602	CLA	C2C-C1C-NC	4.01	113.73	109.97
48	y	605	CHL	CHD-C1D-ND	-4.01	120.77	124.45
51	r1	622	NEX	C38-C25-C24	4.01	118.79	114.28
39	c	524	DGA	OG2-CB1-CB2	4.01	120.14	111.50
39	b1	625	DGA	OG2-CB1-CB2	4.01	120.13	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	N1	612	CLA	C2C-C1C-NC	4.01	113.72	109.97
50	n	622	XAT	C6-C7-C8	-4.00	117.53	125.99
32	c	526	SQD	O7-S-C6	-4.00	102.18	106.94
31	b1	618	BCR	C27-C26-C25	-4.00	116.92	122.73
29	b	617	CLA	CMD-C2D-C1D	3.99	131.75	124.71
48	n	601	CHL	C2C-C3C-C4C	3.99	109.33	106.49
29	c	501	CLA	CHD-C1D-ND	-3.99	120.79	124.45
38	T	101	3PH	O21-C21-C22	3.99	120.10	111.50
39	c1	524	DGA	OG2-CB1-CB2	3.99	120.09	111.50
50	r	621	XAT	C6-C7-C8	-3.98	117.57	125.99
45	H	101	RRX	C15-C14-C13	-3.98	121.62	127.31
29	G1	611	CLA	C1-C2-C3	-3.98	119.15	126.04
48	S1	607	CHL	CHD-C1D-ND	-3.98	120.79	124.45
31	c1	517	BCR	C36-C18-C17	-3.98	117.35	122.92
29	R1	612	CLA	C2C-C1C-NC	3.98	113.70	109.97
49	S	621	LUT	C22-C23-C24	-3.98	107.21	111.74
29	C	508	CLA	C1-C2-C3	-3.98	119.16	126.04
50	R1	621	XAT	C7-C8-C9	-3.97	119.37	125.53
48	r	607	CHL	CHD-C1D-ND	-3.97	120.81	124.45
31	c1	517	BCR	C19-C18-C17	3.97	125.03	118.94
50	y1	622	XAT	C38-C25-C24	3.97	118.74	114.28
37	C1	519	DGD	O2G-C1B-C2B	3.96	120.03	111.50
49	s1	621	LUT	C7-C8-C9	-3.96	120.25	126.23
50	G1	622	XAT	C27-C28-C29	3.96	131.67	125.53
40	D1	410	LHG	O7-C7-C8	3.95	120.02	111.50
36	b1	620	C7Z	C22-C23-C24	3.95	115.72	110.30
29	D1	402	CLA	C1-C2-C3	-3.95	119.21	126.04
51	r	622	NEX	C2-C1-C6	3.95	113.05	109.21
48	G1	601	CHL	CHD-C1D-ND	-3.95	120.83	124.45
29	S	603	CLA	O2D-CGD-CBD	3.95	118.28	111.27
33	H	102	LMG	O7-C10-C11	3.95	120.01	111.50
29	G1	613	CLA	CMA-C3A-C4A	3.94	122.37	111.77
49	n	620	LUT	C31-C30-C29	-3.94	121.69	127.31
48	G	606	CHL	CHD-C1D-ND	-3.94	120.83	124.45
49	y	620	LUT	C35-C34-C33	-3.94	121.69	127.31
29	B1	615	CLA	O2A-C1-C2	3.94	118.99	108.64
29	s	617	CLA	CMA-C3A-C4A	3.94	122.36	111.77
50	y	622	XAT	C38-C25-C24	3.94	118.71	114.28
47	I	102	4RF	O21-C22-C24	3.93	119.98	111.50
29	C1	512	CLA	CMB-C2B-C3B	3.93	132.04	124.68
48	g1	601	CHL	CHD-C1D-ND	-3.93	120.84	124.45
48	Y	609	CHL	C4D-CHA-C1A	3.93	126.03	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	B1	620	C7Z	C1-C6-C5	-3.93	117.08	122.61
51	Y1	623	NEX	C31-C30-C29	3.93	132.92	127.31
48	g	609	CHL	C1-O2A-CGA	3.93	126.75	116.44
37	c	520	DGD	O2G-C1B-C2B	3.93	119.97	111.50
29	R	609	CLA	CMA-C3A-C4A	3.93	122.33	111.77
33	b1	622	LMG	O7-C10-C11	3.92	119.96	111.50
29	Y	602	CLA	C2C-C1C-NC	3.92	113.64	109.97
51	Y	623	NEX	C17-C1-C6	-3.92	106.97	110.47
37	c1	519	DGD	O2G-C1B-C2B	3.92	119.94	111.50
29	s1	612	CLA	CMD-C2D-C1D	3.91	131.61	124.71
50	Y1	622	XAT	O24-C25-C38	-3.91	110.37	115.06
29	A	406	CLA	C2C-C1C-NC	3.91	113.64	109.97
31	C1	515	BCR	C23-C24-C25	-3.91	116.22	127.20
29	A1	406	CLA	O2A-C1-C2	3.91	118.90	108.64
40	G1	624	LHG	O7-C7-C8	3.91	119.92	111.50
29	A1	406	CLA	C2C-C1C-NC	3.91	113.63	109.97
29	r1	602	CLA	C1-C2-C3	-3.90	119.29	126.04
40	S	624	LHG	O7-C7-C8	3.90	119.92	111.50
29	C	507	CLA	C2C-C1C-NC	3.90	113.63	109.97
50	r	621	XAT	C31-C30-C29	-3.90	121.74	127.31
29	C1	513	CLA	CAA-C2A-C3A	-3.90	102.11	112.78
48	s	608	CHL	CHD-C1D-ND	-3.89	120.88	124.45
31	A1	411	BCR	C33-C5-C6	-3.89	120.16	124.53
29	Y	608	CLA	C1-C2-C3	-3.89	120.46	126.75
49	S1	621	LUT	C18-C5-C6	-3.89	120.16	124.53
29	C	508	CLA	CHD-C1D-ND	-3.89	120.88	124.45
49	y1	620	LUT	C11-C10-C9	-3.89	121.76	127.31
48	g	605	CHL	C2C-C3C-C4C	3.89	109.26	106.49
29	b1	613	CLA	C2C-C1C-NC	3.88	113.61	109.97
39	j	101	DGA	OG2-CB1-CB2	3.88	119.87	111.50
29	G1	603	CLA	O2D-CGD-CBD	3.88	118.17	111.27
31	C	515	BCR	C33-C5-C4	3.88	121.07	113.62
31	C1	516	BCR	C27-C26-C25	-3.88	117.10	122.73
39	C	524	DGA	OG2-CB1-CB2	3.88	119.86	111.50
29	b1	615	CLA	OBD-CAD-C3D	-3.88	119.19	128.52
49	G	621	LUT	C11-C10-C9	-3.88	121.78	127.31
49	n	620	LUT	C7-C8-C9	-3.87	120.38	126.23
29	B	612	CLA	C1-C2-C3	-3.87	119.34	126.04
29	b1	617	CLA	C2C-C1C-NC	3.87	113.60	109.97
37	c	519	DGD	O2G-C1B-C2B	3.87	119.85	111.50
29	b	613	CLA	O2A-C1-C2	3.87	118.81	108.64
49	S1	621	LUT	C22-C23-C24	-3.87	107.33	111.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	N	624	LHG	O7-C7-C8	3.87	119.84	111.50
48	n	601	CHL	C3C-C4C-NC	-3.87	106.23	110.57
49	S	621	LUT	C35-C34-C33	-3.87	121.79	127.31
29	A1	410	CLA	O2A-C1-C2	3.87	118.80	108.64
29	g1	610	CLA	C1-C2-C3	-3.87	119.36	126.04
47	k1	101	4RF	O21-C22-C24	3.87	119.83	111.50
29	b1	604	CLA	C1-C2-C3	-3.87	119.36	126.04
49	s	620	LUT	C22-C23-C24	-3.86	107.34	111.74
29	S	602	CLA	C2C-C1C-NC	3.86	113.59	109.97
48	g	605	CHL	C3C-C4C-NC	-3.86	106.24	110.57
48	Y	607	CHL	C4A-NA-C1A	3.86	108.44	106.71
29	n	602	CLA	C1-C2-C3	-3.86	119.37	126.04
48	g1	605	CHL	C2C-C3C-C4C	3.86	109.24	106.49
32	b	621	SQD	O7-S-C6	-3.86	102.35	106.94
50	n	622	XAT	C38-C25-C24	3.86	118.62	114.28
29	S	603	CLA	CMA-C3A-C4A	3.85	122.13	111.77
48	n	609	CHL	CHD-C1D-ND	-3.85	120.91	124.45
40	C1	525	LHG	O7-C7-C8	3.85	119.80	111.50
49	n1	621	LUT	C11-C10-C9	-3.85	121.81	127.31
50	G	622	XAT	C19-C9-C10	-3.85	117.53	122.92
49	n	620	LUT	C35-C34-C33	-3.85	121.81	127.31
29	b	609	CLA	CMB-C2B-C3B	3.85	131.88	124.68
32	c1	526	SQD	O7-S-C6	-3.85	102.36	106.94
29	C1	512	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
51	Y1	623	NEX	C20-C13-C14	-3.85	117.53	122.92
33	C	523	LMG	O7-C10-C11	3.85	119.79	111.50
29	B	609	CLA	CMB-C2B-C1B	-3.85	122.55	128.46
49	g1	620	LUT	C18-C5-C6	-3.85	120.21	124.53
29	c1	502	CLA	C2C-C1C-NC	3.85	113.58	109.97
29	b1	612	CLA	O2D-CGD-O1D	-3.84	116.32	123.84
37	C1	520	DGD	O2G-C1B-C2B	3.84	119.78	111.50
48	G1	601	CHL	C3C-C4C-NC	-3.84	106.26	110.57
29	c1	504	CLA	C2C-C1C-NC	3.84	113.57	109.97
29	y	608	CLA	C1-C2-C3	-3.84	120.54	126.75
40	D1	409	LHG	O7-C7-C8	3.84	119.78	111.50
49	Y	621	LUT	C15-C14-C13	-3.84	121.83	127.31
29	c	502	CLA	C1-C2-C3	-3.84	119.40	126.04
29	C1	505	CLA	CMB-C2B-C3B	3.84	131.86	124.68
51	N	623	NEX	C27-C28-C29	-3.84	119.57	125.53
29	y	614	CLA	CHD-C1D-ND	-3.84	120.93	124.45
30	a	409	PHO	CMB-C2B-C3B	3.83	131.85	124.68
50	N1	622	XAT	C40-C33-C34	-3.83	117.56	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	G1	622	XAT	C7-C8-C9	-3.83	119.59	125.53
29	g1	610	CLA	CHD-C1D-ND	-3.83	120.94	124.45
48	N	601	CHL	C1-C2-C3	-3.83	119.42	126.04
29	N1	604	CLA	C2C-C1C-NC	3.83	113.56	109.97
31	c1	516	BCR	C33-C5-C6	-3.83	120.23	124.53
48	S	608	CHL	CHD-C1D-ND	-3.83	120.94	124.45
31	B1	618	BCR	C36-C18-C17	-3.83	117.56	122.92
50	Y	622	XAT	C36-C21-C26	3.82	120.37	110.05
29	S1	610	CLA	CHD-C1D-ND	-3.82	120.94	124.45
51	s	623	NEX	O24-C25-C24	-3.82	110.51	113.38
29	S	605	CLA	C2C-C1C-NC	3.82	113.55	109.97
29	c	504	CLA	C1-C2-C3	-3.82	119.44	126.04
50	r1	621	XAT	C31-C30-C29	-3.82	121.86	127.31
48	Y1	601	CHL	CHD-C1D-ND	-3.82	120.95	124.45
29	c1	513	CLA	C2D-C1D-ND	3.82	112.92	110.10
31	B	618	BCR	C23-C24-C25	-3.82	116.48	127.20
29	c	512	CLA	CMD-C2D-C1D	3.82	131.44	124.71
29	C	513	CLA	CAA-C2A-C3A	-3.81	102.34	112.78
31	b1	618	BCR	C4-C5-C6	-3.81	117.20	122.73
31	d1	404	BCR	C8-C9-C10	3.81	124.79	118.94
29	A	407	CLA	C2C-C1C-NC	3.81	113.54	109.97
36	B	620	C7Z	C15-C14-C13	-3.81	121.87	127.31
48	g	607	CHL	CHD-C1D-ND	-3.81	120.95	124.45
31	D1	404	BCR	C35-C13-C14	-3.81	117.59	122.92
53	R1	626	ERG	C18-C13-C12	-3.81	104.58	110.59
40	c1	525	LHG	O7-C7-C8	3.81	119.70	111.50
48	n	606	CHL	C1-C2-C3	-3.81	119.46	126.04
40	g	624	LHG	O7-C7-C8	3.80	119.70	111.50
29	a1	407	CLA	C2D-C1D-ND	3.80	112.91	110.10
36	B	620	C7Z	C1-C6-C5	-3.80	117.26	122.61
43	d1	405	PL9	C7-C3-C2	-3.80	118.30	123.30
29	s	612	CLA	CMB-C2B-C3B	3.80	131.78	124.68
29	c	512	CLA	CMB-C2B-C3B	3.80	131.78	124.68
29	c	506	CLA	CHD-C1D-ND	-3.80	120.97	124.45
29	r	602	CLA	CMB-C2B-C1B	-3.79	122.63	128.46
50	N1	622	XAT	C6-C7-C8	-3.79	117.97	125.99
50	n	622	XAT	C7-C8-C9	-3.79	119.65	125.53
29	a1	410	CLA	C2C-C1C-NC	3.79	113.52	109.97
29	Y1	608	CLA	O2A-C1-C2	3.79	118.59	108.64
48	r1	607	CHL	C2C-C3C-C4C	3.79	109.19	106.49
38	T1	101	3PH	O21-C21-C22	3.79	119.66	111.50
45	H	101	RRX	C2-C1-C6	3.79	116.31	110.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	N1	608	CHL	CHD-C1D-ND	-3.78	120.98	124.45
29	Y1	602	CLA	C2C-C1C-NC	3.78	113.52	109.97
30	A	408	PHO	CMB-C2B-C3B	3.78	131.76	124.68
55	Y1	626	PTY	O7-C8-C11	3.78	119.65	111.50
49	S	620	LUT	C2-C3-C4	-3.78	105.13	110.30
48	N1	605	CHL	C1-C2-C3	-3.78	119.50	126.04
40	D	409	LHG	O7-C7-C8	3.78	119.65	111.50
47	i	101	4RF	O21-C22-C24	3.78	119.65	111.50
36	B	620	C7Z	C35-C15-C14	-3.78	115.73	123.47
48	y	609	CHL	CHD-C1D-ND	-3.78	120.98	124.45
29	c	508	CLA	CHD-C1D-ND	-3.77	120.99	124.45
29	B	616	CLA	C2D-C1D-ND	3.77	112.88	110.10
51	n1	623	NEX	C19-C9-C10	-3.77	117.64	122.92
29	b	614	CLA	CHD-C1D-ND	-3.77	120.99	124.45
51	n1	623	NEX	C39-C29-C30	-3.77	117.65	122.92
50	y1	622	XAT	C36-C21-C26	3.76	120.21	110.05
48	y	601	CHL	CHD-C1D-ND	-3.76	121.00	124.45
49	G1	620	LUT	C15-C14-C13	-3.76	121.94	127.31
48	y1	607	CHL	CHD-C1D-ND	-3.76	121.00	124.45
32	a1	412	SQD	O7-S-C6	-3.76	102.47	106.94
51	R1	622	NEX	C27-C28-C29	-3.76	119.69	125.53
48	g	601	CHL	CHD-C1D-ND	-3.76	121.00	124.45
29	a	405	CLA	CHD-C1D-ND	-3.76	121.00	124.45
51	s	623	NEX	C27-C28-C29	-3.76	119.70	125.53
36	B1	620	C7Z	C27-C28-C29	-3.76	120.56	126.23
47	I1	102	4RF	O21-C22-C24	3.76	119.60	111.50
53	r1	626	ERG	C2-C1-C10	3.76	120.88	112.74
29	c	504	CLA	CHD-C1D-ND	-3.76	121.00	124.45
32	B	621	SQD	O7-S-C6	-3.76	102.48	106.94
29	B1	609	CLA	C1-C2-C3	-3.75	119.55	126.04
48	Y	609	CHL	C1B-CHB-C4A	-3.75	122.68	130.12
29	C1	509	CLA	C2C-C1C-NC	3.75	113.49	109.97
48	N	601	CHL	C3C-C4C-NC	-3.75	106.37	110.57
49	y	620	LUT	C15-C14-C13	-3.75	121.96	127.31
29	b1	605	CLA	C1-C2-C3	-3.75	119.56	126.04
50	g	622	XAT	C26-C27-C28	-3.75	118.07	125.99
48	S	606	CHL	CHD-C1D-ND	-3.75	121.01	124.45
29	d1	403	CLA	CMB-C2B-C1B	-3.75	122.71	128.46
48	r1	607	CHL	C3C-C4C-NC	-3.74	106.37	110.57
29	s1	604	CLA	C1-C2-C3	-3.74	119.57	126.04
29	s1	609	CLA	C2D-C1D-ND	3.74	112.86	110.10
29	g	610	CLA	CHD-C1D-ND	-3.74	121.02	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	y	623	NEX	C27-C28-C29	-3.74	119.72	125.53
29	y	603	CLA	C2C-C1C-NC	3.74	113.48	109.97
55	y1	626	PTY	O7-C8-C11	3.74	119.56	111.50
51	y1	623	NEX	C5-C4-C3	3.74	116.17	111.75
29	b	611	CLA	C2C-C1C-NC	3.74	113.47	109.97
37	C	520	DGD	O2G-C1B-C2B	3.74	119.56	111.50
48	Y	601	CHL	CHD-C1D-ND	-3.73	121.02	124.45
48	n1	605	CHL	C2C-C3C-C4C	3.73	109.15	106.49
37	C1	518	DGD	O2G-C1B-C2B	3.73	119.55	111.50
53	r1	626	ERG	C18-C13-C14	-3.73	104.19	110.24
29	s	617	CLA	C1-C2-C3	-3.73	120.71	126.75
48	N	608	CHL	CHD-C1D-ND	-3.73	121.03	124.45
49	g	620	LUT	C7-C8-C9	-3.73	120.60	126.23
49	S1	621	LUT	C1-C6-C5	-3.73	117.36	122.61
29	N	604	CLA	C1-C2-C3	-3.73	119.59	126.04
29	B	606	CLA	C1-C2-C3	-3.73	119.60	126.04
29	B	605	CLA	C1-C2-C3	-3.73	119.60	126.04
29	C1	506	CLA	C2C-C1C-NC	3.73	113.46	109.97
48	Y1	601	CHL	C1B-CHB-C4A	-3.72	122.74	130.12
48	n1	601	CHL	C2C-C3C-C4C	3.72	109.14	106.49
44	F1	101	HEM	CAD-CBD-CGD	-3.72	105.60	113.60
48	n1	605	CHL	C3C-C4C-NC	-3.72	106.40	110.57
49	N1	621	LUT	C38-C25-C24	-3.72	115.61	123.56
30	A1	409	PHO	C4A-C3A-C2A	-3.72	99.30	102.84
32	C	526	SQD	O7-S-C6	-3.71	102.53	106.94
33	d1	411	LMG	O7-C10-C11	3.71	119.50	111.50
32	M	101	SQD	O7-S-C6	-3.71	102.53	106.94
36	B	620	C7Z	C2-C3-C4	3.71	115.38	110.30
50	Y	622	XAT	C38-C25-C26	-3.71	116.05	122.26
36	B	620	C7Z	C22-C23-C24	3.71	115.38	110.30
29	A	410	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
49	s	621	LUT	C22-C23-C24	-3.71	107.52	111.74
49	g	620	LUT	C22-C23-C24	-3.70	107.53	111.74
53	R	626	ERG	C16-C17-C13	3.70	108.31	103.84
29	A	406	CLA	C1C-C2C-C3C	-3.70	103.06	106.96
29	y1	602	CLA	C2D-C1D-ND	3.70	112.83	110.10
48	n	601	CHL	CHD-C1D-ND	-3.70	121.05	124.45
48	g1	608	CHL	CHD-C1D-ND	-3.70	121.05	124.45
49	R1	620	LUT	C15-C14-C13	-3.70	122.03	127.31
49	r1	620	LUT	C18-C5-C6	-3.70	120.37	124.53
29	N	602	CLA	C2D-C1D-ND	3.70	112.83	110.10
29	c	510	CLA	C1C-C2C-C3C	-3.70	103.07	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	g	623	NEX	C5-C6-C1	3.70	123.37	119.70
51	G	623	NEX	C27-C28-C29	-3.70	119.79	125.53
29	n	613	CLA	CBA-CAA-C2A	3.70	124.78	113.86
49	s1	620	LUT	C11-C10-C9	-3.70	122.03	127.31
51	n1	623	NEX	C31-C30-C29	3.69	132.58	127.31
29	s1	605	CLA	C2C-C1C-NC	3.69	113.43	109.97
49	r1	620	LUT	C21-C26-C25	3.69	118.03	111.42
50	r1	621	XAT	C15-C14-C13	-3.69	122.04	127.31
29	b1	608	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
48	g1	607	CHL	C1-C2-C3	-3.69	119.67	126.04
32	a	412	SQD	O7-S-C6	-3.69	102.56	106.94
48	N	601	CHL	C2C-C3C-C4C	3.69	109.12	106.49
55	Y	626	PTY	O7-C8-C11	3.68	119.44	111.50
49	N1	620	LUT	C15-C14-C13	-3.68	122.05	127.31
51	N1	623	NEX	C38-C25-C24	3.68	118.42	114.28
29	N	614	CLA	C2C-C1C-NC	3.68	113.42	109.97
29	a	405	CLA	CMB-C2B-C3B	3.68	131.57	124.68
29	c	510	CLA	C1-C2-C3	-3.68	119.67	126.04
29	g	611	CLA	C2C-C1C-NC	3.68	113.42	109.97
49	s1	620	LUT	C1-C6-C5	-3.68	117.43	122.61
48	R	606	CHL	CHD-C1D-ND	-3.68	121.07	124.45
48	s	601	CHL	C3C-C4C-NC	-3.68	106.45	110.57
48	n1	609	CHL	CMA-C3A-C4A	3.68	121.66	111.77
32	b1	626	SQD	O7-S-C6	-3.68	102.57	106.94
29	S	613	CLA	C2C-C1C-NC	3.68	113.42	109.97
29	B	611	CLA	C2C-C1C-NC	3.67	113.41	109.97
29	g1	602	CLA	CMA-C3A-C4A	3.67	121.64	111.77
29	n	614	CLA	CHD-C1D-ND	-3.67	121.08	124.45
51	y1	623	NEX	C2-C1-C6	3.67	112.78	109.21
48	y1	609	CHL	CHD-C4C-C3C	3.67	130.24	124.84
33	B1	622	LMG	O7-C10-C11	3.67	119.41	111.50
48	y	609	CHL	C2C-C3C-C4C	3.67	109.10	106.49
29	b	614	CLA	C1-C2-C3	-3.66	119.70	126.04
29	B	609	CLA	C1-C2-C3	-3.66	119.71	126.04
29	s	610	CLA	C1-C2-C3	-3.66	119.71	126.04
29	C1	511	CLA	C2C-C1C-NC	3.66	113.40	109.97
51	n1	623	NEX	C38-C25-C24	3.66	118.40	114.28
31	b1	618	BCR	C33-C5-C4	3.66	120.65	113.62
32	B1	626	SQD	O7-S-C6	-3.66	102.59	106.94
48	N1	608	CHL	C3C-C4C-NC	-3.66	106.47	110.57
29	c1	508	CLA	C1-C2-C3	-3.66	119.71	126.04
45	H1	101	RRX	C1-C6-C5	-3.66	117.46	122.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
53	r1	626	ERG	C7-C6-C5	-3.66	116.78	123.20
51	g	623	NEX	O24-C25-C38	-3.66	110.67	115.06
29	G	613	CLA	C1-C2-C3	-3.66	119.72	126.04
29	r	609	CLA	CHD-C1D-ND	-3.66	121.09	124.45
48	Y	601	CHL	C1-C2-C3	-3.65	119.72	126.04
29	C1	508	CLA	CMB-C2B-C3B	3.65	131.51	124.68
48	G1	608	CHL	CHD-C1D-ND	-3.65	121.10	124.45
33	c1	523	LMG	O7-C10-C11	3.65	119.37	111.50
31	a1	411	BCR	C33-C5-C4	3.65	120.63	113.62
29	s1	617	CLA	C1-C2-C3	-3.65	120.85	126.75
48	S	601	CHL	CHD-C1D-ND	-3.65	121.10	124.45
29	n1	603	CLA	C2C-C1C-NC	3.65	113.39	109.97
48	N	609	CHL	CMA-C3A-C4A	3.65	121.58	111.77
48	y1	607	CHL	C4A-NA-C1A	3.65	108.34	106.71
48	G	607	CHL	CHD-C1D-ND	-3.64	121.11	124.45
51	g	623	NEX	C27-C28-C29	-3.64	119.88	125.53
29	n	602	CLA	C2C-C1C-NC	3.64	113.38	109.97
29	Y1	613	CLA	CMA-C3A-C4A	3.64	121.55	111.77
50	g	622	XAT	C6-C7-C8	-3.64	118.30	125.99
29	a1	410	CLA	CMB-C2B-C3B	3.63	131.48	124.68
48	n1	607	CHL	CMA-C3A-C4A	3.63	121.53	111.77
48	G1	601	CHL	C2C-C3C-C4C	3.63	109.08	106.49
29	G1	612	CLA	C2D-C1D-ND	3.63	112.78	110.10
29	y	610	CLA	CHD-C1D-ND	-3.63	121.12	124.45
32	A1	412	SQD	O7-S-C6	-3.63	102.63	106.94
53	r	626	ERG	C1-C10-C5	3.63	115.39	108.75
29	c1	511	CLA	C2C-C1C-NC	3.63	113.37	109.97
40	y1	624	LHG	O7-C7-C8	3.62	119.31	111.50
29	c	512	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
48	S	607	CHL	C2C-C3C-C4C	3.62	109.07	106.49
48	n	607	CHL	CHD-C1D-ND	-3.62	121.13	124.45
29	b1	608	CLA	CMB-C2B-C3B	3.62	131.45	124.68
32	M1	101	SQD	O7-S-C6	-3.62	102.64	106.94
29	a	407	CLA	C2C-C1C-NC	3.62	113.36	109.97
48	g1	605	CHL	C3C-C4C-NC	-3.62	106.51	110.57
32	A	412	SQD	O7-S-C6	-3.62	102.64	106.94
48	S1	608	CHL	C4A-NA-C1A	3.62	108.33	106.71
49	n	621	LUT	C22-C23-C24	-3.62	107.62	111.74
29	a	410	CLA	CMB-C2B-C3B	3.61	131.44	124.68
37	C	518	DGD	O2G-C1B-C2B	3.61	119.29	111.50
43	d	405	PL9	C7-C3-C2	-3.61	118.55	123.30
32	m	101	SQD	O7-S-C6	-3.61	102.65	106.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	s	606	CHL	C3C-C4C-NC	-3.61	106.52	110.57
29	B1	609	CLA	C2C-C1C-NC	3.61	113.35	109.97
31	c	515	BCR	C35-C13-C12	3.61	123.76	118.08
49	y	621	LUT	C15-C14-C13	-3.61	122.16	127.31
36	b	620	C7Z	C11-C12-C13	-3.61	116.28	126.42
31	c1	517	BCR	C33-C5-C6	-3.61	120.48	124.53
29	b1	606	CLA	C2C-C1C-NC	3.61	113.35	109.97
48	s	606	CHL	C2C-C3C-C4C	3.61	109.06	106.49
29	N1	611	CLA	C2C-C1C-NC	3.60	113.35	109.97
29	s	605	CLA	C2C-C1C-NC	3.60	113.35	109.97
29	g1	604	CLA	C2D-C1D-ND	3.60	112.76	110.10
51	G	623	NEX	C39-C29-C30	-3.60	117.88	122.92
48	N1	609	CHL	C3C-C4C-NC	-3.60	106.53	110.57
29	A1	406	CLA	C1-C2-C3	-3.60	119.82	126.04
29	C1	511	CLA	C1-C2-C3	-3.60	119.82	126.04
48	N1	608	CHL	C2C-C3C-C4C	3.60	109.05	106.49
29	n1	602	CLA	C2D-C1D-ND	3.59	112.75	110.10
51	R1	622	NEX	C38-C25-C26	-3.59	116.24	122.26
48	s1	601	CHL	C1B-CHB-C4A	-3.59	123.00	130.12
49	n1	621	LUT	C22-C23-C24	-3.59	107.65	111.74
29	y	612	CLA	C2D-C1D-ND	3.59	112.75	110.10
40	d1	410	LHG	O7-C7-C8	3.59	119.23	111.50
40	d	409	LHG	O7-C7-C8	3.59	119.23	111.50
32	B	626	SQD	O7-S-C6	-3.58	102.68	106.94
29	B	615	CLA	OBD-CAD-C3D	-3.58	119.90	128.52
50	y1	622	XAT	C18-C5-C6	-3.58	116.26	122.26
31	B	618	BCR	C33-C5-C6	-3.58	120.50	124.53
51	g1	623	NEX	C39-C29-C30	-3.58	117.91	122.92
48	g	601	CHL	C2C-C3C-C4C	3.58	109.04	106.49
29	S	602	CLA	O2A-CGA-CBA	3.58	123.14	111.91
29	g	612	CLA	C2C-C1C-NC	3.58	113.33	109.97
50	y1	622	XAT	C38-C25-C26	-3.58	116.26	122.26
29	A1	410	CLA	CHD-C1D-ND	-3.58	121.17	124.45
29	D	402	CLA	C2D-C1D-ND	3.58	112.74	110.10
51	R	622	NEX	C27-C28-C29	-3.58	119.98	125.53
48	N1	609	CHL	CMA-C3A-C4A	3.58	121.38	111.77
29	s1	612	CLA	C2C-C1C-NC	3.57	113.32	109.97
29	c	513	CLA	CMB-C2B-C3B	3.57	131.37	124.68
48	R	607	CHL	C3C-C4C-NC	-3.57	106.56	110.57
31	A	411	BCR	C35-C13-C12	3.57	123.71	118.08
29	c1	509	CLA	O2A-C1-C2	3.57	118.02	108.64
29	s1	617	CLA	CHD-C1D-ND	-3.57	121.17	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
41	c1	527	LMK	O3-C4-C3	-3.57	110.73	122.98
29	b	606	CLA	C1-C2-C3	-3.57	119.87	126.04
29	c1	510	CLA	C1-C2-C3	-3.57	119.87	126.04
29	N1	603	CLA	C2C-C1C-NC	3.57	113.32	109.97
29	b	611	CLA	CHD-C1D-ND	-3.57	121.17	124.45
51	r1	622	NEX	C27-C28-C29	-3.57	119.99	125.53
29	A	406	CLA	C1-C2-C3	-3.57	119.87	126.04
48	n	609	CHL	C4D-CHA-C1A	3.57	125.59	121.25
45	h1	101	RRX	C15-C14-C13	-3.57	122.22	127.31
29	R	610	CLA	C2D-C1D-ND	3.56	112.73	110.10
29	D1	403	CLA	C1-C2-C3	-3.56	119.88	126.04
36	b1	620	C7Z	C11-C10-C9	-3.56	122.22	127.31
29	y	608	CLA	C2C-C1C-NC	3.56	113.31	109.97
48	y1	605	CHL	CHD-C1D-ND	-3.56	121.18	124.45
51	S	623	NEX	C5-C4-C3	3.56	115.96	111.75
31	D1	404	BCR	C36-C18-C17	-3.56	117.94	122.92
50	G1	622	XAT	C15-C14-C13	-3.56	122.23	127.31
50	G1	622	XAT	C38-C25-C24	3.56	118.28	114.28
29	b1	612	CLA	C2D-C1D-ND	3.56	112.73	110.10
29	N	611	CLA	C2C-C1C-NC	3.56	113.30	109.97
29	N1	610	CLA	C2D-C1D-ND	3.56	112.72	110.10
29	B	607	CLA	CMB-C2B-C3B	3.55	131.33	124.68
48	N1	609	CHL	CHD-C1D-ND	-3.55	121.19	124.45
29	d	403	CLA	CHD-C1D-ND	-3.55	121.19	124.45
48	n	605	CHL	C3C-C4C-NC	-3.55	106.59	110.57
29	Y1	614	CLA	CMD-C2D-C3D	-3.55	119.45	127.61
31	B	619	BCR	C33-C5-C4	3.55	120.44	113.62
31	C	516	BCR	C36-C18-C17	-3.55	117.95	122.92
31	C1	517	BCR	C37-C22-C21	-3.55	117.95	122.92
48	N1	601	CHL	CHD-C1D-ND	-3.55	121.19	124.45
29	C1	510	CLA	C2D-C1D-ND	3.55	112.72	110.10
48	s1	608	CHL	C1-O2A-CGA	3.55	125.75	116.44
29	b	614	CLA	C1C-C2C-C3C	-3.55	103.23	106.96
31	B	618	BCR	C4-C5-C6	-3.55	117.58	122.73
31	C	515	BCR	C23-C24-C25	-3.55	117.24	127.20
32	B1	621	SQD	O7-S-C6	-3.54	102.73	106.94
29	A1	407	CLA	C1-C2-C3	-3.54	121.02	126.75
49	R	620	LUT	C18-C5-C6	-3.54	120.55	124.53
48	G1	609	CHL	CHD-C1D-ND	-3.54	121.20	124.45
29	G1	604	CLA	C2C-C1C-NC	3.54	113.29	109.97
51	S	623	NEX	C39-C29-C30	-3.54	117.96	122.92
48	N1	609	CHL	C4A-NA-C1A	3.54	108.30	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	g1	622	XAT	C18-C5-C4	3.54	118.27	114.28
30	A	409	PHO	CMB-C2B-C3B	3.54	131.31	124.68
40	D1	408	LHG	O7-C7-C8	3.54	119.13	111.50
48	S	607	CHL	C3C-C4C-NC	-3.54	106.60	110.57
29	C1	513	CLA	CHD-C1D-ND	-3.54	121.20	124.45
29	Y	611	CLA	CHD-C1D-ND	-3.54	121.20	124.45
29	Y1	611	CLA	CHD-C1D-ND	-3.53	121.21	124.45
49	S	620	LUT	C10-C11-C12	-3.53	112.19	123.22
29	r1	608	CLA	C2C-C1C-NC	3.53	113.28	109.97
48	y	607	CHL	CHD-C1D-ND	-3.53	121.21	124.45
29	s	613	CLA	CHD-C1D-ND	-3.53	121.21	124.45
29	y1	602	CLA	CHD-C1D-ND	-3.53	121.21	124.45
29	B1	612	CLA	C1-C2-C3	-3.53	119.94	126.04
29	N1	611	CLA	CHD-C1D-ND	-3.53	121.21	124.45
49	g1	620	LUT	C21-C26-C27	3.53	117.16	112.70
29	G1	603	CLA	C2D-C1D-ND	3.53	112.70	110.10
29	G1	613	CLA	C1-C2-C3	-3.53	119.94	126.04
29	b1	612	CLA	CMA-C3A-C4A	3.53	121.25	111.77
29	D1	402	CLA	C2D-C1D-ND	3.53	112.70	110.10
50	Y1	622	XAT	C26-C27-C28	-3.53	118.54	125.99
49	n1	621	LUT	C7-C8-C9	-3.53	120.91	126.23
48	r	607	CHL	C2C-C3C-C4C	3.53	109.00	106.49
48	Y1	606	CHL	C1-O2A-CGA	3.52	125.68	116.44
29	D1	403	CLA	CMB-C2B-C3B	3.52	131.26	124.68
29	a	405	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
29	r	603	CLA	CMD-C2D-C1D	3.52	130.91	124.71
33	D1	411	LMG	O7-C10-C11	3.52	119.08	111.50
48	g	609	CHL	CMA-C3A-C4A	3.51	121.22	111.77
29	R	602	CLA	CMA-C3A-C4A	3.51	121.22	111.77
49	G	620	LUT	C15-C14-C13	-3.51	122.30	127.31
29	s1	602	CLA	CMB-C2B-C3B	3.51	131.24	124.68
48	g1	607	CHL	C4A-NA-C1A	3.51	108.28	106.71
29	S1	611	CLA	C2C-C1C-NC	3.51	113.26	109.97
48	n1	607	CHL	C2C-C3C-C4C	3.51	108.99	106.49
29	c	508	CLA	C1-C2-C3	-3.51	119.98	126.04
29	n1	613	CLA	CBA-CAA-C2A	3.51	124.21	113.86
40	d	408	LHG	O7-C7-C8	3.50	119.05	111.50
29	g	611	CLA	CHD-C1D-ND	-3.50	121.24	124.45
29	N1	613	CLA	CHD-C1D-ND	-3.50	121.24	124.45
29	Y1	614	CLA	CHD-C1D-ND	-3.50	121.24	124.45
51	N1	623	NEX	C38-C25-C26	-3.50	116.40	122.26
29	C1	508	CLA	C1-C2-C3	-3.50	120.00	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	C1	523	LMG	O7-C10-C11	3.49	119.03	111.50
49	s1	621	LUT	C18-C5-C6	-3.49	120.61	124.53
53	r1	626	ERG	C14-C8-C7	-3.49	117.50	124.38
48	N	605	CHL	C3C-C4C-NC	-3.49	106.66	110.57
29	B	603	CLA	C1-C2-C3	-3.49	120.01	126.04
49	y1	620	LUT	C18-C5-C6	-3.49	120.61	124.53
29	A	407	CLA	CHD-C1D-ND	-3.49	121.25	124.45
29	y1	604	CLA	CHD-C1D-ND	-3.49	121.25	124.45
29	c	507	CLA	C1C-C2C-C3C	-3.49	103.29	106.96
29	S	613	CLA	CMA-C3A-C4A	3.49	121.14	111.77
29	s	614	CLA	C1-C2-C3	-3.49	120.01	126.04
48	G	606	CHL	C3C-C4C-NC	-3.48	106.66	110.57
48	N1	609	CHL	C2C-C3C-C4C	3.48	108.97	106.49
48	n1	606	CHL	CHD-C1D-ND	-3.48	121.25	124.45
29	r	602	CLA	CMB-C2B-C3B	3.48	131.19	124.68
48	G	606	CHL	CMA-C3A-C4A	3.48	121.13	111.77
29	c1	511	CLA	CHD-C1D-ND	-3.48	121.25	124.45
29	S	602	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
31	C1	514	BCR	C19-C18-C17	3.48	124.28	118.94
49	S1	620	LUT	C35-C15-C14	-3.48	116.34	123.47
29	C1	503	CLA	CMA-C3A-C4A	3.48	121.13	111.77
45	H	101	RRX	C7-C8-C9	-3.48	120.98	126.23
29	S	604	CLA	CHD-C1D-ND	-3.48	121.26	124.45
29	G	610	CLA	C1-C2-C3	-3.48	120.03	126.04
29	D	403	CLA	CHD-C1D-ND	-3.48	121.26	124.45
48	N1	607	CHL	CHD-C1D-ND	-3.48	121.26	124.45
29	g	610	CLA	CAA-C2A-C3A	-3.48	103.26	112.78
29	C	509	CLA	C2C-C1C-NC	3.48	113.23	109.97
31	A	411	BCR	C12-C13-C14	-3.48	113.61	118.94
29	n1	611	CLA	C2C-C1C-NC	3.48	113.23	109.97
29	s	613	CLA	C2D-C1D-ND	3.48	112.67	110.10
31	C1	515	BCR	C34-C9-C10	-3.47	118.06	122.92
29	B	607	CLA	CMB-C2B-C1B	-3.47	123.13	128.46
29	S	613	CLA	C1-C2-C3	-3.47	120.04	126.04
31	C	517	BCR	C28-C27-C26	-3.47	107.88	114.08
48	G	601	CHL	C3C-C4C-NC	-3.47	106.68	110.57
45	h1	101	RRX	C4-C5-C6	-3.47	117.70	122.73
29	r	612	CLA	C2C-C1C-NC	3.47	113.22	109.97
29	g	613	CLA	C2D-C1D-ND	3.47	112.66	110.10
41	c	527	LMK	O3-C4-C3	-3.47	111.09	122.98
49	R1	620	LUT	C18-C5-C6	-3.46	120.64	124.53
29	b1	616	CLA	C1-C2-C3	-3.46	120.05	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B1	619	BCR	C33-C5-C4	3.46	120.27	113.62
49	S	620	LUT	C22-C23-C24	-3.46	107.80	111.74
45	h	101	RRX	C20-C21-C22	3.46	132.25	127.31
48	S1	607	CHL	C2C-C3C-C4C	3.46	108.95	106.49
29	C	501	CLA	CHD-C1D-ND	-3.46	121.28	124.45
48	s	601	CHL	CHD-C1D-ND	-3.45	121.28	124.45
29	s	617	CLA	C2C-C1C-NC	3.45	113.21	109.97
29	N1	603	CLA	CHD-C1D-ND	-3.45	121.28	124.45
49	s	620	LUT	C15-C14-C13	-3.45	122.38	127.31
31	c	517	BCR	C3-C4-C5	-3.45	107.91	114.08
50	n1	622	XAT	C38-C25-C26	-3.45	116.48	122.26
29	B	606	CLA	CHD-C1D-ND	-3.45	121.28	124.45
29	B	609	CLA	CMB-C2B-C3B	3.45	131.13	124.68
29	y1	610	CLA	C1-C2-C3	-3.45	120.08	126.04
29	b	612	CLA	C1-C2-C3	-3.45	120.08	126.04
29	n	610	CLA	CHD-C1D-ND	-3.45	121.29	124.45
29	g1	613	CLA	CMA-C3A-C4A	3.45	121.04	111.77
29	g	603	CLA	C2C-C1C-NC	3.44	113.20	109.97
29	S	612	CLA	C2C-C1C-NC	3.44	113.20	109.97
48	G	609	CHL	CHD-C1D-ND	-3.44	121.29	124.45
29	b	610	CLA	C2D-C1D-ND	3.44	112.64	110.10
45	h1	101	RRX	C23-C22-C21	-3.44	113.66	118.94
29	y1	613	CLA	CHD-C1D-ND	-3.44	121.29	124.45
48	s	606	CHL	CHD-C1D-ND	-3.44	121.29	124.45
49	s	621	LUT	C10-C11-C12	-3.44	112.48	123.22
29	a	405	CLA	C2D-C1D-ND	3.44	112.64	110.10
29	r	603	CLA	C2D-C1D-ND	3.44	112.64	110.10
29	S1	617	CLA	CMA-C3A-C4A	3.44	121.02	111.77
29	c	501	CLA	C1-C2-C3	-3.44	120.09	126.04
29	B1	607	CLA	CHD-C1D-ND	-3.44	121.29	124.45
48	G1	608	CHL	C2C-C3C-C4C	3.44	108.94	106.49
29	b1	605	CLA	C2D-C1D-ND	3.44	112.64	110.10
48	G	601	CHL	CHB-C4A-NA	3.44	129.26	124.51
48	Y	605	CHL	C3C-C4C-NC	-3.44	106.72	110.57
48	y	606	CHL	CHD-C1D-ND	-3.44	121.30	124.45
29	C	508	CLA	CAC-C3C-C4C	3.43	129.27	124.81
48	g1	601	CHL	C2C-C3C-C4C	3.43	108.94	106.49
29	b1	603	CLA	C1-C2-C3	-3.43	120.10	126.04
48	n1	608	CHL	CMA-C3A-C4A	3.43	121.00	111.77
29	Y	610	CLA	C2D-C1D-ND	3.43	112.63	110.10
29	B	605	CLA	C2C-C1C-NC	3.43	113.19	109.97
29	Y1	604	CLA	C2C-C1C-NC	3.43	113.19	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	R1	607	CHL	C3C-C4C-NC	-3.43	106.72	110.57
49	Y1	620	LUT	C2-C3-C4	-3.43	105.61	110.30
29	G1	611	CLA	C2C-C1C-NC	3.43	113.19	109.97
29	b	615	CLA	C1-C2-C3	-3.43	120.11	126.04
29	g1	612	CLA	C2C-C1C-NC	3.43	113.19	109.97
31	d1	404	BCR	C4-C5-C6	-3.43	117.75	122.73
29	C	512	CLA	C2C-C1C-NC	3.43	113.19	109.97
29	G	612	CLA	C2C-C1C-NC	3.43	113.19	109.97
29	c	506	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
48	s1	608	CHL	C3C-C4C-NC	-3.43	106.73	110.57
48	y	605	CHL	C3C-C4C-NC	-3.43	106.73	110.57
29	c1	513	CLA	C1-C2-C3	-3.43	120.12	126.04
29	Y	612	CLA	C2D-C1D-ND	3.43	112.63	110.10
29	G1	603	CLA	CHD-C1D-ND	-3.43	121.31	124.45
48	r1	607	CHL	C4A-NA-C1A	3.43	108.25	106.71
29	G1	610	CLA	C2D-C1D-ND	3.42	112.63	110.10
29	C	510	CLA	C1-C2-C3	-3.42	120.12	126.04
29	Y1	608	CLA	C2D-C1D-ND	3.42	112.63	110.10
29	Y1	612	CLA	C2D-C1D-ND	3.42	112.63	110.10
29	g1	614	CLA	C2C-C1C-NC	3.42	113.18	109.97
29	N1	610	CLA	C1-C2-C3	-3.42	120.13	126.04
29	Y	608	CLA	C2C-C1C-NC	3.42	113.18	109.97
29	y	612	CLA	C2C-C1C-NC	3.42	113.18	109.97
29	N1	602	CLA	C1-C2-C3	-3.42	120.13	126.04
48	g	606	CHL	CMA-C3A-C4A	3.42	120.96	111.77
29	R	603	CLA	C1-C2-C3	-3.42	120.13	126.04
48	y	606	CHL	C1-O2A-CGA	3.42	125.42	116.44
29	B1	608	CLA	C2C-C1C-NC	3.42	113.17	109.97
29	b1	604	CLA	C2D-C1D-ND	3.42	112.62	110.10
29	g1	613	CLA	C2D-C1D-ND	3.42	112.62	110.10
29	n1	610	CLA	CAA-C2A-C3A	-3.42	103.42	112.78
29	C1	505	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
29	c	504	CLA	C2D-C1D-ND	3.42	112.62	110.10
48	N1	601	CHL	C2C-C3C-C4C	3.42	108.92	106.49
29	S1	604	CLA	C2C-C1C-NC	3.41	113.17	109.97
29	a	406	CLA	C2C-C1C-NC	3.41	113.17	109.97
33	D	411	LMG	O7-C10-C11	3.41	118.86	111.50
29	B	609	CLA	O2D-CGD-O1D	-3.41	117.17	123.84
29	c	508	CLA	CMB-C2B-C3B	3.41	131.06	124.68
29	R1	610	CLA	O1D-CGD-CBD	-3.41	117.51	124.48
29	b1	604	CLA	CHD-C1D-ND	-3.41	121.32	124.45
29	n	603	CLA	C2D-C1D-ND	3.41	112.62	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S	621	LUT	C2-C3-C4	-3.41	105.64	110.30
29	N1	613	CLA	CMA-C3A-C4A	3.41	120.93	111.77
49	y1	620	LUT	C35-C34-C33	-3.41	122.45	127.31
29	b	606	CLA	CHD-C1D-ND	-3.41	121.32	124.45
31	B	619	BCR	C36-C18-C17	-3.41	118.15	122.92
29	S	617	CLA	C2C-C1C-NC	3.41	113.16	109.97
48	g	606	CHL	C4D-CHA-C1A	3.41	125.39	121.25
29	G	610	CLA	CHD-C1D-ND	-3.40	121.33	124.45
29	y	613	CLA	C1-C2-C3	-3.40	120.16	126.04
29	s1	610	CLA	C1-C2-C3	-3.40	120.16	126.04
48	y	609	CHL	C3C-C4C-NC	-3.40	106.76	110.57
29	b	614	CLA	C2C-C1C-NC	3.40	113.16	109.97
29	Y	602	CLA	C1-C2-C3	-3.40	120.17	126.04
29	G1	603	CLA	C2C-C1C-NC	3.40	113.16	109.97
29	y	602	CLA	C1-C2-C3	-3.40	120.17	126.04
45	H1	101	RRX	C4-C5-C6	-3.40	117.80	122.73
29	R	604	CLA	C2C-C1C-NC	3.40	113.15	109.97
29	c1	501	CLA	C2C-C1C-NC	3.40	113.15	109.97
39	B	625	DGA	OG2-CB1-CB2	3.40	118.82	111.50
29	c1	503	CLA	CHD-C1D-ND	-3.40	121.33	124.45
29	G	612	CLA	C2D-C1D-ND	3.40	112.61	110.10
29	c1	510	CLA	CHD-C1D-ND	-3.40	121.33	124.45
39	b	625	DGA	OG2-CB1-CB2	3.39	118.81	111.50
51	y	623	NEX	C2-C1-C6	3.39	112.51	109.21
29	c	506	CLA	C2C-C1C-NC	3.39	113.15	109.97
48	n	606	CHL	C3C-C4C-NC	-3.39	106.77	110.57
29	N	603	CLA	CHD-C1D-ND	-3.39	121.34	124.45
29	s1	614	CLA	C2C-C1C-NC	3.39	113.15	109.97
29	n	614	CLA	CMA-C3A-C4A	3.39	120.88	111.77
29	c1	508	CLA	CHD-C1D-ND	-3.39	121.34	124.45
48	Y1	605	CHL	CHD-C1D-ND	-3.39	121.34	124.45
31	c1	515	BCR	C33-C5-C4	3.39	120.12	113.62
29	S1	617	CLA	C2C-C1C-NC	3.39	113.14	109.97
29	R	612	CLA	C1-O2A-CGA	3.39	125.33	116.44
49	s1	620	LUT	C15-C14-C13	-3.39	122.48	127.31
29	B1	613	CLA	C2C-C1C-NC	3.38	113.14	109.97
48	S1	606	CHL	CHD-C1D-ND	-3.38	121.34	124.45
50	r1	621	XAT	C26-C27-C28	-3.38	118.84	125.99
29	c1	510	CLA	C2C-C1C-NC	3.38	113.14	109.97
48	n	605	CHL	C2C-C3C-C4C	3.38	108.90	106.49
48	N1	606	CHL	CHD-C1D-ND	-3.38	121.35	124.45
29	C1	512	CLA	CHD-C1D-ND	-3.38	121.35	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	r	608	CLA	CHD-C1D-ND	-3.38	121.35	124.45
44	F	101	HEM	CMC-C2C-C3C	3.38	131.00	124.68
29	s1	609	CLA	CHD-C1D-ND	-3.38	121.35	124.45
31	C	516	BCR	C19-C18-C17	3.38	124.12	118.94
29	C1	504	CLA	C2C-C1C-NC	3.38	113.14	109.97
42	D1	401	BCT	O2-C-O1	-3.38	110.79	119.55
49	n1	621	LUT	C3-C4-C5	-3.38	105.13	111.85
29	c	508	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
29	C	502	CLA	C2C-C1C-NC	3.37	113.13	109.97
29	s	612	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
29	c	503	CLA	CHD-C1D-ND	-3.37	121.36	124.45
29	B	605	CLA	CMA-C3A-C4A	3.37	120.83	111.77
49	N	620	LUT	C11-C10-C9	-3.37	122.50	127.31
49	y	620	LUT	C22-C23-C24	-3.37	107.91	111.74
29	G	611	CLA	C2C-C1C-NC	3.37	113.13	109.97
48	Y1	605	CHL	CMA-C3A-C4A	3.37	120.82	111.77
29	c1	503	CLA	CMA-C3A-C4A	3.37	120.82	111.77
48	N1	601	CHL	C3C-C4C-NC	-3.37	106.80	110.57
29	S	605	CLA	C1-C2-C3	-3.37	121.31	126.75
29	A	405	CLA	CHD-C1D-ND	-3.37	121.36	124.45
48	r	606	CHL	CHD-C1D-ND	-3.37	121.36	124.45
29	s	604	CLA	C2C-C1C-NC	3.37	113.12	109.97
31	d1	404	BCR	C15-C14-C13	-3.36	122.51	127.31
29	D	403	CLA	C1-C2-C3	-3.36	120.22	126.04
49	y	620	LUT	C21-C26-C27	3.36	116.95	112.70
48	y	601	CHL	C1-C2-C3	-3.36	120.22	126.04
29	G1	613	CLA	C2D-C1D-ND	3.36	112.58	110.10
49	s1	620	LUT	C7-C8-C9	-3.36	121.15	126.23
36	b	620	C7Z	C38-C25-C24	3.36	120.59	114.36
29	B	614	CLA	CHD-C1D-ND	-3.36	121.36	124.45
29	N1	610	CLA	CHD-C1D-ND	-3.36	121.36	124.45
32	b	626	SQD	O7-S-C6	-3.36	102.94	106.94
29	A	407	CLA	C1C-C2C-C3C	-3.36	103.42	106.96
29	d	403	CLA	CMB-C2B-C3B	3.36	130.97	124.68
31	d1	404	BCR	C36-C18-C17	-3.36	118.21	122.92
32	b1	621	SQD	O7-S-C6	-3.36	102.95	106.94
29	c1	512	CLA	CMB-C2B-C3B	3.36	130.96	124.68
29	s	603	CLA	C2C-C1C-NC	3.36	113.12	109.97
29	g	614	CLA	C2C-C1C-NC	3.36	113.12	109.97
29	B	615	CLA	C1-C2-C3	-3.36	120.24	126.04
51	Y	623	NEX	C27-C28-C29	-3.36	120.32	125.53
48	y1	607	CHL	C3C-C4C-NC	-3.36	106.81	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	d	411	LMG	O7-C10-C11	3.36	118.73	111.50
31	d1	404	BCR	C33-C5-C4	3.35	120.06	113.62
52	r	625	LMT	O5B-C1B-C2B	3.35	117.45	110.35
29	c1	506	CLA	CMB-C2B-C1B	-3.35	123.31	128.46
47	k	101	4RF	O21-C22-C24	3.35	118.73	111.50
29	b	603	CLA	C1-C2-C3	-3.35	120.25	126.04
37	c1	520	DGD	O2G-C1B-C2B	3.35	118.72	111.50
29	b	615	CLA	CHD-C1D-ND	-3.35	121.37	124.45
50	R	621	XAT	C38-C25-C24	3.35	118.05	114.28
29	s1	604	CLA	CHD-C1D-ND	-3.35	121.38	124.45
48	Y1	609	CHL	CHD-C1D-ND	-3.35	121.38	124.45
29	n1	610	CLA	C2D-C1D-ND	3.35	112.57	110.10
48	g	607	CHL	CMA-C3A-C4A	3.35	120.77	111.77
51	R1	622	NEX	C39-C29-C30	-3.35	118.23	122.92
29	g1	610	CLA	CMD-C2D-C3D	-3.35	119.92	127.61
29	A	405	CLA	CMB-C2B-C3B	3.35	130.94	124.68
48	y1	601	CHL	C1-O2A-CGA	3.34	125.22	116.44
29	s1	605	CLA	C1-C2-C3	-3.34	121.34	126.75
31	C	517	BCR	C34-C9-C10	-3.34	118.24	122.92
29	c	502	CLA	C2C-C1C-NC	3.34	113.11	109.97
48	y	607	CHL	C2C-C3C-C4C	3.34	108.87	106.49
50	g1	622	XAT	C7-C8-C9	-3.34	120.34	125.53
29	B1	604	CLA	CHD-C1D-ND	-3.34	121.38	124.45
29	C1	508	CLA	CHD-C1D-ND	-3.34	121.38	124.45
43	d1	405	PL9	C7-C8-C9	-3.34	121.23	126.79
29	a	410	CLA	C2C-C1C-NC	3.34	113.10	109.97
47	K1	101	4RF	O21-C22-C24	3.34	118.70	111.50
48	g1	608	CHL	C3C-C4C-NC	-3.34	106.82	110.57
29	n	604	CLA	C2D-C1D-ND	3.34	112.57	110.10
29	n	603	CLA	C1-C2-C3	-3.34	120.27	126.04
49	Y	620	LUT	C10-C11-C12	-3.34	112.79	123.22
29	B1	615	CLA	C2D-C1D-ND	3.34	112.56	110.10
29	N1	613	CLA	C2C-C1C-NC	3.34	113.10	109.97
29	r1	603	CLA	CHD-C1D-ND	-3.34	121.39	124.45
29	d1	403	CLA	C1-C2-C3	-3.34	120.27	126.04
48	g1	606	CHL	C3C-C4C-NC	-3.34	106.83	110.57
29	G	613	CLA	CHD-C1D-ND	-3.34	121.39	124.45
48	Y	605	CHL	C2C-C3C-C4C	3.33	108.87	106.49
31	C	515	BCR	C4-C5-C6	-3.33	117.89	122.73
48	g	601	CHL	C3C-C4C-NC	-3.33	106.83	110.57
29	s1	602	CLA	CHD-C1D-ND	-3.33	121.39	124.45
48	s	608	CHL	C1-C2-C3	-3.33	120.28	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	N	620	LUT	C35-C34-C33	-3.33	122.55	127.31
29	Y1	608	CLA	CMA-C3A-C4A	3.33	120.73	111.77
29	c1	506	CLA	CMB-C2B-C3B	3.33	130.91	124.68
29	R	604	CLA	CHD-C1D-ND	-3.33	121.39	124.45
29	C1	510	CLA	CHD-C1D-ND	-3.33	121.39	124.45
49	g	621	LUT	C15-C14-C13	-3.33	122.56	127.31
49	G	621	LUT	C7-C8-C9	-3.33	121.20	126.23
49	G	620	LUT	C11-C10-C9	-3.33	122.56	127.31
29	B1	615	CLA	CHD-C1D-ND	-3.33	121.40	124.45
45	H1	101	RRX	C37-C22-C23	3.33	123.32	118.08
43	d	405	PL9	C7-C8-C9	-3.32	121.26	126.79
29	N1	602	CLA	CAA-C2A-C3A	-3.32	103.69	112.78
29	C	502	CLA	C1-C2-C3	-3.32	120.30	126.04
29	C	501	CLA	CMA-C3A-C4A	3.32	120.70	111.77
29	Y1	614	CLA	C2C-C1C-NC	3.32	113.08	109.97
48	g1	608	CHL	C2C-C3C-C4C	3.32	108.86	106.49
29	B	613	CLA	CMB-C2B-C3B	3.32	130.89	124.68
31	d	404	BCR	C1-C6-C5	-3.32	117.94	122.61
48	s1	601	CHL	CHD-C1D-ND	-3.32	121.41	124.45
29	a1	407	CLA	C2C-C1C-NC	3.32	113.08	109.97
47	K	101	4RF	O21-C22-C24	3.32	118.65	111.50
49	g1	620	LUT	C15-C14-C13	-3.31	122.58	127.31
48	R	606	CHL	CHB-C4A-NA	3.31	129.09	124.51
49	G	621	LUT	C35-C15-C14	-3.31	116.69	123.47
48	n1	601	CHL	C3C-C4C-NC	-3.31	106.86	110.57
29	g1	612	CLA	CHD-C1D-ND	-3.31	121.41	124.45
29	g	611	CLA	C1-C2-C3	-3.31	120.31	126.04
48	g1	601	CHL	C3C-C4C-NC	-3.31	106.86	110.57
29	B	602	CLA	C2C-C1C-NC	3.31	113.08	109.97
29	N	613	CLA	C2C-C1C-NC	3.31	113.08	109.97
29	Y	611	CLA	C2C-C1C-NC	3.31	113.08	109.97
31	A	411	BCR	C33-C5-C6	-3.31	120.81	124.53
48	G1	605	CHL	C2C-C3C-C4C	3.31	108.85	106.49
33	d	411	LMG	O8-C28-C29	3.31	122.30	111.91
48	n1	607	CHL	CHD-C1D-ND	-3.31	121.41	124.45
29	N	613	CLA	CMA-C3A-C4A	3.31	120.67	111.77
29	S1	609	CLA	CHD-C1D-ND	-3.31	121.41	124.45
49	y1	621	LUT	C35-C15-C14	-3.31	116.70	123.47
47	K	101	4RF	O40-C41-C43	3.31	122.29	111.91
50	g	622	XAT	C38-C25-C26	-3.31	116.72	122.26
29	S1	614	CLA	O2D-CGD-O1D	-3.31	117.37	123.84
29	S	614	CLA	CHD-C1D-ND	-3.31	121.42	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	g1	606	CHL	CHD-C1D-ND	-3.31	121.42	124.45
48	S1	607	CHL	C3C-C4C-NC	-3.31	106.86	110.57
31	A1	411	BCR	C33-C5-C4	3.31	119.97	113.62
29	C1	506	CLA	CHD-C1D-ND	-3.31	121.42	124.45
31	D	404	BCR	C38-C26-C25	-3.31	120.82	124.53
51	S	623	NEX	C27-C28-C29	-3.31	120.40	125.53
48	r	607	CHL	C3C-C4C-NC	-3.31	106.86	110.57
29	s1	609	CLA	C2C-C1C-NC	3.30	113.07	109.97
29	C	513	CLA	C2D-C1D-ND	3.30	112.54	110.10
29	b	613	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
29	S	602	CLA	CAA-C2A-C3A	-3.30	103.73	112.78
29	S	611	CLA	C2C-C1C-NC	3.30	113.07	109.97
29	C	510	CLA	CHD-C1D-ND	-3.30	121.42	124.45
29	y	602	CLA	CHD-C1D-ND	-3.30	121.42	124.45
29	n	612	CLA	C2C-C1C-NC	3.30	113.06	109.97
29	b1	606	CLA	C1-C2-C3	-3.30	120.34	126.04
29	C1	511	CLA	CHD-C1D-ND	-3.30	121.42	124.45
29	b	612	CLA	CHD-C1D-ND	-3.29	121.43	124.45
29	B1	616	CLA	CHD-C1D-ND	-3.29	121.43	124.45
31	C1	516	BCR	C38-C26-C27	3.29	119.94	113.62
29	C1	513	CLA	CMB-C2B-C3B	3.29	130.84	124.68
29	d	403	CLA	CAA-C2A-C3A	-3.29	103.76	112.78
48	G	608	CHL	CMA-C3A-C4A	3.29	120.62	111.77
29	B1	616	CLA	C2C-C1C-NC	3.29	113.06	109.97
29	y1	603	CLA	C2C-C1C-NC	3.29	113.06	109.97
29	b	615	CLA	CMB-C2B-C3B	3.29	130.84	124.68
48	s1	606	CHL	C2C-C3C-C4C	3.29	108.83	106.49
29	g	604	CLA	CHD-C1D-ND	-3.29	121.43	124.45
29	A	407	CLA	C1-C2-C3	-3.29	121.43	126.75
31	d1	404	BCR	C1-C6-C5	-3.29	117.98	122.61
29	b1	614	CLA	OBD-CAD-C3D	-3.29	120.61	128.52
29	r1	612	CLA	CHD-C1D-ND	-3.29	121.43	124.45
31	C1	514	BCR	C36-C18-C17	-3.29	118.32	122.92
29	a1	406	CLA	CMB-C2B-C3B	3.29	130.83	124.68
53	R	626	ERG	C17-C20-C22	-3.29	104.01	110.27
48	g1	605	CHL	CMA-C3A-C4A	3.29	120.61	111.77
29	R	609	CLA	CAA-C2A-C3A	-3.29	103.78	112.78
29	S	605	CLA	O2D-CGD-O1D	-3.29	117.42	123.84
29	n1	614	CLA	C2C-C1C-NC	3.28	113.05	109.97
31	B	619	BCR	C23-C24-C25	-3.28	117.99	127.20
48	G1	605	CHL	C3C-C4C-NC	-3.28	106.89	110.57
29	R1	609	CLA	CAA-C2A-C3A	-3.28	103.80	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	Y	620	LUT	C22-C23-C24	-3.28	108.01	111.74
29	s	617	CLA	CHD-C1D-ND	-3.28	121.44	124.45
29	B1	605	CLA	C2C-C1C-NC	3.28	113.04	109.97
31	a1	411	BCR	C23-C24-C25	-3.28	118.00	127.20
29	B1	606	CLA	CHD-C1D-ND	-3.28	121.44	124.45
29	n	611	CLA	C2C-C1C-NC	3.27	113.04	109.97
50	R	621	XAT	C18-C5-C4	3.27	117.96	114.28
48	y	607	CHL	C3C-C4C-NC	-3.27	106.90	110.57
49	N	620	LUT	C21-C26-C27	3.27	116.84	112.70
29	B	603	CLA	C2C-C1C-NC	3.27	113.04	109.97
49	S	620	LUT	C21-C26-C27	3.27	116.84	112.70
29	n1	602	CLA	C1-C2-C3	-3.27	120.38	126.04
29	G	612	CLA	CHD-C1D-ND	-3.27	121.45	124.45
29	G1	603	CLA	C1-C2-C3	-3.27	120.38	126.04
29	R1	602	CLA	C1-C2-C3	-3.27	120.38	126.04
51	Y	623	NEX	C38-C25-C26	-3.27	116.78	122.26
29	N	610	CLA	C2D-C1D-ND	3.27	112.52	110.10
48	s	607	CHL	C3C-C4C-NC	-3.27	106.90	110.57
48	s	601	CHL	C2C-C3C-C4C	3.27	108.82	106.49
29	Y	608	CLA	CHD-C1D-ND	-3.27	121.45	124.45
29	G1	604	CLA	OBD-CAD-C3D	-3.27	120.65	128.52
40	S1	624	LHG	C5-O7-C7	-3.27	109.74	117.79
29	Y	603	CLA	C1-C2-C3	-3.27	120.39	126.04
29	B	609	CLA	C2D-C1D-ND	3.27	112.51	110.10
29	c	509	CLA	CMB-C2B-C3B	3.27	130.79	124.68
49	G1	620	LUT	C35-C34-C33	-3.27	122.64	127.31
49	N1	621	LUT	C7-C8-C9	-3.27	121.30	126.23
29	Y	602	CLA	C1C-C2C-C3C	-3.27	103.52	106.96
50	n1	622	XAT	C18-C5-C6	-3.27	116.78	122.26
31	c	515	BCR	C23-C24-C25	-3.27	118.02	127.20
29	b	603	CLA	CHD-C1D-ND	-3.27	121.45	124.45
29	G1	614	CLA	C2C-C1C-NC	3.27	113.03	109.97
29	Y	610	CLA	CAA-C2A-C3A	-3.27	103.83	112.78
29	B1	604	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
29	D1	403	CLA	CHD-C1D-ND	-3.27	121.45	124.45
29	y1	611	CLA	CMA-C3A-C4A	3.26	120.55	111.77
29	G1	613	CLA	CHD-C1D-ND	-3.26	121.45	124.45
29	d1	403	CLA	CHD-C1D-ND	-3.26	121.45	124.45
48	G1	607	CHL	CHD-C1D-ND	-3.26	121.45	124.45
29	a1	406	CLA	C2C-C1C-NC	3.26	113.03	109.97
48	Y1	609	CHL	C1-C2-C3	-3.26	120.40	126.04
40	D1	409	LHG	C5-O7-C7	-3.26	109.76	117.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	C1	526	SQD	O7-S-C6	-3.26	103.06	106.94
29	R1	608	CLA	C2C-C1C-NC	3.26	113.03	109.97
29	r1	610	CLA	C1-C2-C3	-3.26	120.40	126.04
48	s1	607	CHL	C4A-NA-C1A	3.26	108.17	106.71
36	b	620	C7Z	C1-C6-C5	-3.26	118.02	122.61
50	R	621	XAT	C7-C8-C9	-3.26	120.47	125.53
29	G	614	CLA	CMB-C2B-C3B	3.26	130.78	124.68
48	g	608	CHL	CHD-C1D-ND	-3.26	121.46	124.45
49	R	620	LUT	C15-C14-C13	-3.26	122.66	127.31
48	N	605	CHL	C2C-C3C-C4C	3.26	108.81	106.49
29	r	610	CLA	CHD-C1D-ND	-3.26	121.46	124.45
31	B1	618	BCR	C33-C5-C6	-3.26	120.87	124.53
49	S1	620	LUT	C35-C34-C33	-3.26	122.66	127.31
29	N1	603	CLA	CMA-C3A-C4A	3.26	120.53	111.77
29	y	610	CLA	C1-C2-C3	-3.26	120.41	126.04
29	s	604	CLA	CHD-C1D-ND	-3.26	121.46	124.45
29	R1	610	CLA	CHD-C1D-ND	-3.26	121.46	124.45
29	y	610	CLA	C2D-C1D-ND	3.26	112.50	110.10
45	h	101	RRX	C15-C16-C17	-3.26	116.80	123.47
51	G	623	NEX	O24-C25-C38	-3.26	111.15	115.06
29	r1	604	CLA	C2D-C1D-ND	3.26	112.50	110.10
29	c	505	CLA	C1-C2-C3	-3.25	120.41	126.04
29	G	604	CLA	C2C-C1C-NC	3.25	113.02	109.97
53	r1	626	ERG	C18-C13-C12	-3.25	105.45	110.59
31	C1	516	BCR	C35-C13-C14	-3.25	118.36	122.92
48	s1	601	CHL	CMA-C3A-C4A	3.25	120.52	111.77
50	G	622	XAT	C7-C8-C9	-3.25	120.48	125.53
31	A	411	BCR	C23-C24-C25	-3.25	118.07	127.20
49	g1	621	LUT	C31-C32-C33	-3.25	117.28	126.42
29	C	507	CLA	C1C-C2C-C3C	-3.25	103.54	106.96
30	a	409	PHO	O2D-CGD-O1D	-3.25	117.48	123.84
45	h1	101	RRX	C30-C25-C26	-3.25	118.04	122.61
29	s	603	CLA	C1-C2-C3	-3.25	120.42	126.04
29	b	615	CLA	O2D-CGD-O1D	-3.25	117.49	123.84
29	B	613	CLA	C2C-C1C-NC	3.25	113.02	109.97
29	a	410	CLA	CHD-C1D-ND	-3.25	121.47	124.45
51	n1	623	NEX	C40-C33-C34	-3.25	118.37	122.92
29	Y	614	CLA	CHD-C1D-ND	-3.24	121.47	124.45
51	s1	623	NEX	C31-C30-C29	3.24	131.94	127.31
50	R1	621	XAT	O4-C5-C4	-3.24	110.94	113.38
29	G1	612	CLA	C2C-C1C-NC	3.24	113.01	109.97
29	s1	611	CLA	C2C-C1C-NC	3.24	113.01	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Y1	610	CLA	CMA-C3A-C4A	3.24	120.49	111.77
29	c1	507	CLA	CHD-C1D-ND	-3.24	121.47	124.45
48	r1	607	CHL	C1B-CHB-C4A	-3.24	123.70	130.12
29	g1	613	CLA	C2C-C1C-NC	3.24	113.01	109.97
29	n	604	CLA	C1-C2-C3	-3.24	120.44	126.04
29	A1	405	CLA	CHD-C1D-ND	-3.24	121.48	124.45
48	N1	609	CHL	CHD-C4C-C3C	3.24	129.60	124.84
50	g	622	XAT	C19-C9-C10	-3.24	118.38	122.92
29	Y	613	CLA	C2C-C1C-NC	3.24	113.01	109.97
29	S1	612	CLA	O2D-CGD-O1D	-3.24	117.50	123.84
29	A1	410	CLA	C2D-C1D-ND	3.24	112.49	110.10
29	n1	613	CLA	C2C-C1C-NC	3.24	113.01	109.97
48	n1	606	CHL	C2C-C3C-C4C	3.24	108.80	106.49
29	y1	612	CLA	C2D-C1D-ND	3.24	112.49	110.10
48	G	605	CHL	CHB-C4A-NA	3.24	128.99	124.51
48	N	609	CHL	CHD-C1D-ND	-3.24	121.48	124.45
29	C	503	CLA	C1-C2-C3	-3.24	120.44	126.04
49	S	621	LUT	C10-C11-C12	-3.24	113.12	123.22
29	C	503	CLA	CMA-C3A-C4A	3.24	120.47	111.77
48	N	606	CHL	CHD-C1D-ND	-3.24	121.48	124.45
49	n	620	LUT	C21-C26-C27	3.23	116.79	112.70
49	G	621	LUT	C35-C34-C33	-3.23	122.69	127.31
48	r	606	CHL	C4A-NA-C1A	3.23	108.16	106.71
29	r	602	CLA	CHD-C1D-ND	-3.23	121.48	124.45
48	N1	608	CHL	CMA-C3A-C4A	3.23	120.47	111.77
30	a1	409	PHO	CMC-C2C-C3C	3.23	131.04	124.94
29	G	602	CLA	CMA-C3A-C4A	3.23	120.46	111.77
29	B1	617	CLA	C1-C2-C3	-3.23	120.45	126.04
29	C	504	CLA	CHD-C1D-ND	-3.23	121.48	124.45
29	N	610	CLA	CHD-C1D-ND	-3.23	121.48	124.45
29	g	611	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
29	C1	507	CLA	C2C-C1C-NC	3.23	113.00	109.97
29	b	605	CLA	C1-C2-C3	-3.23	120.45	126.04
49	Y	620	LUT	C35-C34-C33	-3.23	122.70	127.31
50	r1	621	XAT	C18-C5-C6	-3.23	116.85	122.26
29	n1	612	CLA	C2C-C1C-NC	3.23	113.00	109.97
29	B1	611	CLA	O2D-CGD-O1D	-3.23	117.53	123.84
29	a	410	CLA	C1C-C2C-C3C	-3.23	103.56	106.96
29	Y	602	CLA	CHD-C1D-ND	-3.23	121.49	124.45
44	f	101	HEM	CMC-C2C-C3C	3.23	130.71	124.68
29	a1	405	CLA	C2D-C1D-ND	3.23	112.48	110.10
48	g1	601	CHL	CMA-C3A-C4A	3.23	120.44	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B1	606	CLA	C2C-C1C-NC	3.22	112.99	109.97
29	S1	605	CLA	CMA-C3A-C4A	3.22	120.44	111.77
50	Y1	622	XAT	C40-C33-C34	-3.22	118.41	122.92
48	n	607	CHL	C3C-C4C-NC	-3.22	106.96	110.57
29	R1	602	CLA	C2C-C1C-NC	3.22	112.99	109.97
29	c1	512	CLA	C2C-C1C-NC	3.22	112.99	109.97
29	r1	609	CLA	CMA-C3A-C4A	3.22	120.43	111.77
48	N1	609	CHL	C1-O2A-CGA	3.22	124.89	116.44
49	Y	620	LUT	C15-C14-C13	-3.22	122.71	127.31
29	s1	603	CLA	CMA-C3A-C4A	3.22	120.43	111.77
29	C1	512	CLA	C1-C2-C3	-3.22	120.47	126.04
49	n1	620	LUT	C7-C8-C9	-3.22	121.37	126.23
29	A	407	CLA	C1-O2A-CGA	3.22	124.89	116.44
29	Y1	612	CLA	C2C-C1C-NC	3.22	112.99	109.97
51	n	623	NEX	C27-C28-C29	-3.22	120.54	125.53
48	g1	609	CHL	C3C-C4C-NC	-3.22	106.96	110.57
49	N	620	LUT	C7-C8-C9	-3.22	121.37	126.23
29	B1	616	CLA	C1-C2-C3	-3.22	120.48	126.04
29	r1	610	CLA	C2D-C1D-ND	3.22	112.47	110.10
29	S1	613	CLA	CHD-C1D-ND	-3.22	121.50	124.45
48	y	606	CHL	C3C-C4C-NC	-3.22	106.97	110.57
29	Y	614	CLA	CMA-C3A-C4A	3.22	120.41	111.77
29	a	406	CLA	CMB-C2B-C3B	3.21	130.69	124.68
48	n1	607	CHL	C3C-C4C-NC	-3.21	106.97	110.57
49	N1	621	LUT	C35-C34-C33	-3.21	122.72	127.31
49	Y1	621	LUT	C30-C31-C32	-3.21	113.19	123.22
51	s1	623	NEX	C39-C29-C30	-3.21	118.42	122.92
29	s1	617	CLA	CMB-C2B-C3B	3.21	130.69	124.68
48	N1	601	CHL	C1B-CHB-C4A	-3.21	123.76	130.12
42	D	401	BCT	O2-C-O1	-3.21	111.22	119.55
29	c1	507	CLA	C2C-C1C-NC	3.21	112.98	109.97
29	y	604	CLA	C1-C2-C3	-3.21	120.49	126.04
48	Y1	606	CHL	C3C-C4C-NC	-3.21	106.97	110.57
51	N	623	NEX	C5-C4-C3	3.21	115.55	111.75
48	G	605	CHL	C2C-C3C-C4C	3.21	108.78	106.49
29	s1	603	CLA	C2D-C1D-ND	3.21	112.47	110.10
45	H	101	RRX	C8-C7-C6	-3.21	118.19	127.20
29	y1	604	CLA	C2C-C1C-NC	3.21	112.98	109.97
53	R1	626	ERG	C13-C17-C20	-3.21	115.29	119.43
29	Y	613	CLA	CMA-C3A-C4A	3.21	120.39	111.77
29	C	512	CLA	C2D-C1D-ND	3.21	112.47	110.10
31	b	618	BCR	C15-C14-C13	-3.20	122.74	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	N	613	CLA	C1-C2-C3	-3.20	120.50	126.04
29	S1	602	CLA	O2A-CGA-CBA	3.20	121.96	111.91
33	D1	411	LMG	O8-C28-C29	3.20	121.96	111.91
29	A	406	CLA	CMB-C2B-C3B	3.20	130.67	124.68
48	Y1	605	CHL	C2C-C3C-C4C	3.20	108.77	106.49
48	Y1	609	CHL	C2C-C3C-C4C	3.20	108.77	106.49
29	C	505	CLA	CHD-C1D-ND	-3.20	121.51	124.45
33	W1	201	LMG	O8-C28-C29	3.20	121.95	111.91
31	c	514	BCR	C38-C26-C25	-3.20	120.93	124.53
29	c1	504	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
51	N	623	NEX	C39-C29-C30	-3.20	118.44	122.92
29	n	602	CLA	C1C-C2C-C3C	-3.20	103.59	106.96
29	B	612	CLA	CMB-C2B-C1B	-3.20	123.55	128.46
45	H1	101	RRX	C33-C5-C6	-3.20	120.94	124.53
29	S	614	CLA	C1-C2-C3	-3.20	120.51	126.04
48	y	601	CHL	C3C-C4C-NC	-3.20	106.98	110.57
29	n	610	CLA	C2D-C1D-ND	3.20	112.46	110.10
51	s1	623	NEX	O24-C25-C38	-3.20	111.22	115.06
29	s1	602	CLA	O1D-CGD-CBD	-3.20	117.94	124.48
29	a	405	CLA	C1-O2A-CGA	3.20	124.83	116.44
31	d1	404	BCR	C19-C18-C17	3.20	123.85	118.94
29	g1	613	CLA	CHD-C1D-ND	-3.20	121.52	124.45
29	Y	612	CLA	C2C-C1C-NC	3.20	112.97	109.97
29	S1	605	CLA	C2C-C1C-NC	3.20	112.97	109.97
29	G1	610	CLA	O2A-CGA-CBA	3.20	121.94	111.91
34	A1	414	SPH	C3-C4-C5	-3.20	117.66	124.79
29	B	614	CLA	C1-C2-C3	-3.20	120.52	126.04
48	s1	607	CHL	C3C-C4C-NC	-3.19	106.99	110.57
29	s	609	CLA	C2C-C1C-NC	3.19	112.97	109.97
29	g1	602	CLA	CHD-C1D-ND	-3.19	121.52	124.45
29	B1	608	CLA	CMA-C3A-C4A	3.19	120.36	111.77
40	n1	624	LHG	C5-O7-C7	-3.19	109.93	117.79
29	S1	613	CLA	C1-C2-C3	-3.19	120.52	126.04
31	C1	517	BCR	C36-C18-C17	-3.19	118.45	122.92
36	b1	620	C7Z	C31-C30-C29	-3.19	122.75	127.31
43	D	405	PL9	C7-C8-C9	-3.19	121.48	126.79
48	s1	606	CHL	C3C-C4C-NC	-3.19	106.99	110.57
29	B	606	CLA	C2C-C1C-NC	3.19	112.96	109.97
51	N1	623	NEX	C39-C29-C30	-3.19	118.45	122.92
49	n1	621	LUT	C35-C15-C14	-3.19	116.94	123.47
31	B1	618	BCR	C19-C18-C17	3.19	123.84	118.94
29	n	613	CLA	C2C-C1C-NC	3.19	112.96	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	610	CLA	C2D-C1D-ND	3.19	112.46	110.10
48	Y	609	CHL	C3C-C4C-NC	-3.19	106.99	110.57
50	G1	622	XAT	O24-C25-C24	3.19	115.78	113.38
29	Y1	613	CLA	C1-C2-C3	-3.19	120.53	126.04
29	r1	602	CLA	CHD-C1D-ND	-3.19	121.52	124.45
51	s	623	NEX	C39-C29-C30	-3.19	118.45	122.92
29	S1	614	CLA	C2D-C1D-ND	3.19	112.45	110.10
48	y	606	CHL	C2C-C3C-C4C	3.19	108.76	106.49
49	S	621	LUT	C18-C5-C6	-3.19	120.95	124.53
48	g	608	CHL	CMA-C3A-C4A	3.19	120.35	111.77
50	n1	622	XAT	O24-C25-C24	3.19	115.78	113.38
29	s1	603	CLA	C2C-C1C-NC	3.19	112.96	109.97
29	y1	602	CLA	C1-C2-C3	-3.19	120.53	126.04
48	N1	609	CHL	C1B-CHB-C4A	-3.19	123.80	130.12
29	B1	614	CLA	CMD-C2D-C3D	-3.19	120.28	127.61
48	g1	607	CHL	CHB-C4A-NA	3.19	128.92	124.51
49	G1	620	LUT	C22-C23-C24	-3.19	108.11	111.74
52	r	625	LMT	C3B-C4B-C5B	-3.19	104.56	110.24
48	n1	607	CHL	C1-O2A-CGA	3.18	124.80	116.44
31	b	618	BCR	C4-C5-C6	-3.18	118.11	122.73
43	D	405	PL9	C7-C3-C2	-3.18	119.11	123.30
48	g	607	CHL	C1-C2-C3	-3.18	120.54	126.04
29	s1	602	CLA	O2D-CGD-O1D	-3.18	117.61	123.84
29	C	504	CLA	C1-O2A-CGA	3.18	124.80	116.44
29	C1	509	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
29	S	617	CLA	C1-O2A-CGA	3.18	124.79	116.44
48	y1	609	CHL	C1B-CHB-C4A	-3.18	123.81	130.12
29	B	608	CLA	C2D-C1D-ND	3.18	112.45	110.10
29	S	610	CLA	C2D-C1D-ND	3.18	112.45	110.10
29	D1	402	CLA	CHD-C1D-ND	-3.18	121.53	124.45
29	N1	612	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
29	s	614	CLA	CHD-C1D-ND	-3.18	121.53	124.45
29	c	510	CLA	C2C-C1C-NC	3.18	112.95	109.97
49	S1	620	LUT	C22-C23-C24	-3.18	108.12	111.74
29	B1	609	CLA	C1C-C2C-C3C	-3.18	103.61	106.96
29	G	603	CLA	C2D-C1D-ND	3.18	112.45	110.10
29	Y1	603	CLA	C2C-C1C-NC	3.18	112.95	109.97
29	N1	602	CLA	C2D-C1D-ND	3.18	112.44	110.10
29	R1	604	CLA	CHD-C1D-ND	-3.18	121.53	124.45
29	B1	615	CLA	C2C-C1C-NC	3.17	112.95	109.97
29	c	509	CLA	C2C-C1C-NC	3.17	112.94	109.97
51	N	623	NEX	C31-C30-C29	3.17	131.83	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	N1	607	CHL	C3C-C4C-NC	-3.17	107.02	110.57
29	R1	612	CLA	C1-C2-C3	-3.17	120.56	126.04
29	c1	511	CLA	CMA-C3A-C4A	3.17	120.29	111.77
29	b	603	CLA	C2C-C1C-NC	3.17	112.94	109.97
29	D	402	CLA	CHD-C1D-ND	-3.17	121.54	124.45
29	N	612	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
31	D1	404	BCR	C19-C18-C17	3.17	123.80	118.94
29	c	511	CLA	CMA-C3A-C4A	3.17	120.28	111.77
29	n1	611	CLA	C2D-C1D-ND	3.17	112.44	110.10
29	n	611	CLA	CHD-C1D-ND	-3.17	121.55	124.45
29	r	602	CLA	C6-C5-C3	-3.17	105.16	113.45
29	S1	602	CLA	C2D-C1D-ND	3.16	112.44	110.10
29	c	510	CLA	CHD-C1D-ND	-3.16	121.55	124.45
29	N1	613	CLA	C2D-C1D-ND	3.16	112.44	110.10
29	n1	603	CLA	C1C-C2C-C3C	-3.16	103.63	106.96
29	R	612	CLA	C2C-C1C-NC	3.16	112.94	109.97
48	s1	608	CHL	C1B-CHB-C4A	-3.16	123.85	130.12
51	R1	622	NEX	C17-C1-C6	-3.16	107.64	110.47
48	R	607	CHL	C2C-C3C-C4C	3.16	108.74	106.49
29	B1	602	CLA	CMA-C3A-C4A	3.16	120.27	111.77
49	y	621	LUT	C38-C25-C24	-3.16	116.80	123.56
48	Y	601	CHL	CMA-C3A-C4A	3.16	120.27	111.77
29	s	610	CLA	CHD-C1D-ND	-3.16	121.55	124.45
29	B	602	CLA	C1C-C2C-C3C	-3.16	103.63	106.96
29	B1	612	CLA	CHD-C1D-ND	-3.16	121.55	124.45
29	d	403	CLA	CMA-C3A-C4A	3.16	120.26	111.77
48	r1	606	CHL	CHB-C4A-NA	3.16	128.88	124.51
29	B	610	CLA	C2C-C1C-NC	3.16	112.93	109.97
34	y1	625	SPH	C3-C4-C5	-3.16	117.75	124.79
29	C	503	CLA	CHD-C1D-ND	-3.16	121.55	124.45
29	S1	617	CLA	CHD-C1D-ND	-3.16	121.55	124.45
29	c	505	CLA	C2C-C1C-NC	3.16	112.93	109.97
29	R1	610	CLA	C1D-ND-C4D	-3.16	104.09	106.33
48	g	606	CHL	C3C-C4C-NC	-3.16	107.03	110.57
31	C	515	BCR	C8-C7-C6	-3.16	118.33	127.20
31	D	404	BCR	C19-C18-C17	3.16	123.78	118.94
29	S1	603	CLA	C2C-C1C-NC	3.16	112.93	109.97
49	N1	620	LUT	C18-C5-C6	-3.16	120.98	124.53
48	Y1	606	CHL	CHD-C1D-ND	-3.16	121.55	124.45
50	G	622	XAT	C26-C27-C28	-3.16	119.32	125.99
29	c1	506	CLA	C2C-C1C-NC	3.16	112.93	109.97
50	N	622	XAT	C38-C25-C26	-3.15	116.97	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	s1	614	CLA	CHD-C1D-ND	-3.15	121.56	124.45
48	s	606	CHL	CHB-C4A-NA	3.15	128.87	124.51
29	b1	615	CLA	CHD-C1D-ND	-3.15	121.56	124.45
29	d	403	CLA	C2C-C1C-NC	3.15	112.92	109.97
29	R1	604	CLA	C2C-C1C-NC	3.15	112.92	109.97
29	c	512	CLA	C2C-C1C-NC	3.15	112.92	109.97
29	y1	611	CLA	C2C-C1C-NC	3.15	112.92	109.97
29	b1	602	CLA	C2D-C1D-ND	3.15	112.43	110.10
48	s	607	CHL	CMA-C3A-C4A	3.15	120.24	111.77
29	c1	506	CLA	CHD-C1D-ND	-3.15	121.56	124.45
29	c1	506	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
29	y	613	CLA	C2C-C1C-NC	3.15	112.92	109.97
29	n	610	CLA	O2A-CGA-CBA	3.15	121.79	111.91
48	G1	607	CHL	CMA-C3A-C4A	3.15	120.24	111.77
29	S1	604	CLA	CHD-C1D-ND	-3.15	121.56	124.45
29	R	610	CLA	CMA-C3A-C4A	3.15	120.23	111.77
48	s	607	CHL	CHB-C4A-NA	3.15	128.86	124.51
29	c	513	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
29	R	610	CLA	CMC-C2C-C1C	3.15	129.83	125.04
29	B	612	CLA	CHD-C1D-ND	-3.15	121.56	124.45
48	G	601	CHL	CHD-C1D-ND	-3.15	121.56	124.45
29	B1	605	CLA	CMA-C3A-C4A	3.15	120.23	111.77
53	R	626	ERG	C1-C10-C5	3.15	114.51	108.75
29	S1	612	CLA	CMB-C2B-C3B	3.15	130.56	124.68
29	r	609	CLA	C1-C2-C3	-3.15	120.60	126.04
29	A	405	CLA	CAC-C3C-C4C	3.15	128.89	124.81
29	n1	610	CLA	CMA-C3A-C4A	3.15	120.23	111.77
29	C	513	CLA	O2D-CGD-O1D	-3.15	117.69	123.84
29	s1	604	CLA	CMB-C2B-C3B	3.14	130.56	124.68
29	B1	605	CLA	CHD-C1D-ND	-3.14	121.56	124.45
29	r1	609	CLA	C2C-C1C-NC	3.14	112.92	109.97
29	a	407	CLA	O1D-CGD-CBD	-3.14	118.05	124.48
49	g	620	LUT	C31-C32-C33	-3.14	117.58	126.42
48	s	601	CHL	CHB-C4A-NA	3.14	128.86	124.51
29	y	614	CLA	C2D-C1D-ND	3.14	112.42	110.10
29	y1	613	CLA	C2D-C1D-ND	3.14	112.42	110.10
29	S	617	CLA	CHD-C1D-ND	-3.14	121.56	124.45
29	n1	613	CLA	CHD-C1D-ND	-3.14	121.56	124.45
29	r	602	CLA	CMA-C3A-C4A	3.14	120.22	111.77
48	Y1	607	CHL	C1-O2A-CGA	3.14	124.69	116.44
31	C	517	BCR	C37-C22-C21	-3.14	118.52	122.92
31	d	404	BCR	C34-C9-C10	-3.14	118.52	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	n1	602	CLA	C1D-ND-C4D	-3.14	104.10	106.33
49	S	620	LUT	C30-C31-C32	-3.14	113.42	123.22
49	g1	621	LUT	C35-C15-C14	-3.14	117.05	123.47
29	N	604	CLA	CHD-C1D-ND	-3.14	121.57	124.45
48	y1	607	CHL	C2C-C3C-C4C	3.14	108.73	106.49
49	g	620	LUT	C15-C35-C34	-3.14	117.05	123.47
42	d	401	BCT	O2-C-O1	-3.14	111.41	119.55
48	G	609	CHL	CMA-C3A-C4A	3.14	120.20	111.77
40	l	101	LHG	O8-C23-C24	3.14	121.75	111.91
29	Y1	603	CLA	C1-C2-C3	-3.14	120.62	126.04
29	B1	607	CLA	CMD-C2D-C3D	-3.14	120.40	127.61
48	g1	601	CHL	C4D-CHA-C1A	3.13	125.06	121.25
48	G	601	CHL	C2C-C3C-C4C	3.13	108.72	106.49
49	g1	620	LUT	C31-C32-C33	-3.13	117.62	126.42
33	a1	413	LMG	C8-O7-C10	-3.13	110.08	117.79
50	N1	622	XAT	C28-C29-C30	3.13	123.75	118.94
29	r1	603	CLA	C1-C2-C3	-3.13	120.63	126.04
29	b	606	CLA	C2C-C1C-NC	3.13	112.91	109.97
29	b	616	CLA	C2D-C1D-ND	3.13	112.41	110.10
31	c	515	BCR	C33-C5-C6	-3.13	121.01	124.53
29	B	615	CLA	O2D-CGD-O1D	-3.13	117.72	123.84
29	g	612	CLA	CMA-C3A-C4A	3.13	120.18	111.77
48	S1	606	CHL	C3C-C4C-NC	-3.13	107.06	110.57
49	N1	620	LUT	C38-C25-C24	-3.13	116.86	123.56
29	B1	602	CLA	C1C-C2C-C3C	-3.13	103.67	106.96
29	y	603	CLA	CHD-C1D-ND	-3.13	121.58	124.45
51	r1	622	NEX	C5-C6-C1	3.13	122.80	119.70
29	g1	612	CLA	C2D-C1D-ND	3.13	112.41	110.10
29	A1	410	CLA	C2C-C1C-NC	3.13	112.90	109.97
29	C	510	CLA	C1C-C2C-C3C	-3.13	103.67	106.96
29	A1	406	CLA	CMA-C3A-C4A	3.13	120.17	111.77
29	a	407	CLA	O2D-CGD-O1D	-3.13	117.73	123.84
29	G	613	CLA	CMA-C3A-C4A	3.12	120.17	111.77
49	S1	620	LUT	C18-C5-C6	-3.12	121.02	124.53
51	n1	623	NEX	C20-C13-C14	-3.12	118.55	122.92
29	B1	604	CLA	CMB-C2B-C3B	3.12	130.52	124.68
48	n	607	CHL	CHB-C4A-NA	3.12	128.83	124.51
48	s1	606	CHL	CHB-C4A-NA	3.12	128.83	124.51
29	B	612	CLA	CMB-C2B-C3B	3.12	130.52	124.68
48	N	601	CHL	CMA-C3A-C4A	3.12	120.17	111.77
48	N1	605	CHL	C1B-CHB-C4A	-3.12	123.94	130.12
53	R1	626	ERG	C7-C6-C5	-3.12	117.72	123.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B1	617	CLA	CMA-C3A-C4A	3.12	120.16	111.77
29	s1	613	CLA	CMA-C3A-C4A	3.12	120.16	111.77
49	r	620	LUT	C22-C23-C24	-3.12	108.19	111.74
31	A1	411	BCR	C23-C24-C25	-3.12	118.44	127.20
48	g	606	CHL	C1B-CHB-C4A	-3.12	123.94	130.12
45	h1	101	RRX	C36-C18-C19	3.12	122.99	118.08
49	G1	620	LUT	C31-C30-C29	-3.12	122.86	127.31
48	N1	606	CHL	C2C-C3C-C4C	3.12	108.71	106.49
29	b1	611	CLA	C1C-C2C-C3C	-3.12	103.68	106.96
29	A1	410	CLA	CMA-C3A-C4A	3.12	120.15	111.77
48	Y1	609	CHL	C3C-C4C-NC	-3.12	107.08	110.57
48	Y1	605	CHL	C3C-C4C-NC	-3.12	107.08	110.57
48	y1	605	CHL	C3C-C4C-NC	-3.12	107.08	110.57
51	g1	623	NEX	C17-C1-C6	-3.12	107.68	110.47
33	c1	521	LMG	O8-C28-C29	3.11	121.68	111.91
29	D1	403	CLA	CMB-C2B-C1B	-3.11	123.68	128.46
29	G	614	CLA	CMA-C3A-C4A	3.11	120.14	111.77
29	N1	604	CLA	CHD-C1D-ND	-3.11	121.59	124.45
29	y	613	CLA	CMA-C3A-C4A	3.11	120.14	111.77
31	a	411	BCR	C23-C24-C25	-3.11	118.46	127.20
29	c	509	CLA	CHD-C1D-ND	-3.11	121.59	124.45
31	C	515	BCR	C33-C5-C6	-3.11	121.03	124.53
29	c1	509	CLA	C2C-C1C-NC	3.11	112.89	109.97
45	h	101	RRX	C4-C5-C6	-3.11	118.22	122.73
29	B1	613	CLA	CMD-C2D-C3D	-3.11	120.46	127.61
29	y	604	CLA	C2D-C1D-ND	3.11	112.40	110.10
29	y1	604	CLA	CMA-C3A-C4A	3.11	120.13	111.77
48	R	607	CHL	CMA-C3A-C4A	3.11	120.13	111.77
31	d	404	BCR	C38-C26-C25	-3.11	121.04	124.53
29	n	614	CLA	C2D-C1D-ND	3.11	112.39	110.10
29	B1	614	CLA	CHD-C1D-ND	-3.11	121.60	124.45
29	c	502	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
29	b1	611	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
29	a1	405	CLA	C2C-C1C-NC	3.11	112.88	109.97
29	n1	613	CLA	C1-C2-C3	-3.11	120.67	126.04
48	R1	606	CHL	CHB-C4A-NA	3.11	128.81	124.51
31	B1	618	BCR	C38-C26-C25	-3.11	121.04	124.53
48	s1	607	CHL	CHB-C4A-NA	3.11	128.81	124.51
51	y1	623	NEX	C20-C13-C14	-3.10	118.57	122.92
49	S	620	LUT	C35-C15-C14	-3.10	117.11	123.47
48	S1	601	CHL	CMA-C3A-C4A	3.10	120.12	111.77
29	y	611	CLA	C1-C2-C3	-3.10	120.67	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	r1	604	CLA	C2C-C1C-NC	3.10	112.88	109.97
29	B	609	CLA	O1D-CGD-CBD	-3.10	118.14	124.48
49	n	620	LUT	C18-C5-C6	-3.10	121.04	124.53
29	S	604	CLA	C2D-C1D-ND	3.10	112.39	110.10
29	s	605	CLA	C1-C2-C3	-3.10	121.73	126.75
29	Y	610	CLA	CHD-C1D-ND	-3.10	121.60	124.45
29	G1	603	CLA	C1C-C2C-C3C	-3.10	103.70	106.96
29	R	608	CLA	C1-O2A-CGA	3.10	124.58	116.44
29	B1	611	CLA	C1C-C2C-C3C	-3.10	103.70	106.96
29	G	614	CLA	CHD-C1D-ND	-3.10	121.61	124.45
29	G1	610	CLA	CHD-C1D-ND	-3.10	121.61	124.45
29	y	608	CLA	CMA-C3A-C4A	3.10	120.10	111.77
47	I1	102	4RF	O18-C16-C15	3.10	121.64	111.91
29	S	612	CLA	CMB-C2B-C3B	3.10	130.48	124.68
29	N	602	CLA	CMA-C3A-C4A	3.10	120.10	111.77
29	b	617	CLA	C1-C2-C3	-3.10	120.68	126.04
29	C1	502	CLA	C2C-C1C-NC	3.10	112.88	109.97
48	S	607	CHL	CHD-C1D-ND	-3.10	121.61	124.45
48	S	608	CHL	C3C-C4C-NC	-3.10	107.10	110.57
29	C	501	CLA	C2C-C1C-NC	3.10	112.87	109.97
29	b1	603	CLA	C2D-C1D-ND	3.10	112.39	110.10
31	C1	516	BCR	C28-C27-C26	-3.10	108.55	114.08
29	A1	405	CLA	C1-C2-C3	-3.10	120.69	126.04
29	s1	617	CLA	C2C-C1C-NC	3.10	112.87	109.97
29	n	602	CLA	CMC-C2C-C1C	3.10	129.75	125.04
29	c1	508	CLA	CMB-C2B-C3B	3.10	130.47	124.68
48	G	608	CHL	CHD-C1D-ND	-3.09	121.61	124.45
49	s	621	LUT	C38-C25-C24	-3.09	116.94	123.56
29	c1	504	CLA	CHD-C1D-ND	-3.09	121.61	124.45
48	S1	608	CHL	CHD-C1D-ND	-3.09	121.61	124.45
45	h1	101	RRX	C19-C18-C17	-3.09	114.20	118.94
48	G1	606	CHL	C1-O2A-CGA	3.09	124.56	116.44
29	b	610	CLA	CHD-C1D-ND	-3.09	121.61	124.45
29	A	410	CLA	CHD-C1D-ND	-3.09	121.61	124.45
29	s1	617	CLA	CMA-C3A-C4A	3.09	120.08	111.77
31	C1	514	BCR	C15-C14-C13	-3.09	122.90	127.31
29	R	612	CLA	CHD-C1D-ND	-3.09	121.61	124.45
50	N	622	XAT	C6-C7-C8	-3.09	119.46	125.99
29	s	603	CLA	CMA-C3A-C4A	3.09	120.07	111.77
29	N	610	CLA	C1-C2-C3	-3.09	120.70	126.04
48	n	601	CHL	CMA-C3A-C4A	3.09	120.07	111.77
50	R1	621	XAT	C38-C25-C26	-3.09	117.08	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S1	621	LUT	C15-C14-C13	-3.09	122.90	127.31
29	N1	603	CLA	C1-O2A-CGA	3.09	124.54	116.44
31	a1	411	BCR	C8-C7-C6	-3.09	118.53	127.20
33	c	521	LMG	O8-C28-C29	3.09	121.59	111.91
29	y	612	CLA	CHD-C1D-ND	-3.09	121.62	124.45
29	R1	608	CLA	CHD-C1D-ND	-3.09	121.62	124.45
48	Y	609	CHL	C1-C2-C3	-3.09	120.71	126.04
48	s	607	CHL	C4A-NA-C1A	3.09	108.09	106.71
29	A	406	CLA	CHD-C1D-ND	-3.08	121.62	124.45
50	N1	622	XAT	O24-C25-C24	3.08	115.70	113.38
31	b1	619	BCR	C33-C5-C4	3.08	119.54	113.62
29	a1	406	CLA	CHD-C1D-ND	-3.08	121.62	124.45
51	n	623	NEX	C26-C27-C28	-3.08	119.47	125.99
29	d	403	CLA	CMB-C2B-C1B	-3.08	123.73	128.46
29	C	511	CLA	CHD-C1D-ND	-3.08	121.62	124.45
29	g1	614	CLA	CHD-C1D-ND	-3.08	121.62	124.45
29	B	614	CLA	C1C-C2C-C3C	-3.08	103.72	106.96
48	y	605	CHL	C2C-C3C-C4C	3.08	108.69	106.49
29	D	402	CLA	C1D-ND-C4D	-3.08	104.15	106.33
29	B	609	CLA	C2C-C1C-NC	3.08	112.86	109.97
29	Y	610	CLA	O2A-CGA-CBA	3.08	121.57	111.91
30	A	409	PHO	O2D-CGD-O1D	-3.08	117.82	123.84
29	G1	610	CLA	CMA-C3A-C4A	3.08	120.05	111.77
29	C	505	CLA	C2C-C1C-NC	3.08	112.86	109.97
29	b1	609	CLA	C2C-C1C-NC	3.08	112.86	109.97
29	G	611	CLA	CHD-C1D-ND	-3.08	121.63	124.45
29	C	512	CLA	CMB-C2B-C3B	3.08	130.43	124.68
48	G	606	CHL	C2C-C3C-C4C	3.08	108.68	106.49
29	g	612	CLA	C2D-C1D-ND	3.08	112.37	110.10
29	G1	611	CLA	CMA-C3A-C4A	3.08	120.04	111.77
29	S1	609	CLA	C2D-C1D-ND	3.07	112.37	110.10
29	y	611	CLA	CMB-C2B-C3B	3.07	130.43	124.68
29	G	602	CLA	CHD-C1D-ND	-3.07	121.63	124.45
51	y1	623	NEX	C31-C32-C33	3.07	135.05	126.42
29	g	610	CLA	C1-C2-C3	-3.07	120.73	126.04
39	c1	524	DGA	OG1-CA1-CA2	3.07	121.55	111.91
29	N	611	CLA	CHD-C1D-ND	-3.07	121.63	124.45
29	Y	604	CLA	CHD-C1D-ND	-3.07	121.63	124.45
29	c	502	CLA	CHD-C1D-ND	-3.07	121.63	124.45
29	c	511	CLA	CHD-C1D-ND	-3.07	121.63	124.45
29	s1	614	CLA	C1-C2-C3	-3.07	120.73	126.04
31	a1	411	BCR	C4-C5-C6	-3.07	118.27	122.73

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	612	CLA	C2C-C1C-NC	3.07	112.85	109.97
29	s1	603	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
29	C1	501	CLA	C2D-C1D-ND	3.07	112.37	110.10
30	a	408	PHO	CMB-C2B-C3B	3.07	130.42	124.68
48	s	608	CHL	C3C-C4C-NC	-3.07	107.13	110.57
48	g	609	CHL	C2C-C3C-C4C	3.07	108.68	106.49
51	G1	623	NEX	C27-C28-C29	-3.07	120.77	125.53
29	s1	603	CLA	CHD-C1D-ND	-3.07	121.63	124.45
51	G1	623	NEX	C31-C30-C29	3.07	131.69	127.31
29	s	605	CLA	O2D-CGD-O1D	-3.07	117.84	123.84
51	R	622	NEX	C39-C29-C30	-3.07	118.62	122.92
29	B1	610	CLA	C2D-C1D-ND	3.07	112.36	110.10
31	C	517	BCR	C19-C18-C17	3.07	123.65	118.94
29	g1	610	CLA	CMB-C2B-C3B	3.07	130.42	124.68
29	B1	606	CLA	C1-C2-C3	-3.07	120.74	126.04
51	r	622	NEX	C39-C29-C30	-3.07	118.63	122.92
29	c	507	CLA	CHD-C1D-ND	-3.07	121.64	124.45
29	C	507	CLA	C1-C2-C3	-3.07	120.74	126.04
29	Y	603	CLA	C2D-C1D-ND	3.07	112.36	110.10
49	N1	621	LUT	C16-C1-C6	-3.07	105.33	110.30
48	n1	609	CHL	C4D-CHA-C1A	3.07	124.98	121.25
48	S	607	CHL	CMA-C3A-C4A	3.07	120.01	111.77
29	y	613	CLA	CMB-C2B-C3B	3.06	130.41	124.68
29	g	613	CLA	C1-C2-C3	-3.06	120.74	126.04
29	r1	602	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
29	G	614	CLA	C2C-C1C-NC	3.06	112.84	109.97
29	S	609	CLA	C2C-C1C-NC	3.06	112.84	109.97
48	N	607	CHL	CHB-C4A-NA	3.06	128.75	124.51
29	Y1	608	CLA	CMC-C2C-C1C	3.06	129.70	125.04
29	a	406	CLA	C1C-C2C-C3C	-3.06	103.74	106.96
29	a	407	CLA	C1C-C2C-C3C	-3.06	103.74	106.96
29	R	602	CLA	C2D-C1D-ND	3.06	112.36	110.10
29	g	611	CLA	C2D-C1D-ND	3.06	112.36	110.10
31	d1	404	BCR	C34-C9-C10	-3.06	118.63	122.92
29	b1	606	CLA	C1C-C2C-C3C	-3.06	103.74	106.96
29	g1	612	CLA	CMA-C3A-C4A	3.06	120.00	111.77
31	C1	514	BCR	C38-C26-C25	-3.06	121.09	124.53
29	A	410	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
31	D	404	BCR	C36-C18-C17	-3.06	118.64	122.92
29	b1	614	CLA	CHD-C1D-ND	-3.06	121.64	124.45
29	c1	502	CLA	C1-C2-C3	-3.06	120.75	126.04
29	b1	615	CLA	C2C-C1C-NC	3.06	112.84	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	B	620	C7Z	C8-C7-C6	-3.06	118.61	127.20
29	b	606	CLA	C2D-C1D-ND	3.06	112.36	110.10
29	C1	503	CLA	C1-C2-C3	-3.06	120.75	126.04
29	B	604	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
51	y	623	NEX	C20-C13-C14	-3.06	118.64	122.92
29	g	613	CLA	C2C-C1C-NC	3.06	112.84	109.97
29	S	603	CLA	C1-C2-C3	-3.06	120.75	126.04
29	A	405	CLA	CMB-C2B-C1B	-3.06	123.76	128.46
29	R1	608	CLA	C2D-C1D-ND	3.06	112.36	110.10
29	b	611	CLA	C1-C2-C3	-3.06	120.76	126.04
49	G1	621	LUT	C7-C8-C9	-3.06	121.62	126.23
29	b1	603	CLA	CHD-C1D-ND	-3.06	121.64	124.45
31	a1	411	BCR	C33-C5-C6	-3.06	121.10	124.53
49	s	621	LUT	C18-C5-C6	-3.06	121.10	124.53
48	N1	601	CHL	CHB-C4A-NA	3.06	128.74	124.51
48	g1	607	CHL	C1-O2A-CGA	3.06	124.46	116.44
29	s1	610	CLA	CAC-C3C-C4C	3.06	128.78	124.81
31	d	404	BCR	C19-C18-C17	3.06	123.63	118.94
51	Y1	623	NEX	C39-C29-C30	-3.06	118.64	122.92
29	g1	614	CLA	CMA-C3A-C4A	3.06	119.98	111.77
29	S1	610	CLA	CMD-C2D-C3D	-3.05	120.59	127.61
29	B	604	CLA	C2C-C1C-NC	3.05	112.83	109.97
29	y1	608	CLA	C2C-C1C-NC	3.05	112.83	109.97
29	a1	410	CLA	OBD-CAD-C3D	-3.05	121.17	128.52
47	I	102	4RF	O40-C41-C43	3.05	121.49	111.91
50	r	621	XAT	C18-C5-C6	-3.05	117.14	122.26
29	g1	603	CLA	C2C-C1C-NC	3.05	112.83	109.97
48	Y1	606	CHL	CHB-C4A-NA	3.05	128.73	124.51
29	y1	602	CLA	C1D-ND-C4D	-3.05	104.17	106.33
29	D1	403	CLA	C2C-C1C-NC	3.05	112.83	109.97
48	Y1	601	CHL	C1-C2-C3	-3.05	120.77	126.04
29	s1	614	CLA	C1C-C2C-C3C	-3.05	103.75	106.96
29	c1	505	CLA	CHD-C1D-ND	-3.05	121.65	124.45
29	C1	513	CLA	C2D-C1D-ND	3.05	112.35	110.10
45	H	101	RRX	C16-C17-C18	-3.05	122.96	127.31
48	S1	606	CHL	C2C-C3C-C4C	3.05	108.66	106.49
51	s1	623	NEX	C40-C33-C34	-3.05	118.65	122.92
45	H	101	RRX	C15-C16-C17	-3.05	117.23	123.47
29	c	502	CLA	CMA-C3A-C4A	3.05	119.97	111.77
29	g1	604	CLA	CHD-C1D-ND	-3.05	121.65	124.45
29	r1	608	CLA	C1-O2A-CGA	3.05	124.44	116.44
29	S	603	CLA	C2C-C1C-NC	3.05	112.83	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c1	510	CLA	C1C-C2C-C3C	-3.05	103.75	106.96
29	s1	613	CLA	CHD-C1D-ND	-3.05	121.65	124.45
29	y1	611	CLA	C7-C6-C5	-3.05	105.09	113.36
51	g	623	NEX	C31-C30-C29	3.05	131.66	127.31
48	Y1	609	CHL	CHB-C4A-NA	3.05	128.72	124.51
29	b	602	CLA	C2D-C1D-ND	3.05	112.35	110.10
29	N	613	CLA	O2A-CGA-CBA	3.04	121.46	111.91
29	B	617	CLA	C2C-C1C-NC	3.04	112.82	109.97
29	b1	612	CLA	CMB-C2B-C1B	-3.04	123.78	128.46
29	n	603	CLA	CBC-CAC-C3C	-3.04	104.04	112.43
29	C1	507	CLA	C1C-C2C-C3C	-3.04	103.76	106.96
51	n	623	NEX	C39-C29-C30	-3.04	118.66	122.92
29	c	507	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
29	y1	608	CLA	CHD-C1D-ND	-3.04	121.66	124.45
29	S1	612	CLA	C2D-C1D-ND	3.04	112.35	110.10
45	h1	101	RRX	C15-C16-C17	-3.04	117.24	123.47
48	S1	601	CHL	C2C-C3C-C4C	3.04	108.66	106.49
29	B1	614	CLA	C1C-C2C-C3C	-3.04	103.76	106.96
29	S	612	CLA	C2D-C1D-ND	3.04	112.34	110.10
29	S1	603	CLA	C2D-C1D-ND	3.04	112.34	110.10
48	n1	609	CHL	C3C-C4C-NC	-3.04	107.16	110.57
29	c1	509	CLA	CHD-C1D-ND	-3.04	121.66	124.45
48	G1	605	CHL	CHD-C1D-ND	-3.04	121.66	124.45
49	n1	620	LUT	C35-C34-C33	-3.04	122.97	127.31
29	s1	605	CLA	CMA-C3A-C4A	3.04	119.94	111.77
29	R1	603	CLA	C2C-C1C-NC	3.04	112.82	109.97
29	c1	508	CLA	CMA-C3A-C4A	3.04	119.94	111.77
29	Y	604	CLA	C2D-C1D-ND	3.04	112.34	110.10
48	S	606	CHL	C1B-CHB-C4A	-3.04	124.10	130.12
29	B1	610	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
51	S1	623	NEX	C39-C29-C30	-3.04	118.67	122.92
29	b	602	CLA	CHD-C1D-ND	-3.04	121.66	124.45
29	C1	507	CLA	CHD-C1D-ND	-3.04	121.66	124.45
29	B1	608	CLA	C2D-C1D-ND	3.04	112.34	110.10
29	A	410	CLA	C2C-C1C-NC	3.04	112.82	109.97
48	N	601	CHL	CHB-C4A-NA	3.04	128.71	124.51
29	N1	603	CLA	C1C-C2C-C3C	-3.04	103.76	106.96
29	S	617	CLA	C1-C2-C3	-3.04	121.84	126.75
29	r1	603	CLA	CMA-C3A-C4A	3.04	119.93	111.77
29	S1	613	CLA	C2D-C1D-ND	3.04	112.34	110.10
31	C	517	BCR	C23-C22-C21	3.04	123.60	118.94
29	Y1	604	CLA	O2D-CGD-O1D	-3.04	117.90	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A1	406	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
48	N1	607	CHL	C2C-C3C-C4C	3.03	108.65	106.49
29	c1	511	CLA	C1-C2-C3	-3.03	120.80	126.04
33	H1	102	LMG	O7-C10-C11	3.03	118.04	111.50
29	G	613	CLA	C2C-C1C-NC	3.03	112.81	109.97
29	G	612	CLA	CMA-C3A-C4A	3.03	119.92	111.77
48	n1	601	CHL	CMA-C3A-C4A	3.03	119.92	111.77
36	B1	620	C7Z	C7-C8-C9	-3.03	121.65	126.23
29	Y	613	CLA	C1-C2-C3	-3.03	120.80	126.04
48	n1	607	CHL	C1-C2-C3	-3.03	120.80	126.04
29	c	509	CLA	CMB-C2B-C1B	-3.03	123.81	128.46
29	Y	613	CLA	CHD-C1D-ND	-3.03	121.67	124.45
51	g1	623	NEX	C38-C25-C26	-3.03	117.18	122.26
29	b1	613	CLA	C1-C2-C3	-3.03	120.80	126.04
49	S	621	LUT	C7-C8-C9	-3.03	121.66	126.23
29	B1	603	CLA	C2C-C1C-NC	3.03	112.81	109.97
29	a1	407	CLA	C1C-C2C-C3C	-3.03	103.77	106.96
48	n	601	CHL	CHB-C4A-NA	3.03	128.70	124.51
29	b	608	CLA	O2D-CGD-O1D	-3.03	117.92	123.84
49	S1	621	LUT	C21-C26-C27	3.03	116.53	112.70
45	H1	101	RRX	C33-C5-C4	3.03	119.43	113.62
29	R1	608	CLA	C1-C2-C3	-3.03	120.81	126.04
29	B	608	CLA	C2C-C1C-NC	3.03	112.81	109.97
29	r1	602	CLA	C2D-C1D-ND	3.03	112.33	110.10
30	A1	409	PHO	C1A-C2A-C3A	-3.03	99.96	102.84
48	n1	606	CHL	C3C-C4C-NC	-3.03	107.18	110.57
29	g	602	CLA	CMB-C2B-C3B	3.03	130.34	124.68
29	b	607	CLA	O2A-CGA-CBA	3.03	121.40	111.91
29	b	603	CLA	C1-O2A-CGA	3.02	124.38	116.44
29	c1	505	CLA	C2D-C1D-ND	3.02	112.33	110.10
29	S1	611	CLA	CMA-C3A-C4A	3.02	119.90	111.77
29	Y1	608	CLA	C2C-C1C-NC	3.02	112.81	109.97
29	g	602	CLA	CHD-C1D-ND	-3.02	121.67	124.45
29	s	612	CLA	CHD-C1D-ND	-3.02	121.67	124.45
29	y1	603	CLA	C1C-C2C-C3C	-3.02	103.78	106.96
29	G	602	CLA	CMB-C2B-C3B	3.02	130.33	124.68
29	S1	602	CLA	CHD-C1D-ND	-3.02	121.68	124.45
29	Y	603	CLA	C2C-C1C-NC	3.02	112.80	109.97
48	Y	607	CHL	C3C-C4C-NC	-3.02	107.18	110.57
49	S	621	LUT	C15-C14-C13	-3.02	123.00	127.31
29	c1	512	CLA	CMB-C2B-C1B	-3.02	123.82	128.46
29	g1	614	CLA	CMD-C2D-C3D	-3.02	120.67	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	y	625	SPH	C3-C4-C5	-3.02	118.05	124.79
29	A1	405	CLA	C2C-C1C-NC	3.02	112.80	109.97
29	c1	503	CLA	C2C-C1C-NC	3.02	112.80	109.97
45	H	101	RRX	C30-C29-C28	-3.02	106.82	113.64
51	g	623	NEX	C1-C2-C3	3.02	120.46	113.64
29	c	511	CLA	CMB-C2B-C3B	3.02	130.33	124.68
29	r1	612	CLA	C1-C2-C3	-3.02	120.82	126.04
29	Y1	610	CLA	CMB-C2B-C3B	3.02	130.32	124.68
29	R1	609	CLA	C2C-C1C-NC	3.02	112.80	109.97
49	s1	620	LUT	C19-C9-C10	-3.02	118.70	122.92
48	y	601	CHL	CHC-C1C-NC	3.02	128.78	124.20
49	y	620	LUT	C2-C3-C4	-3.02	106.17	110.30
29	a1	410	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
49	g	621	LUT	C31-C30-C29	-3.02	123.01	127.31
48	G	605	CHL	C3C-C4C-NC	-3.01	107.19	110.57
29	r	604	CLA	CHD-C1D-ND	-3.01	121.68	124.45
29	y	608	CLA	CHD-C1D-ND	-3.01	121.68	124.45
48	N1	607	CHL	CMA-C3A-C4A	3.01	119.87	111.77
29	b1	609	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
48	r1	607	CHL	C4D-CHA-C1A	3.01	124.92	121.25
29	Y	603	CLA	CHD-C1D-ND	-3.01	121.69	124.45
29	s1	617	CLA	C2D-C1D-ND	3.01	112.32	110.10
29	g	614	CLA	C2D-C1D-ND	3.01	112.32	110.10
51	r	622	NEX	C40-C33-C34	-3.01	118.71	122.92
29	s1	611	CLA	C1-C2-C3	-3.01	120.84	126.04
29	n1	603	CLA	CMA-C3A-C4A	3.01	119.86	111.77
29	s1	602	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
29	B	602	CLA	C2D-C1D-ND	3.01	112.32	110.10
29	s	612	CLA	C2D-C1D-ND	3.01	112.32	110.10
29	y1	610	CLA	C2C-C1C-NC	3.01	112.79	109.97
29	a	406	CLA	CMB-C2B-C1B	-3.01	123.84	128.46
29	S	605	CLA	CHD-C1D-ND	-3.01	121.69	124.45
29	R	612	CLA	C2D-C1D-ND	3.01	112.32	110.10
31	C	514	BCR	C12-C13-C14	-3.01	114.33	118.94
48	Y	607	CHL	CMA-C3A-C4A	3.01	119.85	111.77
29	G	602	CLA	C1-C2-C3	-3.01	120.84	126.04
29	B	602	CLA	CHD-C1D-ND	-3.01	121.69	124.45
29	C1	501	CLA	CHD-C1D-ND	-3.01	121.69	124.45
51	g	623	NEX	C39-C29-C30	-3.01	118.71	122.92
29	b1	607	CLA	C1-C2-C3	-3.01	120.84	126.04
29	b1	608	CLA	C1-O2A-CGA	3.01	124.33	116.44
29	B1	611	CLA	C2D-C1D-ND	3.01	112.32	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	r1	609	CLA	CHD-C1D-ND	-3.01	121.69	124.45
29	S	602	CLA	C1C-C2C-C3C	-3.01	103.80	106.96
29	b1	603	CLA	C2C-C1C-NC	3.00	112.79	109.97
49	s1	621	LUT	C35-C15-C14	-3.00	117.32	123.47
29	R1	609	CLA	C2D-C1D-ND	3.00	112.32	110.10
29	g1	603	CLA	C2D-C1D-ND	3.00	112.32	110.10
48	G1	605	CHL	CHB-C4A-NA	3.00	128.67	124.51
29	B	614	CLA	CMB-C2B-C3B	3.00	130.30	124.68
48	y	605	CHL	CMA-C3A-C4A	3.00	119.84	111.77
29	b	611	CLA	C2D-C1D-ND	3.00	112.32	110.10
49	s	620	LUT	C38-C25-C24	-3.00	117.14	123.56
53	r	626	ERG	C19-C10-C1	-3.00	104.69	109.43
50	y	622	XAT	C19-C9-C10	-3.00	118.72	122.92
29	N	614	CLA	C1C-C2C-C3C	-3.00	103.80	106.96
29	a1	410	CLA	C1-C2-C3	-3.00	120.85	126.04
29	b	611	CLA	C1C-C2C-C3C	-3.00	103.80	106.96
29	s	602	CLA	C2D-C1D-ND	3.00	112.31	110.10
40	s1	624	LHG	O8-C23-C24	3.00	121.32	111.91
29	B	611	CLA	CHD-C1D-ND	-3.00	121.70	124.45
48	g	608	CHL	C3C-C4C-NC	-3.00	107.21	110.57
50	r1	621	XAT	C19-C9-C10	-3.00	118.72	122.92
51	n	623	NEX	C31-C30-C29	3.00	131.59	127.31
52	R	625	LMT	C3'-C4'-C5'	-3.00	104.05	110.93
48	Y1	609	CHL	C1-O2A-CGA	3.00	124.31	116.44
30	a	408	PHO	O1D-CGD-CBD	3.00	129.73	124.74
48	G1	609	CHL	CMA-C3A-C4A	3.00	119.83	111.77
48	N1	607	CHL	C1-O2A-CGA	3.00	124.31	116.44
29	N	602	CLA	C1D-ND-C4D	-3.00	104.21	106.33
29	B1	614	CLA	C1-C2-C3	-3.00	120.86	126.04
29	A	406	CLA	CMB-C2B-C1B	-3.00	123.86	128.46
29	B1	612	CLA	CAC-C3C-C4C	3.00	128.70	124.81
29	y	604	CLA	CHD-C1D-ND	-3.00	121.70	124.45
29	n1	610	CLA	C2C-C1C-NC	3.00	112.78	109.97
38	b1	624	3PH	O31-C31-C32	3.00	121.31	111.91
29	N	614	CLA	C2D-C1D-ND	2.99	112.31	110.10
31	B	619	BCR	C4-C5-C6	-2.99	118.38	122.73
29	N1	614	CLA	C2C-C1C-NC	2.99	112.78	109.97
29	y1	613	CLA	C2C-C1C-NC	2.99	112.78	109.97
29	B	603	CLA	CMA-C3A-C4A	2.99	119.82	111.77
29	b	608	CLA	CHD-C1D-ND	-2.99	121.70	124.45
51	s	623	NEX	C31-C30-C29	2.99	131.58	127.31
50	G1	622	XAT	C40-C33-C34	-2.99	118.73	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a	406	CLA	CMD-C2D-C3D	-2.99	120.73	127.61
49	s	620	LUT	C10-C11-C12	-2.99	113.88	123.22
29	A1	406	CLA	CMB-C2B-C3B	2.99	130.28	124.68
36	B1	620	C7Z	C23-C24-C25	2.99	117.81	111.85
48	Y	607	CHL	C2C-C3C-C4C	2.99	108.62	106.49
29	B1	616	CLA	C1C-C2C-C3C	-2.99	103.81	106.96
29	B	608	CLA	CHD-C1D-ND	-2.99	121.70	124.45
29	B1	608	CLA	CHD-C1D-ND	-2.99	121.70	124.45
29	G	602	CLA	C2C-C1C-NC	2.99	112.77	109.97
29	A	406	CLA	C2D-C1D-ND	2.99	112.31	110.10
48	N	606	CHL	C1B-CHB-C4A	-2.99	124.19	130.12
29	B	607	CLA	CHD-C1D-ND	-2.99	121.71	124.45
29	r1	604	CLA	CHD-C1D-ND	-2.99	121.71	124.45
29	n	613	CLA	O2D-CGD-O1D	-2.99	117.99	123.84
49	S	621	LUT	C35-C15-C14	-2.99	117.35	123.47
29	R	609	CLA	CHD-C1D-ND	-2.99	121.71	124.45
29	Y1	610	CLA	CHD-C1D-ND	-2.99	121.71	124.45
48	G1	608	CHL	C3C-C4C-NC	-2.99	107.22	110.57
29	B1	607	CLA	O1D-CGD-CBD	-2.99	118.37	124.48
52	R	625	LMT	C3B-C4B-C5B	-2.99	104.91	110.24
48	N1	605	CHL	CHB-C4A-NA	2.99	128.64	124.51
29	a	407	CLA	CHD-C1D-ND	-2.99	121.71	124.45
48	y1	606	CHL	CMA-C3A-C4A	2.99	119.80	111.77
29	S1	612	CLA	C2C-C1C-NC	2.99	112.77	109.97
29	c	513	CLA	CMB-C2B-C1B	-2.99	123.87	128.46
48	S	608	CHL	CMA-C3A-C4A	2.99	119.80	111.77
44	F1	101	HEM	CMC-C2C-C3C	2.99	130.26	124.68
29	s	613	CLA	C2C-C1C-NC	2.99	112.77	109.97
37	b1	623	DGD	O5D-C6D-C5D	2.99	114.57	109.05
29	B1	611	CLA	C1-C2-C3	-2.99	120.88	126.04
29	B	611	CLA	C1C-C2C-C3C	-2.99	103.82	106.96
48	Y	606	CHL	CHD-C1D-ND	-2.98	121.71	124.45
55	Y1	627	PTY	C6-O7-C8	-2.98	112.33	117.90
29	n1	604	CLA	C2C-C1C-NC	2.98	112.77	109.97
29	n1	614	CLA	CAA-C2A-C3A	-2.98	104.61	112.78
29	Y1	604	CLA	CHD-C1D-ND	-2.98	121.71	124.45
49	n1	620	LUT	C22-C23-C24	-2.98	108.34	111.74
50	G1	622	XAT	O24-C25-C38	-2.98	111.48	115.06
29	A1	407	CLA	CMA-C3A-C4A	2.98	119.79	111.77
48	S1	608	CHL	C3C-C4C-NC	-2.98	107.23	110.57
29	a	410	CLA	CMB-C2B-C1B	-2.98	123.88	128.46
45	h	101	RRX	C33-C5-C4	2.98	119.34	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	G	603	CLA	C1-C2-C3	-2.98	120.89	126.04
31	B	619	BCR	C33-C5-C6	-2.98	121.18	124.53
29	B	615	CLA	CHD-C1D-ND	-2.98	121.72	124.45
48	S1	601	CHL	CHD-C1D-ND	-2.98	121.72	124.45
29	s	611	CLA	C2C-C1C-NC	2.98	112.76	109.97
29	C1	510	CLA	C1-C2-C3	-2.98	120.89	126.04
31	d	404	BCR	C4-C5-C6	-2.98	118.41	122.73
29	s	611	CLA	CMA-C3A-C4A	2.98	119.78	111.77
29	B	616	CLA	CHD-C1D-ND	-2.98	121.72	124.45
29	D	403	CLA	C2D-C1D-ND	2.98	112.30	110.10
29	g	610	CLA	C2D-C1D-ND	2.98	112.30	110.10
29	y1	604	CLA	C2D-C1D-ND	2.98	112.30	110.10
48	y	601	CHL	CMA-C3A-C4A	2.98	119.77	111.77
49	S	620	LUT	C38-C25-C24	-2.98	117.19	123.56
49	Y1	620	LUT	C7-C8-C9	-2.98	121.74	126.23
29	G1	611	CLA	C2D-C1D-ND	2.98	112.30	110.10
48	Y1	606	CHL	C2C-C3C-C4C	2.98	108.61	106.49
36	B	620	C7Z	C27-C28-C29	-2.98	121.74	126.23
53	r	626	ERG	C14-C8-C7	-2.98	118.52	124.38
29	Y1	603	CLA	CHD-C1D-ND	-2.98	121.72	124.45
51	n1	623	NEX	C27-C28-C29	-2.97	120.91	125.53
48	S	606	CHL	C3C-C4C-NC	-2.97	107.23	110.57
29	y	604	CLA	CMB-C2B-C1B	-2.97	123.89	128.46
48	s1	601	CHL	C4D-CHA-C1A	2.97	124.87	121.25
31	B	619	BCR	C37-C22-C23	2.97	122.76	118.08
29	B	605	CLA	O2A-CGA-CBA	2.97	121.23	111.91
29	g	602	CLA	O2A-CGA-CBA	2.97	121.23	111.91
29	d1	403	CLA	CMA-C3A-C4A	2.97	119.76	111.77
49	y	620	LUT	C11-C10-C9	-2.97	123.07	127.31
29	a	405	CLA	C1D-ND-C4D	-2.97	104.22	106.33
29	y1	612	CLA	C1-C2-C3	-2.97	120.90	126.04
29	C	501	CLA	C1C-C2C-C3C	-2.97	103.83	106.96
29	g	613	CLA	CHD-C1D-ND	-2.97	121.72	124.45
29	y1	610	CLA	C2D-C1D-ND	2.97	112.29	110.10
49	s1	620	LUT	C18-C5-C6	-2.97	121.19	124.53
29	r1	604	CLA	CMB-C2B-C3B	2.97	130.23	124.68
29	b	605	CLA	C11-C12-C13	-2.97	106.32	115.92
29	R1	612	CLA	C2D-C1D-ND	2.97	112.29	110.10
48	y1	609	CHL	CHB-C4A-NA	2.97	128.62	124.51
49	y	620	LUT	C38-C25-C24	-2.97	117.21	123.56
29	b	607	CLA	C1-C2-C3	-2.97	120.91	126.04
48	N1	608	CHL	CHB-C4A-NA	2.97	128.62	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	n1	614	CLA	CHD-C1D-ND	-2.97	121.73	124.45
29	b1	615	CLA	C1-C2-C3	-2.97	120.91	126.04
49	s1	620	LUT	C38-C25-C24	-2.97	117.21	123.56
48	y1	607	CHL	CHB-C4A-NA	2.97	128.61	124.51
48	R	607	CHL	CHD-C4C-C3C	2.97	129.20	124.84
49	r	620	LUT	C15-C14-C13	-2.96	123.08	127.31
48	y	609	CHL	CMA-C3A-C4A	2.96	119.74	111.77
53	r	626	ERG	C2-C1-C10	2.96	119.16	112.74
29	C	507	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
29	y	612	CLA	C1C-C2C-C3C	-2.96	103.84	106.96
29	R1	612	CLA	CMA-C3A-C4A	2.96	119.74	111.77
48	G1	608	CHL	CMA-C3A-C4A	2.96	119.73	111.77
29	b	617	CLA	CAA-C2A-C3A	-2.96	104.67	112.78
29	r1	609	CLA	C2D-C1D-ND	2.96	112.29	110.10
29	R	609	CLA	C2C-C1C-NC	2.96	112.75	109.97
31	c	517	BCR	C19-C18-C17	2.96	123.49	118.94
50	y	622	XAT	C38-C25-C26	-2.96	117.30	122.26
29	n	613	CLA	CMA-C3A-C4A	2.96	119.73	111.77
48	N	608	CHL	C3C-C4C-NC	-2.96	107.25	110.57
48	g1	607	CHL	CMA-C3A-C4A	2.96	119.73	111.77
29	b1	602	CLA	CHD-C1D-ND	-2.96	121.73	124.45
48	N	609	CHL	C3C-C4C-NC	-2.96	107.25	110.57
29	s	602	CLA	O2A-CGA-CBA	2.96	121.19	111.91
45	H	101	RRX	C20-C21-C22	2.96	131.53	127.31
50	r1	621	XAT	C27-C28-C29	2.96	130.12	125.53
29	n	610	CLA	O1D-CGD-CBD	-2.96	118.43	124.48
29	n	611	CLA	C2D-C1D-ND	2.96	112.28	110.10
51	G1	623	NEX	C17-C1-C6	-2.96	107.83	110.47
29	y	610	CLA	O2A-CGA-CBA	2.96	121.19	111.91
29	b	607	CLA	CMB-C2B-C3B	2.96	130.21	124.68
29	a1	407	CLA	CMA-C3A-C4A	2.96	119.72	111.77
51	r	622	NEX	C19-C9-C10	-2.96	118.78	122.92
48	Y	607	CHL	CHB-C4A-NA	2.95	128.60	124.51
29	y	604	CLA	CMB-C2B-C3B	2.95	130.21	124.68
29	Y1	602	CLA	O1D-CGD-CBD	-2.95	118.44	124.48
51	R1	622	NEX	C1-C2-C3	2.95	120.31	113.64
51	N1	623	NEX	C27-C28-C29	-2.95	120.95	125.53
48	n	609	CHL	C3C-C4C-NC	-2.95	107.26	110.57
29	c1	503	CLA	C1-C2-C3	-2.95	120.94	126.04
29	b1	614	CLA	C2C-C1C-NC	2.95	112.74	109.97
48	G1	601	CHL	C1-C2-C3	-2.95	120.94	126.04
29	N1	612	CLA	CHD-C1D-ND	-2.95	121.74	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	b1	620	C7Z	C18-C5-C6	-2.95	121.21	124.53
48	r1	607	CHL	CMA-C3A-C4A	2.95	119.71	111.77
29	g1	610	CLA	C2D-C1D-ND	2.95	112.28	110.10
29	s1	605	CLA	O2A-CGA-CBA	2.95	121.17	111.91
29	y	614	CLA	C2C-C1C-NC	2.95	112.74	109.97
29	b	610	CLA	CMB-C2B-C3B	2.95	130.20	124.68
29	A	410	CLA	C2D-C1D-ND	2.95	112.28	110.10
29	b1	612	CLA	CMB-C2B-C3B	2.95	130.20	124.68
29	N1	604	CLA	C1C-C2C-C3C	-2.95	103.86	106.96
29	S1	614	CLA	CHD-C1D-ND	-2.95	121.74	124.45
29	n1	611	CLA	CHD-C1D-ND	-2.95	121.74	124.45
49	Y1	621	LUT	C3-C4-C5	-2.95	105.98	111.85
29	G1	612	CLA	CMA-C3A-C4A	2.95	119.70	111.77
29	a1	406	CLA	O2A-CGA-CBA	2.95	121.16	111.91
29	S1	614	CLA	C1-C2-C3	-2.95	120.95	126.04
48	n1	601	CHL	C1-C2-C3	-2.95	120.95	126.04
37	c1	519	DGD	O1G-C1A-C2A	2.95	121.15	111.91
29	D	403	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
29	n	602	CLA	CHD-C1D-ND	-2.95	121.75	124.45
29	c	501	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
29	y1	603	CLA	C1-C2-C3	-2.95	120.95	126.04
48	Y	606	CHL	C1-O2A-CGA	2.95	124.17	116.44
48	N	606	CHL	C4D-CHA-C1A	2.94	124.83	121.25
51	y1	623	NEX	C12-C13-C14	2.94	123.46	118.94
29	C1	509	CLA	C1-C2-C3	-2.94	120.95	126.04
29	n	610	CLA	C1-O2A-CGA	2.94	124.17	116.44
29	b1	602	CLA	CMA-C3A-C4A	2.94	119.68	111.77
48	S1	608	CHL	CMA-C3A-C4A	2.94	119.68	111.77
49	G1	621	LUT	C18-C5-C6	-2.94	121.22	124.53
29	r	603	CLA	C2C-C1C-NC	2.94	112.73	109.97
29	S1	613	CLA	C2C-C1C-NC	2.94	112.73	109.97
48	n	608	CHL	CMA-C3A-C4A	2.94	119.68	111.77
48	N1	605	CHL	C3C-C4C-NC	-2.94	107.27	110.57
31	C	515	BCR	C1-C6-C5	-2.94	118.47	122.61
48	r	607	CHL	CMA-C3A-C4A	2.94	119.68	111.77
29	G	603	CLA	C1C-C2C-C3C	-2.94	103.86	106.96
29	b1	616	CLA	C1C-C2C-C3C	-2.94	103.86	106.96
29	s1	614	CLA	C2D-C1D-ND	2.94	112.27	110.10
29	G	610	CLA	C2C-C1C-NC	2.94	112.73	109.97
29	b	613	CLA	CMD-C2D-C3D	-2.94	120.85	127.61
29	B1	610	CLA	C2C-C1C-NC	2.94	112.73	109.97
29	B1	605	CLA	C1C-C2C-C3C	-2.94	103.86	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	g	601	CHL	C1-O2A-CGA	2.94	124.16	116.44
29	B	611	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
49	N	620	LUT	C22-C23-C24	-2.94	108.39	111.74
29	C1	508	CLA	C2C-C1C-NC	2.94	112.73	109.97
29	g1	610	CLA	CMC-C2C-C1C	2.94	129.51	125.04
29	S	617	CLA	C1C-C2C-C3C	-2.94	103.87	106.96
29	s	613	CLA	C1C-C2C-C3C	-2.94	103.87	106.96
29	N	610	CLA	C2C-C1C-NC	2.94	112.72	109.97
29	b	608	CLA	C2C-C1C-NC	2.94	112.72	109.97
48	s1	607	CHL	C2C-C3C-C4C	2.94	108.58	106.49
48	y	601	CHL	C4A-NA-C1A	2.94	108.03	106.71
36	b	620	C7Z	C28-C27-C26	-2.94	118.96	127.20
49	N	620	LUT	C38-C25-C24	-2.94	117.28	123.56
29	s	614	CLA	O2D-CGD-O1D	-2.94	118.10	123.84
29	b	617	CLA	C2D-C1D-ND	2.94	112.27	110.10
29	d	402	CLA	CHD-C1D-ND	-2.93	121.76	124.45
29	R1	612	CLA	CHD-C1D-ND	-2.93	121.76	124.45
31	C	514	BCR	C35-C13-C12	2.93	122.70	118.08
48	s1	601	CHL	C3C-C4C-NC	-2.93	107.28	110.57
48	r	606	CHL	CMA-C3A-C4A	2.93	119.66	111.77
48	r1	607	CHL	C1-O2A-CGA	2.93	124.14	116.44
31	b	618	BCR	C1-C6-C7	2.93	124.08	115.78
49	g1	620	LUT	C39-C29-C28	2.93	122.70	118.08
29	s	612	CLA	C2C-C1C-NC	2.93	112.72	109.97
29	c	504	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
29	s	602	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
29	B1	609	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
29	G1	614	CLA	CHD-C1D-ND	-2.93	121.76	124.45
29	y1	603	CLA	CHD-C1D-ND	-2.93	121.76	124.45
29	a1	407	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
31	D1	404	BCR	C38-C26-C25	-2.93	121.24	124.53
29	b1	615	CLA	CMB-C2B-C3B	2.93	130.16	124.68
29	B1	605	CLA	O2A-CGA-CBA	2.93	121.10	111.91
29	s	611	CLA	C1-C2-C3	-2.93	120.97	126.04
29	y	604	CLA	C2C-C1C-NC	2.93	112.72	109.97
29	c	512	CLA	C2D-C1D-ND	2.93	112.26	110.10
29	b	609	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
48	G	607	CHL	CHB-C4A-NA	2.93	128.56	124.51
29	s1	602	CLA	O2A-CGA-CBA	2.93	121.10	111.91
29	s1	603	CLA	C1-C2-C3	-2.93	120.98	126.04
29	n	604	CLA	CHD-C1D-ND	-2.93	121.76	124.45
49	R1	620	LUT	C18-C5-C4	2.93	119.78	114.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	G	622	XAT	C38-C25-C26	-2.93	117.36	122.26
48	G	608	CHL	C2C-C3C-C4C	2.93	108.58	106.49
29	c	513	CLA	C2C-C1C-NC	2.93	112.71	109.97
29	G1	602	CLA	C2A-C1A-CHA	2.93	128.97	123.86
29	s	613	CLA	C1-O2A-CGA	2.93	124.12	116.44
29	G	613	CLA	C2D-C1D-ND	2.93	112.26	110.10
29	g	611	CLA	CMA-C3A-C4A	2.92	119.63	111.77
48	n	609	CHL	CHD-C4C-C3C	2.92	129.14	124.84
29	s1	602	CLA	C6-C5-C3	-2.92	105.79	113.45
29	Y1	613	CLA	O2A-CGA-CBA	2.92	121.08	111.91
29	b	607	CLA	CHD-C1D-ND	-2.92	121.77	124.45
31	C	517	BCR	C33-C5-C6	-2.92	121.25	124.53
29	b1	603	CLA	O2A-CGA-CBA	2.92	121.08	111.91
29	B1	605	CLA	C1-C2-C3	-2.92	120.99	126.04
29	S1	605	CLA	C1-C2-C3	-2.92	122.02	126.75
29	B1	613	CLA	C1C-C2C-C3C	-2.92	103.88	106.96
51	n1	623	NEX	C38-C25-C26	-2.92	117.36	122.26
43	D1	405	PL9	C8-C7-C3	2.92	120.24	111.98
40	D	409	LHG	O8-C23-C24	2.92	121.07	111.91
29	b1	603	CLA	C1-O2A-CGA	2.92	124.10	116.44
29	y1	610	CLA	CHD-C1D-ND	-2.92	121.77	124.45
29	y1	611	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
29	G	603	CLA	C2C-C1C-NC	2.92	112.71	109.97
48	Y1	607	CHL	CMA-C3A-C4A	2.92	119.62	111.77
29	Y1	613	CLA	C2D-C1D-ND	2.92	112.25	110.10
48	n1	609	CHL	C1-O2A-CGA	2.92	124.10	116.44
33	h1	102	LMG	O8-C28-C29	2.92	121.07	111.91
40	N1	624	LHG	O8-C23-C24	2.92	121.07	111.91
53	R	626	ERG	C19-C10-C1	-2.92	104.82	109.43
29	C	505	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
29	y1	612	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
29	s1	617	CLA	CMB-C2B-C1B	-2.92	123.98	128.46
29	s	605	CLA	CHD-C1D-ND	-2.92	121.77	124.45
31	C1	515	BCR	C33-C5-C4	2.92	119.22	113.62
43	D1	405	PL9	C40-C39-C41	2.92	120.18	115.27
29	n	613	CLA	C1-C2-C3	-2.92	121.00	126.04
29	c	503	CLA	C2C-C1C-NC	2.92	112.70	109.97
40	C	525	LHG	O8-C23-C24	2.91	121.06	111.91
29	G	614	CLA	CAA-C2A-C3A	-2.91	104.80	112.78
48	g	609	CHL	C3C-C4C-NC	-2.91	107.30	110.57
29	s1	604	CLA	C2C-C1C-NC	2.91	112.70	109.97
31	c	515	BCR	C34-C9-C10	-2.91	118.84	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	514	BCR	C23-C24-C25	-2.91	119.02	127.20
29	c1	507	CLA	CMA-C3A-C4A	2.91	119.60	111.77
29	b	607	CLA	C2C-C1C-NC	2.91	112.70	109.97
29	s1	611	CLA	C1C-C2C-C3C	-2.91	103.89	106.96
29	a	407	CLA	CMA-C3A-C4A	2.91	119.60	111.77
29	b1	608	CLA	C2D-C1D-ND	2.91	112.25	110.10
47	i	101	4RF	O40-C41-C43	2.91	121.04	111.91
29	r	604	CLA	C2C-C1C-NC	2.91	112.70	109.97
29	C1	503	CLA	CMB-C2B-C3B	2.91	130.12	124.68
29	C	513	CLA	CBA-CAA-C2A	2.91	122.45	113.86
29	g	603	CLA	C1C-C2C-C3C	-2.91	103.90	106.96
51	g	623	NEX	C2-C1-C6	2.91	112.04	109.21
29	N	604	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
29	b	602	CLA	CMA-C3A-C4A	2.91	119.59	111.77
48	g	606	CHL	C2C-C3C-C4C	2.91	108.56	106.49
49	Y	621	LUT	C38-C25-C24	-2.91	117.34	123.56
48	N	607	CHL	C3C-C4C-NC	-2.91	107.31	110.57
29	C	503	CLA	C2C-C1C-NC	2.91	112.70	109.97
51	r	622	NEX	C5-C6-C1	2.91	122.58	119.70
49	g	621	LUT	C38-C25-C24	-2.91	117.34	123.56
29	C1	513	CLA	CMA-C3A-C4A	2.91	119.58	111.77
48	g1	608	CHL	CMA-C3A-C4A	2.91	119.58	111.77
29	B	610	CLA	CHD-C1D-ND	-2.91	121.78	124.45
29	Y	614	CLA	C2C-C1C-NC	2.90	112.69	109.97
29	S	610	CLA	CHD-C1D-ND	-2.90	121.78	124.45
29	c1	511	CLA	C1C-C2C-C3C	-2.90	103.90	106.96
29	C1	505	CLA	C2D-C1D-ND	2.90	112.24	110.10
48	Y	609	CHL	CMA-C3A-C4A	2.90	119.58	111.77
29	a1	410	CLA	C1C-C2C-C3C	-2.90	103.90	106.96
29	B	609	CLA	CMA-C3A-C4A	2.90	119.58	111.77
29	r1	603	CLA	C1-O2A-CGA	2.90	124.06	116.44
47	I1	102	4RF	O40-C41-C43	2.90	121.02	111.91
45	h	101	RRX	C36-C18-C19	2.90	122.65	118.08
49	Y	620	LUT	C31-C30-C29	-2.90	123.17	127.31
29	b	616	CLA	CHD-C1D-ND	-2.90	121.79	124.45
29	Y1	613	CLA	CHD-C1D-ND	-2.90	121.79	124.45
29	B	616	CLA	C6-C5-C3	-2.90	105.85	113.45
29	r1	612	CLA	CMB-C2B-C3B	2.90	130.11	124.68
29	C1	509	CLA	CHD-C1D-ND	-2.90	121.79	124.45
48	n	605	CHL	C1-C2-C3	-2.90	121.03	126.04
29	S1	611	CLA	CHA-C4D-ND	2.90	138.57	132.50
48	Y1	607	CHL	C3C-C4C-NC	-2.90	107.32	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	R1	607	CHL	CMA-C3A-C4A	2.90	119.57	111.77
29	C	511	CLA	CMB-C2B-C3B	2.90	130.10	124.68
29	y	614	CLA	CMA-C3A-C4A	2.90	119.56	111.77
53	r	626	ERG	C6-C7-C8	-2.90	116.36	122.07
29	B	610	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
29	g1	604	CLA	CMB-C2B-C3B	2.90	130.10	124.68
29	r	610	CLA	C2D-C1D-ND	2.90	112.24	110.10
29	b1	609	CLA	CMA-C3A-C4A	2.90	119.56	111.77
29	B	613	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
48	y	607	CHL	C1-C2-C3	-2.90	121.03	126.04
29	s	617	CLA	C1C-C2C-C3C	-2.90	103.91	106.96
48	G	607	CHL	CMA-C3A-C4A	2.90	119.56	111.77
30	A1	408	PHO	O2D-CGD-O1D	-2.90	118.17	123.84
48	G1	605	CHL	C4A-NA-C1A	2.90	108.01	106.71
29	b	605	CLA	CMA-C3A-C4A	2.90	119.56	111.77
29	C	509	CLA	CHD-C1D-ND	-2.90	121.79	124.45
29	C1	504	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
29	a1	410	CLA	O2A-CGA-CBA	2.90	120.99	111.91
50	G	622	XAT	O24-C25-C24	2.90	115.56	113.38
48	N1	607	CHL	CHB-C4A-NA	2.89	128.51	124.51
33	C	521	LMG	O8-C28-C29	2.89	120.99	111.91
37	c	519	DGD	O1G-C1A-C2A	2.89	120.99	111.91
29	C	502	CLA	C2D-C1D-ND	2.89	112.24	110.10
38	t	101	3PH	O31-C31-C32	2.89	120.98	111.91
29	s	603	CLA	C2D-C1D-ND	2.89	112.23	110.10
29	b	604	CLA	O2A-CGA-CBA	2.89	120.98	111.91
29	g	603	CLA	CHD-C1D-ND	-2.89	121.80	124.45
48	g1	609	CHL	CHB-C4A-NA	2.89	128.51	124.51
29	s	617	CLA	O2A-CGA-CBA	2.89	120.98	111.91
29	c1	501	CLA	C1-C2-C3	-2.89	121.04	126.04
29	y	602	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
29	s1	611	CLA	OBD-CAD-C3D	-2.89	121.56	128.52
29	y1	612	CLA	CMA-C3A-C4A	2.89	119.54	111.77
51	S	623	NEX	C19-C9-C10	-2.89	118.88	122.92
51	n	623	NEX	C5-C4-C3	2.89	115.17	111.75
29	G1	613	CLA	CMB-C2B-C3B	2.89	130.08	124.68
29	B1	603	CLA	C2D-C1D-ND	2.89	112.23	110.10
29	b	616	CLA	C2C-C1C-NC	2.89	112.68	109.97
29	B1	613	CLA	CHD-C1D-ND	-2.89	121.80	124.45
48	S	606	CHL	C4D-CHA-C1A	2.89	124.76	121.25
31	c	515	BCR	C37-C22-C23	2.89	122.62	118.08
29	s1	609	CLA	C1-C2-C3	-2.89	121.05	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	614	CLA	O2D-CGD-O1D	-2.89	118.19	123.84
51	R1	622	NEX	C40-C33-C34	-2.89	118.88	122.92
29	r1	608	CLA	CMA-C3A-C4A	2.89	119.53	111.77
29	r	603	CLA	CMA-C3A-C4A	2.88	119.53	111.77
29	b	609	CLA	C2D-C1D-ND	2.88	112.23	110.10
29	n	603	CLA	C1C-C2C-C3C	-2.88	103.92	106.96
48	y1	609	CHL	C1-C2-C3	-2.88	121.06	126.04
29	G1	602	CLA	O1D-CGD-CBD	-2.88	118.58	124.48
31	C	516	BCR	C27-C26-C25	-2.88	118.54	122.73
48	y	607	CHL	C4D-CHA-C1A	2.88	124.76	121.25
48	y1	601	CHL	CMA-C3A-C4A	2.88	119.52	111.77
30	a1	409	PHO	O2D-CGD-O1D	-2.88	118.20	123.84
29	b	603	CLA	O2A-CGA-CBA	2.88	120.95	111.91
29	C	511	CLA	C2C-C1C-NC	2.88	112.67	109.97
29	B1	617	CLA	C2C-C1C-NC	2.88	112.67	109.97
29	g	611	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
29	c	504	CLA	C1D-ND-C4D	-2.88	104.29	106.33
29	g	610	CLA	O1D-CGD-CBD	-2.88	118.59	124.48
48	s	607	CHL	C2C-C3C-C4C	2.88	108.54	106.49
29	G	614	CLA	CMB-C2B-C1B	-2.88	124.04	128.46
49	S	620	LUT	C40-C33-C32	2.88	122.61	118.08
29	S1	617	CLA	C1C-C2C-C3C	-2.88	103.93	106.96
31	b1	618	BCR	C36-C18-C17	-2.88	118.89	122.92
51	N1	623	NEX	C40-C33-C34	-2.88	118.89	122.92
29	c	511	CLA	O2A-CGA-CBA	2.88	120.94	111.91
51	Y	623	NEX	C31-C30-C29	2.88	131.42	127.31
54	s1	625	LPX	O3-P1-O4	2.88	126.46	112.24
29	c1	501	CLA	O2A-CGA-CBA	2.88	120.94	111.91
48	S	601	CHL	C3C-C4C-NC	-2.88	107.34	110.57
48	S1	601	CHL	C1B-CHB-C4A	-2.88	124.42	130.12
29	b1	606	CLA	CHD-C1D-ND	-2.88	121.81	124.45
29	b	614	CLA	C2D-C1D-ND	2.88	112.22	110.10
29	g1	611	CLA	C2D-C1D-ND	2.88	112.22	110.10
29	s1	610	CLA	CHD-C1D-ND	-2.87	121.81	124.45
48	N	606	CHL	C3C-C4C-NC	-2.87	107.35	110.57
29	n	614	CLA	CAA-C2A-C3A	-2.87	104.91	112.78
48	s1	608	CHL	C1-C2-C3	-2.87	121.07	126.04
29	R1	610	CLA	CMA-C3A-C4A	2.87	119.50	111.77
29	B	609	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
29	a	410	CLA	C1-C2-C3	-2.87	121.07	126.04
29	s1	614	CLA	CMA-C3A-C4A	2.87	119.49	111.77
29	b	609	CLA	C1-C2-C3	-2.87	121.08	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	N1	611	CLA	CMD-C2D-C3D	-2.87	121.01	127.61
29	g1	610	CLA	O1D-CGD-CBD	-2.87	118.61	124.48
45	H1	101	RRX	C36-C18-C19	2.87	122.60	118.08
29	G	612	CLA	C1D-ND-C4D	-2.87	104.30	106.33
29	B	607	CLA	CMA-C3A-C4A	2.87	119.49	111.77
29	B1	612	CLA	C2C-C1C-NC	2.87	112.66	109.97
29	C1	501	CLA	C2C-C1C-NC	2.87	112.66	109.97
29	N	611	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
29	n1	610	CLA	C1D-ND-C4D	-2.87	104.30	106.33
29	S	617	CLA	O2D-CGD-O1D	-2.87	118.23	123.84
29	Y	608	CLA	C2D-C1D-ND	2.87	112.22	110.10
29	c1	504	CLA	C1-O2A-CGA	2.87	123.97	116.44
29	B	603	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
45	h1	101	RRX	C8-C9-C10	-2.87	114.54	118.94
29	B	604	CLA	CHD-C1D-ND	-2.87	121.82	124.45
29	b	605	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
29	a	405	CLA	CMC-C2C-C1C	2.87	129.41	125.04
51	g1	623	NEX	C27-C28-C29	-2.87	121.08	125.53
31	b	618	BCR	C23-C24-C25	-2.87	119.15	127.20
29	c1	501	CLA	C1C-C2C-C3C	-2.87	103.94	106.96
48	G1	607	CHL	C1-C2-C3	-2.87	121.09	126.04
29	R	602	CLA	O2A-CGA-CBA	2.87	120.90	111.91
29	s1	609	CLA	C1D-ND-C4D	-2.87	104.30	106.33
29	b1	612	CLA	OBD-CAD-C3D	-2.87	121.62	128.52
45	H	101	RRX	C30-C25-C26	-2.87	118.58	122.61
48	N	606	CHL	CMA-C3A-C4A	2.86	119.47	111.77
29	S1	605	CLA	C1-O2A-CGA	2.86	123.96	116.44
37	C	519	DGD	O1G-C1A-C2A	2.86	120.89	111.91
29	R	604	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
29	R	608	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
29	N	603	CLA	C2D-C1D-ND	2.86	112.21	110.10
48	y1	609	CHL	CMA-C3A-C4A	2.86	119.47	111.77
29	n	614	CLA	C2C-C1C-NC	2.86	112.65	109.97
29	g1	612	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
29	g1	603	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
38	S	626	3PH	O31-C31-C32	2.86	120.89	111.91
29	C	506	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
29	s	602	CLA	CHD-C1D-ND	-2.86	121.82	124.45
29	n1	603	CLA	C2D-C1D-ND	2.86	112.21	110.10
50	r1	621	XAT	C20-C13-C14	-2.86	118.92	122.92
29	s1	602	CLA	CMA-C3A-C4A	2.86	119.46	111.77
29	b1	605	CLA	C2C-C1C-NC	2.86	112.65	109.97

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b1	607	CLA	C2C-C1C-NC	2.86	112.65	109.97
51	r1	622	NEX	C39-C29-C30	-2.86	118.92	122.92
29	b1	610	CLA	CHD-C1D-ND	-2.86	121.83	124.45
48	s	607	CHL	CHD-C1D-ND	-2.86	121.83	124.45
29	r	609	CLA	C2C-C1C-NC	2.86	112.65	109.97
49	s	620	LUT	C7-C8-C9	-2.86	121.91	126.23
50	R	621	XAT	C38-C25-C26	-2.86	117.47	122.26
29	Y1	610	CLA	C1-C2-C3	-2.86	121.10	126.04
29	B1	613	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
29	R	602	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
31	C	514	BCR	C38-C26-C25	-2.86	121.32	124.53
48	y1	606	CHL	C2C-C3C-C4C	2.86	108.53	106.49
29	N1	611	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
51	r	622	NEX	C31-C30-C29	2.86	131.39	127.31
29	s1	613	CLA	C2D-C1D-ND	2.86	112.21	110.10
29	s	613	CLA	CMA-C3A-C4A	2.86	119.45	111.77
49	R	620	LUT	C8-C7-C6	-2.86	119.18	127.20
29	y1	604	CLA	C1-O2A-CGA	2.86	123.94	116.44
29	n1	614	CLA	C1C-C2C-C3C	-2.86	103.95	106.96
29	a1	407	CLA	O1D-CGD-CBD	-2.86	118.64	124.48
29	Y	614	CLA	C1-C2-C3	-2.86	121.11	126.04
29	G	613	CLA	C1C-C2C-C3C	-2.85	103.95	106.96
29	b	617	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
30	A	408	PHO	O2D-CGD-O1D	-2.85	118.26	123.84
48	S1	607	CHL	CMA-C3A-C4A	2.85	119.44	111.77
29	r1	612	CLA	C2D-C1D-ND	2.85	112.21	110.10
29	S	609	CLA	CHD-C1D-ND	-2.85	121.83	124.45
37	C1	519	DGD	O1G-C1A-C2A	2.85	120.86	111.91
29	b	602	CLA	C2C-C1C-NC	2.85	112.64	109.97
31	a	411	BCR	C33-C5-C6	-2.85	121.33	124.53
29	N	613	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
29	r1	610	CLA	CMC-C2C-C1C	2.85	129.38	125.04
29	D	403	CLA	C2C-C1C-NC	2.85	112.64	109.97
29	B	615	CLA	CMB-C2B-C3B	2.85	130.01	124.68
51	R	622	NEX	C40-C33-C34	-2.85	118.93	122.92
53	r	626	ERG	C16-C17-C13	2.85	107.28	103.84
29	B1	605	CLA	C2D-C1D-ND	2.85	112.20	110.10
48	y	601	CHL	CHD-C4C-C3C	2.85	129.03	124.84
48	G	608	CHL	C3C-C4C-NC	-2.85	107.38	110.57
49	R	620	LUT	C1-C6-C5	-2.85	118.60	122.61
48	Y	605	CHL	CMA-C3A-C4A	2.85	119.43	111.77
29	G	604	CLA	CHD-C1D-ND	-2.85	121.84	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b1	610	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
29	Y	604	CLA	CMB-C2B-C3B	2.85	130.00	124.68
31	B	619	BCR	C23-C22-C21	-2.85	114.57	118.94
29	c	513	CLA	CBA-CAA-C2A	2.85	122.27	113.86
29	A1	407	CLA	CHD-C1D-ND	-2.85	121.84	124.45
29	Y1	612	CLA	C1C-C2C-C3C	-2.85	103.96	106.96
29	B1	614	CLA	CHA-C4D-ND	2.85	138.45	132.50
29	N	603	CLA	C1-O2A-CGA	2.85	123.91	116.44
29	B	612	CLA	O2D-CGD-O1D	-2.85	118.28	123.84
29	y	603	CLA	C1C-C2C-C3C	-2.85	103.97	106.96
29	B1	612	CLA	CMB-C2B-C3B	2.85	130.00	124.68
29	c1	506	CLA	C2D-C1D-ND	2.84	112.20	110.10
29	c1	501	CLA	CMA-C3A-C4A	2.84	119.42	111.77
29	N	612	CLA	C2C-C1C-NC	2.84	112.64	109.97
48	Y	609	CHL	C2C-C3C-C4C	2.84	108.52	106.49
29	s1	617	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
30	a1	408	PHO	O2D-CGD-O1D	-2.84	118.28	123.84
29	Y1	602	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
48	g	608	CHL	C2C-C3C-C4C	2.84	108.52	106.49
51	Y1	623	NEX	C27-C28-C29	-2.84	121.12	125.53
48	S1	606	CHL	CHB-C4A-NA	2.84	128.44	124.51
29	S	614	CLA	C2C-C1C-NC	2.84	112.63	109.97
29	S1	609	CLA	C2C-C1C-NC	2.84	112.63	109.97
29	B	606	CLA	C2D-C1D-ND	2.84	112.20	110.10
29	c	502	CLA	C2D-C1D-ND	2.84	112.20	110.10
29	c1	506	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
29	y1	614	CLA	CHD-C1D-ND	-2.84	121.84	124.45
48	Y1	606	CHL	CMA-C3A-C4A	2.84	119.41	111.77
31	d	404	BCR	C35-C13-C12	2.84	122.55	118.08
29	g	614	CLA	CMA-C3A-C4A	2.84	119.41	111.77
29	g	610	CLA	C1C-C2C-C3C	-2.84	103.97	106.96
29	S	611	CLA	C2D-C1D-ND	2.84	112.20	110.10
29	Y1	611	CLA	C1-C2-C3	-2.84	121.13	126.04
48	n	606	CHL	C2C-C3C-C4C	2.84	108.51	106.49
29	C	501	CLA	CAA-C2A-C3A	-2.84	105.00	112.78
29	C	503	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
29	a	410	CLA	CAA-C2A-C3A	-2.84	105.00	112.78
29	N	604	CLA	CHA-C4D-ND	2.84	138.44	132.50
48	Y1	605	CHL	C4A-NA-C1A	2.84	107.98	106.71
51	n1	623	NEX	C5-C4-C3	2.84	115.11	111.75
31	C1	517	BCR	C19-C18-C17	2.84	123.30	118.94
43	D1	405	PL9	C22-C23-C24	-2.84	120.83	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	G1	605	CHL	CMA-C3A-C4A	2.84	119.40	111.77
29	G1	610	CLA	C1-C2-C3	-2.84	121.14	126.04
31	a	411	BCR	C38-C26-C25	-2.84	121.34	124.53
31	B1	618	BCR	C37-C22-C21	-2.84	118.95	122.92
29	Y	612	CLA	C1-C2-C3	-2.84	121.14	126.04
29	c1	512	CLA	CMA-C3A-C4A	2.84	119.40	111.77
49	N1	621	LUT	C10-C11-C12	-2.84	114.36	123.22
29	c	506	CLA	CMB-C2B-C3B	2.84	129.98	124.68
29	A1	407	CLA	CMB-C2B-C3B	2.84	129.98	124.68
50	r1	621	XAT	C40-C33-C34	-2.84	118.95	122.92
29	a	406	CLA	C6-C5-C3	-2.84	106.02	113.45
42	d1	401	BCT	O3-C-O1	-2.84	112.19	119.55
31	C	515	BCR	C34-C9-C10	-2.83	118.95	122.92
31	b	618	BCR	C36-C18-C17	-2.83	118.95	122.92
29	s	611	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
40	D	408	LHG	O8-C23-C24	2.83	120.80	111.91
40	S1	624	LHG	O8-C23-C24	2.83	120.80	111.91
29	S1	603	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
29	a1	407	CLA	CMB-C2B-C3B	2.83	129.98	124.68
29	S1	604	CLA	CMA-C3A-C4A	2.83	119.39	111.77
48	g1	609	CHL	CMA-C3A-C4A	2.83	119.39	111.77
29	Y	614	CLA	CMD-C2D-C3D	-2.83	121.10	127.61
29	C	509	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
50	G1	622	XAT	C38-C25-C26	-2.83	117.52	122.26
29	b1	615	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
36	b1	620	C7Z	C3-C4-C5	2.83	117.49	111.85
29	S	605	CLA	C1-O2A-CGA	2.83	123.87	116.44
29	g1	613	CLA	CAC-C3C-C4C	2.83	128.48	124.81
29	B1	615	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
48	y	607	CHL	CMA-C3A-C4A	2.83	119.38	111.77
29	Y1	613	CLA	C2C-C1C-NC	2.83	112.62	109.97
29	N	614	CLA	CHD-C1D-ND	-2.83	121.85	124.45
33	A	413	LMG	O8-C28-C29	2.83	120.79	111.91
29	b	610	CLA	O2A-CGA-CBA	2.83	120.78	111.91
49	S	621	LUT	C16-C1-C6	-2.83	105.71	110.30
49	N1	620	LUT	C11-C10-C9	-2.83	123.27	127.31
51	s	623	NEX	C20-C13-C14	-2.83	118.96	122.92
29	N	610	CLA	CMA-C3A-C4A	2.83	119.37	111.77
29	s	605	CLA	C1C-C2C-C3C	-2.83	103.98	106.96
51	y	623	NEX	C4-C3-C2	2.83	116.23	110.77
29	R	610	CLA	C1-O2A-CGA	2.83	123.86	116.44
29	R1	609	CLA	CHD-C1D-ND	-2.83	121.86	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S	610	CLA	C1-O2A-CGA	2.83	123.86	116.44
29	C1	508	CLA	C2D-C1D-ND	2.83	112.19	110.10
39	j	101	DGA	OG1-CA1-CA2	2.82	120.77	111.91
29	y	612	CLA	O2D-CGD-O1D	-2.82	118.31	123.84
29	n1	604	CLA	CHD-C1D-ND	-2.82	121.86	124.45
29	s1	604	CLA	CMB-C2B-C1B	-2.82	124.12	128.46
29	y1	602	CLA	CMA-C3A-C4A	2.82	119.36	111.77
29	R	612	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
29	Y	608	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
49	G	620	LUT	C18-C5-C6	-2.82	121.36	124.53
48	g	605	CHL	CMA-C3A-C4A	2.82	119.36	111.77
51	R	622	NEX	C19-C9-C10	-2.82	118.97	122.92
48	N	609	CHL	C1-O2A-CGA	2.82	123.85	116.44
48	N1	606	CHL	C3C-C4C-NC	-2.82	107.41	110.57
30	A	409	PHO	O1D-CGD-CBD	2.82	129.44	124.74
48	R	606	CHL	C1B-CHB-C4A	-2.82	124.53	130.12
29	G1	603	CLA	CMA-C3A-C4A	2.82	119.35	111.77
36	B1	620	C7Z	C18-C5-C4	2.82	119.58	114.36
31	c	517	BCR	C36-C18-C17	-2.82	118.97	122.92
29	G1	602	CLA	CHA-C1A-NA	-2.82	119.94	126.40
29	a	410	CLA	CMA-C3A-C4A	2.82	119.35	111.77
29	d	402	CLA	C2D-C1D-ND	2.82	112.18	110.10
48	Y	601	CHL	C3C-C4C-NC	-2.82	107.41	110.57
29	s	603	CLA	C1C-C2C-C3C	-2.82	103.99	106.96
29	C	511	CLA	CMA-C3A-C4A	2.82	119.34	111.77
29	r	612	CLA	CHD-C1D-ND	-2.82	121.86	124.45
29	R	602	CLA	C2C-C1C-NC	2.82	112.61	109.97
29	S1	612	CLA	CMB-C2B-C1B	-2.82	124.14	128.46
29	b	608	CLA	CMB-C2B-C3B	2.82	129.95	124.68
48	s1	607	CHL	CHD-C1D-ND	-2.82	121.87	124.45
29	b	602	CLA	O2A-CGA-CBA	2.82	120.74	111.91
29	s	605	CLA	O2A-CGA-CBA	2.82	120.74	111.91
45	H	101	RRX	C33-C5-C4	2.81	119.02	113.62
29	b1	605	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
29	s1	612	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
29	c1	507	CLA	C1-O2A-CGA	2.81	123.83	116.44
31	c1	516	BCR	C34-C9-C10	-2.81	118.98	122.92
51	y1	623	NEX	C39-C29-C30	-2.81	118.98	122.92
29	S	605	CLA	C1C-C2C-C3C	-2.81	104.00	106.96
48	n1	609	CHL	C1B-CHB-C4A	-2.81	124.55	130.12
34	a	414	SPH	C3-C4-C5	-2.81	118.52	124.79
29	s1	605	CLA	O2D-CGD-O1D	-2.81	118.34	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	g1	609	CHL	CHD-C4C-C3C	2.81	128.97	124.84
29	S1	613	CLA	CMA-C3A-C4A	2.81	119.33	111.77
49	N	620	LUT	C39-C29-C28	2.81	122.51	118.08
49	Y1	621	LUT	C38-C25-C24	-2.81	117.54	123.56
48	n	608	CHL	CHB-C4A-NA	2.81	128.40	124.51
50	n	622	XAT	C38-C25-C26	-2.81	117.55	122.26
51	Y	623	NEX	C39-C29-C30	-2.81	118.98	122.92
49	G	620	LUT	C22-C23-C24	-2.81	108.54	111.74
29	G1	613	CLA	C2C-C1C-NC	2.81	112.61	109.97
37	B1	623	DGD	C2G-O2G-C1B	-2.81	110.87	117.79
48	y	609	CHL	C1-O2A-CGA	2.81	123.82	116.44
37	B1	623	DGD	O1G-C1A-C2A	2.81	120.72	111.91
29	b	604	CLA	C2C-C1C-NC	2.81	112.60	109.97
48	N1	606	CHL	CMA-C3A-C4A	2.81	119.32	111.77
29	b	615	CLA	C1-O2A-CGA	2.81	123.81	116.44
36	B	620	C7Z	C28-C27-C26	-2.81	119.32	127.20
29	N	602	CLA	CHD-C1D-ND	-2.81	121.88	124.45
29	b	616	CLA	C1C-C2C-C3C	-2.81	104.01	106.96
29	B	613	CLA	CMD-C2D-C3D	-2.81	121.16	127.61
29	d	403	CLA	C1-C2-C3	-2.81	121.19	126.04
49	g	620	LUT	C35-C34-C33	-2.80	123.31	127.31
49	g1	621	LUT	C15-C14-C13	-2.80	123.31	127.31
29	C1	502	CLA	CMA-C3A-C4A	2.80	119.31	111.77
29	B1	615	CLA	CMB-C2B-C3B	2.80	129.93	124.68
29	s	604	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
53	r1	626	ERG	C1-C10-C5	2.80	113.89	108.75
29	g	602	CLA	CMB-C2B-C1B	-2.80	124.15	128.46
49	n1	621	LUT	C19-C9-C10	-2.80	119.00	122.92
49	Y	621	LUT	C7-C8-C9	-2.80	122.00	126.23
29	N1	603	CLA	C2D-C1D-ND	2.80	112.17	110.10
29	c1	511	CLA	C2D-C1D-ND	2.80	112.17	110.10
48	g1	609	CHL	C4A-NA-C1A	2.80	107.97	106.71
33	W	201	LMG	O8-C28-C29	2.80	120.70	111.91
33	b1	622	LMG	O8-C28-C29	2.80	120.70	111.91
29	Y	608	CLA	CMA-C3A-C4A	2.80	119.30	111.77
29	s	605	CLA	CMA-C3A-C4A	2.80	119.30	111.77
29	r	603	CLA	C1-C2-C3	-2.80	121.20	126.04
40	C1	525	LHG	O8-C23-C24	2.80	120.70	111.91
49	n	621	LUT	C15-C14-C13	-2.80	123.31	127.31
29	R	610	CLA	CAA-C2A-C3A	-2.80	105.11	112.78
48	n1	608	CHL	CHD-C1D-ND	-2.80	121.88	124.45
29	R	603	CLA	CHA-C4D-ND	2.80	138.36	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b1	605	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
29	y	608	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
29	c1	505	CLA	C1C-C2C-C3C	-2.80	104.01	106.96
31	b1	618	BCR	C38-C26-C27	2.80	118.99	113.62
48	G1	601	CHL	CHB-C4A-NA	2.80	128.38	124.51
29	s1	611	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
29	B	616	CLA	C2C-C1C-NC	2.80	112.59	109.97
29	G1	614	CLA	C2D-C1D-ND	2.80	112.17	110.10
29	B	607	CLA	C2C-C1C-NC	2.80	112.59	109.97
29	r	608	CLA	CMD-C2D-C3D	-2.80	121.18	127.61
40	n	624	LHG	O8-C23-C24	2.80	120.69	111.91
29	g1	610	CLA	C1D-ND-C4D	-2.80	104.35	106.33
51	Y	623	NEX	C20-C13-C14	-2.80	119.00	122.92
29	Y	613	CLA	C2D-C1D-ND	2.80	112.17	110.10
29	G	603	CLA	CHD-C1D-ND	-2.80	121.88	124.45
29	B1	604	CLA	O2A-CGA-CBA	2.80	120.68	111.91
29	b	610	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
29	B	610	CLA	C1-C2-C3	-2.80	121.21	126.04
29	b	612	CLA	O1D-CGD-CBD	-2.80	118.76	124.48
48	n1	601	CHL	CHB-C4A-NA	2.79	128.38	124.51
48	G1	601	CHL	C1B-CHB-C4A	-2.79	124.58	130.12
29	C1	510	CLA	C2C-C1C-NC	2.79	112.59	109.97
48	Y1	607	CHL	CHB-C4A-NA	2.79	128.38	124.51
31	d1	404	BCR	C37-C22-C21	-2.79	119.01	122.92
29	c	503	CLA	CMB-C2B-C3B	2.79	129.91	124.68
43	D1	405	PL9	C37-C38-C39	-2.79	120.94	127.66
29	B	617	CLA	C2D-C1D-ND	2.79	112.16	110.10
29	b1	610	CLA	C2C-C1C-NC	2.79	112.59	109.97
29	n1	610	CLA	CHD-C1D-ND	-2.79	121.89	124.45
29	S	614	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
50	r1	621	XAT	C7-C8-C9	-2.79	121.20	125.53
50	N1	622	XAT	C38-C25-C26	-2.79	117.58	122.26
48	y1	606	CHL	C3C-C4C-NC	-2.79	107.44	110.57
49	s1	621	LUT	C19-C9-C10	-2.79	119.01	122.92
48	s1	607	CHL	CMA-C3A-C4A	2.79	119.27	111.77
29	b1	611	CLA	CMA-C3A-C4A	2.79	119.27	111.77
29	C1	506	CLA	C1C-C2C-C3C	-2.79	104.02	106.96
29	b1	609	CLA	C2D-C1D-ND	2.79	112.16	110.10
40	c	525	LHG	O8-C23-C24	2.79	120.66	111.91
29	r1	602	CLA	C2C-C1C-NC	2.79	112.58	109.97
29	y	613	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
29	n1	602	CLA	CAA-C2A-C3A	-2.79	105.14	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	r	610	CLA	C2C-C1C-NC	2.79	112.58	109.97
51	Y	623	NEX	C26-C27-C28	-2.79	120.10	125.99
51	Y1	623	NEX	C19-C9-C10	-2.79	119.02	122.92
29	a	406	CLA	O2A-CGA-CBA	2.79	120.66	111.91
29	A1	407	CLA	C1C-C2C-C3C	-2.79	104.03	106.96
29	s	614	CLA	C2C-C1C-NC	2.79	112.58	109.97
40	L	101	LHG	O8-C23-C24	2.79	120.65	111.91
48	N	607	CHL	CHD-C1D-ND	-2.79	121.89	124.45
29	Y	610	CLA	O1D-CGD-CBD	-2.79	118.78	124.48
29	Y1	612	CLA	O2A-CGA-CBA	2.79	120.65	111.91
29	c1	502	CLA	O2D-CGD-O1D	-2.78	118.39	123.84
33	H1	102	LMG	O8-C9-C8	2.78	116.54	108.43
29	g1	602	CLA	CMB-C2B-C3B	2.78	129.89	124.68
48	g1	609	CHL	C1B-CHB-C4A	-2.78	124.60	130.12
47	i1	101	4RF	O40-C41-C43	2.78	120.64	111.91
29	C1	506	CLA	CMA-C3A-C4A	2.78	119.25	111.77
29	B	614	CLA	C2C-C1C-NC	2.78	112.58	109.97
29	n	603	CLA	C2C-C1C-NC	2.78	112.58	109.97
29	a1	406	CLA	CMD-C2D-C3D	-2.78	121.21	127.61
29	g	614	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
50	y1	622	XAT	C8-C9-C10	2.78	123.21	118.94
49	g	620	LUT	C18-C5-C6	-2.78	121.40	124.53
29	C	503	CLA	C2D-C1D-ND	2.78	112.15	110.10
29	B	608	CLA	CMA-C3A-C4A	2.78	119.25	111.77
29	Y	613	CLA	O2A-CGA-CBA	2.78	120.63	111.91
48	g	606	CHL	C1-O2A-CGA	2.78	123.74	116.44
29	N1	604	CLA	CMD-C2D-C3D	-2.78	121.22	127.61
29	g1	610	CLA	O2A-CGA-CBA	2.78	120.63	111.91
29	C	505	CLA	C1-C2-C3	-2.78	121.24	126.04
51	S1	623	NEX	C2-C1-C6	2.78	111.91	109.21
51	g1	623	NEX	C16-C1-C6	-2.78	107.98	110.47
29	Y	613	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
29	y1	613	CLA	C1C-C2C-C3C	-2.78	104.03	106.96
29	D	403	CLA	CAA-C2A-C3A	-2.78	105.17	112.78
29	C1	508	CLA	C1C-C2C-C3C	-2.78	104.04	106.96
49	g1	620	LUT	C35-C15-C14	-2.78	117.78	123.47
48	R	606	CHL	C3C-C4C-NC	-2.78	107.46	110.57
48	n	605	CHL	CHB-C4A-NA	2.78	128.35	124.51
29	b	615	CLA	CMB-C2B-C1B	-2.78	124.20	128.46
29	g1	613	CLA	C1C-C2C-C3C	-2.78	104.04	106.96
29	B	613	CLA	CHA-C4D-ND	2.78	138.31	132.50
29	B1	612	CLA	C2D-C1D-ND	2.78	112.15	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	Y	609	CHL	C1-O2A-CGA	2.78	123.73	116.44
29	g1	611	CLA	CMA-C3A-C4A	2.78	119.23	111.77
39	C	524	DGA	OG1-CA1-CA2	2.78	120.62	111.91
29	r1	608	CLA	CHD-C1D-ND	-2.78	121.90	124.45
29	y	611	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
29	b	608	CLA	CMB-C2B-C1B	-2.77	124.20	128.46
29	c	506	CLA	O2D-CGD-O1D	-2.77	118.41	123.84
55	Y	626	PTY	O4-C30-C31	2.77	120.61	111.91
29	S1	614	CLA	C2C-C1C-NC	2.77	112.57	109.97
50	g1	622	XAT	C12-C13-C14	2.77	123.20	118.94
29	Y	603	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
48	y1	606	CHL	C4A-NA-C1A	2.77	107.95	106.71
29	b	608	CLA	C2D-C1D-ND	2.77	112.15	110.10
31	C	514	BCR	C36-C18-C17	-2.77	119.04	122.92
29	y1	602	CLA	O2A-CGA-CBA	2.77	120.61	111.91
29	y1	612	CLA	C2C-C1C-NC	2.77	112.57	109.97
29	g1	604	CLA	C1D-ND-C4D	-2.77	104.36	106.33
29	Y1	614	CLA	C1-C2-C3	-2.77	121.25	126.04
44	f1	101	HEM	CMC-C2C-C3C	2.77	129.87	124.68
29	b	613	CLA	CHA-C4D-ND	2.77	138.30	132.50
29	s1	617	CLA	O2A-CGA-CBA	2.77	120.61	111.91
29	N1	611	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
29	r1	603	CLA	C2C-C1C-NC	2.77	112.57	109.97
29	B	604	CLA	O2A-CGA-CBA	2.77	120.61	111.91
43	d	405	PL9	C22-C23-C24	-2.77	120.99	127.66
29	N	603	CLA	C1C-C2C-C3C	-2.77	104.04	106.96
29	B1	603	CLA	CMA-C3A-C4A	2.77	119.22	111.77
29	B	610	CLA	O2A-CGA-CBA	2.77	120.60	111.91
29	b1	617	CLA	CHD-C1D-ND	-2.77	121.91	124.45
48	r	606	CHL	CHB-C4A-NA	2.77	128.34	124.51
29	N1	604	CLA	CHA-C4D-ND	2.77	138.29	132.50
29	s	614	CLA	CAA-C2A-C3A	-2.77	105.19	112.78
31	C	517	BCR	C36-C18-C17	-2.77	119.04	122.92
38	s1	626	3PH	O31-C31-C32	2.77	120.60	111.91
29	r1	603	CLA	C2D-C1D-ND	2.77	112.14	110.10
29	Y1	614	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
29	N1	614	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
48	n1	605	CHL	C1-O2A-CGA	2.77	123.71	116.44
29	S	605	CLA	O2A-CGA-CBA	2.77	120.60	111.91
29	B	607	CLA	O2A-CGA-CBA	2.77	120.60	111.91
29	S	611	CLA	CMA-C3A-C4A	2.77	119.21	111.77
29	S1	605	CLA	C2D-C1D-ND	2.77	112.14	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	R1	604	CLA	C1C-C2C-C3C	-2.77	104.05	106.96
29	C	501	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
29	G1	614	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
48	n1	608	CHL	C2C-C3C-C4C	2.77	108.46	106.49
51	r1	622	NEX	C16-C1-C6	-2.77	108.00	110.47
29	B	603	CLA	CHD-C1D-ND	-2.77	121.91	124.45
29	n	612	CLA	C2D-C1D-ND	2.77	112.14	110.10
51	G	623	NEX	C16-C1-C6	-2.77	108.00	110.47
44	f	101	HEM	C4C-CHD-C1D	2.77	126.21	122.56
29	C1	504	CLA	CAC-C3C-C4C	2.77	128.40	124.81
48	R1	606	CHL	CMA-C3A-C4A	2.77	119.21	111.77
29	y	603	CLA	C2D-C1D-ND	2.77	112.14	110.10
29	N1	604	CLA	OBD-CAD-C3D	-2.76	121.87	128.52
30	a	409	PHO	O1D-CGD-CBD	2.76	129.34	124.74
29	S	605	CLA	CMA-C3A-C4A	2.76	119.20	111.77
31	C	516	BCR	C35-C13-C12	2.76	122.43	118.08
55	y	626	PTY	O4-C30-C31	2.76	120.58	111.91
29	B1	607	CLA	CAA-C2A-C3A	-2.76	105.21	112.78
29	s	609	CLA	C1-C2-C3	-2.76	121.26	126.04
29	B	607	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
29	C	512	CLA	O2D-CGD-O1D	-2.76	118.43	123.84
29	a1	406	CLA	CMB-C2B-C1B	-2.76	124.22	128.46
49	n	620	LUT	C31-C32-C33	-2.76	118.65	126.42
49	Y1	620	LUT	C18-C5-C6	-2.76	121.42	124.53
29	S	610	CLA	CMB-C2B-C3B	2.76	129.85	124.68
29	N	602	CLA	C1-C2-C3	-2.76	121.26	126.04
29	Y1	604	CLA	C1-O2A-CGA	2.76	123.69	116.44
29	y1	612	CLA	CHD-C1D-ND	-2.76	121.92	124.45
29	G1	604	CLA	C2D-C1D-ND	2.76	112.14	110.10
29	s1	612	CLA	CMA-C3A-C4A	2.76	119.20	111.77
48	Y1	607	CHL	C2C-C3C-C4C	2.76	108.46	106.49
29	G1	614	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
29	B	611	CLA	C2D-C1D-ND	2.76	112.14	110.10
29	y1	608	CLA	CMA-C3A-C4A	2.76	119.19	111.77
38	s	626	3PH	O31-C31-C32	2.76	120.57	111.91
29	s	602	CLA	C1-C2-C3	-2.76	121.27	126.04
29	N1	613	CLA	C1C-C2C-C3C	-2.76	104.05	106.96
48	Y1	609	CHL	CMA-C3A-C4A	2.76	119.19	111.77
48	S	607	CHL	CHB-C4A-NA	2.76	128.33	124.51
29	c	506	CLA	C1C-C2C-C3C	-2.76	104.06	106.96
29	Y1	608	CLA	C1C-C2C-C3C	-2.76	104.06	106.96
29	c	503	CLA	C1-C2-C3	-2.76	121.27	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S	612	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
29	B1	603	CLA	CHD-C1D-ND	-2.76	121.92	124.45
48	R1	606	CHL	CHD-C1D-ND	-2.76	121.92	124.45
29	s1	604	CLA	CMD-C2D-C3D	-2.76	121.27	127.61
40	d1	409	LHG	O8-C23-C24	2.76	120.56	111.91
29	g	613	CLA	CMA-C3A-C4A	2.76	119.18	111.77
29	y	603	CLA	CMA-C3A-C4A	2.76	119.18	111.77
29	Y	610	CLA	C1D-ND-C4D	-2.76	104.38	106.33
48	n1	606	CHL	C4D-CHA-C1A	2.76	124.60	121.25
29	s1	604	CLA	CMA-C3A-C4A	2.76	119.18	111.77
29	B1	615	CLA	CMA-C3A-C4A	2.76	119.18	111.77
29	r	602	CLA	C2C-C1C-NC	2.76	112.55	109.97
29	C1	512	CLA	C2D-C1D-ND	2.75	112.13	110.10
51	Y	623	NEX	C1-C2-C3	2.75	119.86	113.64
29	a1	405	CLA	CMB-C2B-C3B	2.75	129.83	124.68
29	n	603	CLA	CHD-C1D-ND	-2.75	121.92	124.45
29	C1	506	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
31	d	404	BCR	C33-C5-C4	2.75	118.91	113.62
52	r1	625	LMT	C3'-C4'-C5'	-2.75	104.61	110.93
29	g	602	CLA	CMA-C3A-C4A	2.75	119.17	111.77
29	C1	504	CLA	C1C-C2C-C3C	-2.75	104.06	106.96
50	y	622	XAT	C26-C27-C28	-2.75	120.17	125.99
49	R	620	LUT	C7-C8-C9	-2.75	122.08	126.23
29	S1	611	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
29	N	604	CLA	OBD-CAD-C3D	-2.75	121.90	128.52
29	N	604	CLA	C2C-C1C-NC	2.75	112.55	109.97
48	R1	607	CHL	C1-O2A-CGA	2.75	123.66	116.44
31	C	517	BCR	C31-C1-C6	-2.75	105.84	110.30
29	C	506	CLA	C1C-C2C-C3C	-2.75	104.07	106.96
29	Y	602	CLA	O2A-CGA-CBA	2.75	120.53	111.91
29	D1	403	CLA	CMA-C3A-C4A	2.75	119.16	111.77
40	g1	624	LHG	C6-C5-C4	-2.75	105.29	111.79
49	n	621	LUT	C38-C25-C24	-2.75	117.68	123.56
49	r	620	LUT	C37-C21-C22	-2.75	104.23	109.44
49	S	621	LUT	C38-C25-C24	-2.75	117.68	123.56
48	G1	606	CHL	CMA-C3A-C4A	2.75	119.16	111.77
29	C	512	CLA	CMB-C2B-C1B	-2.75	124.24	128.46
48	N	605	CHL	CMA-C3A-C4A	2.75	119.16	111.77
29	Y1	614	CLA	OBD-CAD-C3D	-2.75	121.91	128.52
29	y	602	CLA	C2C-C1C-NC	2.75	112.54	109.97
29	b1	615	CLA	CHA-C4D-ND	2.74	138.24	132.50
48	s	601	CHL	C4A-NA-C1A	2.74	107.94	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	R1	603	CLA	CMA-C3A-C4A	2.74	119.15	111.77
48	R	607	CHL	CHD-C1D-ND	-2.74	121.93	124.45
55	y1	627	PTY	C6-O7-C8	-2.74	112.78	117.90
29	n	611	CLA	C1C-C2C-C3C	-2.74	104.07	106.96
29	R	609	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
29	C	502	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
29	c1	513	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
29	S1	603	CLA	CMA-C3A-C4A	2.74	119.14	111.77
53	R1	626	ERG	C13-C14-C8	2.74	118.80	113.48
29	B	617	CLA	C1-C2-C3	-2.74	121.30	126.04
40	d	409	LHG	C5-O7-C7	-2.74	111.04	117.79
54	s	625	LPX	O3-P1-O4	2.74	125.79	112.24
50	r	621	XAT	O24-C25-C38	-2.74	111.77	115.06
48	G	601	CHL	CMA-C3A-C4A	2.74	119.14	111.77
48	Y1	601	CHL	C3C-C4C-NC	-2.74	107.50	110.57
49	Y1	620	LUT	C35-C15-C14	-2.74	117.86	123.47
29	N1	614	CLA	C2D-C1D-ND	2.74	112.12	110.10
29	r1	603	CLA	O2A-CGA-CBA	2.74	120.50	111.91
29	S1	604	CLA	CAA-CBA-CGA	-2.74	105.25	113.25
48	N1	608	CHL	C1-O2A-CGA	2.74	123.63	116.44
29	D1	403	CLA	O2D-CGD-O1D	-2.74	118.48	123.84
29	b1	605	CLA	CHA-C1A-NA	-2.74	120.13	126.40
29	D1	402	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
40	d	408	LHG	O8-C23-C24	2.74	120.50	111.91
29	n1	613	CLA	C1-O2A-CGA	2.74	123.62	116.44
29	C1	503	CLA	C2C-C1C-NC	2.74	112.54	109.97
29	Y	604	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
29	Y	604	CLA	O1D-CGD-CBD	-2.74	118.88	124.48
29	S	604	CLA	C1-O2A-CGA	2.74	123.62	116.44
29	y	614	CLA	C1C-C2C-C3C	-2.74	104.08	106.96
29	y	602	CLA	O2A-CGA-CBA	2.74	120.49	111.91
48	S	601	CHL	C2C-C3C-C4C	2.74	108.44	106.49
29	C	510	CLA	CMD-C2D-C3D	-2.74	121.32	127.61
53	r1	626	ERG	C4-C5-C10	2.74	120.05	116.42
29	R1	612	CLA	C1C-C2C-C3C	-2.73	104.08	106.96
51	y	623	NEX	C39-C29-C30	-2.73	119.09	122.92
29	y1	602	CLA	CMB-C2B-C3B	2.73	129.79	124.68
29	c1	503	CLA	C2D-C1D-ND	2.73	112.12	110.10
29	c1	513	CLA	CBA-CAA-C2A	2.73	121.93	113.86
29	G	610	CLA	CMA-C3A-C4A	2.73	119.12	111.77
29	S1	604	CLA	C1-C2-C3	-2.73	121.32	126.04
33	w1	201	LMG	O8-C28-C29	2.73	120.48	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a1	410	CLA	CMB-C2B-C1B	-2.73	124.26	128.46
48	S	606	CHL	CMA-C3A-C4A	2.73	119.11	111.77
29	s	605	CLA	C1-O2A-CGA	2.73	123.61	116.44
29	y1	611	CLA	C2D-C1D-ND	2.73	112.12	110.10
48	y1	607	CHL	C1B-CHB-C4A	-2.73	124.71	130.12
29	c	511	CLA	CMB-C2B-C1B	-2.73	124.27	128.46
48	S	608	CHL	C1-O2A-CGA	2.73	123.60	116.44
29	y	608	CLA	C2D-C1D-ND	2.73	112.11	110.10
29	n1	613	CLA	C2D-C1D-ND	2.73	112.11	110.10
29	b	605	CLA	CMD-C2D-C3D	-2.73	121.34	127.61
29	c	510	CLA	CMD-C2D-C3D	-2.73	121.34	127.61
29	C	511	CLA	C1-C2-C3	-2.73	121.33	126.04
48	S1	607	CHL	CHB-C4A-NA	2.73	128.28	124.51
29	n	612	CLA	CHD-C1D-ND	-2.73	121.95	124.45
29	S1	609	CLA	CAA-C2A-C3A	-2.73	105.31	112.78
31	c1	514	BCR	C15-C14-C13	-2.73	123.42	127.31
51	R1	622	NEX	C15-C14-C13	2.73	131.20	127.31
29	B	615	CLA	C2C-C1C-NC	2.73	112.53	109.97
31	D	404	BCR	C33-C5-C6	-2.73	121.47	124.53
29	B	605	CLA	CHA-C4D-ND	2.73	138.20	132.50
29	S1	602	CLA	CAA-C2A-C3A	-2.73	105.31	112.78
29	N	611	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
29	c1	512	CLA	C1-C2-C3	-2.73	121.33	126.04
29	N	614	CLA	CMA-C3A-C4A	2.73	119.10	111.77
33	d1	411	LMG	O8-C28-C29	2.73	120.46	111.91
29	s	617	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
29	N1	603	CLA	C1-C2-C3	-2.73	121.33	126.04
31	C	514	BCR	C33-C5-C6	-2.72	121.47	124.53
36	B1	620	C7Z	C18-C5-C6	-2.72	121.47	124.53
29	b	604	CLA	O2D-CGD-O1D	-2.72	118.51	123.84
29	g	602	CLA	C1-C2-C3	-2.72	121.33	126.04
29	c1	505	CLA	C2C-C1C-NC	2.72	112.52	109.97
48	N1	601	CHL	C4D-CHA-C1A	2.72	124.56	121.25
40	Y1	624	LHG	C5-O7-C7	-2.72	111.08	117.79
29	A	410	CLA	CAA-C2A-C3A	-2.72	105.32	112.78
48	g	601	CHL	CHB-C4A-NA	2.72	128.28	124.51
48	s	608	CHL	CMA-C3A-C4A	2.72	119.09	111.77
33	c1	523	LMG	O8-C28-C29	2.72	120.45	111.91
48	Y	601	CHL	CHB-C4A-NA	2.72	128.28	124.51
31	b1	619	BCR	C1-C6-C5	-2.72	118.78	122.61
48	g	608	CHL	C4D-CHA-C1A	2.72	124.56	121.25
38	t1	101	3PH	O31-C31-C32	2.72	120.45	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	619	BCR	C12-C13-C14	-2.72	114.76	118.94
29	c1	506	CLA	CMA-C3A-C4A	2.72	119.09	111.77
29	s	603	CLA	C1-O2A-CGA	2.72	123.58	116.44
48	Y1	606	CHL	C1-C2-C3	-2.72	121.34	126.04
49	s	620	LUT	C40-C33-C32	2.72	122.36	118.08
29	S1	605	CLA	O2A-CGA-CBA	2.72	120.44	111.91
29	S	604	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
29	B1	603	CLA	O2A-CGA-CBA	2.72	120.44	111.91
29	a	410	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
29	b1	613	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
48	g	607	CHL	C1B-CHB-C4A	-2.72	124.73	130.12
50	G	622	XAT	C11-C10-C9	-2.72	123.43	127.31
31	B1	618	BCR	C33-C5-C4	2.72	118.84	113.62
29	C1	512	CLA	CMA-C3A-C4A	2.72	119.08	111.77
29	N	611	CLA	C2D-C1D-ND	2.72	112.11	110.10
29	c	503	CLA	C2D-C1D-ND	2.72	112.11	110.10
31	b	619	BCR	C33-C5-C6	-2.72	121.48	124.53
48	n1	606	CHL	C1B-CHB-C4A	-2.72	124.73	130.12
51	N1	623	NEX	C1-C2-C3	2.72	119.78	113.64
29	b1	609	CLA	C1C-C2C-C3C	-2.72	104.10	106.96
29	s1	611	CLA	CMA-C3A-C4A	2.72	119.08	111.77
29	B1	604	CLA	C2C-C1C-NC	2.72	112.52	109.97
29	s1	611	CLA	C2D-C1D-ND	2.72	112.11	110.10
29	s1	614	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
29	C1	513	CLA	CMB-C2B-C1B	-2.71	124.29	128.46
31	B1	618	BCR	C8-C9-C10	2.71	123.11	118.94
49	y	620	LUT	C10-C11-C12	-2.71	114.75	123.22
29	r	610	CLA	O2A-CGA-CBA	2.71	120.42	111.91
29	R1	609	CLA	O2A-CGA-CBA	2.71	120.42	111.91
29	g	610	CLA	CMB-C2B-C3B	2.71	129.75	124.68
48	y1	609	CHL	CHC-C1C-NC	2.71	128.32	124.20
49	n1	620	LUT	C38-C25-C24	-2.71	117.76	123.56
29	b1	617	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
29	a1	407	CLA	C3D-C2D-C1D	-2.71	102.13	105.83
48	N1	609	CHL	C4D-CHA-C1A	2.71	124.55	121.25
29	N	603	CLA	C2C-C1C-NC	2.71	112.51	109.97
29	C1	507	CLA	C1-C2-C3	-2.71	121.35	126.04
40	G1	624	LHG	C6-C5-C4	-2.71	105.38	111.79
49	N	620	LUT	C15-C14-C13	-2.71	123.44	127.31
29	C	506	CLA	O2A-CGA-CBA	2.71	120.41	111.91
29	B1	613	CLA	CHA-C4D-ND	2.71	138.17	132.50
29	n	611	CLA	CAA-C2A-C3A	-2.71	105.36	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	b	618	BCR	C19-C18-C17	2.71	123.10	118.94
29	g1	613	CLA	CMC-C2C-C1C	2.71	129.17	125.04
29	B	616	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
29	s	604	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
29	s	610	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
29	Y	610	CLA	C2C-C1C-NC	2.71	112.51	109.97
29	G1	604	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
29	B	614	CLA	CMB-C2B-C1B	-2.71	124.30	128.46
29	y	611	CLA	C2C-C1C-NC	2.71	112.51	109.97
29	R	608	CLA	CHA-C4D-ND	2.71	138.16	132.50
29	b1	612	CLA	CHA-C4D-ND	2.71	138.16	132.50
29	n1	614	CLA	CMA-C3A-C4A	2.71	119.05	111.77
48	y1	609	CHL	C4D-CHA-C1A	2.71	124.54	121.25
29	C	501	CLA	C2D-C1D-ND	2.71	112.10	110.10
29	C1	510	CLA	C1C-C2C-C3C	-2.71	104.11	106.96
29	s	604	CLA	C1-C2-C3	-2.71	121.36	126.04
54	S	625	LPX	O3-P1-O4	2.71	125.61	112.24
29	s	611	CLA	CHD-C1D-ND	-2.71	121.97	124.45
29	C	513	CLA	C2C-C1C-NC	2.70	112.51	109.97
47	K1	101	4RF	O40-C41-C43	2.70	120.40	111.91
29	b1	605	CLA	CHA-C4D-ND	2.70	138.16	132.50
48	N	605	CHL	C1-O2A-CGA	2.70	123.54	116.44
29	G	604	CLA	CMA-C3A-C4A	2.70	119.04	111.77
48	G	606	CHL	C4D-CHA-C1A	2.70	124.54	121.25
29	b	604	CLA	CHA-C4D-ND	2.70	138.16	132.50
29	G	610	CLA	CAA-C2A-C3A	-2.70	105.37	112.78
29	B	609	CLA	CHD-C1D-ND	-2.70	121.97	124.45
29	C	506	CLA	CHD-C1D-ND	-2.70	121.97	124.45
29	c	509	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
29	d	403	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
29	g1	612	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
29	S	610	CLA	OBD-CAD-C3D	-2.70	122.01	128.52
29	B	611	CLA	C1-O2A-CGA	2.70	123.54	116.44
29	b1	614	CLA	C2D-C1D-ND	2.70	112.10	110.10
29	G1	613	CLA	C1D-ND-C4D	-2.70	104.42	106.33
29	d	403	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
29	S	613	CLA	C1C-C2C-C3C	-2.70	104.11	106.96
51	s	623	NEX	C19-C9-C10	-2.70	119.14	122.92
31	B	618	BCR	C19-C18-C17	2.70	123.09	118.94
48	S1	608	CHL	C1-O2A-CGA	2.70	123.53	116.44
29	n	612	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
47	i	101	4RF	O18-C16-C15	2.70	120.38	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	N	609	CHL	C1B-CHB-C4A	-2.70	124.77	130.12
29	s1	610	CLA	O2A-CGA-CBA	2.70	120.38	111.91
29	B	613	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
31	c	515	BCR	C33-C5-C4	2.70	118.80	113.62
40	s	624	LHG	O8-C23-C24	2.70	120.38	111.91
29	c1	507	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
48	y1	606	CHL	CHD-C1D-ND	-2.70	121.97	124.45
49	r1	620	LUT	C31-C32-C33	-2.70	118.83	126.42
29	B1	609	CLA	C1-O2A-CGA	2.70	123.53	116.44
31	d	404	BCR	C36-C18-C17	-2.70	119.14	122.92
49	S	620	LUT	C31-C30-C29	-2.70	123.46	127.31
29	A	407	CLA	CMA-C3A-C4A	2.70	119.03	111.77
29	S1	602	CLA	C1-C2-C3	-2.70	121.38	126.04
49	r1	620	LUT	C1-C6-C5	-2.70	118.81	122.61
29	r1	609	CLA	C1-C2-C3	-2.70	121.38	126.04
29	d1	403	CLA	C2C-C1C-NC	2.70	112.50	109.97
29	S	604	CLA	O2A-CGA-CBA	2.70	120.37	111.91
37	c	520	DGD	O1G-C1A-C2A	2.70	120.37	111.91
48	g	601	CHL	CMA-C3A-C4A	2.70	119.02	111.77
29	c	513	CLA	C1C-C2C-C3C	-2.70	104.12	106.96
29	y	611	CLA	CHD-C1D-ND	-2.70	121.98	124.45
29	c	511	CLA	C2C-C1C-NC	2.70	112.50	109.97
29	s	610	CLA	C2C-C1C-NC	2.70	112.50	109.97
43	D1	405	PL9	C36-C34-C33	-2.70	115.66	121.12
29	N	612	CLA	CHA-C4D-ND	2.70	138.14	132.50
29	r1	610	CLA	CAA-C2A-C3A	-2.70	105.40	112.78
29	C1	504	CLA	C2D-C1D-ND	2.69	112.09	110.10
29	g1	602	CLA	C2D-C1D-ND	2.69	112.09	110.10
50	R	621	XAT	C40-C33-C34	-2.69	119.15	122.92
29	B1	603	CLA	C1-O2A-CGA	2.69	123.51	116.44
43	d1	405	PL9	C40-C39-C41	2.69	119.80	115.27
29	N	603	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
29	S	611	CLA	C1-C2-C3	-2.69	121.38	126.04
48	N	607	CHL	C1-C2-C3	-2.69	121.38	126.04
29	C	507	CLA	CHD-C1D-ND	-2.69	121.98	124.45
55	Y1	626	PTY	O4-C30-C31	2.69	120.36	111.91
29	b	612	CLA	C2D-C1D-ND	2.69	112.09	110.10
29	R1	602	CLA	CHD-C1D-ND	-2.69	121.98	124.45
29	b	614	CLA	CMD-C2D-C3D	-2.69	121.42	127.61
29	D	402	CLA	O2A-CGA-CBA	2.69	120.36	111.91
49	r1	620	LUT	C18-C5-C4	2.69	119.34	114.36
48	S	601	CHL	CMA-C3A-C4A	2.69	119.01	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	603	CLA	C2D-C1D-ND	2.69	112.09	110.10
29	s	605	CLA	CAA-C2A-C3A	-2.69	105.41	112.78
51	N1	623	NEX	C31-C30-C29	2.69	131.15	127.31
51	N	623	NEX	C38-C25-C26	-2.69	117.75	122.26
29	Y1	603	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
29	n1	612	CLA	CHD-C1D-ND	-2.69	121.98	124.45
29	A1	410	CLA	CAA-C2A-C3A	-2.69	105.41	112.78
48	R	607	CHL	C1-O2A-CGA	2.69	123.50	116.44
49	Y	621	LUT	C18-C5-C6	-2.69	121.51	124.53
50	n1	622	XAT	C26-C27-C28	-2.69	120.31	125.99
29	y	610	CLA	CAA-C2A-C3A	-2.69	105.42	112.78
30	A1	409	PHO	O2D-CGD-O1D	-2.69	118.58	123.84
29	B	604	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
29	S1	603	CLA	C1-O2A-CGA	2.69	123.50	116.44
31	C1	517	BCR	C23-C22-C21	2.69	123.07	118.94
29	s1	602	CLA	C2D-C1D-ND	2.69	112.08	110.10
48	R1	607	CHL	CHB-C4A-NA	2.69	128.23	124.51
29	A	410	CLA	O2A-CGA-CBA	2.69	120.34	111.91
29	c1	504	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
48	g	601	CHL	C1-C2-C3	-2.69	121.39	126.04
29	b1	604	CLA	C1D-ND-C4D	-2.69	104.43	106.33
48	Y	606	CHL	CHB-C4A-NA	2.69	128.23	124.51
31	C	516	BCR	C28-C27-C26	-2.69	109.28	114.08
29	c	501	CLA	CMA-C3A-C4A	2.69	119.00	111.77
29	G	611	CLA	C1-C2-C3	-2.69	121.40	126.04
29	S	603	CLA	C2D-C1D-ND	2.69	112.08	110.10
29	Y1	610	CLA	O1D-CGD-CBD	-2.69	118.99	124.48
29	n	604	CLA	C1C-C2C-C3C	-2.69	104.13	106.96
29	s	613	CLA	C1D-ND-C4D	-2.69	104.43	106.33
48	s	608	CHL	CHB-C4A-NA	2.69	128.22	124.51
48	y1	601	CHL	C3C-C4C-NC	-2.68	107.56	110.57
31	b1	619	BCR	C4-C5-C6	-2.68	118.83	122.73
48	g	607	CHL	C4A-NA-C1A	2.68	107.91	106.71
29	S	602	CLA	CMB-C2B-C1B	-2.68	124.34	128.46
29	B	602	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
29	c1	504	CLA	CMD-C2D-C3D	-2.68	121.44	127.61
29	R	603	CLA	C2C-C1C-NC	2.68	112.48	109.97
29	Y1	602	CLA	CHA-C4D-ND	2.68	138.11	132.50
29	r	602	CLA	O2A-CGA-CBA	2.68	120.32	111.91
29	G1	610	CLA	O1D-CGD-CBD	-2.68	119.00	124.48
29	s1	611	CLA	CHA-C4D-ND	2.68	138.11	132.50
29	C	512	CLA	C1C-C2C-C3C	-2.68	104.14	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	N	607	CHL	CMA-C3A-C4A	2.68	118.98	111.77
29	c	508	CLA	C2C-C1C-NC	2.68	112.48	109.97
31	B	619	BCR	C35-C13-C12	2.68	122.30	118.08
48	y	605	CHL	CHD-C4C-C3C	2.68	128.78	124.84
29	R1	609	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
31	c	517	BCR	C2-C1-C6	2.68	114.61	110.48
29	r	608	CLA	C2C-C1C-NC	2.68	112.48	109.97
29	r1	604	CLA	CMB-C2B-C1B	-2.68	124.35	128.46
50	g1	622	XAT	C39-C29-C30	-2.68	119.17	122.92
48	n	608	CHL	C3C-C4C-NC	-2.68	107.57	110.57
49	n1	621	LUT	C10-C11-C12	-2.68	114.86	123.22
29	n1	613	CLA	CMA-C3A-C4A	2.68	118.97	111.77
48	n	607	CHL	C2C-C3C-C4C	2.68	108.40	106.49
48	N	608	CHL	CHB-C4A-NA	2.68	128.22	124.51
50	y1	622	XAT	C40-C33-C34	-2.68	119.17	122.92
45	H	101	RRX	C32-C1-C6	-2.68	105.96	110.30
29	B	614	CLA	C1D-ND-C4D	-2.68	104.43	106.33
29	G	614	CLA	C1-O2A-CGA	2.68	123.47	116.44
48	R	607	CHL	CHB-C4A-NA	2.68	128.21	124.51
29	a1	406	CLA	CHA-C4D-ND	2.68	138.10	132.50
29	b1	614	CLA	CMA-C3A-C4A	2.68	118.97	111.77
38	T1	101	3PH	O31-C31-C32	2.68	120.31	111.91
48	y	609	CHL	CHD-C4C-C3C	2.68	128.77	124.84
29	n1	611	CLA	C1C-C2C-C3C	-2.68	104.14	106.96
50	r1	621	XAT	C38-C25-C26	-2.68	117.78	122.26
29	c	501	CLA	C2C-C1C-NC	2.68	112.48	109.97
29	R1	608	CLA	C1C-C2C-C3C	-2.67	104.14	106.96
29	y1	611	CLA	C1C-C2C-C3C	-2.67	104.14	106.96
29	C1	511	CLA	C1C-C2C-C3C	-2.67	104.14	106.96
29	B1	607	CLA	C2C-C1C-NC	2.67	112.48	109.97
29	s1	612	CLA	C2D-C1D-ND	2.67	112.07	110.10
29	a1	406	CLA	OBD-CAD-C3D	-2.67	122.09	128.52
29	r	608	CLA	CMB-C2B-C3B	2.67	129.68	124.68
37	b1	623	DGD	C4E-C3E-C2E	2.67	115.49	110.82
50	Y1	622	XAT	C19-C9-C10	-2.67	119.18	122.92
29	C1	502	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
29	y	613	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
51	r	622	NEX	C5-C4-C3	-2.67	108.58	111.75
51	g	623	NEX	C15-C14-C13	2.67	131.12	127.31
29	A	405	CLA	CMD-C2D-C3D	-2.67	121.47	127.61
29	B1	614	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
48	s1	601	CHL	CHD-C4C-C3C	2.67	128.76	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	n1	602	CLA	CMB-C2B-C3B	2.67	129.67	124.68
30	A	409	PHO	C1-C2-C3	-2.67	121.43	126.04
29	S1	603	CLA	CHA-C4D-ND	2.67	138.08	132.50
29	G1	611	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
29	Y1	608	CLA	CHD-C1D-ND	-2.67	122.00	124.45
36	B	620	C7Z	C24-C25-C26	-2.67	114.90	120.85
48	G	601	CHL	CHD-C4C-C3C	2.67	128.76	124.84
29	r	603	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
29	S	605	CLA	CHA-C4D-ND	2.67	138.08	132.50
31	c1	514	BCR	C34-C9-C10	-2.67	119.19	122.92
48	G	601	CHL	C1-C2-C3	-2.67	121.43	126.04
29	B1	607	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
29	G1	613	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
51	S	623	NEX	C31-C30-C29	2.67	131.12	127.31
29	y1	608	CLA	CMD-C2D-C3D	-2.67	121.48	127.61
29	n1	610	CLA	O2A-CGA-CBA	2.67	120.28	111.91
29	c	505	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
29	n	611	CLA	CMA-C3A-C4A	2.67	118.94	111.77
31	A1	411	BCR	C35-C13-C12	2.67	122.28	118.08
29	B	616	CLA	C1D-ND-C4D	-2.67	104.44	106.33
29	G1	614	CLA	CMA-C3A-C4A	2.67	118.94	111.77
29	y1	608	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
29	r	603	CLA	C1C-C2C-C3C	-2.67	104.15	106.96
29	s	614	CLA	O2A-CGA-CBA	2.67	120.28	111.91
29	b	607	CLA	CMB-C2B-C1B	-2.67	124.37	128.46
36	B1	620	C7Z	C21-C26-C27	2.67	123.32	115.78
29	S	609	CLA	CAA-C2A-C3A	-2.67	105.48	112.78
29	A	410	CLA	C1-C2-C3	-2.67	121.43	126.04
29	b1	611	CLA	C1-C2-C3	-2.67	121.43	126.04
29	b1	612	CLA	C3D-C2D-C1D	-2.67	102.19	105.83
48	y1	601	CHL	C4D-CHA-C1A	2.67	124.49	121.25
48	G1	606	CHL	C3C-C4C-NC	-2.67	107.58	110.57
51	S1	623	NEX	C38-C25-C26	-2.67	117.79	122.26
50	r1	621	XAT	C15-C35-C34	2.66	128.93	123.47
49	r1	620	LUT	C20-C13-C14	-2.66	119.19	122.92
39	c	524	DGA	OG1-CA1-CA2	2.66	120.27	111.91
48	g1	606	CHL	CMA-C3A-C4A	2.66	118.93	111.77
29	C1	503	CLA	CHD-C1D-ND	-2.66	122.01	124.45
48	N1	607	CHL	C1-C2-C3	-2.66	121.44	126.04
47	K	101	4RF	O18-C16-C15	2.66	120.27	111.91
29	r1	608	CLA	C2D-C1D-ND	2.66	112.07	110.10
29	n	614	CLA	C1D-ND-C4D	-2.66	104.44	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	G1	610	CLA	C2C-C1C-NC	2.66	112.47	109.97
31	c1	517	BCR	C23-C22-C21	2.66	123.03	118.94
29	s1	605	CLA	CHD-C1D-ND	-2.66	122.01	124.45
29	y1	603	CLA	CHA-C4D-ND	2.66	138.07	132.50
29	c	512	CLA	O2A-CGA-CBA	2.66	120.26	111.91
31	b	619	BCR	C35-C13-C12	2.66	122.27	118.08
29	b1	616	CLA	CHD-C1D-ND	-2.66	122.01	124.45
29	g1	613	CLA	C1D-ND-C4D	-2.66	104.44	106.33
29	g1	610	CLA	CMB-C2B-C1B	-2.66	124.38	128.46
48	R1	606	CHL	C4A-NA-C1A	2.66	107.90	106.71
29	n1	604	CLA	CHA-C4D-ND	2.66	138.06	132.50
29	c1	503	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
48	y1	605	CHL	CHB-C4A-NA	2.66	128.19	124.51
50	n1	622	XAT	O4-C5-C4	-2.66	111.38	113.38
29	N	602	CLA	O2A-CGA-CBA	2.66	120.25	111.91
29	s1	611	CLA	O2A-CGA-CBA	2.66	120.25	111.91
29	R1	609	CLA	CMA-C3A-C4A	2.66	118.92	111.77
29	g1	603	CLA	CHD-C1D-ND	-2.66	122.01	124.45
29	y1	608	CLA	CHA-C4D-ND	2.66	138.06	132.50
29	y1	614	CLA	CHA-C4D-ND	2.66	138.06	132.50
45	h1	101	RRX	C1-C6-C5	-2.66	118.87	122.61
29	c1	511	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
29	y	614	CLA	C1-C2-C3	-2.66	121.44	126.04
29	Y	612	CLA	O2A-CGA-CBA	2.66	120.25	111.91
29	b	602	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
29	c1	513	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
29	r1	603	CLA	C1C-C2C-C3C	-2.66	104.16	106.96
49	n1	621	LUT	C40-C33-C34	-2.66	119.20	122.92
29	Y1	602	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
29	g1	613	CLA	O2A-CGA-CBA	2.66	120.25	111.91
29	y	614	CLA	CAA-C2A-C3A	-2.66	105.50	112.78
29	R1	604	CLA	C2D-C1D-ND	2.66	112.06	110.10
41	C	527	LMK	O3-C4-C3	-2.66	113.87	122.98
29	G1	613	CLA	O2A-CGA-CBA	2.66	120.24	111.91
49	s1	621	LUT	C2-C3-C4	-2.66	106.67	110.30
29	A1	406	CLA	OBD-CAD-C3D	-2.66	122.13	128.52
29	r1	612	CLA	C2C-C1C-NC	2.66	112.46	109.97
29	s	614	CLA	CMD-C2D-C3D	-2.66	121.50	127.61
29	B	615	CLA	CHA-C4D-ND	2.66	138.05	132.50
37	C	520	DGD	O1G-C1A-C2A	2.66	120.24	111.91
53	r1	626	ERG	C6-C7-C8	-2.66	116.84	122.07
45	H1	101	RRX	C15-C16-C17	-2.66	118.03	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S	621	LUT	C39-C29-C28	2.65	122.26	118.08
29	n1	604	CLA	C2D-C1D-ND	2.65	112.06	110.10
51	s	623	NEX	C17-C1-C6	-2.65	108.10	110.47
29	n	612	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
29	R	610	CLA	O1D-CGD-CBD	-2.65	119.06	124.48
29	c	513	CLA	CMA-C3A-C4A	2.65	118.90	111.77
29	g1	612	CLA	C1D-ND-C4D	-2.65	104.45	106.33
50	R	621	XAT	C10-C11-C12	-2.65	114.94	123.22
29	s	614	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
45	h1	101	RRX	C2-C1-C6	2.65	114.56	110.48
48	S1	601	CHL	C3C-C4C-NC	-2.65	107.60	110.57
29	C1	511	CLA	CMD-C2D-C3D	-2.65	121.52	127.61
29	s	609	CLA	CMA-C3A-C4A	2.65	118.90	111.77
49	n	620	LUT	C22-C23-C24	-2.65	108.72	111.74
29	Y	613	CLA	C1-O2A-CGA	2.65	123.39	116.44
29	B1	610	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
50	Y1	622	XAT	C20-C13-C14	-2.65	119.21	122.92
29	S	614	CLA	CMD-C2D-C3D	-2.65	121.52	127.61
48	n	606	CHL	CHB-C4A-NA	2.65	128.18	124.51
49	s	621	LUT	C7-C8-C9	-2.65	122.23	126.23
48	S1	606	CHL	CMA-C3A-C4A	2.65	118.89	111.77
48	y1	601	CHL	CHB-C4A-NA	2.65	128.17	124.51
29	B	607	CLA	CHA-C4D-ND	2.65	138.04	132.50
51	g	623	NEX	C40-C33-C34	-2.65	119.21	122.92
48	Y	609	CHL	C1D-CHD-C4C	-2.65	120.35	126.06
29	A	405	CLA	C2D-C1D-ND	2.65	112.06	110.10
29	c	501	CLA	O2A-CGA-CBA	2.65	120.22	111.91
29	A	405	CLA	CMC-C2C-C1C	2.65	129.07	125.04
29	s1	604	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
29	S	613	CLA	CHD-C1D-ND	-2.65	122.02	124.45
31	c1	514	BCR	C36-C18-C17	-2.65	119.22	122.92
29	C	509	CLA	CMD-C2D-C3D	-2.65	121.53	127.61
31	c	515	BCR	C23-C22-C21	-2.65	114.88	118.94
49	N1	621	LUT	C1-C6-C5	-2.65	118.89	122.61
29	c	512	CLA	C1C-C2C-C3C	-2.65	104.17	106.96
29	b1	616	CLA	O2D-CGD-O1D	-2.65	118.67	123.84
29	S	603	CLA	CHD-C1D-ND	-2.65	122.02	124.45
29	r	612	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
29	a	407	CLA	C1-O2A-CGA	2.64	123.38	116.44
29	b1	607	CLA	CAA-C2A-C3A	-2.64	105.54	112.78
29	b1	617	CLA	OBD-CAD-C3D	-2.64	122.16	128.52
31	b	619	BCR	C33-C5-C4	2.64	118.70	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	r	602	CLA	CAA-C2A-C3A	-2.64	105.54	112.78
29	c1	513	CLA	C2C-C1C-NC	2.64	112.45	109.97
51	y1	623	NEX	C27-C28-C29	-2.64	121.43	125.53
29	G	611	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
29	c	503	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
29	S	617	CLA	C2D-C1D-ND	2.64	112.05	110.10
29	S	612	CLA	CMB-C2B-C1B	-2.64	124.40	128.46
29	c1	512	CLA	C1C-C2C-C3C	-2.64	104.18	106.96
51	n	623	NEX	C17-C1-C6	-2.64	108.11	110.47
48	Y	605	CHL	C1B-CHB-C4A	-2.64	124.88	130.12
29	s	603	CLA	CHA-C4D-ND	2.64	138.03	132.50
51	g	623	NEX	C26-C27-C28	-2.64	120.41	125.99
29	g	610	CLA	C2C-C1C-NC	2.64	112.45	109.97
29	b	606	CLA	O2A-CGA-CBA	2.64	120.20	111.91
29	b	603	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
39	J	101	DGA	OG1-CA1-CA2	2.64	120.20	111.91
49	Y1	620	LUT	C1-C2-C3	-2.64	107.68	113.64
29	d1	402	CLA	C2D-C1D-ND	2.64	112.05	110.10
29	Y1	603	CLA	CHA-C4D-ND	2.64	138.02	132.50
48	G1	609	CHL	CHB-C4A-NA	2.64	128.16	124.51
31	b1	619	BCR	C8-C7-C6	-2.64	119.79	127.20
40	G	624	LHG	C6-C5-C4	-2.64	105.55	111.79
51	y	623	NEX	C38-C25-C26	-2.64	117.84	122.26
29	C1	511	CLA	CMA-C3A-C4A	2.64	118.86	111.77
29	b1	606	CLA	CAC-C3C-C4C	2.64	128.23	124.81
49	G	621	LUT	C31-C30-C29	-2.64	123.55	127.31
29	a1	405	CLA	CMD-C2D-C3D	-2.64	121.55	127.61
29	b	605	CLA	CHA-C4D-ND	2.64	138.02	132.50
29	C1	509	CLA	CMA-C3A-C4A	2.64	118.86	111.77
49	G	621	LUT	C20-C13-C12	2.64	122.23	118.08
48	g1	601	CHL	CHD-C4C-C3C	2.64	128.72	124.84
29	S	610	CLA	O2A-CGA-CBA	2.64	120.18	111.91
29	b1	605	CLA	C2A-C1A-CHA	2.64	128.47	123.86
31	B1	619	BCR	C36-C18-C17	-2.64	119.23	122.92
29	n1	602	CLA	O1D-CGD-CBD	-2.64	119.09	124.48
51	s1	623	NEX	C12-C13-C14	2.64	122.99	118.94
29	C1	501	CLA	C2A-C1A-CHA	2.64	128.47	123.86
37	C	518	DGD	O1G-C1A-C2A	2.64	120.18	111.91
29	C	502	CLA	CHD-C1D-ND	-2.64	122.03	124.45
29	B1	607	CLA	C1D-ND-C4D	-2.64	104.46	106.33
49	n	621	LUT	C16-C1-C6	-2.64	106.03	110.30
29	D1	403	CLA	C1C-C2C-C3C	-2.64	104.19	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	s	620	LUT	C30-C31-C32	-2.63	115.00	123.22
49	S1	620	LUT	C10-C11-C12	-2.63	115.00	123.22
29	C1	501	CLA	O1D-CGD-CBD	-2.63	119.09	124.48
29	R	610	CLA	O2A-CGA-CBA	2.63	120.17	111.91
29	b	613	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
29	C	504	CLA	C2D-C1D-ND	2.63	112.05	110.10
29	N1	614	CLA	CMA-C3A-C4A	2.63	118.85	111.77
29	B1	610	CLA	O2A-CGA-CBA	2.63	120.17	111.91
29	G	604	CLA	CHA-C4D-ND	2.63	138.01	132.50
50	n	622	XAT	C18-C5-C6	-2.63	117.85	122.26
29	S	617	CLA	CMA-C3A-C4A	2.63	118.85	111.77
29	Y	613	CLA	CHA-C4D-ND	2.63	138.01	132.50
29	Y1	610	CLA	O2A-CGA-CBA	2.63	120.17	111.91
29	s1	613	CLA	C2C-C1C-NC	2.63	112.44	109.97
38	T	101	3PH	O31-C31-C32	2.63	120.17	111.91
29	s1	605	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
29	c1	501	CLA	CHA-C4D-ND	2.63	138.00	132.50
29	r1	609	CLA	O2A-CGA-CBA	2.63	120.17	111.91
29	g	603	CLA	CHA-C4D-ND	2.63	138.00	132.50
29	S1	602	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
29	g	604	CLA	OBD-CAD-C3D	-2.63	122.19	128.52
29	S	614	CLA	CHA-C4D-ND	2.63	138.00	132.50
29	G	611	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
29	Y	611	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
29	r	610	CLA	CMA-C3A-C4A	2.63	118.84	111.77
50	G	622	XAT	C6-C7-C8	-2.63	120.43	125.99
29	Y1	604	CLA	O2A-CGA-CBA	2.63	120.16	111.91
29	y	613	CLA	CMB-C2B-C1B	-2.63	124.42	128.46
29	C	505	CLA	O2A-CGA-CBA	2.63	120.16	111.91
33	B	622	LMG	O8-C28-C29	2.63	120.16	111.91
29	y1	604	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
50	Y	622	XAT	C19-C9-C10	-2.63	119.24	122.92
29	g1	611	CLA	C2C-C1C-NC	2.63	112.44	109.97
29	C1	503	CLA	CHA-C4D-ND	2.63	138.00	132.50
29	Y1	614	CLA	CHA-C4D-ND	2.63	138.00	132.50
29	y1	604	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
29	r	612	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
29	C1	507	CLA	OBD-CAD-C3D	-2.63	122.20	128.52
29	c1	505	CLA	OBD-CAD-C3D	-2.63	122.20	128.52
29	b	604	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
29	c1	503	CLA	C1C-C2C-C3C	-2.63	104.19	106.96
29	n1	614	CLA	O2D-CGD-O1D	-2.63	118.70	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	613	CLA	C2C-C1C-NC	2.63	112.43	109.97
29	R1	603	CLA	C2D-C1D-ND	2.63	112.04	110.10
29	S	617	CLA	O2A-CGA-CBA	2.63	120.15	111.91
29	S1	603	CLA	C1C-C2C-C3C	-2.63	104.20	106.96
48	Y	607	CHL	C1-O2A-CGA	2.62	123.33	116.44
29	c1	502	CLA	CHA-C4D-ND	2.62	137.99	132.50
29	B	604	CLA	CHA-C4D-ND	2.62	137.99	132.50
48	n1	605	CHL	CMA-C3A-C4A	2.62	118.83	111.77
29	c1	510	CLA	CMD-C2D-C3D	-2.62	121.58	127.61
29	g1	602	CLA	CMC-C2C-C1C	2.62	129.03	125.04
29	B	612	CLA	O2A-CGA-CBA	2.62	120.14	111.91
29	y	612	CLA	O2A-CGA-CBA	2.62	120.14	111.91
29	s	614	CLA	CMB-C2B-C3B	2.62	129.59	124.68
29	s1	602	CLA	CAA-C2A-C3A	-2.62	105.59	112.78
29	C1	503	CLA	C2D-C1D-ND	2.62	112.04	110.10
29	S1	602	CLA	CHA-C4D-ND	2.62	137.99	132.50
29	s1	609	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
29	y	612	CLA	C1D-ND-C4D	-2.62	104.47	106.33
50	n	622	XAT	C19-C9-C10	-2.62	119.25	122.92
49	y	621	LUT	C11-C10-C9	-2.62	123.57	127.31
36	b1	620	C7Z	C23-C24-C25	2.62	117.08	111.85
53	r	626	ERG	C13-C14-C8	2.62	118.56	113.48
29	B1	603	CLA	CHA-C4D-ND	2.62	137.98	132.50
29	s	617	CLA	CAA-C2A-C3A	-2.62	105.60	112.78
29	C	510	CLA	CMB-C2B-C3B	2.62	129.58	124.68
45	h1	101	RRX	C35-C13-C12	2.62	122.21	118.08
29	g	604	CLA	CMA-C3A-C4A	2.62	118.81	111.77
48	N1	601	CHL	CHD-C4C-C3C	2.62	128.69	124.84
48	n1	609	CHL	CHD-C4C-C3C	2.62	128.69	124.84
29	R	609	CLA	C2D-C1D-ND	2.62	112.03	110.10
48	n1	607	CHL	CHB-C4A-NA	2.62	128.13	124.51
29	n	604	CLA	C2C-C1C-NC	2.62	112.42	109.97
29	n	613	CLA	CHA-C4D-ND	2.62	137.98	132.50
29	g	614	CLA	C1C-C2C-C3C	-2.62	104.20	106.96
29	c	512	CLA	CMA-C3A-C4A	2.62	118.81	111.77
48	n	609	CHL	C1-O2A-CGA	2.62	123.31	116.44
30	a1	408	PHO	CMB-C2B-C3B	2.62	129.57	124.68
29	B	605	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
29	c	506	CLA	CAA-C2A-C3A	-2.62	105.61	112.78
29	C	511	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
29	C1	501	CLA	CHA-C1A-NA	-2.62	120.41	126.40
29	B1	604	CLA	C1C-C2C-C3C	-2.62	104.21	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	g	614	CLA	O2A-CGA-CBA	2.62	120.12	111.91
29	S	604	CLA	C1D-ND-C4D	-2.62	104.48	106.33
29	b	610	CLA	C1D-ND-C4D	-2.62	104.48	106.33
31	C1	515	BCR	C38-C26-C25	-2.62	121.59	124.53
29	B1	602	CLA	C2D-C1D-ND	2.61	112.03	110.10
29	c1	510	CLA	CHA-C4D-ND	2.61	137.97	132.50
29	b1	607	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
29	C	509	CLA	CHA-C4D-ND	2.61	137.97	132.50
29	S	605	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
36	b	620	C7Z	C24-C25-C26	-2.61	115.02	120.85
29	r	609	CLA	C2D-C1D-ND	2.61	112.03	110.10
29	S1	610	CLA	C2D-C1D-ND	2.61	112.03	110.10
29	B1	617	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
44	f	101	HEM	C4D-ND-C1D	2.61	107.77	105.07
36	B	620	C7Z	C11-C12-C13	-2.61	119.08	126.42
29	b1	616	CLA	C6-C5-C3	-2.61	106.60	113.45
47	I	102	4RF	O18-C16-C15	2.61	120.11	111.91
29	b	610	CLA	C1-C2-C3	-2.61	121.53	126.04
29	r1	612	CLA	CMB-C2B-C1B	-2.61	124.45	128.46
29	s	603	CLA	CHA-C1A-NA	-2.61	120.42	126.40
29	Y	608	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
48	S1	608	CHL	CHB-C4A-NA	2.61	128.12	124.51
29	b1	616	CLA	CHA-C4D-ND	2.61	137.96	132.50
29	C1	501	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
49	g1	621	LUT	C38-C25-C24	-2.61	117.97	123.56
29	Y1	604	CLA	CMA-C3A-C4A	2.61	118.79	111.77
29	B1	616	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
49	s1	621	LUT	C31-C32-C33	-2.61	119.08	126.42
29	C1	509	CLA	CHA-C4D-ND	2.61	137.96	132.50
48	n	607	CHL	CMA-C3A-C4A	2.61	118.79	111.77
29	Y	612	CLA	CHD-C1D-ND	-2.61	122.06	124.45
29	r1	604	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
48	g1	605	CHL	C1-O2A-CGA	2.61	124.31	116.73
29	c1	506	CLA	O2A-CGA-CBA	2.61	120.10	111.91
31	B1	619	BCR	C34-C9-C10	-2.61	119.27	122.92
48	S	601	CHL	C1B-CHB-C4A	-2.61	124.95	130.12
29	G	610	CLA	CMB-C2B-C3B	2.61	129.56	124.68
51	Y1	623	NEX	C11-C10-C9	2.61	131.03	127.31
29	C	511	CLA	CAA-CBA-CGA	-2.61	105.63	113.25
29	n1	603	CLA	CHA-C4D-ND	2.61	137.96	132.50
29	r1	610	CLA	CHA-C4D-ND	2.61	137.96	132.50
29	C1	510	CLA	C1D-ND-C4D	-2.61	104.48	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	501	CLA	C1C-C2C-C3C	-2.61	104.21	106.96
33	C1	521	LMG	O8-C28-C29	2.61	120.09	111.91
29	n	613	CLA	C2D-C1D-ND	2.61	112.03	110.10
29	Y1	611	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
29	C1	509	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
29	r1	603	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
29	A1	407	CLA	CMB-C2B-C1B	-2.61	124.46	128.46
31	B	618	BCR	C23-C22-C21	-2.61	114.94	118.94
29	d1	403	CLA	O2A-CGA-CBA	2.61	120.09	111.91
29	S	602	CLA	CHA-C4D-ND	2.61	137.95	132.50
29	B1	616	CLA	C2D-C1D-ND	2.61	112.03	110.10
29	b	617	CLA	C2C-C1C-NC	2.61	112.41	109.97
29	b1	602	CLA	C2C-C1C-NC	2.61	112.41	109.97
48	y1	605	CHL	CMA-C3A-C4A	2.61	118.78	111.77
29	b	612	CLA	CMB-C2B-C3B	2.61	129.56	124.68
45	H	101	RRX	C36-C18-C19	2.61	122.18	118.08
48	N1	609	CHL	CHB-C4A-NA	2.61	128.12	124.51
29	b1	607	CLA	CMA-C3A-C4A	2.61	118.78	111.77
29	C1	503	CLA	O2A-CGA-CBA	2.61	120.08	111.91
48	y1	609	CHL	CHD-C1D-ND	-2.61	122.06	124.45
31	a1	411	BCR	C29-C28-C27	2.60	117.20	111.38
29	Y1	608	CLA	CHA-C4D-ND	2.60	137.95	132.50
42	D1	401	BCT	O3-C-O1	-2.60	112.79	119.55
29	C	510	CLA	C2C-C1C-NC	2.60	112.41	109.97
29	b1	613	CLA	CHA-C4D-ND	2.60	137.95	132.50
29	R1	603	CLA	C1-C2-C3	-2.60	121.54	126.04
48	y	606	CHL	CHB-C4A-NA	2.60	128.11	124.51
29	B1	602	CLA	CHA-C4D-ND	2.60	137.94	132.50
29	G1	612	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
29	b1	617	CLA	C2D-C1D-ND	2.60	112.02	110.10
48	y1	606	CHL	CHB-C4A-NA	2.60	128.11	124.51
29	r	608	CLA	CMB-C2B-C1B	-2.60	124.46	128.46
29	B	609	CLA	OBD-CAD-C3D	-2.60	122.26	128.52
49	G	620	LUT	C18-C5-C4	2.60	119.17	114.36
29	S1	609	CLA	C1D-ND-C4D	-2.60	104.49	106.33
29	Y1	613	CLA	C1-O2A-CGA	2.60	123.27	116.44
29	b1	609	CLA	CHD-C1D-ND	-2.60	122.06	124.45
29	S1	610	CLA	C1D-ND-C4D	-2.60	104.49	106.33
29	a	410	CLA	C2D-C1D-ND	2.60	112.02	110.10
29	y	604	CLA	C1C-C2C-C3C	-2.60	104.22	106.96
29	R1	603	CLA	CAC-C3C-C4C	2.60	128.18	124.81
40	c	525	LHG	C6-C5-C4	-2.60	105.64	111.79

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	617	CLA	CMB-C2B-C3B	2.60	129.54	124.68
29	S1	617	CLA	C2D-C1D-ND	2.60	112.02	110.10
29	C	506	CLA	C6-C5-C3	-2.60	106.64	113.45
40	g	624	LHG	O8-C23-C24	2.60	120.06	111.91
29	S1	613	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
31	C1	514	BCR	C33-C5-C6	-2.60	121.61	124.53
36	b	620	C7Z	C15-C35-C34	-2.60	118.15	123.47
49	r	620	LUT	C30-C31-C32	-2.60	115.11	123.22
29	b1	607	CLA	CHD-C1D-ND	-2.60	122.07	124.45
50	N1	622	XAT	O4-C5-C18	-2.60	111.94	115.06
48	y	601	CHL	C1B-CHB-C4A	-2.60	124.97	130.12
29	c1	508	CLA	CMB-C2B-C1B	-2.60	124.47	128.46
49	n	620	LUT	C8-C7-C6	-2.60	119.91	127.20
48	y	601	CHL	CHB-C4A-NA	2.60	128.10	124.51
29	d	402	CLA	C1D-ND-C4D	-2.60	104.49	106.33
52	R1	625	LMT	C3'-C4'-C5'	-2.60	104.97	110.93
29	B1	616	CLA	CMD-C2D-C3D	-2.60	121.64	127.61
29	G1	614	CLA	CMB-C2B-C3B	2.60	129.53	124.68
29	S1	617	CLA	CMB-C2B-C3B	2.60	129.53	124.68
48	n1	609	CHL	C2C-C3C-C4C	2.60	108.34	106.49
29	c	503	CLA	CMA-C3A-C4A	2.60	118.75	111.77
37	b	623	DGD	O1G-C1A-C2A	2.59	120.05	111.91
29	C	506	CLA	CHA-C4D-ND	2.59	137.93	132.50
29	c	512	CLA	C1-C2-C3	-2.59	121.56	126.04
29	b1	615	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
33	c	523	LMG	O8-C28-C29	2.59	120.05	111.91
29	N	603	CLA	CBC-CAC-C3C	-2.59	105.28	112.43
48	G	609	CHL	C3C-C4C-NC	-2.59	107.66	110.57
29	g	604	CLA	CHA-C4D-ND	2.59	137.93	132.50
29	y	603	CLA	O1D-CGD-CBD	-2.59	119.18	124.48
29	Y	614	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
29	R	603	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
29	b	617	CLA	OBD-CAD-C3D	-2.59	122.28	128.52
29	b1	610	CLA	C1-C2-C3	-2.59	121.56	126.04
29	c	510	CLA	CHA-C4D-ND	2.59	137.92	132.50
48	N	608	CHL	CMA-C3A-C4A	2.59	118.74	111.77
29	c1	512	CLA	CHA-C4D-ND	2.59	137.92	132.50
29	G	602	CLA	C2D-C1D-ND	2.59	112.01	110.10
29	c	513	CLA	C2D-C1D-ND	2.59	112.01	110.10
29	g	610	CLA	O2A-CGA-CBA	2.59	120.04	111.91
29	y	610	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
29	B	606	CLA	C1C-C2C-C3C	-2.59	104.23	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	s1	610	CLA	CHA-C4D-ND	2.59	137.92	132.50
29	d1	402	CLA	C2C-C1C-NC	2.59	112.40	109.97
29	g	603	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
29	s	605	CLA	CHA-C4D-ND	2.59	137.92	132.50
29	a1	405	CLA	C1D-ND-C4D	-2.59	104.50	106.33
29	n1	602	CLA	CMA-C3A-C4A	2.59	118.73	111.77
29	c1	501	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
48	G	607	CHL	C1-C2-C3	-2.59	121.56	126.04
29	S	604	CLA	C2C-C1C-NC	2.59	112.40	109.97
29	B	607	CLA	CMD-C2D-C3D	-2.59	121.66	127.61
29	y1	603	CLA	CMD-C2D-C3D	-2.59	121.66	127.61
29	G	602	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
49	s1	621	LUT	C1-C6-C7	2.59	123.10	115.78
29	C	509	CLA	C1C-C2C-C3C	-2.59	104.23	106.96
29	B	617	CLA	CAA-C2A-C3A	-2.59	105.69	112.78
29	Y	613	CLA	O1D-CGD-CBD	-2.59	119.19	124.48
48	G1	606	CHL	CHB-C4A-NA	2.59	128.09	124.51
29	c	505	CLA	CHA-C4D-ND	2.59	137.91	132.50
29	c1	501	CLA	CHD-C1D-ND	-2.59	122.08	124.45
29	S	609	CLA	C1-O2A-CGA	2.59	123.23	116.44
29	s	612	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
29	y	603	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
29	C1	512	CLA	C1C-C2C-C3C	-2.59	104.24	106.96
29	b1	603	CLA	C1C-C2C-C3C	-2.59	104.24	106.96
29	C	501	CLA	C1-C2-C3	-2.59	121.57	126.04
40	s	624	LHG	C5-O7-C7	-2.59	111.42	117.79
29	Y	614	CLA	CHA-C4D-ND	2.59	137.91	132.50
29	g1	604	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
48	G	608	CHL	C4A-NA-C1A	2.59	107.87	106.71
48	r	607	CHL	C4D-CHA-C1A	2.59	124.40	121.25
49	R	620	LUT	C18-C5-C4	2.59	119.15	114.36
29	s1	604	CLA	O2D-CGD-O1D	-2.59	118.78	123.84
29	c1	509	CLA	C1C-C2C-C3C	-2.59	104.24	106.96
29	c	506	CLA	C1-O2A-CGA	2.59	123.23	116.44
29	c1	504	CLA	CHA-C4D-ND	2.59	137.91	132.50
31	b1	619	BCR	C33-C5-C6	-2.59	121.62	124.53
48	g	605	CHL	CHB-C4A-NA	2.59	128.09	124.51
29	g1	610	CLA	CMA-C3A-C4A	2.58	118.72	111.77
31	A1	411	BCR	C36-C18-C17	-2.58	119.30	122.92
29	r1	602	CLA	O2A-CGA-CBA	2.58	120.02	111.91
29	b	607	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
29	B	606	CLA	CHA-C4D-ND	2.58	137.90	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	R1	621	XAT	C19-C9-C10	-2.58	119.30	122.92
29	c1	513	CLA	CHA-C4D-ND	2.58	137.90	132.50
29	R	612	CLA	CMA-C3A-C4A	2.58	118.72	111.77
29	n	610	CLA	CMB-C2B-C3B	2.58	129.51	124.68
47	K1	101	4RF	O18-C16-C15	2.58	120.01	111.91
31	C1	517	BCR	C23-C24-C25	-2.58	119.95	127.20
29	G	612	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
29	R1	610	CLA	CMC-C2C-C1C	2.58	128.97	125.04
48	s1	608	CHL	CMA-C3A-C4A	2.58	118.71	111.77
31	c	516	BCR	C19-C18-C17	2.58	122.90	118.94
29	y	604	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
29	R1	602	CLA	CMA-C3A-C4A	2.58	118.71	111.77
29	d1	402	CLA	O1D-CGD-CBD	-2.58	119.20	124.48
48	Y	606	CHL	C3C-C4C-NC	-2.58	107.68	110.57
29	d	402	CLA	C2C-C1C-NC	2.58	112.39	109.97
51	R	622	NEX	C26-C27-C28	-2.58	120.54	125.99
37	B	623	DGD	O1G-C1A-C2A	2.58	120.01	111.91
29	s1	609	CLA	CMA-C3A-C4A	2.58	118.71	111.77
29	g	614	CLA	CHD-C1D-ND	-2.58	122.08	124.45
29	G1	602	CLA	CHA-C4D-ND	2.58	137.90	132.50
29	G	610	CLA	C1C-C2C-C3C	-2.58	104.24	106.96
29	C	510	CLA	CHA-C4D-ND	2.58	137.90	132.50
29	B	606	CLA	O2A-CGA-CBA	2.58	120.00	111.91
29	d1	403	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
29	D1	402	CLA	C1D-ND-C4D	-2.58	104.50	106.33
29	c	501	CLA	CAA-C2A-C3A	-2.58	105.72	112.78
29	s	611	CLA	C2D-C1D-ND	2.58	112.00	110.10
29	B1	606	CLA	CMD-C2D-C3D	-2.58	121.69	127.61
29	r1	612	CLA	CMD-C2D-C3D	-2.58	121.69	127.61
50	N1	622	XAT	C7-C8-C9	-2.58	121.53	125.53
53	r	626	ERG	C18-C13-C14	-2.58	106.07	110.24
29	C	509	CLA	C6-C5-C3	-2.58	106.70	113.45
29	d	402	CLA	CHA-C4D-ND	2.58	137.89	132.50
29	y1	610	CLA	CMA-C3A-C4A	2.58	118.70	111.77
29	b1	613	CLA	CHD-C1D-ND	-2.58	122.09	124.45
29	c1	506	CLA	C1-C2-C3	-2.58	121.59	126.04
29	B	614	CLA	C3D-C2D-C1D	-2.58	102.31	105.83
29	N	610	CLA	C1C-C2C-C3C	-2.58	104.25	106.96
29	d	402	CLA	C1-C2-C3	-2.58	121.59	126.04
48	n	607	CHL	C1-O2A-CGA	2.58	123.20	116.44
29	Y1	610	CLA	C2C-C1C-NC	2.58	112.39	109.97
51	G	623	NEX	C31-C30-C29	2.57	130.98	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
51	R	622	NEX	C31-C30-C29	2.57	130.98	127.31
31	c	514	BCR	C36-C18-C17	-2.57	119.32	122.92
37	b1	623	DGD	O1G-C1A-C2A	2.57	119.99	111.91
29	Y	614	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
29	R	604	CLA	CMB-C2B-C3B	2.57	129.49	124.68
29	B	614	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
48	Y	605	CHL	C4D-CHA-C1A	2.57	124.38	121.25
29	a1	410	CLA	CHD-C1D-ND	-2.57	122.09	124.45
48	n	609	CHL	C1B-CHB-C4A	-2.57	125.02	130.12
30	A	408	PHO	O1D-CGD-CBD	2.57	129.03	124.74
29	B	607	CLA	CAA-C2A-C3A	-2.57	105.73	112.78
29	C1	502	CLA	CHA-C4D-ND	2.57	137.88	132.50
29	y1	608	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
29	b1	608	CLA	CHA-C4D-ND	2.57	137.88	132.50
30	A1	408	PHO	CMB-C2B-C3B	2.57	129.49	124.68
48	n	606	CHL	CHD-C1D-ND	-2.57	122.09	124.45
29	s1	604	CLA	CHA-C4D-ND	2.57	137.88	132.50
29	b	603	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
29	s	609	CLA	C2D-C1D-ND	2.57	112.00	110.10
29	g1	610	CLA	CHA-C4D-ND	2.57	137.88	132.50
29	r1	602	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
49	S	620	LUT	C15-C35-C34	-2.57	118.21	123.47
29	y1	610	CLA	O2A-CGA-CBA	2.57	119.98	111.91
29	b1	613	CLA	CMD-C2D-C3D	-2.57	121.70	127.61
48	S	601	CHL	CHB-C4A-NA	2.57	128.07	124.51
29	r1	608	CLA	C1C-C2C-C3C	-2.57	104.25	106.96
29	N1	602	CLA	CHD-C1D-ND	-2.57	122.09	124.45
50	g	622	XAT	C39-C29-C30	-2.57	119.32	122.92
29	B1	616	CLA	CHA-C4D-ND	2.57	137.88	132.50
29	d1	402	CLA	CHA-C4D-ND	2.57	137.88	132.50
29	c1	509	CLA	CMB-C2B-C3B	2.57	129.49	124.68
29	C1	502	CLA	C1-C2-C3	-2.57	121.60	126.04
48	y	601	CHL	C4D-CHA-C1A	2.57	124.38	121.25
48	s1	608	CHL	C4D-CHA-C1A	2.57	124.38	121.25
29	G	602	CLA	CMB-C2B-C1B	-2.57	124.52	128.46
29	R	608	CLA	CMD-C2D-C3D	-2.57	121.70	127.61
49	n1	621	LUT	C38-C25-C24	-2.57	118.06	123.56
48	S1	606	CHL	CHD-C4C-C3C	2.57	128.62	124.84
49	S1	621	LUT	C18-C5-C4	2.57	119.11	114.36
33	H1	102	LMG	O8-C28-C29	2.57	119.97	111.91
29	y1	613	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
48	S	606	CHL	CHB-C4A-NA	2.57	128.06	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	N	624	LHG	O8-C23-C24	2.57	119.97	111.91
29	Y	602	CLA	CMA-C3A-C4A	2.57	118.67	111.77
29	R1	608	CLA	C1D-ND-C4D	-2.57	104.51	106.33
29	r	602	CLA	CHA-C4D-ND	2.57	137.87	132.50
38	S1	626	3PH	O31-C31-C32	2.57	119.97	111.91
49	g1	620	LUT	C11-C10-C9	-2.57	123.65	127.31
29	b1	606	CLA	CMB-C2B-C3B	2.57	129.48	124.68
45	H1	101	RRX	C11-C12-C13	-2.57	119.20	126.42
29	C	504	CLA	C1-C2-C3	-2.57	121.60	126.04
29	G	613	CLA	O2A-CGA-CBA	2.57	119.96	111.91
39	b1	625	DGA	OG1-CA1-CA2	2.57	119.96	111.91
29	R	609	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
49	n	621	LUT	C18-C5-C6	-2.57	121.65	124.53
29	A	407	CLA	CAA-C2A-C3A	-2.57	105.75	112.78
48	g	605	CHL	C4D-CHA-C1A	2.57	124.37	121.25
29	S	612	CLA	CHA-C4D-ND	2.57	137.87	132.50
29	r	602	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
29	B1	603	CLA	C1C-C2C-C3C	-2.57	104.26	106.96
29	B1	607	CLA	O2A-CGA-CBA	2.56	119.96	111.91
29	c1	504	CLA	C1-C2-C3	-2.56	121.61	126.04
29	y	610	CLA	C2C-C1C-NC	2.56	112.37	109.97
29	d1	402	CLA	CHD-C1D-ND	-2.56	122.10	124.45
29	S	603	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
29	g	611	CLA	CAA-C2A-C3A	-2.56	105.76	112.78
49	y	621	LUT	C2-C3-C4	-2.56	106.80	110.30
48	S	608	CHL	C2C-C3C-C4C	2.56	108.32	106.49
29	g1	613	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
29	y1	612	CLA	CHA-C4D-ND	2.56	137.86	132.50
29	B1	610	CLA	CHA-C4D-ND	2.56	137.86	132.50
29	Y	612	CLA	C1C-C2C-C3C	-2.56	104.26	106.96
48	s1	606	CHL	CHD-C1D-ND	-2.56	122.10	124.45
29	B1	605	CLA	CHA-C4D-ND	2.56	137.86	132.50
29	N1	612	CLA	CHA-C4D-ND	2.56	137.86	132.50
29	B	615	CLA	C2D-C1D-ND	2.56	111.99	110.10
29	r	612	CLA	C2D-C1D-ND	2.56	111.99	110.10
29	G	603	CLA	CMA-C3A-C4A	2.56	118.65	111.77
29	n1	614	CLA	C1-O2A-CGA	2.56	123.16	116.44
29	C1	507	CLA	O2A-CGA-CBA	2.56	119.94	111.91
29	B	611	CLA	C1-C2-C3	-2.56	121.62	126.04
29	b1	606	CLA	CHA-C4D-ND	2.56	137.85	132.50
29	A	405	CLA	C1D-ND-C4D	-2.56	104.52	106.33
29	s1	613	CLA	C1-C2-C3	-2.56	121.62	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	s	620	LUT	C20-C13-C12	2.56	122.11	118.08
29	b1	612	CLA	O2A-CGA-CBA	2.56	119.94	111.91
29	B	613	CLA	C1-C2-C3	-2.56	121.62	126.04
29	Y1	612	CLA	CHA-C4D-ND	2.56	137.85	132.50
48	n	606	CHL	CMA-C3A-C4A	2.56	118.65	111.77
29	N1	614	CLA	CHD-C1D-ND	-2.56	122.10	124.45
48	N	609	CHL	CHD-C4C-C3C	2.56	128.60	124.84
37	B	623	DGD	O2G-C1B-O1B	-2.56	117.52	123.70
29	C1	505	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
29	d1	402	CLA	O2A-CGA-CBA	2.56	119.94	111.91
29	s	617	CLA	C2D-C1D-ND	2.56	111.99	110.10
48	n	609	CHL	C2C-C3C-C4C	2.56	108.31	106.49
29	s	609	CLA	CHA-C4D-ND	2.56	137.85	132.50
29	S1	609	CLA	CMD-C2D-C3D	-2.56	121.73	127.61
36	b	620	C7Z	C21-C26-C27	2.56	123.01	115.78
29	S1	605	CLA	CAA-C2A-C3A	-2.56	105.78	112.78
29	c1	507	CLA	CMD-C2D-C3D	-2.56	121.73	127.61
36	B1	620	C7Z	C20-C13-C14	-2.56	119.34	122.92
29	c	511	CLA	C1-C2-C3	-2.56	121.62	126.04
34	A	414	SPH	C3-C4-C5	-2.56	119.09	124.79
29	A1	406	CLA	CHD-C1D-ND	-2.56	122.11	124.45
29	R1	608	CLA	CMA-C3A-C4A	2.56	118.64	111.77
29	B1	608	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
29	c1	507	CLA	C1C-C2C-C3C	-2.56	104.27	106.96
29	c1	503	CLA	O2A-CGA-CBA	2.56	119.93	111.91
40	D1	408	LHG	O8-C23-C24	2.55	119.92	111.91
29	b1	602	CLA	CHA-C4D-ND	2.55	137.84	132.50
48	S1	607	CHL	C1B-CHB-C4A	-2.55	125.06	130.12
29	R	610	CLA	CHA-C4D-ND	2.55	137.84	132.50
29	C1	505	CLA	O1D-CGD-CBD	-2.55	119.26	124.48
29	y1	602	CLA	C16-C15-C13	-2.55	107.66	115.92
29	B	610	CLA	CAA-CBA-CGA	-2.55	105.79	113.25
29	b1	617	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
48	G1	609	CHL	C3C-C4C-NC	-2.55	107.71	110.57
29	B1	617	CLA	CHA-C4D-ND	2.55	137.84	132.50
29	G1	604	CLA	CHA-C4D-ND	2.55	137.84	132.50
29	R	603	CLA	C6-C5-C3	-2.55	106.76	113.45
29	N1	602	CLA	O2A-CGA-CBA	2.55	119.92	111.91
29	Y1	610	CLA	CMB-C2B-C1B	-2.55	124.54	128.46
29	y1	603	CLA	OBD-CAD-C3D	-2.55	122.38	128.52
29	b	611	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
32	B1	621	SQD	O3-C3-C2	-2.55	104.45	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Y1	613	CLA	CHA-C4D-ND	2.55	137.84	132.50
29	R	608	CLA	CHD-C1D-ND	-2.55	122.11	124.45
29	G1	604	CLA	CHD-C1D-ND	-2.55	122.11	124.45
29	b	609	CLA	O1D-CGD-CBD	-2.55	119.26	124.48
29	b1	602	CLA	C1-C2-C3	-2.55	121.63	126.04
29	r1	612	CLA	CHA-C1A-NA	-2.55	120.56	126.40
48	S1	607	CHL	C4D-CHA-C1A	2.55	124.35	121.25
29	c	511	CLA	C2D-C1D-ND	2.55	111.98	110.10
29	A1	406	CLA	C2D-C1D-ND	2.55	111.98	110.10
29	C1	511	CLA	C2D-C1D-ND	2.55	111.98	110.10
29	c	509	CLA	CMD-C2D-C3D	-2.55	121.75	127.61
29	C	511	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
29	n	613	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
29	b	605	CLA	O2A-CGA-CBA	2.55	119.91	111.91
31	c	517	BCR	C34-C9-C10	-2.55	119.35	122.92
29	N1	614	CLA	CHA-C4D-ND	2.55	137.83	132.50
29	y	611	CLA	CMB-C2B-C1B	-2.55	124.55	128.46
29	b	604	CLA	CHD-C1D-ND	-2.55	122.11	124.45
40	Y	624	LHG	C6-C5-C4	-2.55	105.76	111.79
29	b1	605	CLA	C3D-C2D-C1D	-2.55	102.35	105.83
31	c	514	BCR	C15-C14-C13	-2.55	123.67	127.31
29	c	503	CLA	CAA-C2A-C3A	-2.55	105.80	112.78
29	r	609	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
29	b1	608	CLA	C2C-C1C-NC	2.55	112.36	109.97
48	Y1	601	CHL	CHD-C4C-C3C	2.55	128.59	124.84
29	y1	613	CLA	C1-O2A-CGA	2.55	123.13	116.44
48	Y1	601	CHL	C4D-CHA-C1A	2.55	124.35	121.25
29	b1	606	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
29	b1	615	CLA	CMD-C2D-C3D	-2.55	121.75	127.61
29	d	403	CLA	CMD-C2D-C3D	-2.55	121.76	127.61
29	c	506	CLA	CMD-C2D-C3D	-2.55	121.76	127.61
29	c1	512	CLA	O2A-CGA-CBA	2.55	119.90	111.91
29	R1	602	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
29	S1	614	CLA	C1C-C2C-C3C	-2.55	104.28	106.96
29	G	614	CLA	CHA-C4D-ND	2.55	137.82	132.50
54	S1	625	LPX	O3-P1-O4	2.55	124.82	112.24
29	A1	406	CLA	CHA-C4D-ND	2.55	137.82	132.50
48	N1	605	CHL	C4D-CHA-C1A	2.54	124.35	121.25
29	n1	604	CLA	O2A-CGA-CBA	2.54	119.89	111.91
49	y1	620	LUT	C31-C30-C29	-2.54	123.68	127.31
29	C1	507	CLA	O2D-CGD-O1D	-2.54	118.86	123.84
29	B	614	CLA	O2A-CGA-CBA	2.54	119.89	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	g	612	CLA	C1C-C2C-C3C	-2.54	104.28	106.96
37	C	520	DGD	O6D-C5D-C6D	2.54	111.80	106.67
31	c1	516	BCR	C19-C18-C17	2.54	122.84	118.94
49	N	620	LUT	C10-C11-C12	-2.54	115.28	123.22
29	S	602	CLA	CHD-C1D-ND	-2.54	122.12	124.45
29	a	407	CLA	C2D-C1D-ND	2.54	111.98	110.10
49	s	621	LUT	C20-C13-C12	2.54	122.08	118.08
48	Y1	609	CHL	C4A-NA-C1A	2.54	107.85	106.71
51	r	622	NEX	C16-C1-C6	-2.54	108.20	110.47
29	B	611	CLA	O2A-CGA-CBA	2.54	119.89	111.91
38	B	624	3PH	O31-C31-C32	2.54	119.89	111.91
51	y1	623	NEX	C1-C2-C3	2.54	119.38	113.64
29	S1	611	CLA	O2A-CGA-CBA	2.54	119.88	111.91
29	y1	608	CLA	OBD-CAD-C3D	-2.54	122.41	128.52
40	c1	525	LHG	O8-C23-C24	2.54	119.88	111.91
29	s	614	CLA	CHA-C4D-ND	2.54	137.81	132.50
40	L	101	LHG	C5-O7-C7	-2.54	111.54	117.79
53	R	626	ERG	C13-C14-C8	2.54	118.41	113.48
29	C	505	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
48	N	607	CHL	C4D-CHA-C1A	2.54	124.34	121.25
29	b	613	CLA	CHD-C1D-ND	-2.54	122.12	124.45
48	r1	607	CHL	CHB-C4A-NA	2.54	128.02	124.51
29	C	504	CLA	C2C-C1C-NC	2.54	112.35	109.97
31	A1	411	BCR	C12-C13-C14	-2.54	115.05	118.94
29	c1	507	CLA	CHA-C4D-ND	2.54	137.81	132.50
40	d	410	LHG	O8-C23-C24	2.54	119.88	111.91
29	s1	605	CLA	C1-O2A-CGA	2.54	123.11	116.44
29	S	611	CLA	CHD-C1D-ND	-2.54	122.12	124.45
29	S	603	CLA	CHA-C1A-NA	-2.54	120.58	126.40
29	B1	613	CLA	C1-C2-C3	-2.54	121.65	126.04
29	Y1	610	CLA	CAA-C2A-C3A	-2.54	105.83	112.78
29	B1	607	CLA	CHA-C4D-ND	2.54	137.81	132.50
29	G	610	CLA	C2D-C1D-ND	2.54	111.97	110.10
29	C1	508	CLA	CMA-C3A-C4A	2.54	118.59	111.77
29	C	507	CLA	CHA-C4D-ND	2.54	137.81	132.50
29	n1	612	CLA	CHA-C4D-ND	2.54	137.81	132.50
29	y1	610	CLA	CHA-C4D-ND	2.54	137.81	132.50
33	d	411	LMG	C6-C5-C4	-2.54	107.06	113.00
29	Y1	611	CLA	C2C-C1C-NC	2.54	112.35	109.97
29	N1	612	CLA	C2D-C1D-ND	2.54	111.97	110.10
29	S1	610	CLA	OBD-CAD-C3D	-2.54	122.42	128.52
29	Y1	612	CLA	O2D-CGD-O1D	-2.54	118.88	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	R	603	CLA	CHA-C1A-NA	-2.54	120.59	126.40
29	s1	612	CLA	CHA-C4D-ND	2.54	137.80	132.50
29	Y	603	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
29	b	609	CLA	C2C-C1C-NC	2.54	112.35	109.97
29	b	607	CLA	C1C-C2C-C3C	-2.54	104.29	106.96
48	r	607	CHL	CHD-C4C-C3C	2.53	128.57	124.84
29	G	611	CLA	C2D-C1D-ND	2.53	111.97	110.10
29	Y1	610	CLA	C2D-C1D-ND	2.53	111.97	110.10
33	W1	201	LMG	C4-C3-C2	2.53	115.25	110.82
48	n	608	CHL	C1B-CHB-C4A	-2.53	125.10	130.12
29	b	607	CLA	CHA-C4D-ND	2.53	137.80	132.50
49	Y1	620	LUT	C31-C30-C29	-2.53	123.69	127.31
29	G	604	CLA	C1C-C2C-C3C	-2.53	104.29	106.96
29	B	606	CLA	O1D-CGD-CBD	-2.53	119.30	124.48
29	C	510	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
48	S	606	CHL	C2C-C3C-C4C	2.53	108.30	106.49
29	B	602	CLA	CMA-C3A-C4A	2.53	118.58	111.77
29	B1	602	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
29	R	602	CLA	CAA-C2A-C3A	-2.53	105.84	112.78
29	G	602	CLA	CMD-C2D-C3D	-2.53	121.79	127.61
29	s	617	CLA	CHA-C4D-ND	2.53	137.80	132.50
40	d1	408	LHG	O8-C23-C24	2.53	119.86	111.91
29	N1	614	CLA	CMB-C2B-C3B	2.53	129.42	124.68
29	R	608	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
51	y1	623	NEX	C35-C34-C33	2.53	130.92	127.31
29	a1	410	CLA	CHA-C4D-ND	2.53	137.80	132.50
50	y	622	XAT	O4-C5-C4	-2.53	111.48	113.38
50	g1	622	XAT	C20-C13-C14	-2.53	119.38	122.92
31	c	517	BCR	C35-C13-C12	2.53	122.06	118.08
29	S1	612	CLA	CHD-C1D-ND	-2.53	122.13	124.45
29	n	612	CLA	OBD-CAD-C3D	-2.53	122.43	128.52
29	b1	608	CLA	CMA-C3A-C4A	2.53	118.58	111.77
29	c1	508	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
40	L1	101	LHG	O7-C7-O9	-2.53	117.59	123.70
31	C	514	BCR	C37-C22-C23	2.53	122.06	118.08
29	B	606	CLA	CMD-C2D-C3D	-2.53	121.79	127.61
29	A	406	CLA	O2A-CGA-CBA	2.53	119.85	111.91
29	Y	611	CLA	CMD-C2D-C3D	-2.53	121.80	127.61
48	y1	607	CHL	C4D-CHA-C1A	2.53	124.33	121.25
48	s	608	CHL	C4A-NA-C1A	2.53	107.84	106.71
29	s	613	CLA	C1-C2-C3	-2.53	121.67	126.04
29	D	403	CLA	O2A-CGA-CBA	2.53	119.84	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	G1	622	XAT	C19-C9-C10	-2.53	119.38	122.92
29	s	605	CLA	CMD-C2D-C3D	-2.53	121.80	127.61
29	b	609	CLA	CHA-C4D-ND	2.53	137.79	132.50
29	B1	612	CLA	CMB-C2B-C1B	-2.53	124.58	128.46
29	y	608	CLA	CHA-C4D-ND	2.53	137.79	132.50
29	S	602	CLA	CMB-C2B-C3B	2.53	129.41	124.68
29	c	501	CLA	CMD-C2D-C3D	-2.53	121.80	127.61
29	r	610	CLA	C2A-C1A-CHA	2.53	128.28	123.86
40	D	410	LHG	O8-C23-C24	2.53	119.84	111.91
31	D	404	BCR	C33-C5-C4	2.53	118.47	113.62
29	S1	614	CLA	CHA-C1A-NA	-2.53	120.61	126.40
29	N1	612	CLA	CMA-C3A-C4A	2.53	118.56	111.77
29	s	604	CLA	CHA-C4D-ND	2.53	137.78	132.50
29	y	614	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
49	G1	620	LUT	C2-C3-C4	-2.53	106.85	110.30
29	C1	513	CLA	CHA-C4D-ND	2.52	137.78	132.50
39	j1	101	DGA	OG1-CA1-CA2	2.52	119.83	111.91
29	n1	612	CLA	C1C-C2C-C3C	-2.52	104.30	106.96
29	r1	609	CLA	C1C-C2C-C3C	-2.52	104.30	106.96
48	G	605	CHL	CHD-C1D-ND	-2.52	122.13	124.45
29	b1	610	CLA	CHA-C4D-ND	2.52	137.78	132.50
29	Y1	614	CLA	CAA-C2A-C3A	-2.52	105.86	112.78
45	h	101	RRX	C30-C25-C26	-2.52	119.06	122.61
49	s	621	LUT	C15-C14-C13	-2.52	123.71	127.31
29	b1	613	CLA	C1C-C2C-C3C	-2.52	104.30	106.96
49	N	621	LUT	C3-C4-C5	-2.52	106.83	111.85
53	R1	626	ERG	C20-C22-C23	-2.52	117.84	125.67
29	S1	610	CLA	C2C-C1C-NC	2.52	112.34	109.97
29	N1	610	CLA	C1D-ND-C4D	-2.52	104.54	106.33
29	n	613	CLA	C1-O2A-CGA	2.52	123.06	116.44
29	r	604	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
44	F1	101	HEM	CAD-C3D-C2D	-2.52	123.18	127.88
29	N	603	CLA	C1D-ND-C4D	-2.52	104.54	106.33
33	h	102	LMG	O8-C28-C29	2.52	119.82	111.91
49	G1	620	LUT	C38-C25-C24	-2.52	118.17	123.56
48	Y	607	CHL	C1-C2-C3	-2.52	121.68	126.04
29	n1	613	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
29	A	405	CLA	CAA-C2A-C3A	-2.52	105.88	112.78
29	C1	512	CLA	CHA-C4D-ND	2.52	137.77	132.50
29	R1	602	CLA	C1-O2A-CGA	2.52	123.06	116.44
29	s	611	CLA	O2A-CGA-CBA	2.52	119.82	111.91
29	b1	610	CLA	C2D-C1D-ND	2.52	111.96	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	g	614	CLA	CHA-C4D-ND	2.52	137.77	132.50
29	G	604	CLA	CAA-C2A-C3A	-2.52	105.88	112.78
50	G1	622	XAT	C18-C5-C6	-2.52	118.04	122.26
40	N1	624	LHG	C6-C5-C4	-2.52	105.83	111.79
48	Y	609	CHL	CHC-C1C-NC	2.52	128.03	124.20
33	h1	102	LMG	C8-O7-C10	-2.52	111.59	117.79
29	N	604	CLA	CMD-C2D-C3D	-2.52	121.82	127.61
39	C1	524	DGA	OG1-CA1-CA2	2.52	119.81	111.91
31	c1	514	BCR	C33-C5-C4	2.52	118.45	113.62
29	C	502	CLA	C1-O2A-CGA	2.52	123.05	116.44
29	b	615	CLA	C2D-C1D-ND	2.52	111.96	110.10
52	R	625	LMT	O5B-C1B-C2B	2.52	115.68	110.35
33	D	411	LMG	O8-C28-C29	2.52	119.81	111.91
29	B	609	CLA	CHA-C4D-ND	2.52	137.77	132.50
29	r	612	CLA	CHA-C4D-ND	2.52	137.77	132.50
48	Y	606	CHL	CMA-C3A-C4A	2.52	118.54	111.77
29	N	602	CLA	CAA-C2A-C3A	-2.52	105.88	112.78
49	S1	621	LUT	C7-C8-C9	-2.52	122.43	126.23
51	y1	623	NEX	C17-C1-C6	-2.52	108.22	110.47
29	C1	507	CLA	CHA-C4D-ND	2.52	137.76	132.50
29	y	604	CLA	CAA-C2A-C3A	-2.52	105.89	112.78
45	h1	101	RRX	C10-C11-C12	-2.52	115.36	123.22
48	S1	608	CHL	C4D-CHA-C1A	2.52	124.31	121.25
48	g	607	CHL	CHB-C4A-NA	2.52	127.99	124.51
29	G1	611	CLA	CHA-C4D-ND	2.52	137.76	132.50
29	Y1	603	CLA	O2A-CGA-CBA	2.52	119.80	111.91
29	c1	513	CLA	C1D-ND-C4D	-2.52	104.55	106.33
29	C1	506	CLA	CMD-C2D-C3D	-2.52	121.83	127.61
29	b1	602	CLA	C1C-C2C-C3C	-2.52	104.31	106.96
48	N	605	CHL	C1-C2-C3	-2.52	121.69	126.04
29	c	509	CLA	CHA-C4D-ND	2.51	137.76	132.50
29	N1	602	CLA	CMB-C2B-C3B	2.51	129.38	124.68
29	c	501	CLA	C2D-C1D-ND	2.51	111.96	110.10
48	S1	601	CHL	CHB-C4A-NA	2.51	127.99	124.51
29	G	604	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
29	s	612	CLA	C1C-C2C-C3C	-2.51	104.31	106.96
29	B	611	CLA	CMA-C3A-C4A	2.51	118.53	111.77
29	R1	610	CLA	C2C-C1C-NC	2.51	112.33	109.97
48	r1	607	CHL	CHD-C4C-C3C	2.51	128.53	124.84
31	C1	516	BCR	C34-C9-C10	-2.51	119.40	122.92
29	B	606	CLA	CMB-C2B-C1B	-2.51	124.60	128.46
29	d1	402	CLA	CMA-C3A-C4A	2.51	118.53	111.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c1	513	CLA	C1C-C2C-C3C	-2.51	104.31	106.96
29	s	602	CLA	CHA-C4D-ND	2.51	137.76	132.50
29	b1	602	CLA	CMC-C2C-C1C	2.51	128.87	125.04
40	d1	410	LHG	C5-O7-C7	-2.51	111.61	117.79
29	g1	614	CLA	CHA-C4D-ND	2.51	137.75	132.50
29	C1	505	CLA	C1-O2A-CGA	2.51	123.03	116.44
29	y1	608	CLA	O2A-CGA-CBA	2.51	119.79	111.91
29	b	608	CLA	CHA-C4D-ND	2.51	137.75	132.50
43	d	405	PL9	C27-C28-C29	-2.51	121.61	127.66
29	R	602	CLA	CMB-C2B-C3B	2.51	129.38	124.68
29	g	613	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
43	d1	405	PL9	O2-C1-C6	2.51	124.94	120.59
29	C1	501	CLA	CHA-C4D-ND	2.51	137.75	132.50
29	Y	612	CLA	CHA-C4D-ND	2.51	137.75	132.50
29	y	613	CLA	CHA-C4D-ND	2.51	137.75	132.50
29	r1	603	CLA	CHA-C4D-ND	2.51	137.75	132.50
29	R	608	CLA	O2A-CGA-CBA	2.51	119.78	111.91
29	d	403	CLA	O2A-CGA-CBA	2.51	119.78	111.91
29	b1	614	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
48	g1	609	CHL	CHC-C1C-NC	2.51	128.01	124.20
29	S	603	CLA	CHA-C4D-ND	2.51	137.75	132.50
49	R	620	LUT	C35-C15-C14	-2.51	118.33	123.47
29	R	609	CLA	C1-C2-C3	-2.51	121.70	126.04
29	c	503	CLA	CHA-C4D-ND	2.51	137.75	132.50
29	b	615	CLA	CHA-C4D-ND	2.51	137.75	132.50
29	n	612	CLA	CHA-C4D-ND	2.51	137.75	132.50
29	G1	613	CLA	CMB-C2B-C1B	-2.51	124.61	128.46
51	y1	623	NEX	C26-C27-C28	-2.51	120.69	125.99
29	y1	612	CLA	O2A-CGA-CBA	2.51	119.78	111.91
50	Y	622	XAT	C39-C29-C30	-2.51	119.41	122.92
31	b	619	BCR	C23-C24-C25	-2.51	120.16	127.20
29	Y	604	CLA	CHA-C4D-ND	2.51	137.74	132.50
29	y1	611	CLA	CHA-C4D-ND	2.51	137.74	132.50
29	n	604	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
40	G1	624	LHG	O8-C23-C24	2.51	119.78	111.91
43	D1	405	PL9	C31-C32-C33	-2.51	103.64	111.88
29	y	602	CLA	CHA-C4D-ND	2.51	137.74	132.50
48	N	608	CHL	C1-O2A-CGA	2.51	123.02	116.44
29	y1	611	CLA	CHD-C1D-ND	-2.51	122.15	124.45
48	n	608	CHL	CHD-C1D-ND	-2.51	122.15	124.45
33	C	523	LMG	O8-C28-C29	2.51	119.77	111.91
47	k	101	4RF	O40-C41-C43	2.51	119.77	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	n1	610	CLA	C1-C2-C3	-2.51	121.71	126.04
29	b1	617	CLA	CHA-C4D-ND	2.51	137.74	132.50
48	G1	606	CHL	C1B-CHB-C4A	-2.51	125.15	130.12
48	g1	601	CHL	C1B-CHB-C4A	-2.51	125.15	130.12
51	Y	623	NEX	C4-C3-C2	2.51	115.61	110.77
29	c	511	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
29	A	410	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
29	s1	603	CLA	C1C-C2C-C3C	-2.51	104.32	106.96
29	c1	510	CLA	CHA-C1A-NA	-2.51	120.66	126.40
29	b	603	CLA	CHA-C4D-ND	2.51	137.74	132.50
29	R1	602	CLA	CHA-C4D-ND	2.51	137.74	132.50
29	s1	602	CLA	C2C-C1C-NC	2.51	112.32	109.97
29	N	602	CLA	CMB-C2B-C3B	2.51	129.37	124.68
49	G	621	LUT	C38-C25-C24	-2.51	118.20	123.56
29	G1	610	CLA	CHA-C4D-ND	2.50	137.74	132.50
48	R1	607	CHL	C4A-NA-C1A	2.50	107.83	106.71
29	r	610	CLA	CMD-C2D-C3D	-2.50	121.85	127.61
39	J1	101	DGA	OG1-CA1-CA2	2.50	119.77	111.91
29	s	603	CLA	C2A-C1A-CHA	2.50	128.24	123.86
29	S	609	CLA	C2D-C1D-ND	2.50	111.95	110.10
29	C	513	CLA	CHA-C4D-ND	2.50	137.74	132.50
29	s1	609	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
29	G	614	CLA	CMD-C2D-C3D	-2.50	121.86	127.61
51	Y1	623	NEX	C40-C33-C34	-2.50	119.42	122.92
50	n	622	XAT	O4-C5-C4	-2.50	111.50	113.38
29	r	603	CLA	CHA-C1A-NA	-2.50	120.67	126.40
29	b1	614	CLA	C1-C2-C3	-2.50	121.72	126.04
49	S	620	LUT	C8-C7-C6	-2.50	120.17	127.20
29	R1	608	CLA	CMD-C2D-C3D	-2.50	121.86	127.61
50	y1	622	XAT	C20-C13-C14	-2.50	119.42	122.92
29	B	617	CLA	CHA-C4D-ND	2.50	137.73	132.50
49	G	620	LUT	C3-C4-C5	-2.50	106.87	111.85
48	G	606	CHL	C1-O2A-CGA	2.50	123.01	116.44
29	D	403	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
29	r	604	CLA	CHA-C4D-ND	2.50	137.73	132.50
29	y1	610	CLA	CAA-C2A-C3A	-2.50	105.93	112.78
29	c1	511	CLA	CMD-C2D-C3D	-2.50	121.86	127.61
29	c	506	CLA	CHA-C4D-ND	2.50	137.73	132.50
29	S	605	CLA	CMD-C2D-C3D	-2.50	121.86	127.61
29	C	511	CLA	CMB-C2B-C1B	-2.50	124.62	128.46
29	b	602	CLA	CHA-C4D-ND	2.50	137.73	132.50
31	c1	514	BCR	C40-C30-C25	-2.50	106.25	110.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	605	CLA	CMD-C2D-C3D	-2.50	121.87	127.61
49	N	620	LUT	C18-C5-C6	-2.50	121.72	124.53
29	B	603	CLA	CHA-C4D-ND	2.50	137.72	132.50
29	G	613	CLA	CHA-C4D-ND	2.50	137.72	132.50
29	r1	610	CLA	CMA-C3A-C4A	2.50	118.49	111.77
50	Y	622	XAT	C18-C5-C6	-2.50	118.08	122.26
29	C1	511	CLA	OBD-CAD-C3D	-2.50	122.51	128.52
29	C1	504	CLA	CHD-C1D-ND	-2.50	122.16	124.45
29	G1	602	CLA	C4D-CHA-C1A	2.50	124.29	121.25
29	B1	603	CLA	C6-C5-C3	-2.50	106.91	113.45
48	G	609	CHL	C1-O2A-CGA	2.50	123.00	116.44
29	R1	610	CLA	O2A-CGA-CBA	2.50	119.74	111.91
29	G1	602	CLA	C1-C2-C3	-2.50	121.72	126.04
29	S	602	CLA	CMA-C3A-C4A	2.50	118.48	111.77
29	B	615	CLA	CMB-C2B-C1B	-2.50	124.63	128.46
48	S	608	CHL	CHB-C4A-NA	2.50	127.96	124.51
29	n1	614	CLA	CHA-C4D-ND	2.50	137.72	132.50
48	G	609	CHL	CHC-C1C-NC	2.50	127.99	124.20
29	g1	602	CLA	C1-O2A-CGA	2.50	122.99	116.44
29	c	506	CLA	O2A-CGA-CBA	2.50	119.74	111.91
49	s	621	LUT	C16-C1-C6	-2.50	106.25	110.30
29	B	606	CLA	CMB-C2B-C3B	2.50	129.35	124.68
29	n1	614	CLA	C2D-C1D-ND	2.50	111.94	110.10
29	A1	410	CLA	C1C-C2C-C3C	-2.50	104.33	106.96
50	n1	622	XAT	C39-C29-C30	-2.50	119.43	122.92
29	c1	505	CLA	O1D-CGD-CBD	-2.49	119.38	124.48
29	C1	503	CLA	CMB-C2B-C1B	-2.49	124.63	128.46
29	G	611	CLA	CMA-C3A-C4A	2.49	118.48	111.77
32	m	101	SQD	O3-C3-C2	-2.49	104.58	110.35
29	R1	608	CLA	CHA-C4D-ND	2.49	137.71	132.50
48	S1	608	CHL	C2C-C3C-C4C	2.49	108.27	106.49
40	y1	624	LHG	O8-C23-C24	2.49	119.73	111.91
49	N	621	LUT	C7-C8-C9	-2.49	122.47	126.23
48	y1	609	CHL	C3C-C4C-NC	-2.49	107.78	110.57
29	y1	610	CLA	O1D-CGD-CBD	-2.49	119.39	124.48
40	S	624	LHG	C5-O7-C7	-2.49	111.66	117.79
48	G1	605	CHL	C1-O2A-CGA	2.49	123.97	116.73
29	b	605	CLA	C16-C15-C13	-2.49	107.86	115.92
31	b1	619	BCR	C36-C18-C17	-2.49	119.43	122.92
29	R	610	CLA	C3D-C2D-C1D	-2.49	102.43	105.83
29	b1	604	CLA	C2C-C1C-NC	2.49	112.31	109.97
29	r1	612	CLA	C1C-C2C-C3C	-2.49	104.34	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	g1	603	CLA	CHA-C4D-ND	2.49	137.71	132.50
49	g	620	LUT	C10-C11-C12	-2.49	115.44	123.22
53	R1	626	ERG	C14-C8-C7	-2.49	119.47	124.38
29	r	610	CLA	CHA-C4D-ND	2.49	137.71	132.50
29	C1	506	CLA	CHA-C4D-ND	2.49	137.71	132.50
29	R	602	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
29	C	511	CLA	O2A-CGA-CBA	2.49	119.72	111.91
29	n	603	CLA	CHA-C4D-ND	2.49	137.71	132.50
48	y1	601	CHL	C2C-C3C-C4C	2.49	108.26	106.49
29	s	603	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
29	r	612	CLA	C1-C2-C3	-2.49	121.74	126.04
29	A	405	CLA	CHA-C4D-ND	2.49	137.71	132.50
29	B	607	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
29	C	512	CLA	O2A-CGA-CBA	2.49	119.72	111.91
32	a1	412	SQD	O3-C3-C2	-2.49	104.59	110.35
29	g1	604	CLA	CMB-C2B-C1B	-2.49	124.64	128.46
29	C1	511	CLA	O2A-CGA-CBA	2.49	119.72	111.91
29	B1	611	CLA	C1-O2A-CGA	2.49	122.97	116.44
29	S1	604	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
29	s1	605	CLA	CHA-C4D-ND	2.49	137.71	132.50
29	Y	604	CLA	CMB-C2B-C1B	-2.49	124.64	128.46
29	S	611	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
29	s1	610	CLA	C2C-C1C-NC	2.49	112.30	109.97
29	y1	614	CLA	C2C-C1C-NC	2.49	112.30	109.97
29	N1	611	CLA	CHA-C4D-ND	2.49	137.70	132.50
51	Y1	623	NEX	C26-C27-C28	-2.49	120.73	125.99
29	B1	607	CLA	C1-O2A-CGA	2.49	122.97	116.44
29	r	608	CLA	CHA-C4D-ND	2.49	137.70	132.50
43	D	405	PL9	C22-C23-C24	-2.49	121.67	127.66
29	b	615	CLA	C1C-C2C-C3C	-2.49	104.34	106.96
29	G	602	CLA	CHA-C4D-ND	2.49	137.70	132.50
29	a1	405	CLA	CMB-C2B-C1B	-2.49	124.64	128.46
29	C	513	CLA	C1-O2A-CGA	2.49	122.97	116.44
29	C1	505	CLA	C2C-C1C-NC	2.49	112.30	109.97
29	b	607	CLA	C2D-C1D-ND	2.49	111.94	110.10
29	s	611	CLA	CHA-C4D-ND	2.49	137.70	132.50
29	S	611	CLA	CHA-C4D-ND	2.48	137.70	132.50
29	n	604	CLA	CHA-C4D-ND	2.48	137.70	132.50
48	n	607	CHL	C1B-CHB-C4A	-2.48	125.20	130.12
29	b	608	CLA	C1-O2A-CGA	2.48	122.96	116.44
29	S	609	CLA	CHA-C4D-ND	2.48	137.69	132.50
29	Y	602	CLA	CHA-C4D-ND	2.48	137.69	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B1	609	CLA	CHA-C4D-ND	2.48	137.69	132.50
29	b	608	CLA	O2A-CGA-CBA	2.48	119.70	111.91
29	y	614	CLA	C1D-ND-C4D	-2.48	104.57	106.33
29	C	503	CLA	O2A-CGA-CBA	2.48	119.70	111.91
29	c1	503	CLA	CMD-C2D-C3D	-2.48	121.90	127.61
48	y	605	CHL	C4D-CHA-C1A	2.48	124.27	121.25
48	N1	605	CHL	C4A-NA-C1A	2.48	107.82	106.71
50	G1	622	XAT	O4-C5-C4	-2.48	111.52	113.38
51	G	623	NEX	C40-C33-C34	-2.48	119.45	122.92
29	S1	609	CLA	CHA-C4D-ND	2.48	137.69	132.50
48	n	601	CHL	C1-C2-C3	-2.48	121.75	126.04
29	R	603	CLA	CMB-C2B-C3B	2.48	129.32	124.68
29	y1	614	CLA	C1C-C2C-C3C	-2.48	104.35	106.96
51	g1	623	NEX	C28-C29-C30	2.48	122.75	118.94
41	C1	527	LMK	O3-C4-C3	-2.48	114.47	122.98
31	c	516	BCR	C36-C18-C17	-2.48	119.45	122.92
44	F1	101	HEM	C4B-CHC-C1C	-2.48	119.29	122.56
48	n	606	CHL	C1B-CHB-C4A	-2.48	125.21	130.12
50	G	622	XAT	C8-C9-C10	2.48	122.75	118.94
29	b1	614	CLA	O2A-CGA-CBA	2.48	119.69	111.91
29	R	610	CLA	CHD-C1D-ND	-2.48	122.18	124.45
48	n1	605	CHL	C1B-CHB-C4A	-2.48	125.21	130.12
48	G1	607	CHL	C1-O2A-CGA	2.48	122.94	116.44
31	B	618	BCR	C37-C22-C23	2.48	121.98	118.08
51	R1	622	NEX	C19-C9-C10	-2.48	119.45	122.92
50	G1	622	XAT	C31-C30-C29	-2.48	123.78	127.31
29	N	611	CLA	CMA-C3A-C4A	2.48	118.43	111.77
29	B	613	CLA	O2D-CGD-O1D	-2.48	119.00	123.84
29	B1	604	CLA	C2D-C1D-ND	2.48	111.93	110.10
29	N1	610	CLA	CMB-C2B-C3B	2.48	129.31	124.68
51	s	623	NEX	O24-C25-C38	-2.48	112.09	115.06
51	G1	623	NEX	C38-C25-C26	-2.48	118.11	122.26
29	c	501	CLA	CHA-C4D-ND	2.48	137.68	132.50
49	Y1	621	LUT	C18-C5-C6	-2.48	121.75	124.53
29	s	609	CLA	CHD-C1D-ND	-2.48	122.18	124.45
48	G	608	CHL	CHB-C4A-NA	2.48	127.94	124.51
29	B	610	CLA	CHA-C4D-ND	2.48	137.68	132.50
29	s1	610	CLA	C2D-C1D-ND	2.48	111.93	110.10
48	Y1	607	CHL	C1B-CHB-C4A	-2.47	125.22	130.12
29	S1	604	CLA	O2A-CGA-CBA	2.47	119.67	111.91
29	g1	604	CLA	CHA-C4D-ND	2.47	137.68	132.50
29	Y	603	CLA	CHA-C4D-ND	2.47	137.68	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	s	610	CLA	CHA-C4D-ND	2.47	137.67	132.50
29	C	502	CLA	CMA-C3A-C4A	2.47	118.42	111.77
29	b1	609	CLA	CHA-C4D-ND	2.47	137.67	132.50
29	c1	512	CLA	CMA-C3A-C2A	2.47	123.80	113.83
29	b	612	CLA	CMB-C2B-C1B	-2.47	124.66	128.46
33	A1	413	LMG	O1-C1-C2	2.47	112.16	108.30
29	c1	512	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
48	S1	601	CHL	C4D-CHA-C1A	2.47	124.26	121.25
29	s1	603	CLA	CHA-C4D-ND	2.47	137.67	132.50
29	g1	614	CLA	C2D-C1D-ND	2.47	111.93	110.10
29	B1	615	CLA	CHA-C4D-ND	2.47	137.67	132.50
29	c1	509	CLA	CHA-C4D-ND	2.47	137.67	132.50
29	Y	603	CLA	C1D-ND-C4D	-2.47	104.58	106.33
29	g	603	CLA	CMD-C2D-C3D	-2.47	121.93	127.61
29	N	604	CLA	C2D-C1D-ND	2.47	111.92	110.10
29	B	605	CLA	O1D-CGD-CBD	-2.47	119.43	124.48
29	a	406	CLA	CHA-C4D-ND	2.47	137.67	132.50
48	G1	606	CHL	CHD-C1D-ND	-2.47	122.18	124.45
29	r1	608	CLA	CHA-C4D-ND	2.47	137.67	132.50
29	n	602	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
29	n1	604	CLA	CMB-C2B-C3B	2.47	129.30	124.68
49	g	621	LUT	C16-C1-C6	-2.47	106.29	110.30
29	S	610	CLA	CHA-C4D-ND	2.47	137.66	132.50
29	r	609	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
29	r	610	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
29	b1	606	CLA	O2A-CGA-CBA	2.47	119.66	111.91
29	D1	403	CLA	CHA-C4D-ND	2.47	137.66	132.50
29	a	406	CLA	C2D-C1D-ND	2.47	111.92	110.10
29	c1	508	CLA	C2C-C1C-NC	2.47	112.28	109.97
29	g	612	CLA	CHA-C4D-ND	2.47	137.66	132.50
29	s1	612	CLA	CHA-C1A-NA	-2.47	120.75	126.40
51	G	623	NEX	C20-C13-C14	-2.47	119.47	122.92
29	A1	405	CLA	C2D-C1D-ND	2.47	111.92	110.10
48	G	607	CHL	C4A-NA-C1A	2.47	107.81	106.71
48	n1	606	CHL	CHB-C4A-NA	2.47	127.92	124.51
48	G1	609	CHL	CHC-C1C-NC	2.47	127.94	124.20
29	r1	609	CLA	CAC-C3C-C4C	2.47	128.01	124.81
29	C1	507	CLA	CHA-C1A-NA	-2.47	120.75	126.40
29	g	604	CLA	CMD-C2D-C3D	-2.47	121.94	127.61
29	C	513	CLA	CMA-C3A-C4A	2.47	118.40	111.77
29	c1	507	CLA	C1-C2-C3	-2.47	121.78	126.04
29	a	407	CLA	CHA-C4D-ND	2.47	137.66	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	g	602	CLA	C1C-C2C-C3C	-2.47	104.36	106.96
29	B	612	CLA	C2D-C1D-ND	2.47	111.92	110.10
37	c	518	DGD	O1G-C1A-C2A	2.47	119.64	111.91
40	L1	101	LHG	O8-C23-C24	2.47	119.64	111.91
29	b1	613	CLA	CAC-C3C-C4C	2.47	128.01	124.81
29	N	610	CLA	CHA-C4D-ND	2.47	137.66	132.50
29	c	507	CLA	CHA-C4D-ND	2.47	137.66	132.50
29	Y1	608	CLA	C3D-C2D-C1D	-2.47	102.47	105.83
31	a	411	BCR	C34-C9-C10	-2.47	119.47	122.92
48	r1	606	CHL	CMA-C3A-C4A	2.46	118.40	111.77
29	s1	617	CLA	C1D-ND-C4D	-2.46	104.58	106.33
29	b	614	CLA	CHA-C4D-ND	2.46	137.66	132.50
29	r1	612	CLA	CHA-C4D-ND	2.46	137.65	132.50
29	B1	613	CLA	C1-O2A-CGA	2.46	122.91	116.44
29	y	603	CLA	O2A-CGA-CBA	2.46	119.64	111.91
29	G1	604	CLA	CMA-C3A-C4A	2.46	118.39	111.77
29	N	614	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
29	n1	603	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
37	c	518	DGD	C6E-C5E-C4E	-2.46	107.23	113.00
29	B1	602	CLA	O2A-CGA-CBA	2.46	119.64	111.91
29	y	611	CLA	C2D-C1D-ND	2.46	111.92	110.10
29	C1	509	CLA	CMB-C2B-C3B	2.46	129.29	124.68
29	b1	615	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
33	b	622	LMG	O8-C28-C29	2.46	119.64	111.91
31	A	411	BCR	C38-C26-C25	-2.46	121.76	124.53
29	B1	602	CLA	CMD-C2D-C3D	-2.46	121.95	127.61
29	S1	609	CLA	CMA-C3A-C4A	2.46	118.39	111.77
29	r1	604	CLA	CMA-C3A-C4A	2.46	118.39	111.77
29	Y	610	CLA	CMC-C2C-C3C	2.46	132.80	126.12
29	r	608	CLA	CMA-C3A-C4A	2.46	118.39	111.77
29	n	612	CLA	CHA-C1A-NA	-2.46	120.76	126.40
43	D1	405	PL9	C11-C12-C13	-2.46	103.79	111.88
29	c1	509	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
29	R	603	CLA	CMA-C3A-C4A	2.46	118.39	111.77
49	S1	621	LUT	C20-C13-C14	-2.46	119.48	122.92
40	Y1	624	LHG	O8-C23-C24	2.46	119.63	111.91
29	C1	511	CLA	CHA-C4D-ND	2.46	137.65	132.50
29	B	603	CLA	O2A-CGA-CBA	2.46	119.63	111.91
29	B	615	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
29	d	403	CLA	CHA-C4D-ND	2.46	137.65	132.50
29	c	503	CLA	O2A-CGA-CBA	2.46	119.63	111.91
29	G	613	CLA	CMD-C2D-C3D	-2.46	121.96	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	g	602	CLA	CHA-C4D-ND	2.46	137.64	132.50
29	s1	602	CLA	CHA-C4D-ND	2.46	137.64	132.50
29	S1	602	CLA	O1D-CGD-CBD	-2.46	119.45	124.48
29	c1	512	CLA	CHD-C1D-ND	-2.46	122.19	124.45
29	N	613	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
48	g1	606	CHL	CHD-C4C-C3C	2.46	128.45	124.84
29	Y1	611	CLA	CMD-C2D-C3D	-2.46	121.96	127.61
48	n1	606	CHL	CMA-C3A-C4A	2.46	118.38	111.77
50	r1	621	XAT	C4-C3-C2	-2.46	106.03	110.77
45	h	101	RRX	C16-C15-C14	-2.46	118.44	123.47
29	Y1	612	CLA	CHA-C1A-NA	-2.46	120.77	126.40
48	r	607	CHL	C1B-CHB-C4A	-2.46	125.25	130.12
48	y	606	CHL	C1B-CHB-C4A	-2.46	125.25	130.12
29	B1	612	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
48	n1	605	CHL	CHB-C4A-NA	2.46	127.91	124.51
29	n	602	CLA	CHA-C4D-ND	2.46	137.64	132.50
29	c	513	CLA	CHA-C4D-ND	2.46	137.64	132.50
48	s1	608	CHL	CHC-C1C-NC	2.46	127.93	124.20
31	b	619	BCR	C36-C18-C17	-2.46	119.48	122.92
29	b	606	CLA	C1C-C2C-C3C	-2.46	104.37	106.96
29	S1	611	CLA	C2D-C1D-ND	2.46	111.91	110.10
29	N1	611	CLA	CAA-CBA-CGA	-2.46	106.08	113.25
29	B1	605	CLA	CHA-C1A-NA	-2.46	120.78	126.40
29	C1	507	CLA	CBC-CAC-C3C	-2.46	105.66	112.43
29	c	509	CLA	O2D-CGD-O1D	-2.46	119.04	123.84
29	B	616	CLA	C1-O2A-CGA	2.45	122.89	116.44
49	y	621	LUT	C35-C34-C33	-2.45	123.81	127.31
29	n1	604	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
29	R	602	CLA	CMC-C2C-C1C	2.45	128.78	125.04
29	b	617	CLA	C1-O2A-CGA	2.45	122.88	116.44
29	d1	403	CLA	C2D-C1D-ND	2.45	111.91	110.10
51	n	623	NEX	O24-C25-C24	-2.45	111.54	113.38
29	y1	614	CLA	CAA-C2A-C3A	-2.45	106.06	112.78
31	B	618	BCR	C1-C6-C7	2.45	122.72	115.78
29	B	612	CLA	C2C-C1C-NC	2.45	112.27	109.97
29	C1	504	CLA	CHA-C4D-ND	2.45	137.63	132.50
40	Y	624	LHG	O8-C23-C24	2.45	119.61	111.91
29	b1	612	CLA	CHD-C1D-ND	-2.45	122.20	124.45
29	s1	613	CLA	O2A-CGA-CBA	2.45	119.60	111.91
29	b1	610	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
29	N	611	CLA	CHA-C4D-ND	2.45	137.63	132.50
29	S1	602	CLA	C1D-ND-C4D	-2.45	104.59	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	n1	613	CLA	C1D-ND-C4D	-2.45	104.59	106.33
49	R1	620	LUT	C21-C26-C25	2.45	115.81	111.42
37	C1	520	DGD	O1G-C1A-C2A	2.45	119.60	111.91
40	S	624	LHG	O8-C23-C24	2.45	119.60	111.91
36	B1	620	C7Z	C40-C33-C34	-2.45	119.49	122.92
29	Y1	602	CLA	O2A-CGA-CBA	2.45	119.60	111.91
50	N	622	XAT	O4-C5-C18	-2.45	112.12	115.06
29	S	614	CLA	CMB-C2B-C3B	2.45	129.26	124.68
48	Y	609	CHL	CHA-C4D-ND	2.45	137.63	132.50
29	B1	612	CLA	O2A-CGA-CBA	2.45	119.60	111.91
29	g1	602	CLA	C2C-C1C-NC	2.45	112.27	109.97
29	g1	604	CLA	C2C-C1C-NC	2.45	112.27	109.97
29	b	603	CLA	C2D-C1D-ND	2.45	111.91	110.10
29	d1	403	CLA	CHA-C4D-ND	2.45	137.62	132.50
32	C	526	SQD	O3-C3-C2	-2.45	104.68	110.35
33	c	521	LMG	C8-O7-C10	-2.45	111.76	117.79
30	A1	409	PHO	CMB-C2B-C3B	2.45	129.26	124.68
29	y	604	CLA	O1D-CGD-CBD	-2.45	119.47	124.48
29	G1	602	CLA	O2A-CGA-CBA	2.45	119.59	111.91
29	c1	511	CLA	O2A-CGA-CBA	2.45	119.59	111.91
29	r	604	CLA	CMD-C2D-C3D	-2.45	121.98	127.61
29	g1	602	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
48	g	607	CHL	C3C-C4C-NC	-2.45	107.82	110.57
51	s	623	NEX	C1-C2-C3	2.45	119.17	113.64
30	a	409	PHO	CMC-C2C-C3C	2.45	129.56	124.94
33	C1	523	LMG	O1-C1-C2	2.45	112.13	108.30
29	C	510	CLA	O2A-CGA-CBA	2.45	119.59	111.91
49	S	620	LUT	C8-C9-C10	-2.45	115.18	118.94
29	b	605	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
31	b	618	BCR	C34-C9-C10	-2.45	119.49	122.92
31	c1	517	BCR	C35-C13-C14	-2.45	119.49	122.92
51	y	623	NEX	C19-C9-C10	-2.45	119.49	122.92
51	G1	623	NEX	C4-C3-C2	2.45	115.50	110.77
49	Y	621	LUT	C35-C15-C14	-2.45	118.46	123.47
45	H1	101	RRX	C2-C1-C6	2.45	114.25	110.48
48	n1	608	CHL	C3C-C4C-NC	-2.45	107.83	110.57
29	S1	605	CLA	C1C-C2C-C3C	-2.45	104.38	106.96
37	c1	518	DGD	C3G-C2G-C1G	-2.45	106.00	111.79
29	g1	613	CLA	CHA-C4D-ND	2.45	137.62	132.50
34	y1	625	SPH	C1-C2-C3	-2.45	107.76	113.03
29	B	604	CLA	C1-C2-C3	-2.45	121.81	126.04
29	y1	614	CLA	O2A-CGA-CBA	2.45	119.59	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	r1	602	CLA	C1D-ND-C4D	-2.45	104.60	106.33
29	G1	604	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
29	N	614	CLA	CHA-C4D-ND	2.45	137.62	132.50
48	N1	609	CHL	CHC-C1C-NC	2.45	127.91	124.20
50	N1	622	XAT	C39-C29-C30	-2.45	119.50	122.92
49	y	621	LUT	C18-C5-C6	-2.45	121.78	124.53
29	G1	612	CLA	CHA-C4D-ND	2.45	137.61	132.50
49	r	620	LUT	C18-C5-C4	2.45	118.89	114.36
29	b1	605	CLA	CHD-C1D-ND	-2.45	122.21	124.45
29	D	402	CLA	CHA-C4D-ND	2.44	137.61	132.50
29	y1	613	CLA	CHA-C4D-ND	2.44	137.61	132.50
36	b	620	C7Z	C8-C7-C6	-2.44	120.34	127.20
29	C	502	CLA	CHA-C4D-ND	2.44	137.61	132.50
48	G	607	CHL	C1-O2A-CGA	2.44	122.86	116.44
29	N	604	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
48	N	607	CHL	C2C-C3C-C4C	2.44	108.23	106.49
29	y	611	CLA	CHA-C4D-ND	2.44	137.61	132.50
29	Y1	602	CLA	C1-C2-C3	-2.44	121.82	126.04
52	R1	625	LMT	C1'-O5'-C5'	-2.44	108.89	113.69
29	R	608	CLA	CAC-C3C-C4C	2.44	127.98	124.81
29	s	603	CLA	O1D-CGD-CBD	-2.44	119.48	124.48
49	S	620	LUT	C32-C33-C34	-2.44	115.19	118.94
29	B1	615	CLA	CHA-C1A-NA	-2.44	120.80	126.40
50	n1	622	XAT	C19-C9-C10	-2.44	119.50	122.92
29	G	604	CLA	C2D-C1D-ND	2.44	111.90	110.10
29	y1	613	CLA	CMA-C3A-C4A	2.44	118.34	111.77
51	y	623	NEX	C40-C33-C34	-2.44	119.50	122.92
29	C1	512	CLA	CMD-C2D-C3D	-2.44	122.00	127.61
48	G	609	CHL	C4D-CHA-C1A	2.44	124.22	121.25
29	s	609	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
52	r	625	LMT	C1B-C2B-C3B	2.44	115.08	110.00
29	c1	507	CLA	CMB-C2B-C3B	2.44	129.25	124.68
29	Y1	603	CLA	CMD-C2D-C3D	-2.44	122.00	127.61
31	C1	515	BCR	C8-C9-C10	2.44	122.69	118.94
48	Y	609	CHL	CHD-C4C-C3C	2.44	128.43	124.84
29	g1	604	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
29	g1	614	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
51	r1	622	NEX	C20-C13-C14	-2.44	119.50	122.92
29	C1	501	CLA	CMA-C3A-C4A	2.44	118.33	111.77
29	G	603	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
29	C1	512	CLA	C2C-C1C-NC	2.44	112.26	109.97
29	a1	406	CLA	C2D-C1D-ND	2.44	111.90	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	N	603	CLA	CHA-C4D-ND	2.44	137.60	132.50
29	B	603	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
29	d	402	CLA	CMD-C2D-C3D	-2.44	122.00	127.61
51	S1	623	NEX	C31-C30-C29	2.44	130.79	127.31
29	N1	602	CLA	C1-O2A-CGA	2.44	122.84	116.44
29	Y1	604	CLA	CHA-C4D-ND	2.44	137.60	132.50
49	G1	620	LUT	C30-C31-C32	-2.44	115.61	123.22
48	y	606	CHL	CMA-C3A-C4A	2.44	118.33	111.77
29	B	602	CLA	CHA-C4D-ND	2.44	137.60	132.50
48	G	605	CHL	CMA-C3A-C4A	2.44	118.33	111.77
29	b1	610	CLA	O2A-CGA-CBA	2.44	119.56	111.91
37	c1	520	DGD	O1G-C1A-C2A	2.44	119.56	111.91
29	c	508	CLA	CMA-C3A-C4A	2.44	118.33	111.77
29	g	610	CLA	CHA-C4D-ND	2.44	137.60	132.50
29	Y	608	CLA	C1-O2A-CGA	2.44	122.84	116.44
31	c1	514	BCR	C33-C5-C6	-2.44	121.79	124.53
29	Y1	604	CLA	C1C-C2C-C3C	-2.44	104.39	106.96
40	G	624	LHG	O8-C23-C24	2.44	119.55	111.91
29	S1	611	CLA	CHA-C1A-NA	-2.44	120.82	126.40
29	y	604	CLA	CHA-C4D-ND	2.44	137.59	132.50
29	C1	505	CLA	CHA-C4D-ND	2.44	137.59	132.50
48	G1	607	CHL	C4D-CHA-C1A	2.44	124.21	121.25
29	D1	402	CLA	CHA-C4D-ND	2.44	137.59	132.50
49	y	621	LUT	C35-C15-C14	-2.43	118.49	123.47
29	G	610	CLA	O1D-CGD-CBD	-2.43	119.50	124.48
29	R	609	CLA	CHA-C4D-ND	2.43	137.59	132.50
29	b1	603	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
48	r	607	CHL	CHB-C4A-NA	2.43	127.88	124.51
29	A1	405	CLA	CMB-C2B-C3B	2.43	129.23	124.68
29	a1	406	CLA	C1-O2A-CGA	2.43	122.83	116.44
29	b1	612	CLA	C2C-C1C-NC	2.43	112.25	109.97
32	A1	412	SQD	O8-S-C6	-2.43	101.86	105.74
29	S1	604	CLA	C1-O2A-CGA	2.43	122.83	116.44
29	B1	612	CLA	CHA-C4D-ND	2.43	137.59	132.50
29	b	606	CLA	C1D-ND-C4D	-2.43	104.61	106.33
29	c	511	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
49	y1	621	LUT	C38-C25-C24	-2.43	118.36	123.56
29	s	610	CLA	C2A-C1A-CHA	2.43	128.11	123.86
29	s	612	CLA	CHA-C4D-ND	2.43	137.59	132.50
29	n1	611	CLA	CHA-C4D-ND	2.43	137.58	132.50
29	S1	611	CLA	C1-C2-C3	-2.43	121.84	126.04
29	S1	611	CLA	C1C-C2C-C3C	-2.43	104.40	106.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	R1	604	CLA	CHA-C4D-ND	2.43	137.58	132.50
29	S	613	CLA	CMB-C2B-C3B	2.43	129.22	124.68
29	G1	613	CLA	CHA-C4D-ND	2.43	137.58	132.50
48	y	607	CHL	C1-O2A-CGA	2.43	122.82	116.44
29	C	502	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
29	y	610	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
29	Y1	613	CLA	C1C-C2C-C3C	-2.43	104.40	106.96
29	R	603	CLA	CMB-C2B-C1B	-2.43	124.73	128.46
49	S	621	LUT	C3-C4-C5	-2.43	107.02	111.85
29	y1	611	CLA	CHA-C1A-NA	-2.43	120.84	126.40
31	A	411	BCR	C36-C18-C17	-2.43	119.52	122.92
29	s1	603	CLA	O1D-CGD-CBD	-2.43	119.52	124.48
29	B	617	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
29	D1	402	CLA	C2C-C1C-NC	2.43	112.25	109.97
29	c1	513	CLA	CMC-C2C-C1C	2.43	128.74	125.04
53	R	626	ERG	C11-C9-C8	-2.43	105.89	111.33
29	g1	602	CLA	CHA-C4D-ND	2.43	137.58	132.50
29	b1	611	CLA	C1-O2A-CGA	2.43	122.81	116.44
29	C	511	CLA	CHA-C4D-ND	2.43	137.58	132.50
48	N1	605	CHL	CMA-C3A-C4A	2.43	118.30	111.77
48	G1	607	CHL	C1B-CHB-C4A	-2.43	125.31	130.12
48	G1	609	CHL	C4A-NA-C1A	2.43	107.80	106.71
29	N1	614	CLA	CHA-C1A-NA	-2.43	120.84	126.40
29	r1	608	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
29	n1	611	CLA	O2A-CGA-CBA	2.43	119.52	111.91
29	R	604	CLA	C2D-C1D-ND	2.43	111.89	110.10
29	y1	614	CLA	C2D-C1D-ND	2.43	111.89	110.10
29	g	610	CLA	C3D-C2D-C1D	-2.43	102.52	105.83
29	B	616	CLA	C1-C2-C3	-2.43	121.85	126.04
29	s1	617	CLA	CHA-C4D-ND	2.43	137.57	132.50
48	G	609	CHL	CHD-C4C-C3C	2.43	128.41	124.84
49	Y1	621	LUT	C15-C14-C13	-2.43	123.85	127.31
29	a1	406	CLA	C1C-C2C-C3C	-2.43	104.41	106.96
48	N	609	CHL	C4D-CHA-C1A	2.43	124.20	121.25
50	Y	622	XAT	C28-C29-C30	2.43	122.66	118.94
29	g1	604	CLA	O2A-CGA-CBA	2.43	119.52	111.91
29	y1	612	CLA	C1-O2A-CGA	2.43	122.81	116.44
29	N1	613	CLA	C1-O2A-CGA	2.42	122.81	116.44
29	N1	614	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
29	A	406	CLA	CMA-C3A-C4A	2.42	118.29	111.77
31	C1	516	BCR	C8-C9-C10	2.42	122.66	118.94
53	r	626	ERG	C13-C17-C20	-2.42	116.30	119.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	G1	603	CLA	C3D-C2D-C1D	-2.42	102.52	105.83
29	a1	410	CLA	CMA-C3A-C4A	2.42	118.29	111.77
29	n1	610	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
29	Y1	610	CLA	CHA-C4D-ND	2.42	137.57	132.50
29	N	604	CLA	O2A-CGA-CBA	2.42	119.51	111.91
29	N	603	CLA	C1-C2-C3	-2.42	121.85	126.04
29	G1	610	CLA	C1D-ND-C4D	-2.42	104.61	106.33
29	g1	603	CLA	O2A-CGA-CBA	2.42	119.51	111.91
29	r1	604	CLA	CHA-C4D-ND	2.42	137.57	132.50
42	d	401	BCT	O3-C-O1	-2.42	113.26	119.55
49	Y	621	LUT	C10-C11-C12	-2.42	115.66	123.22
53	R1	626	ERG	C11-C9-C8	-2.42	105.90	111.33
29	G	610	CLA	CHA-C4D-ND	2.42	137.56	132.50
29	S	602	CLA	C2D-C1D-ND	2.42	111.89	110.10
29	a1	405	CLA	CHA-C4D-ND	2.42	137.56	132.50
30	A	409	PHO	CMC-C2C-C3C	2.42	129.51	124.94
29	y1	610	CLA	CMB-C2B-C3B	2.42	129.21	124.68
29	n	604	CLA	OBD-CAD-C3D	-2.42	122.69	128.52
31	b1	618	BCR	C28-C27-C26	-2.42	109.75	114.08
30	a1	408	PHO	CBA-CAA-C2A	-2.42	106.74	113.81
29	Y	611	CLA	CHA-C4D-ND	2.42	137.56	132.50
29	y	611	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
29	S	609	CLA	CHA-C1A-NA	-2.42	120.86	126.40
29	b1	611	CLA	CHA-C4D-ND	2.42	137.56	132.50
29	y	610	CLA	C1D-ND-C4D	-2.42	104.62	106.33
29	G1	612	CLA	C1D-ND-C4D	-2.42	104.62	106.33
29	s1	613	CLA	CHA-C4D-ND	2.42	137.56	132.50
29	b	609	CLA	C1C-C2C-C3C	-2.42	104.41	106.96
29	b1	607	CLA	CHA-C4D-ND	2.42	137.56	132.50
29	Y	608	CLA	O2D-CGD-O1D	-2.42	119.11	123.84
30	A1	409	PHO	O1D-CGD-CBD	2.42	128.77	124.74
29	r	610	CLA	O1D-CGD-CBD	-2.42	119.54	124.48
49	G	621	LUT	C10-C11-C12	-2.42	115.67	123.22
48	G	607	CHL	C1B-CHB-C4A	-2.42	125.33	130.12
36	b1	620	C7Z	C20-C13-C14	-2.42	119.54	122.92
50	R1	621	XAT	C24-C23-C22	-2.42	106.11	110.77
29	r1	610	CLA	C1D-ND-C4D	-2.42	104.62	106.33
51	N	623	NEX	C17-C1-C6	-2.42	108.31	110.47
29	g1	613	CLA	C1-O2A-CGA	2.42	122.78	116.44
53	R	626	ERG	C12-C13-C17	-2.42	112.95	116.57
29	b	611	CLA	CHA-C4D-ND	2.42	137.55	132.50
29	G1	614	CLA	CHA-C4D-ND	2.42	137.55	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S1	610	CLA	CHA-C4D-ND	2.42	137.55	132.50
50	Y1	622	XAT	O24-C25-C24	-2.42	111.57	113.38
29	S1	605	CLA	CHA-C1A-NA	-2.42	120.87	126.40
30	a	408	PHO	CMD-C2D-C3D	2.41	129.20	124.68
29	g	602	CLA	CMC-C2C-C1C	2.41	128.72	125.04
29	r1	612	CLA	C1D-ND-C4D	-2.41	104.62	106.33
29	n	602	CLA	CMA-C3A-C4A	2.41	118.26	111.77
29	A1	410	CLA	O1D-CGD-CBD	-2.41	119.55	124.48
29	C1	505	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
29	c	511	CLA	CHA-C4D-ND	2.41	137.55	132.50
48	s1	601	CHL	C3A-C2A-C1A	2.41	104.95	101.34
49	Y1	620	LUT	C22-C23-C24	-2.41	108.99	111.74
29	C	506	CLA	CMD-C2D-C3D	-2.41	122.06	127.61
29	n	610	CLA	C1C-C2C-C3C	-2.41	104.42	106.96
29	C	503	CLA	CHA-C4D-ND	2.41	137.55	132.50
29	R	604	CLA	CHA-C4D-ND	2.41	137.55	132.50
29	D1	403	CLA	CMD-C2D-C3D	-2.41	122.06	127.61
31	D1	404	BCR	C30-C25-C24	2.41	122.60	115.78
29	C	501	CLA	CHA-C4D-ND	2.41	137.55	132.50
29	N1	602	CLA	O2D-CGD-O1D	-2.41	119.12	123.84
49	y1	621	LUT	C15-C14-C13	-2.41	123.87	127.31
29	r1	609	CLA	C1-O2A-CGA	2.41	122.77	116.44
48	N	605	CHL	CHB-C4A-NA	2.41	127.85	124.51
29	n	611	CLA	CHA-C4D-ND	2.41	137.54	132.50
29	c1	510	CLA	C6-C7-C8	-2.41	108.12	115.92
29	B1	606	CLA	CHA-C4D-ND	2.41	137.54	132.50
29	B1	608	CLA	CHA-C4D-ND	2.41	137.54	132.50
29	r	609	CLA	O2A-CGA-CBA	2.41	119.47	111.91
29	S1	602	CLA	CMA-C3A-C4A	2.41	118.25	111.77
29	B1	602	CLA	CAA-CBA-CGA	-2.41	106.21	113.25
51	g1	623	NEX	C1-C2-C3	2.41	119.09	113.64
29	g	612	CLA	CHD-C1D-ND	-2.41	122.24	124.45
29	s1	614	CLA	CHA-C4D-ND	2.41	137.54	132.50
29	Y	612	CLA	CGD-CBD-CAD	-2.41	102.93	110.73
29	B	610	CLA	CMA-C3A-C4A	2.41	118.25	111.77
48	g1	606	CHL	C2C-C3C-C4C	2.41	108.21	106.49
29	S1	604	CLA	CHA-C4D-ND	2.41	137.54	132.50
49	N	621	LUT	C35-C34-C33	-2.41	123.87	127.31
29	b	603	CLA	CMD-C2D-C3D	-2.41	122.07	127.61
29	B1	606	CLA	O2A-CGA-CBA	2.41	119.47	111.91
29	Y1	614	CLA	O2A-CGA-CBA	2.41	119.47	111.91
33	B1	622	LMG	O8-C28-C29	2.41	119.47	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	N1	608	CHL	CMB-C2B-C1B	-2.41	124.76	128.46
48	y	605	CHL	CHB-C4A-NA	2.41	127.84	124.51
29	r	609	CLA	C1D-ND-C4D	-2.41	104.62	106.33
48	R1	606	CHL	C3C-C4C-NC	-2.41	107.87	110.57
49	y	620	LUT	C7-C8-C9	-2.41	122.60	126.23
37	c1	518	DGD	O1G-C1A-C2A	2.41	119.47	111.91
48	n	609	CHL	C1-C2-C3	-2.41	121.88	126.04
29	Y1	613	CLA	CMD-C2D-C3D	-2.41	122.08	127.61
48	N1	601	CHL	CMA-C3A-C4A	2.41	118.24	111.77
29	b1	617	CLA	O2A-CGA-CBA	2.41	119.46	111.91
29	S1	613	CLA	CHA-C4D-ND	2.41	137.53	132.50
29	C1	510	CLA	O2A-CGA-CBA	2.41	119.46	111.91
29	C1	512	CLA	CHA-C1A-NA	-2.41	120.89	126.40
29	y1	604	CLA	O2A-CGA-CBA	2.41	119.46	111.91
29	Y1	612	CLA	CMA-C3A-C4A	2.41	118.24	111.77
29	g	610	CLA	CMB-C2B-C1B	-2.41	124.77	128.46
44	F	101	HEM	C4D-ND-C1D	2.41	107.56	105.07
29	b1	610	CLA	CAA-C2A-C3A	-2.41	106.19	112.78
29	C	508	CLA	CHA-C4D-ND	2.41	137.53	132.50
48	G1	601	CHL	C4A-NA-C1A	2.40	107.79	106.71
29	r1	602	CLA	C6-C5-C3	-2.40	107.15	113.45
29	R	610	CLA	OBD-CAD-C3D	-2.40	122.73	128.52
29	C	504	CLA	CMB-C2B-C3B	2.40	129.18	124.68
29	C1	513	CLA	CMD-C2D-C3D	-2.40	122.08	127.61
29	R	604	CLA	CMA-C3A-C4A	2.40	118.23	111.77
29	s1	610	CLA	CMA-C3A-C4A	2.40	118.23	111.77
29	N	611	CLA	CHA-C1A-NA	-2.40	120.89	126.40
48	y1	605	CHL	C2C-C3C-C4C	2.40	108.20	106.49
33	A	413	LMG	C8-O7-C10	-2.40	111.88	117.79
29	R	612	CLA	CHA-C4D-ND	2.40	137.53	132.50
29	G	614	CLA	O2A-CGA-CBA	2.40	119.45	111.91
48	S	608	CHL	C4A-NA-C1A	2.40	107.79	106.71
40	N	624	LHG	C5-O7-C7	-2.40	111.88	117.79
29	b1	614	CLA	CHA-C1A-NA	-2.40	120.90	126.40
29	g	602	CLA	C2C-C1C-NC	2.40	112.22	109.97
29	G1	611	CLA	CAA-C2A-C3A	-2.40	106.20	112.78
29	c1	506	CLA	CHA-C4D-ND	2.40	137.52	132.50
29	R	602	CLA	CHD-C1D-ND	-2.40	122.25	124.45
50	R	621	XAT	C11-C10-C9	2.40	130.74	127.31
29	S	613	CLA	CHA-C4D-ND	2.40	137.52	132.50
29	N1	604	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
29	c1	505	CLA	O2D-CGD-O1D	-2.40	119.14	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Y1	611	CLA	O1D-CGD-CBD	-2.40	119.57	124.48
29	B	617	CLA	CHD-C1D-ND	-2.40	122.25	124.45
29	C	512	CLA	CHD-C1D-ND	-2.40	122.25	124.45
37	B	623	DGD	C4E-C3E-C2E	2.40	115.01	110.82
29	G1	612	CLA	C1C-C2C-C3C	-2.40	104.43	106.96
29	N1	612	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
32	b1	626	SQD	O3-C3-C2	-2.40	104.80	110.35
29	N	613	CLA	CHA-C4D-ND	2.40	137.52	132.50
29	R1	603	CLA	CHD-C1D-ND	-2.40	122.25	124.45
49	S	620	LUT	C18-C5-C6	-2.40	121.83	124.53
29	n	614	CLA	C1C-C2C-C3C	-2.40	104.44	106.96
29	S1	610	CLA	C1C-C2C-C3C	-2.40	104.44	106.96
29	y1	614	CLA	CMC-C2C-C1C	2.40	128.69	125.04
45	h1	101	RRX	C16-C15-C14	-2.40	118.56	123.47
29	c	507	CLA	CMA-C3A-C4A	2.40	118.22	111.77
29	y	603	CLA	CHA-C4D-ND	2.40	137.51	132.50
29	c1	501	CLA	OBD-CAD-C3D	-2.40	122.75	128.52
29	N	603	CLA	CMD-C2D-C3D	-2.40	122.10	127.61
51	g1	623	NEX	C26-C27-C28	-2.40	120.92	125.99
51	S	623	NEX	C40-C33-C34	-2.40	119.57	122.92
29	C	504	CLA	CHA-C4D-ND	2.40	137.51	132.50
29	c1	508	CLA	CHA-C4D-ND	2.40	137.51	132.50
29	g	602	CLA	C2D-C1D-ND	2.40	111.87	110.10
29	S1	604	CLA	C2D-C1D-ND	2.40	111.87	110.10
29	C1	503	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
29	g	604	CLA	CMB-C2B-C3B	2.40	129.16	124.68
49	n	621	LUT	C10-C11-C12	-2.40	115.74	123.22
29	b	606	CLA	CHA-C4D-ND	2.40	137.51	132.50
48	N1	606	CHL	CHB-C4A-NA	2.40	127.83	124.51
48	g	608	CHL	C1B-CHB-C4A	-2.40	125.37	130.12
31	c	514	BCR	C33-C5-C6	-2.40	121.84	124.53
29	g1	610	CLA	CAC-C3C-C4C	2.40	127.92	124.81
31	a1	411	BCR	C1-C6-C5	-2.40	119.24	122.61
29	b1	616	CLA	CHA-C1A-NA	-2.40	120.91	126.40
29	c	512	CLA	CHA-C4D-ND	2.39	137.51	132.50
29	B1	604	CLA	CHA-C4D-ND	2.39	137.51	132.50
48	n1	605	CHL	C1-C2-C3	-2.39	121.90	126.04
29	C1	504	CLA	CMA-C3A-C4A	2.39	118.21	111.77
29	A1	407	CLA	O2A-CGA-CBA	2.39	119.42	111.91
29	C1	503	CLA	CMC-C2C-C1C	2.39	128.69	125.04
36	b1	620	C7Z	C11-C12-C13	-2.39	119.69	126.42
31	a1	411	BCR	C38-C26-C25	-2.39	121.84	124.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C	511	CLA	C2D-C1D-ND	2.39	111.87	110.10
29	N1	613	CLA	CMB-C2B-C3B	2.39	129.16	124.68
29	N1	613	CLA	O2A-CGA-CBA	2.39	119.42	111.91
48	g	605	CHL	CMA-C3A-C2A	2.39	123.48	113.83
29	c	503	CLA	C7-C6-C5	-2.39	106.86	113.36
29	s1	610	CLA	CHA-C1A-NA	-2.39	120.92	126.40
29	n	614	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
29	B	608	CLA	CHA-C4D-ND	2.39	137.50	132.50
29	b1	614	CLA	CHA-C4D-ND	2.39	137.50	132.50
29	y	603	CLA	C1-C2-C3	-2.39	121.91	126.04
29	g	603	CLA	CHA-C1A-NA	-2.39	120.92	126.40
29	s	602	CLA	C1-O2A-CGA	2.39	122.72	116.44
29	b1	617	CLA	C1-O2A-CGA	2.39	122.72	116.44
29	r	608	CLA	C1C-C2C-C3C	-2.39	104.44	106.96
29	c	508	CLA	C2D-C1D-ND	2.39	111.87	110.10
29	b1	611	CLA	C2D-C1D-ND	2.39	111.87	110.10
36	b	620	C7Z	C21-C26-C25	-2.39	119.24	122.61
49	Y1	620	LUT	C15-C14-C13	-2.39	123.90	127.31
29	b	612	CLA	O2A-CGA-CBA	2.39	119.41	111.91
36	b1	620	C7Z	C1-C2-C3	2.39	119.04	113.64
29	b1	609	CLA	C1-O2A-CGA	2.39	122.72	116.44
29	G	603	CLA	CBC-CAC-C3C	-2.39	105.84	112.43
29	B1	615	CLA	C3D-C2D-C1D	-2.39	102.57	105.83
49	s1	621	LUT	C32-C33-C34	2.39	122.61	118.94
55	y1	626	PTY	O4-C30-C31	2.39	119.41	111.91
29	r1	609	CLA	CMC-C2C-C1C	2.39	128.68	125.04
29	a1	405	CLA	C1-C2-C3	-2.39	121.91	126.04
38	B1	624	3PH	O31-C31-C32	2.39	119.41	111.91
29	A1	406	CLA	O2A-CGA-CBA	2.39	119.41	111.91
49	n1	621	LUT	C20-C13-C12	2.39	121.84	118.08
29	N	602	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
48	G1	601	CHL	CHD-C4C-C3C	2.39	128.35	124.84
29	G	603	CLA	CHA-C4D-ND	2.39	137.50	132.50
29	g	604	CLA	C2D-C1D-ND	2.39	111.86	110.10
48	Y	607	CHL	CHD-C1D-ND	-2.39	122.26	124.45
29	S	611	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
29	b	615	CLA	CMC-C2C-C1C	2.39	128.68	125.04
29	R	608	CLA	CHA-C1A-NA	-2.39	120.93	126.40
31	D1	404	BCR	C37-C22-C21	-2.39	119.58	122.92
29	n	610	CLA	CHA-C4D-ND	2.39	137.50	132.50
29	C1	513	CLA	C1D-ND-C4D	-2.39	104.64	106.33
29	R1	612	CLA	CHA-C4D-ND	2.39	137.50	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	y	609	CHL	C1B-CHB-C4A	-2.39	125.39	130.12
29	C	504	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
29	r	608	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
29	Y1	603	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
33	c1	523	LMG	C8-O7-C10	-2.39	111.91	117.79
48	y	607	CHL	CHB-C4A-NA	2.39	127.81	124.51
29	n1	612	CLA	CMD-C2D-C3D	-2.39	122.12	127.61
29	g1	612	CLA	CHA-C4D-ND	2.39	137.49	132.50
29	r	610	CLA	CHA-C1A-NA	-2.39	120.93	126.40
29	G	603	CLA	O2A-CGA-CBA	2.39	119.40	111.91
29	R	604	CLA	O2D-CGD-O1D	-2.39	119.17	123.84
29	c	513	CLA	C1-C2-C3	-2.39	121.92	126.04
48	g	606	CHL	CHD-C4C-C3C	2.39	128.35	124.84
29	S1	605	CLA	CHA-C4D-ND	2.39	137.49	132.50
29	r	609	CLA	CAA-C2A-C3A	-2.39	106.24	112.78
29	D1	402	CLA	OBD-CAD-C3D	-2.39	122.78	128.52
29	B	609	CLA	C1D-ND-C4D	-2.39	104.64	106.33
29	G1	610	CLA	C3D-C2D-C1D	-2.39	102.58	105.83
29	B	611	CLA	CHA-C4D-ND	2.39	137.49	132.50
29	a1	405	CLA	C1C-C2C-C3C	-2.39	104.45	106.96
29	b1	607	CLA	C2D-C1D-ND	2.39	111.86	110.10
29	y	610	CLA	CHA-C4D-ND	2.39	137.49	132.50
39	B	625	DGA	OG1-CA1-CA2	2.39	119.39	111.91
47	k1	101	4RF	O40-C41-C43	2.39	119.39	111.91
29	y1	614	CLA	CMD-C2D-C3D	-2.39	122.13	127.61
49	Y1	621	LUT	C20-C13-C12	2.39	121.83	118.08
31	c1	516	BCR	C37-C22-C21	-2.39	119.58	122.92
32	c1	526	SQD	O3-C3-C2	-2.39	104.83	110.35
29	Y1	608	CLA	CHA-C1A-NA	-2.39	120.94	126.40
29	s1	602	CLA	CAC-C3C-C4C	2.38	127.90	124.81
29	c1	509	CLA	C2D-C1D-ND	2.38	111.86	110.10
48	G1	609	CHL	C1B-CHB-C4A	-2.38	125.40	130.12
29	C	505	CLA	CHA-C4D-ND	2.38	137.49	132.50
29	Y1	602	CLA	CMD-C2D-C3D	-2.38	122.13	127.61
29	Y1	602	CLA	CHD-C1D-ND	-2.38	122.26	124.45
29	d	402	CLA	O2A-CGA-CBA	2.38	119.39	111.91
29	A1	405	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
29	c1	501	CLA	O2D-CGD-O1D	-2.38	119.18	123.84
31	B1	619	BCR	C1-C6-C5	-2.38	119.26	122.61
49	N1	621	LUT	C35-C15-C14	-2.38	118.59	123.47
29	C	509	CLA	CMB-C2B-C3B	2.38	129.13	124.68
29	A1	405	CLA	C1-O2A-CGA	2.38	122.69	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B1	610	CLA	CHD-C1D-ND	-2.38	122.27	124.45
29	B1	605	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
45	H1	101	RRX	C8-C7-C6	-2.38	120.51	127.20
29	G1	603	CLA	CHA-C4D-ND	2.38	137.48	132.50
29	S1	611	CLA	C2A-C1A-CHA	2.38	128.02	123.86
29	A1	407	CLA	C4D-CHA-C1A	2.38	124.15	121.25
29	b1	610	CLA	CMB-C2B-C3B	2.38	129.13	124.68
29	b	613	CLA	O2A-CGA-CBA	2.38	119.38	111.91
29	a1	407	CLA	CHA-C4D-ND	2.38	137.48	132.50
29	Y	612	CLA	O1D-CGD-CBD	-2.38	119.61	124.48
29	n	613	CLA	CMB-C2B-C3B	2.38	129.13	124.68
49	s	621	LUT	C35-C34-C33	-2.38	123.91	127.31
29	n	602	CLA	CAA-C2A-C3A	-2.38	106.26	112.78
29	g1	611	CLA	CAA-C2A-C3A	-2.38	106.26	112.78
40	y	624	LHG	O8-C23-C24	2.38	119.38	111.91
29	g1	603	CLA	CMA-C3A-C4A	2.38	118.17	111.77
29	n	610	CLA	CAA-CBA-CGA	2.38	120.21	113.25
29	d1	403	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
29	b	616	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
29	B1	603	CLA	CHA-C1A-NA	-2.38	120.95	126.40
29	G	611	CLA	CHA-C4D-ND	2.38	137.48	132.50
29	S	617	CLA	CHA-C4D-ND	2.38	137.48	132.50
33	C	521	LMG	C8-O7-C10	-2.38	111.93	117.79
29	c	511	CLA	CHA-C1A-NA	-2.38	120.95	126.40
29	B1	610	CLA	CMB-C2B-C3B	2.38	129.13	124.68
29	R	604	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
29	b	615	CLA	CMD-C2D-C3D	-2.38	122.14	127.61
48	y1	607	CHL	CMA-C3A-C4A	2.38	118.17	111.77
31	D	404	BCR	C35-C13-C12	2.38	121.82	118.08
31	c1	517	BCR	C33-C5-C4	2.38	118.18	113.62
49	r	620	LUT	C18-C5-C6	-2.38	121.86	124.53
29	c	512	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
29	B	612	CLA	CAA-C2A-C3A	-2.38	106.27	112.78
29	b1	606	CLA	CMC-C2C-C1C	2.38	128.66	125.04
29	b	604	CLA	CMD-C2D-C3D	-2.38	122.15	127.61
49	s	621	LUT	C39-C29-C28	2.38	121.82	118.08
36	B1	620	C7Z	C11-C12-C13	-2.38	119.74	126.42
29	Y1	611	CLA	C2D-C1D-ND	2.38	111.86	110.10
29	G1	613	CLA	CMC-C2C-C1C	2.38	128.66	125.04
29	S1	605	CLA	CHD-C1D-ND	-2.38	122.27	124.45
29	A1	407	CLA	CHA-C1A-NA	-2.38	120.96	126.40
29	C1	503	CLA	CHA-C1A-NA	-2.38	120.96	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	R1	603	CLA	CHA-C4D-ND	2.38	137.47	132.50
29	s1	609	CLA	CHA-C4D-ND	2.38	137.47	132.50
33	C1	523	LMG	O8-C28-C29	2.38	119.36	111.91
29	B	604	CLA	CMA-C3A-C4A	2.38	118.16	111.77
50	y	622	XAT	C18-C5-C6	-2.38	118.28	122.26
48	s1	601	CHL	C2C-C3C-C4C	2.38	108.18	106.49
48	g	607	CHL	CHC-C1C-NC	2.37	127.81	124.20
29	c	505	CLA	O1D-CGD-CBD	-2.37	119.62	124.48
29	C1	506	CLA	C2D-C1D-ND	2.37	111.85	110.10
40	d	409	LHG	O8-C23-C24	2.37	119.36	111.91
49	y	621	LUT	C10-C11-C12	-2.37	115.81	123.22
29	g1	614	CLA	CHA-C1A-NA	-2.37	120.96	126.40
29	s1	617	CLA	CHA-C1A-NA	-2.37	120.96	126.40
29	n	614	CLA	CMD-C2D-C3D	-2.37	122.15	127.61
49	R1	620	LUT	C35-C15-C14	-2.37	118.61	123.47
29	C	513	CLA	CHD-C1D-ND	-2.37	122.27	124.45
29	S	612	CLA	CHD-C1D-ND	-2.37	122.27	124.45
29	s	610	CLA	O1D-CGD-CBD	-2.37	119.63	124.48
29	g	613	CLA	O2A-CGA-CBA	2.37	119.36	111.91
48	N	607	CHL	C1B-CHB-C4A	-2.37	125.42	130.12
29	Y	604	CLA	C2C-C1C-NC	2.37	112.19	109.97
37	B1	623	DGD	O3G-C1D-C2D	2.37	112.01	108.30
33	w	201	LMG	O8-C28-C29	2.37	119.35	111.91
29	D1	403	CLA	C6-C5-C3	-2.37	107.23	113.45
49	y1	621	LUT	C18-C5-C4	2.37	118.75	114.36
29	n	602	CLA	O2A-CGA-CBA	2.37	119.35	111.91
29	A	407	CLA	CMB-C2B-C3B	2.37	129.12	124.68
29	D1	402	CLA	O2A-CGA-CBA	2.37	119.35	111.91
49	r1	620	LUT	C11-C12-C13	-2.37	119.75	126.42
29	g	604	CLA	C2C-C1C-NC	2.37	112.19	109.97
29	N	613	CLA	C2D-C1D-ND	2.37	111.85	110.10
29	C	506	CLA	CMC-C2C-C3C	2.37	132.55	126.12
53	R	626	ERG	C11-C9-C10	2.37	119.46	113.58
29	A	406	CLA	CHA-C4D-ND	2.37	137.46	132.50
29	d	402	CLA	O2D-CGD-O1D	-2.37	119.20	123.84
32	M1	101	SQD	O3-C3-C2	-2.37	104.87	110.35
29	C	505	CLA	C2D-C1D-ND	2.37	111.85	110.10
29	B1	603	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
44	F1	101	HEM	C4D-ND-C1D	2.37	107.52	105.07
29	c1	503	CLA	CHA-C4D-ND	2.37	137.45	132.50
29	C	503	CLA	C1C-C2C-C3C	-2.37	104.47	106.96
29	y	602	CLA	CAC-C3C-C4C	2.37	127.88	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
50	g1	622	XAT	C26-C27-C28	-2.37	120.99	125.99
29	n	614	CLA	CHA-C4D-ND	2.37	137.45	132.50
50	g1	622	XAT	C38-C25-C26	-2.37	118.30	122.26
29	S	610	CLA	C1-C2-C3	-2.37	121.95	126.04
29	C1	513	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
29	n	604	CLA	O2A-CGA-CBA	2.37	119.33	111.91
29	r1	604	CLA	O2A-CGA-CBA	2.37	119.33	111.91
48	y	607	CHL	CHD-C4C-C3C	2.37	128.32	124.84
50	N1	622	XAT	C40-C33-C32	2.37	121.80	118.08
29	y1	613	CLA	C1-C2-C3	-2.37	121.95	126.04
40	n1	624	LHG	O8-C23-C24	2.37	119.33	111.91
29	B1	604	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
29	S	609	CLA	CMA-C3A-C4A	2.36	118.13	111.77
48	s1	606	CHL	CMA-C3A-C4A	2.36	118.13	111.77
29	B1	612	CLA	CMC-C2C-C1C	2.36	128.64	125.04
30	A	409	PHO	O2A-CGA-O1A	-2.36	117.62	123.59
36	B	620	C7Z	C21-C26-C27	2.36	122.47	115.78
29	C1	510	CLA	CHA-C4D-ND	2.36	137.44	132.50
49	S1	620	LUT	C30-C31-C32	-2.36	115.84	123.22
29	R	608	CLA	C1-C2-C3	-2.36	121.95	126.04
29	c	508	CLA	O2A-CGA-CBA	2.36	119.33	111.91
29	G1	603	CLA	C1D-ND-C4D	-2.36	104.66	106.33
29	y1	604	CLA	CHA-C4D-ND	2.36	137.44	132.50
51	G1	623	NEX	C16-C1-C6	-2.36	108.36	110.47
29	N1	602	CLA	CHA-C4D-ND	2.36	137.44	132.50
29	n1	613	CLA	CHA-C4D-ND	2.36	137.44	132.50
29	b	605	CLA	CHD-C1D-ND	-2.36	122.28	124.45
29	A1	406	CLA	CHA-C1A-NA	-2.36	120.99	126.40
29	Y1	614	CLA	CMA-C3A-C4A	2.36	118.12	111.77
29	b	616	CLA	CHA-C4D-ND	2.36	137.44	132.50
29	C	508	CLA	C6-C5-C3	-2.36	107.26	113.45
29	B	613	CLA	O1D-CGD-CBD	-2.36	119.65	124.48
48	s	606	CHL	CMB-C2B-C1B	-2.36	124.83	128.46
29	S1	604	CLA	C1C-C2C-C3C	-2.36	104.47	106.96
31	A	411	BCR	C37-C22-C23	2.36	121.80	118.08
45	h	101	RRX	C35-C13-C12	2.36	121.80	118.08
29	C1	509	CLA	CMD-C2D-C3D	-2.36	122.18	127.61
51	g1	623	NEX	C40-C33-C34	-2.36	119.62	122.92
29	b	603	CLA	CMB-C2B-C3B	2.36	129.09	124.68
29	B1	616	CLA	CHA-C1A-NA	-2.36	120.99	126.40
48	G1	608	CHL	CHB-C4A-NA	2.36	127.78	124.51
48	g1	605	CHL	CHB-C4A-NA	2.36	127.78	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	R	620	LUT	C30-C31-C32	-2.36	115.85	123.22
31	B	618	BCR	C36-C18-C17	-2.36	119.62	122.92
48	g	607	CHL	C1-O2A-CGA	2.36	122.63	116.44
29	N	604	CLA	CMB-C2B-C3B	2.36	129.09	124.68
29	c1	504	CLA	O2A-CGA-CBA	2.36	119.31	111.91
51	s1	623	NEX	O24-C25-C24	-2.36	111.61	113.38
29	c1	508	CLA	CMD-C2D-C3D	-2.36	122.19	127.61
31	c	516	BCR	C34-C9-C10	-2.36	119.62	122.92
34	y	625	SPH	C1-C2-C3	-2.36	107.95	113.03
29	G	613	CLA	C1-O2A-CGA	2.36	122.63	116.44
50	r	621	XAT	C38-C25-C26	-2.36	118.31	122.26
29	b1	603	CLA	CHA-C4D-ND	2.36	137.43	132.50
29	S	614	CLA	C2D-C1D-ND	2.36	111.84	110.10
29	C1	512	CLA	CAA-C2A-C3A	-2.36	106.32	112.78
29	S	614	CLA	C6-C5-C3	-2.36	107.28	113.45
29	A1	405	CLA	CHA-C4D-ND	2.36	137.43	132.50
29	s1	603	CLA	CHA-C1A-NA	-2.36	121.00	126.40
29	G	604	CLA	CMB-C2B-C3B	2.36	129.09	124.68
29	s	612	CLA	C1D-ND-C4D	-2.36	104.66	106.33
29	B1	606	CLA	C1-O2A-CGA	2.36	122.62	116.44
43	D1	405	PL9	O2-C1-C6	2.36	124.67	120.59
29	S1	613	CLA	C1C-C2C-C3C	-2.36	104.48	106.96
29	s	610	CLA	O2A-CGA-CBA	2.36	119.30	111.91
29	N1	603	CLA	CHA-C4D-ND	2.36	137.43	132.50
29	b	616	CLA	C1D-ND-C4D	-2.36	104.66	106.33
51	R1	622	NEX	O24-C25-C24	-2.35	111.61	113.38
29	y1	602	CLA	O2D-CGD-O1D	-2.35	119.23	123.84
53	R1	626	ERG	C16-C17-C13	2.35	106.68	103.84
29	r	612	CLA	CHA-C1A-NA	-2.35	121.01	126.40
29	B	608	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
29	Y	602	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
29	s	613	CLA	O2A-CGA-CBA	2.35	119.29	111.91
29	s1	610	CLA	CMB-C2B-C3B	2.35	129.08	124.68
29	n1	602	CLA	CMD-C2D-C3D	-2.35	122.20	127.61
50	g	622	XAT	C40-C33-C34	-2.35	119.63	122.92
31	c1	516	BCR	C33-C5-C4	2.35	118.14	113.62
43	d1	405	PL9	C27-C28-C29	-2.35	122.00	127.66
29	b	611	CLA	CMD-C2D-C3D	-2.35	122.20	127.61
29	B1	604	CLA	C1-C2-C3	-2.35	121.97	126.04
29	R	612	CLA	CHA-C1A-NA	-2.35	121.01	126.40
48	Y1	609	CHL	C1B-CHB-C4A	-2.35	125.46	130.12
48	R1	607	CHL	CHD-C1D-ND	-2.35	122.29	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	y	612	CLA	CBC-CAC-C3C	-2.35	105.95	112.43
50	g	622	XAT	C27-C28-C29	2.35	129.18	125.53
31	b	618	BCR	C8-C7-C6	-2.35	120.60	127.20
51	S	623	NEX	O24-C25-C38	-2.35	112.24	115.06
29	b1	611	CLA	CHA-C1A-NA	-2.35	121.01	126.40
29	y1	602	CLA	C3D-C2D-C1D	-2.35	102.62	105.83
29	b	607	CLA	CMA-C3A-C4A	2.35	118.09	111.77
43	d	405	PL9	C20-C19-C21	2.35	119.22	115.27
29	c	512	CLA	CHA-C1A-NA	-2.35	121.02	126.40
29	r	609	CLA	CMD-C2D-C3D	-2.35	122.21	127.61
49	n	620	LUT	C18-C5-C4	2.35	118.71	114.36
29	B1	611	CLA	O2A-CGA-CBA	2.35	119.28	111.91
37	c	520	DGD	C2G-O2G-C1B	-2.35	112.01	117.79
51	Y1	623	NEX	C12-C13-C14	2.35	122.55	118.94
29	n	611	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
29	b1	611	CLA	CAC-C3C-C4C	2.35	127.86	124.81
29	r	609	CLA	CHA-C4D-ND	2.35	137.41	132.50
29	A1	410	CLA	CMB-C2B-C3B	2.35	129.07	124.68
29	D	403	CLA	CMA-C3A-C4A	2.35	118.09	111.77
29	C1	503	CLA	C1C-C2C-C3C	-2.35	104.49	106.96
29	G1	602	CLA	C1C-C2C-C3C	-2.35	104.49	106.96
29	b1	609	CLA	C1-C2-C3	-2.35	121.98	126.04
29	g	604	CLA	O2A-CGA-CBA	2.35	119.28	111.91
29	b	605	CLA	CAA-C2A-C3A	-2.35	106.35	112.78
29	C	511	CLA	CHA-C1A-NA	-2.35	121.02	126.40
29	B1	611	CLA	CHA-C4D-ND	2.35	137.41	132.50
29	b	602	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
29	s	609	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
48	S1	606	CHL	C1B-CHB-C4A	-2.35	125.47	130.12
29	y	614	CLA	CHA-C4D-ND	2.35	137.41	132.50
29	B1	602	CLA	CHD-C1D-ND	-2.35	122.30	124.45
48	n	607	CHL	CHD-C4C-C3C	2.35	128.29	124.84
49	n1	620	LUT	C10-C11-C12	-2.35	115.89	123.22
31	b	619	BCR	C12-C13-C14	-2.35	115.34	118.94
36	B1	620	C7Z	C8-C7-C6	-2.35	120.61	127.20
29	b	607	CLA	O1D-CGD-CBD	-2.35	119.68	124.48
38	b	624	3PH	O31-C31-C32	2.35	119.27	111.91
29	S1	603	CLA	O1D-CGD-CBD	-2.34	119.69	124.48
29	s1	604	CLA	O2A-CGA-CBA	2.34	119.26	111.91
49	y	621	LUT	C7-C8-C9	-2.34	122.69	126.23
29	S1	617	CLA	CHA-C1A-NA	-2.34	121.03	126.40
29	S1	617	CLA	O1D-CGD-CBD	-2.34	119.69	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	s	606	CHL	CHA-C1A-NA	-2.34	121.03	126.40
49	s	621	LUT	C19-C9-C8	2.34	121.77	118.08
29	b1	608	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
29	b1	607	CLA	C1C-C2C-C3C	-2.34	104.49	106.96
29	G1	611	CLA	CHD-C1D-ND	-2.34	122.30	124.45
49	g	620	LUT	C2-C3-C4	-2.34	107.10	110.30
29	S1	609	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
29	C	509	CLA	C1-C2-C3	-2.34	121.99	126.04
29	Y1	604	CLA	C2D-C1D-ND	2.34	111.83	110.10
29	a	410	CLA	CHA-C4D-ND	2.34	137.40	132.50
29	c	505	CLA	C1-O2A-CGA	2.34	122.59	116.44
29	g1	611	CLA	CHA-C4D-ND	2.34	137.40	132.50
29	S1	614	CLA	CMA-C3A-C4A	2.34	118.07	111.77
29	C	501	CLA	CMD-C2D-C3D	-2.34	122.23	127.61
29	r1	610	CLA	O2D-CGD-O1D	-2.34	119.26	123.84
48	G1	609	CHL	C1-O2A-CGA	2.34	122.58	116.44
29	a1	405	CLA	C1-O2A-CGA	2.34	122.58	116.44
29	C	507	CLA	C2A-C1A-CHA	2.34	127.95	123.86
29	b1	602	CLA	CHA-C1A-NA	-2.34	121.04	126.40
48	G	609	CHL	C4A-NA-C1A	2.34	107.76	106.71
29	D1	402	CLA	C3D-C2D-C1D	-2.34	102.64	105.83
50	R1	621	XAT	C39-C29-C30	-2.34	119.65	122.92
29	B	614	CLA	CHA-C4D-ND	2.34	137.39	132.50
29	Y	614	CLA	CAA-C2A-C3A	-2.34	106.37	112.78
31	B1	619	BCR	C19-C18-C17	2.34	122.53	118.94
48	Y1	601	CHL	CHC-C1C-NC	2.34	127.75	124.20
29	n1	603	CLA	CHD-C1D-ND	-2.34	122.31	124.45
29	y1	608	CLA	C1-O2A-CGA	2.34	122.58	116.44
32	a	412	SQD	O3-C3-C2	-2.34	104.94	110.35
29	B	617	CLA	C1-O2A-CGA	2.34	122.58	116.44
29	A1	407	CLA	CHA-C4D-ND	2.34	137.39	132.50
29	Y	603	CLA	CMA-C3A-C4A	2.34	118.05	111.77
29	c1	508	CLA	CHA-C1A-NA	-2.34	121.05	126.40
49	G	620	LUT	C35-C15-C14	-2.34	118.69	123.47
48	G1	606	CHL	C4D-CHA-C1A	2.34	124.09	121.25
50	g	622	XAT	O4-C5-C18	-2.34	112.26	115.06
29	G1	610	CLA	CMB-C2B-C3B	2.33	129.05	124.68
48	n	606	CHL	C4D-CHA-C1A	2.33	124.09	121.25
31	b1	618	BCR	C37-C22-C21	-2.33	119.65	122.92
48	n	609	CHL	CHC-C1C-NC	2.33	127.74	124.20
29	c1	512	CLA	C2D-C1D-ND	2.33	111.82	110.10
29	Y1	602	CLA	CAC-C3C-C4C	2.33	127.84	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	606	CLA	CMB-C2B-C3B	2.33	129.04	124.68
48	N	608	CHL	C2C-C3C-C4C	2.33	108.15	106.49
29	b1	603	CLA	OBD-CAD-C3D	-2.33	122.91	128.52
29	R1	603	CLA	CHA-C1A-NA	-2.33	121.06	126.40
50	R1	621	XAT	C20-C13-C14	-2.33	119.66	122.92
29	b1	603	CLA	CMA-C3A-C4A	2.33	118.04	111.77
49	s	621	LUT	C15-C35-C34	-2.33	118.70	123.47
29	b1	606	CLA	CMA-C3A-C4A	2.33	118.04	111.77
29	G	602	CLA	O1D-CGD-CBD	-2.33	119.71	124.48
29	S1	610	CLA	O2A-CGA-CBA	2.33	119.22	111.91
40	y	624	LHG	C6-C5-C4	-2.33	106.27	111.79
29	Y	612	CLA	C1D-ND-C4D	-2.33	104.68	106.33
29	B1	610	CLA	C1D-ND-C4D	-2.33	104.68	106.33
49	s	620	LUT	C35-C15-C14	-2.33	118.70	123.47
48	N1	607	CHL	CMB-C2B-C1B	-2.33	124.88	128.46
49	g1	621	LUT	C18-C5-C6	-2.33	121.91	124.53
29	R	602	CLA	CHA-C4D-ND	2.33	137.37	132.50
29	G	611	CLA	O1D-CGD-CBD	-2.33	119.72	124.48
29	A	405	CLA	C6-C5-C3	-2.33	107.34	113.45
29	a	407	CLA	O2A-CGA-CBA	2.33	119.22	111.91
29	R1	612	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
29	Y1	613	CLA	C1D-ND-C4D	-2.33	104.68	106.33
29	n	603	CLA	CMA-C3A-C4A	2.33	118.03	111.77
29	c	510	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
29	r	604	CLA	C2D-C1D-ND	2.33	111.82	110.10
29	y	613	CLA	O2A-CGA-CBA	2.33	119.22	111.91
29	N1	602	CLA	C1D-ND-C4D	-2.33	104.68	106.33
29	g	614	CLA	CHA-C1A-NA	-2.33	121.07	126.40
29	A1	407	CLA	O2D-CGD-O1D	-2.33	119.29	123.84
52	R1	625	LMT	O5'-C1'-O1'	-2.33	104.46	109.97
29	G	604	CLA	CMB-C2B-C1B	-2.33	124.89	128.46
29	S	612	CLA	C1C-C2C-C3C	-2.33	104.51	106.96
43	d1	405	PL9	C35-C34-C36	2.33	119.19	115.27
48	n	608	CHL	CMB-C2B-C1B	-2.33	124.89	128.46
48	S1	608	CHL	C1-C2-C3	-2.33	122.02	126.04
29	A	407	CLA	CHA-C4D-ND	2.33	137.37	132.50
29	g1	610	CLA	CAA-C2A-C3A	-2.33	106.41	112.78
29	n1	613	CLA	CMD-C2D-C3D	-2.33	122.26	127.61
29	s1	604	CLA	C2D-C1D-ND	2.33	111.82	110.10
29	g	613	CLA	CAA-C2A-C3A	-2.33	106.41	112.78
31	B1	618	BCR	C31-C1-C6	-2.33	106.53	110.30
29	D	403	CLA	CHA-C4D-ND	2.33	137.36	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S1	621	LUT	C39-C29-C30	-2.33	119.67	122.92
29	B	608	CLA	O2A-CGA-CBA	2.32	119.20	111.91
29	Y1	611	CLA	O2D-CGD-O1D	-2.32	119.29	123.84
29	s1	605	CLA	C2D-C1D-ND	2.32	111.82	110.10
29	B1	606	CLA	CHA-C1A-NA	-2.32	121.08	126.40
29	b	612	CLA	C1C-C2C-C3C	-2.32	104.51	106.96
29	b1	608	CLA	C1C-C2C-C3C	-2.32	104.51	106.96
29	r1	610	CLA	CMB-C2B-C3B	2.32	129.03	124.68
29	N1	610	CLA	C2C-C1C-NC	2.32	112.15	109.97
29	S	604	CLA	CHA-C4D-ND	2.32	137.36	132.50
43	d1	405	PL9	C32-C33-C34	-2.32	122.06	127.66
29	R1	604	CLA	CMB-C2B-C3B	2.32	129.03	124.68
48	G1	607	CHL	CMB-C2B-C1B	-2.32	124.89	128.46
48	Y1	601	CHL	CMB-C2B-C1B	-2.32	124.89	128.46
29	s	613	CLA	CBC-CAC-C3C	-2.32	106.03	112.43
47	k1	101	4RF	O18-C16-C15	2.32	119.20	111.91
29	g	604	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
29	r	602	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
29	c1	511	CLA	CHA-C4D-ND	2.32	137.36	132.50
29	r1	609	CLA	CHA-C4D-ND	2.32	137.36	132.50
29	b1	608	CLA	O2A-CGA-CBA	2.32	119.20	111.91
36	b1	620	C7Z	C21-C26-C25	-2.32	119.34	122.61
50	G1	622	XAT	C6-C7-C8	-2.32	121.08	125.99
29	b	606	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
29	Y1	613	CLA	O2D-CGD-O1D	-2.32	119.30	123.84
49	Y1	620	LUT	C38-C25-C24	-2.32	118.59	123.56
48	N	607	CHL	C1-O2A-CGA	2.32	122.54	116.44
29	G1	614	CLA	O2A-CGA-CBA	2.32	119.19	111.91
29	B1	609	CLA	C2D-C1D-ND	2.32	111.81	110.10
29	Y	613	CLA	CMD-C2D-C3D	-2.32	122.27	127.61
29	g	602	CLA	CAA-C2A-C3A	-2.32	106.42	112.78
33	B1	622	LMG	C8-O7-C10	-2.32	112.08	117.79
49	g	621	LUT	C19-C9-C8	2.32	121.73	118.08
29	C	512	CLA	CHA-C4D-ND	2.32	137.35	132.50
29	R	610	CLA	C1D-ND-C4D	-2.32	104.69	106.33
29	b1	602	CLA	C1D-ND-C4D	-2.32	104.69	106.33
29	S1	609	CLA	C1C-C2C-C3C	-2.32	104.52	106.96
49	N	620	LUT	C37-C21-C26	2.32	113.06	109.55
29	N	604	CLA	O1D-CGD-CBD	-2.32	119.73	124.48
29	G	602	CLA	O2A-CGA-CBA	2.32	119.19	111.91
48	S	601	CHL	C4D-CHA-C1A	2.32	124.07	121.25
53	r1	626	ERG	C12-C13-C17	-2.32	113.10	116.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	Y1	620	LUT	C11-C10-C9	-2.32	124.00	127.31
29	B	616	CLA	C3D-C2D-C1D	-2.32	102.67	105.83
29	g1	603	CLA	CHA-C1A-NA	-2.32	121.08	126.40
29	b	602	CLA	C1-C2-C3	-2.32	122.03	126.04
29	N	610	CLA	O1D-CGD-CBD	-2.32	119.74	124.48
29	b	611	CLA	C3D-C2D-C1D	-2.32	102.67	105.83
29	s1	610	CLA	O1D-CGD-CBD	-2.32	119.74	124.48
48	G1	606	CHL	C2C-C3C-C4C	2.32	108.14	106.49
50	g1	622	XAT	C6-C7-C8	-2.32	121.09	125.99
51	n1	623	NEX	C28-C29-C30	2.32	122.50	118.94
29	B	616	CLA	CHA-C4D-ND	2.32	137.35	132.50
49	Y	620	LUT	C16-C1-C6	-2.32	106.54	110.30
48	n	605	CHL	CMA-C3A-C4A	2.32	118.00	111.77
29	b	615	CLA	C2C-C1C-NC	2.32	112.14	109.97
29	G	610	CLA	O2A-CGA-CBA	2.32	119.18	111.91
53	R1	626	ERG	C11-C12-C13	2.32	116.75	112.78
48	s	606	CHL	CMA-C3A-C4A	2.32	118.00	111.77
48	N	601	CHL	CHD-C4C-C3C	2.32	128.25	124.84
29	y	612	CLA	CHA-C4D-ND	2.32	137.35	132.50
49	G1	620	LUT	C10-C11-C12	-2.32	115.99	123.22
29	S	604	CLA	CMD-C2D-C3D	-2.32	122.29	127.61
29	c1	509	CLA	CMD-C2D-C3D	-2.32	122.29	127.61
40	g1	624	LHG	O8-C23-C24	2.32	119.17	111.91
31	c1	517	BCR	C12-C13-C14	2.32	122.49	118.94
29	b	610	CLA	C2C-C1C-NC	2.32	112.14	109.97
29	A	410	CLA	CHA-C4D-ND	2.32	137.34	132.50
29	G1	603	CLA	CHA-C1A-NA	-2.32	121.10	126.40
29	B	608	CLA	CMB-C2B-C3B	2.31	129.01	124.68
29	n	610	CLA	C3D-C2D-C1D	-2.31	102.67	105.83
48	G1	606	CHL	CHD-C4C-C3C	2.31	128.24	124.84
29	B1	606	CLA	C1C-C2C-C3C	-2.31	104.52	106.96
29	G	603	CLA	C1D-ND-C4D	-2.31	104.69	106.33
29	r	603	CLA	CHA-C4D-ND	2.31	137.34	132.50
48	g	608	CHL	CHB-C4A-NA	2.31	127.71	124.51
29	n	603	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
48	s1	606	CHL	CMB-C2B-C1B	-2.31	124.91	128.46
49	n1	621	LUT	C18-C5-C6	-2.31	121.93	124.53
29	g	611	CLA	CHA-C4D-ND	2.31	137.34	132.50
48	N1	605	CHL	CHD-C4C-C3C	2.31	128.24	124.84
48	g1	605	CHL	CHD-C4C-C3C	2.31	128.24	124.84
29	N1	613	CLA	C1D-ND-C4D	-2.31	104.69	106.33
48	n	601	CHL	C1-O2A-CGA	2.31	122.51	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Y1	611	CLA	CMB-C2B-C3B	2.31	129.00	124.68
29	R	603	CLA	O2A-CGA-CBA	2.31	119.17	111.91
49	Y	621	LUT	C16-C1-C6	-2.31	106.55	110.30
29	G	611	CLA	O2A-CGA-CBA	2.31	119.16	111.91
29	s1	611	CLA	C2A-C1A-CHA	2.31	127.90	123.86
29	N	612	CLA	CHA-C1A-NA	-2.31	121.10	126.40
29	N1	614	CLA	C1-O2A-CGA	2.31	122.51	116.44
29	g	603	CLA	CMA-C3A-C4A	2.31	117.99	111.77
29	B	604	CLA	CAA-C2A-C3A	-2.31	106.45	112.78
48	y1	601	CHL	C1B-CHB-C4A	-2.31	125.54	130.12
29	Y1	610	CLA	CMD-C2D-C3D	-2.31	122.30	127.61
49	G	620	LUT	C31-C32-C33	-2.31	119.92	126.42
29	y	610	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
29	b1	611	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
29	C	509	CLA	C11-C12-C13	-2.31	108.45	115.92
49	g	620	LUT	C38-C25-C24	-2.31	118.61	123.56
29	C1	506	CLA	O2A-CGA-CBA	2.31	119.16	111.91
53	R	626	ERG	C1-C10-C9	-2.31	103.50	108.28
29	S	604	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
48	y	607	CHL	C1B-CHB-C4A	-2.31	125.54	130.12
29	Y1	603	CLA	CHA-C1A-NA	-2.31	121.11	126.40
43	d	405	PL9	C31-C32-C33	-2.31	104.29	111.88
49	y	620	LUT	C18-C5-C6	-2.31	121.93	124.53
29	b	614	CLA	C1D-ND-C4D	-2.31	104.69	106.33
49	N	620	LUT	C37-C21-C22	-2.31	105.06	109.44
29	N	610	CLA	C3D-C2D-C1D	-2.31	102.68	105.83
29	y1	614	CLA	CHA-C1A-NA	-2.31	121.11	126.40
29	b1	604	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
29	S1	604	CLA	CAC-C3C-C4C	2.31	127.81	124.81
29	C1	505	CLA	O2A-CGA-CBA	2.31	119.15	111.91
43	D	405	PL9	C37-C38-C39	-2.31	122.10	127.66
29	s1	609	CLA	O2A-CGA-CBA	2.31	119.15	111.91
29	n	614	CLA	CMC-C2C-C1C	2.31	128.55	125.04
29	r	603	CLA	CHD-C1D-ND	-2.31	122.33	124.45
29	b1	608	CLA	CHD-C1D-ND	-2.31	122.33	124.45
29	B1	609	CLA	CHA-C1A-NA	-2.31	121.11	126.40
31	A	411	BCR	C33-C5-C4	2.31	118.05	113.62
29	R1	602	CLA	CMD-C2D-C3D	-2.31	122.31	127.61
30	A1	409	PHO	CMC-C2C-C3C	2.31	129.29	124.94
29	b	606	CLA	CMD-C2D-C3D	-2.31	122.31	127.61
29	s	617	CLA	CHA-C1A-NA	-2.31	121.12	126.40
49	G	620	LUT	C10-C11-C12	-2.31	116.02	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	N1	611	CLA	CAC-C3C-C4C	2.31	127.80	124.81
33	b1	622	LMG	C7-O1-C1	-2.31	109.23	113.74
29	c1	513	CLA	CHA-C1A-NA	-2.31	121.12	126.40
29	Y	611	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
29	b1	606	CLA	CMD-C2D-C3D	-2.31	122.31	127.61
50	R	621	XAT	C26-C27-C28	-2.31	121.12	125.99
29	C1	501	CLA	O2A-CGA-CBA	2.31	119.14	111.91
29	S1	604	CLA	CMD-C2D-C3D	-2.31	122.31	127.61
29	S	614	CLA	O2D-CGD-O1D	-2.31	119.33	123.84
37	C1	518	DGD	O1G-C1A-C2A	2.30	119.14	111.91
48	N	609	CHL	CHB-C4A-NA	2.30	127.70	124.51
29	b1	606	CLA	CHA-C1A-NA	-2.30	121.12	126.40
29	b1	608	CLA	CHA-C1A-NA	-2.30	121.12	126.40
29	c1	507	CLA	C2D-C1D-ND	2.30	111.80	110.10
29	R1	602	CLA	O2A-CGA-CBA	2.30	119.14	111.91
39	B1	625	DGA	OG1-CA1-CA2	2.30	119.14	111.91
29	r1	603	CLA	CMD-C2D-C3D	-2.30	122.31	127.61
48	y1	601	CHL	CMB-C2B-C1B	-2.30	124.92	128.46
29	S	614	CLA	CHA-C1A-NA	-2.30	121.12	126.40
29	c	507	CLA	CHA-C1A-NA	-2.30	121.12	126.40
29	c	511	CLA	C6-C5-C3	-2.30	107.41	113.45
36	b1	620	C7Z	C18-C5-C4	2.30	118.62	114.36
29	C	506	CLA	CHD-C4C-C3C	2.30	128.23	124.84
29	r	610	CLA	CAA-C2A-C3A	-2.30	106.47	112.78
32	M	101	SQD	O3-C3-C2	-2.30	105.02	110.35
48	y	607	CHL	CMB-C2B-C1B	-2.30	124.92	128.46
29	c	511	CLA	CAA-CBA-CGA	-2.30	106.52	113.25
29	N	612	CLA	CHD-C1D-ND	-2.30	122.34	124.45
29	s	610	CLA	CHA-C1A-NA	-2.30	121.12	126.40
29	b	616	CLA	C1-C2-C3	-2.30	122.06	126.04
51	y1	623	NEX	C38-C25-C26	-2.30	118.40	122.26
48	g1	606	CHL	C1B-CHB-C4A	-2.30	125.56	130.12
29	s1	614	CLA	CHA-C1A-NA	-2.30	121.13	126.40
29	Y	608	CLA	CHA-C4D-ND	2.30	137.31	132.50
51	S	623	NEX	C5-C6-C1	2.30	121.98	119.70
48	Y1	605	CHL	CHB-C4A-NA	2.30	127.69	124.51
29	y	614	CLA	O2A-CGA-CBA	2.30	119.13	111.91
50	N	622	XAT	C4-C3-C2	-2.30	106.33	110.77
29	n	610	CLA	CMA-C3A-C4A	2.30	117.95	111.77
49	y	621	LUT	C19-C9-C8	2.30	121.70	118.08
29	C1	506	CLA	C6-C5-C3	-2.30	107.42	113.45
31	B	618	BCR	C15-C14-C13	-2.30	124.03	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	G1	620	LUT	C16-C1-C6	-2.30	106.57	110.30
29	B1	617	CLA	CAA-CBA-CGA	-2.30	106.53	113.25
29	b	609	CLA	O2A-CGA-CBA	2.30	119.12	111.91
29	a	406	CLA	C1-O2A-CGA	2.30	122.48	116.44
36	b1	620	C7Z	C40-C33-C34	-2.30	119.70	122.92
31	d1	404	BCR	C38-C26-C25	-2.30	121.95	124.53
48	G1	606	CHL	CMB-C2B-C1B	-2.30	124.93	128.46
51	R1	622	NEX	C4-C3-C2	2.30	115.21	110.77
29	A1	407	CLA	O1D-CGD-CBD	-2.30	119.78	124.48
29	Y1	612	CLA	C1D-ND-C4D	-2.30	104.70	106.33
29	c	507	CLA	C2D-C1D-ND	2.30	111.80	110.10
51	R1	622	NEX	C24-C23-C22	-2.30	106.33	110.77
29	s	602	CLA	CAA-C2A-C3A	-2.30	106.48	112.78
29	s	602	CLA	CMB-C2B-C3B	2.30	128.98	124.68
29	Y1	612	CLA	CHD-C1D-ND	-2.30	122.34	124.45
29	C1	502	CLA	CHA-C1A-NA	-2.30	121.14	126.40
29	D1	402	CLA	CHA-C1A-NA	-2.30	121.14	126.40
31	c	516	BCR	C37-C22-C23	2.30	121.70	118.08
48	n1	608	CHL	C4D-CHA-C1A	2.30	124.05	121.25
31	C1	516	BCR	C37-C22-C21	-2.30	119.70	122.92
48	y	605	CHL	C1B-CHB-C4A	-2.30	125.57	130.12
29	y1	602	CLA	CMB-C2B-C1B	-2.30	124.93	128.46
29	G	604	CLA	OBD-CAD-C3D	-2.30	122.99	128.52
34	A	414	SPH	O3-C3-C2	2.30	110.96	107.31
48	y	605	CHL	CHC-C1C-NC	2.30	127.69	124.20
29	S1	612	CLA	CHA-C1A-NA	-2.30	121.14	126.40
29	G	602	CLA	C1C-C2C-C3C	-2.30	104.54	106.96
31	C	517	BCR	C23-C24-C25	-2.30	120.75	127.20
29	Y1	611	CLA	CHA-C4D-ND	2.30	137.30	132.50
29	A1	410	CLA	C1-O2A-CGA	2.30	122.47	116.44
29	S1	603	CLA	CHD-C1D-ND	-2.30	122.34	124.45
50	g	622	XAT	C20-C13-C14	-2.30	119.71	122.92
29	R1	610	CLA	C3D-C2D-C1D	-2.30	102.70	105.83
51	S1	623	NEX	C1-C2-C3	2.30	118.83	113.64
30	a	408	PHO	CMC-C2C-C3C	2.30	129.27	124.94
29	B	615	CLA	CMD-C2D-C3D	-2.30	122.33	127.61
32	A	412	SQD	O3-C3-C2	-2.30	105.04	110.35
29	Y	602	CLA	CAA-C2A-C3A	-2.30	106.49	112.78
29	B	616	CLA	CHA-C1A-NA	-2.30	121.14	126.40
49	s1	620	LUT	C40-C33-C32	2.29	121.69	118.08
48	Y1	607	CHL	CMB-C2B-C1B	-2.29	124.94	128.46
48	G1	609	CHL	CHD-C4C-C3C	2.29	128.21	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	g1	611	CLA	O1D-CGD-CBD	-2.29	119.79	124.48
29	c	505	CLA	C1C-C2C-C3C	-2.29	104.54	106.96
32	C1	526	SQD	O3-C3-C2	-2.29	105.05	110.35
29	c1	512	CLA	CHA-C1A-NA	-2.29	121.14	126.40
29	y	608	CLA	CHA-C1A-NA	-2.29	121.14	126.40
29	y1	608	CLA	CHA-C1A-NA	-2.29	121.15	126.40
48	g1	607	CHL	CMB-C2B-C1B	-2.29	124.94	128.46
31	C	515	BCR	C1-C6-C7	2.29	122.26	115.78
29	G	604	CLA	CHA-C1A-NA	-2.29	121.15	126.40
29	R1	604	CLA	O2A-CGA-CBA	2.29	119.10	111.91
29	R1	604	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
29	s1	613	CLA	C1-O2A-CGA	2.29	122.46	116.44
29	b1	607	CLA	O1D-CGD-CBD	-2.29	119.80	124.48
48	G	607	CHL	CMB-C2B-C1B	-2.29	124.94	128.46
48	Y	607	CHL	CMB-C2B-C1B	-2.29	124.94	128.46
29	N	613	CLA	CHD-C1D-ND	-2.29	122.35	124.45
29	Y	613	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
29	c	508	CLA	CHA-C4D-ND	2.29	137.29	132.50
29	g1	603	CLA	C1-C2-C3	-2.29	122.08	126.04
48	n	607	CHL	CMB-C2B-C1B	-2.29	124.94	128.46
36	b	620	C7Z	C31-C32-C33	-2.29	119.98	126.42
29	G1	604	CLA	CHA-C1A-NA	-2.29	121.15	126.40
29	r	604	CLA	C1C-C2C-C3C	-2.29	104.55	106.96
29	c	504	CLA	C2C-C1C-NC	2.29	112.12	109.97
29	A1	406	CLA	CMB-C2B-C1B	-2.29	124.94	128.46
29	c	504	CLA	C1-O2A-CGA	2.29	122.45	116.44
29	C	512	CLA	CMA-C3A-C4A	2.29	117.92	111.77
29	N1	613	CLA	CHA-C4D-ND	2.29	137.29	132.50
49	N	621	LUT	C38-C25-C24	-2.29	118.66	123.56
51	g1	623	NEX	C31-C32-C33	2.29	132.84	126.42
29	B1	610	CLA	C1-O2A-CGA	2.29	122.45	116.44
29	g	603	CLA	O2A-CGA-CBA	2.29	119.09	111.91
50	y1	622	XAT	O24-C25-C24	2.29	115.10	113.38
29	c	502	CLA	CHA-C4D-ND	2.29	137.28	132.50
41	C	527	LMK	C9-O8-C28	-2.29	109.39	113.80
51	G	623	NEX	C4-C3-C2	2.29	115.19	110.77
29	C	508	CLA	C2C-C1C-NC	2.29	112.11	109.97
48	G	605	CHL	C1-O2A-CGA	2.29	123.38	116.73
29	G1	604	CLA	CMD-C2D-C3D	-2.29	122.35	127.61
29	A1	406	CLA	C6-C5-C3	-2.29	107.46	113.45
29	R	604	CLA	O2A-CGA-CBA	2.29	119.08	111.91
48	G	607	CHL	C4D-CHA-C1A	2.29	124.03	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	a	411	BCR	C35-C13-C12	2.29	121.68	118.08
29	R1	602	CLA	CHA-C1A-NA	-2.29	121.16	126.40
29	R	604	CLA	CMB-C2B-C1B	-2.29	124.95	128.46
31	B	619	BCR	C8-C7-C6	-2.29	120.78	127.20
29	b	617	CLA	CHA-C4D-ND	2.29	137.28	132.50
29	b	605	CLA	CHA-C1A-NA	-2.29	121.16	126.40
48	N	608	CHL	CMB-C2B-C1B	-2.29	124.95	128.46
29	s1	603	CLA	C3D-C2D-C1D	-2.29	102.71	105.83
29	S	603	CLA	C1-O2A-CGA	2.29	122.44	116.44
29	y	614	CLA	OBD-CAD-C3D	-2.29	123.02	128.52
29	B1	614	CLA	CMC-C2C-C3C	2.29	132.32	126.12
29	S	602	CLA	O1D-CGD-CBD	-2.28	119.81	124.48
29	S1	614	CLA	CHA-C4D-ND	2.28	137.28	132.50
29	b	604	CLA	CAA-C2A-C3A	-2.28	106.52	112.78
48	G	609	CHL	CHB-C4A-NA	2.28	127.67	124.51
48	n	608	CHL	C2C-C3C-C4C	2.28	108.12	106.49
29	s	602	CLA	O1D-CGD-CBD	-2.28	119.81	124.48
29	B1	617	CLA	C2D-C1D-ND	2.28	111.79	110.10
50	G	622	XAT	C39-C29-C30	-2.28	119.72	122.92
31	B1	619	BCR	C35-C13-C12	2.28	121.67	118.08
29	a	407	CLA	CHA-C1A-NA	-2.28	121.17	126.40
31	C	517	BCR	C27-C26-C25	-2.28	119.42	122.73
29	B	616	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
48	s1	606	CHL	C1B-CHB-C4A	-2.28	125.60	130.12
51	N	623	NEX	C31-C32-C33	2.28	132.83	126.42
48	Y	601	CHL	CMB-C2B-C1B	-2.28	124.96	128.46
29	n1	602	CLA	O2A-CGA-CBA	2.28	119.07	111.91
48	Y1	601	CHL	CHB-C4A-NA	2.28	127.67	124.51
29	y1	612	CLA	C1C-C2C-C3C	-2.28	104.56	106.96
48	n1	605	CHL	C3A-C2A-C1A	2.28	104.76	101.34
29	b	607	CLA	CAA-C2A-C3A	-2.28	106.53	112.78
29	S1	612	CLA	CMA-C3A-C4A	2.28	117.91	111.77
29	N	611	CLA	OBD-CAD-C3D	-2.28	123.03	128.52
29	r1	608	CLA	O2A-CGA-CBA	2.28	119.07	111.91
29	y1	612	CLA	CMB-C2B-C3B	2.28	128.95	124.68
43	d1	405	PL9	C22-C23-C24	-2.28	122.17	127.66
51	G1	623	NEX	C40-C33-C34	-2.28	119.73	122.92
48	G1	606	CHL	CHA-C1A-NA	-2.28	121.17	126.40
49	G1	620	LUT	C18-C5-C6	-2.28	121.97	124.53
29	C1	511	CLA	CAA-CBA-CGA	-2.28	106.59	113.25
33	A1	413	LMG	O6-C5-C4	2.28	113.84	109.69
53	R1	626	ERG	C11-C9-C10	2.28	119.24	113.58

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	605	CLA	C1C-C2C-C3C	-2.28	104.56	106.96
29	C	507	CLA	CHA-C1A-NA	-2.28	121.17	126.40
29	s	604	CLA	CMD-C2D-C3D	-2.28	122.37	127.61
29	Y1	602	CLA	CMA-C3A-C4A	2.28	117.90	111.77
49	N	620	LUT	C20-C13-C12	2.28	121.67	118.08
51	g	623	NEX	O24-C25-C24	-2.28	111.67	113.38
29	B1	614	CLA	CHA-C1A-NA	-2.28	121.18	126.40
29	N	612	CLA	C1C-C2C-C3C	-2.28	104.56	106.96
49	r	620	LUT	C38-C25-C24	-2.28	118.68	123.56
29	R1	609	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
29	C1	503	CLA	CMD-C2D-C3D	-2.28	122.37	127.61
29	b	609	CLA	CHD-C1D-ND	-2.28	122.36	124.45
29	B	608	CLA	C1C-C2C-C3C	-2.28	104.56	106.96
29	y1	613	CLA	C1D-ND-C4D	-2.28	104.72	106.33
29	A1	410	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
29	G1	602	CLA	C3D-C2D-C1D	-2.28	102.72	105.83
29	G	614	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
48	g	605	CHL	C1-O2A-CGA	2.28	123.34	116.73
29	B1	604	CLA	CHA-C1A-NA	-2.28	121.19	126.40
32	b	621	SQD	O3-C3-C2	-2.28	105.09	110.35
29	r	602	CLA	OBD-CAD-C3D	-2.28	123.04	128.52
29	g1	604	CLA	CMA-C3A-C4A	2.28	117.89	111.77
29	a	407	CLA	C2A-C1A-CHA	2.27	127.84	123.86
29	B1	616	CLA	OBD-CAD-C3D	-2.27	123.05	128.52
29	Y	604	CLA	C1-C2-C3	-2.27	122.11	126.04
29	B1	612	CLA	C1C-C2C-C3C	-2.27	104.56	106.96
29	Y1	611	CLA	C1C-C2C-C3C	-2.27	104.56	106.96
45	H1	101	RRX	C23-C22-C21	-2.27	115.45	118.94
29	g1	611	CLA	CHD-C1D-ND	-2.27	122.36	124.45
51	r1	622	NEX	O24-C25-C38	-2.27	112.33	115.06
29	s1	613	CLA	CHA-C1A-NA	-2.27	121.19	126.40
29	N	612	CLA	CMD-C2D-C3D	-2.27	122.38	127.61
48	n1	608	CHL	CMB-C2B-C1B	-2.27	124.97	128.46
29	b1	616	CLA	CMA-C3A-C4A	2.27	117.88	111.77
29	g1	611	CLA	C1C-C2C-C3C	-2.27	104.57	106.96
29	S1	610	CLA	CHA-C1A-NA	-2.27	121.19	126.40
29	b	610	CLA	CHA-C4D-ND	2.27	137.25	132.50
29	C1	507	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
29	n1	612	CLA	CHA-C1A-NA	-2.27	121.19	126.40
29	c	508	CLA	O2D-CGD-O1D	-2.27	119.39	123.84
29	G	610	CLA	CMD-C2D-C3D	-2.27	122.39	127.61
29	c	504	CLA	CHA-C4D-ND	2.27	137.25	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c1	511	CLA	C1D-ND-C4D	-2.27	104.72	106.33
29	b	609	CLA	CHA-C1A-NA	-2.27	121.19	126.40
29	N	604	CLA	CMA-C3A-C4A	2.27	117.88	111.77
29	c	503	CLA	CHA-C1A-NA	-2.27	121.20	126.40
29	n1	602	CLA	CMC-C2C-C1C	2.27	128.50	125.04
48	n1	608	CHL	C4A-NA-C1A	2.27	107.73	106.71
29	R1	612	CLA	C6-C5-C3	-2.27	107.50	113.45
39	b	625	DGA	OG1-CA1-CA2	2.27	119.03	111.91
29	C1	511	CLA	CAC-C3C-C4C	2.27	127.76	124.81
29	r	603	CLA	OBD-CAD-C3D	-2.27	123.06	128.52
29	y	613	CLA	C6-C5-C3	-2.27	107.50	113.45
29	G1	602	CLA	C2D-C1D-ND	2.27	111.78	110.10
29	r1	612	CLA	C1-O2A-CGA	2.27	122.40	116.44
29	B1	609	CLA	CMB-C2B-C1B	-2.27	124.97	128.46
29	r	608	CLA	C1-C2-C3	-2.27	122.12	126.04
43	D	405	PL9	O1-C4-C3	-2.27	118.22	120.72
29	R1	609	CLA	CHA-C4D-ND	2.27	137.25	132.50
29	S1	612	CLA	CHA-C4D-ND	2.27	137.25	132.50
29	B	602	CLA	C1D-ND-C4D	-2.27	104.72	106.33
45	h	101	RRX	C19-C18-C17	-2.27	115.46	118.94
29	s1	617	CLA	O2D-CGD-O1D	-2.27	119.40	123.84
29	r1	602	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
29	n1	610	CLA	C1C-C2C-C3C	-2.27	104.57	106.96
51	G	623	NEX	C19-C9-C10	-2.27	119.75	122.92
48	Y	606	CHL	C1B-CHB-C4A	-2.27	125.62	130.12
49	S1	621	LUT	C38-C25-C24	-2.27	118.71	123.56
29	s1	614	CLA	O2A-CGA-CBA	2.27	119.03	111.91
29	s1	611	CLA	CHA-C1A-NA	-2.27	121.20	126.40
48	y	606	CHL	C4D-CHA-C1A	2.27	124.01	121.25
29	a	407	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
29	G1	613	CLA	CMD-C2D-C3D	-2.27	122.40	127.61
51	y	623	NEX	C40-C33-C32	2.27	121.65	118.08
29	b1	616	CLA	C2D-C1D-ND	2.27	111.78	110.10
32	B	621	SQD	O3-C3-C2	-2.27	105.11	110.35
29	B	606	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
29	S	613	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
29	b1	611	CLA	O2A-CGA-CBA	2.27	119.02	111.91
48	g	607	CHL	CMB-C2B-C1B	-2.27	124.98	128.46
29	n1	612	CLA	O2D-CGD-O1D	-2.27	119.41	123.84
29	b	610	CLA	CMB-C2B-C1B	-2.27	124.98	128.46
49	y1	621	LUT	C40-C33-C34	-2.27	119.75	122.92
29	S1	602	CLA	CMB-C2B-C3B	2.27	128.92	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
43	d	405	PL9	C36-C34-C33	-2.27	116.53	121.12
29	r1	602	CLA	CHA-C4D-ND	2.26	137.24	132.50
29	c	503	CLA	CMB-C2B-C1B	-2.26	124.98	128.46
37	c	518	DGD	C1E-C2E-C3E	-2.26	105.28	110.00
29	S	610	CLA	C2C-C1C-NC	2.26	112.09	109.97
43	D1	405	PL9	O2-C1-C2	-2.26	116.59	121.78
29	B	609	CLA	O2A-CGA-CBA	2.26	119.01	111.91
29	r1	610	CLA	O2A-CGA-CBA	2.26	119.01	111.91
29	N1	610	CLA	CMA-C3A-C4A	2.26	117.86	111.77
29	R1	608	CLA	O2D-CGD-O1D	-2.26	119.41	123.84
29	c	507	CLA	C1-C2-C3	-2.26	122.13	126.04
29	Y	611	CLA	CMB-C2B-C3B	2.26	128.91	124.68
29	r1	609	CLA	O2D-CGD-O1D	-2.26	119.42	123.84
29	C1	505	CLA	C1D-ND-C4D	-2.26	104.73	106.33
48	n	608	CHL	C4A-NA-C1A	2.26	107.72	106.71
48	G	609	CHL	C1B-CHB-C4A	-2.26	125.64	130.12
29	R	603	CLA	OBD-CAD-C3D	-2.26	123.08	128.52
49	g	621	LUT	C1-C6-C5	-2.26	119.43	122.61
31	a1	411	BCR	C36-C18-C17	-2.26	119.75	122.92
44	F1	101	HEM	CMA-C3A-C4A	-2.26	124.99	128.46
29	Y	610	CLA	C3D-C2D-C1D	-2.26	102.75	105.83
29	n	602	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
48	G1	609	CHL	C4D-CHA-C1A	2.26	124.00	121.25
40	Y1	624	LHG	C6-C5-C4	-2.26	106.44	111.79
29	Y	608	CLA	CHA-C1A-NA	-2.26	121.22	126.40
29	n1	603	CLA	CMD-C2D-C3D	-2.26	122.41	127.61
29	B1	609	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
29	g	604	CLA	CAA-C2A-C3A	-2.26	106.59	112.78
49	g1	620	LUT	C7-C8-C9	-2.26	122.82	126.23
31	B	619	BCR	C19-C18-C17	2.26	122.41	118.94
29	c	505	CLA	OBD-CAD-C3D	-2.26	123.08	128.52
29	B1	608	CLA	CAC-C3C-C4C	2.26	127.74	124.81
29	N	602	CLA	O1D-CGD-CBD	-2.26	119.86	124.48
48	N	607	CHL	CMB-C2B-C1B	-2.26	124.99	128.46
29	c1	508	CLA	C1C-C2C-C3C	-2.26	104.58	106.96
40	D1	409	LHG	O8-C23-C24	2.26	119.00	111.91
45	H	101	RRX	C19-C18-C17	-2.26	115.47	118.94
37	C1	518	DGD	O6D-C5D-C6D	2.26	111.23	106.67
29	N1	610	CLA	CHA-C4D-ND	2.26	137.23	132.50
29	c1	512	CLA	C1-O2A-CGA	2.26	122.37	116.44
29	D	403	CLA	C1D-ND-C4D	-2.26	104.73	106.33
48	y	606	CHL	C1-C2-C3	-2.26	122.14	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	r1	620	LUT	C35-C15-C14	-2.26	118.85	123.47
29	y1	610	CLA	C6-C5-C3	-2.26	107.53	113.45
29	A1	406	CLA	C2A-C1A-CHA	2.26	127.81	123.86
29	c1	510	CLA	O2A-CGA-CBA	2.26	118.99	111.91
48	Y	609	CHL	CHD-C1D-C2D	2.26	130.22	125.48
29	S	602	CLA	CHA-C1A-NA	-2.26	121.23	126.40
49	S1	620	LUT	C1-C6-C5	-2.26	119.43	122.61
48	G1	608	CHL	CHA-C1A-NA	-2.26	121.23	126.40
29	r1	608	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
29	c1	511	CLA	CHA-C1A-NA	-2.26	121.23	126.40
32	B1	626	SQD	O3-C3-C2	-2.26	105.13	110.35
29	C	505	CLA	CMD-C2D-C3D	-2.26	122.42	127.61
29	C	507	CLA	C2D-C1D-ND	2.26	111.77	110.10
29	S1	613	CLA	C1D-ND-C4D	-2.26	104.73	106.33
29	B	611	CLA	CMB-C2B-C3B	2.25	128.90	124.68
29	R1	608	CLA	CHA-C1A-NA	-2.25	121.23	126.40
29	b1	604	CLA	C3D-C2D-C1D	-2.25	102.75	105.83
29	S	611	CLA	O2A-CGA-CBA	2.25	118.98	111.91
29	R	610	CLA	C1C-C2C-C3C	-2.25	104.59	106.96
29	b	608	CLA	C1C-C2C-C3C	-2.25	104.59	106.96
29	S1	613	CLA	CMD-C2D-C3D	-2.25	122.43	127.61
29	G	614	CLA	CHA-C1A-NA	-2.25	121.24	126.40
48	N1	609	CHL	C1D-CHD-C4C	-2.25	121.20	126.06
29	S	609	CLA	O1D-CGD-CBD	-2.25	119.87	124.48
29	N1	610	CLA	O1D-CGD-CBD	-2.25	119.87	124.48
29	b	608	CLA	CMA-C3A-C4A	2.25	117.83	111.77
49	Y	621	LUT	C11-C10-C9	-2.25	124.09	127.31
29	A	406	CLA	C6-C5-C3	-2.25	107.55	113.45
29	B	612	CLA	CHA-C4D-ND	2.25	137.21	132.50
29	S1	617	CLA	CHA-C4D-ND	2.25	137.21	132.50
50	y1	622	XAT	C39-C29-C30	-2.25	119.77	122.92
29	Y	604	CLA	CAA-C2A-C3A	-2.25	106.61	112.78
29	b	602	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
29	s1	610	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
29	a	405	CLA	CHA-C4D-ND	2.25	137.21	132.50
49	G1	620	LUT	C15-C35-C34	-2.25	118.86	123.47
29	s	614	CLA	C6-C5-C3	-2.25	107.55	113.45
29	G1	602	CLA	C16-C15-C13	-2.25	108.64	115.92
29	A1	410	CLA	CHA-C4D-ND	2.25	137.21	132.50
29	A1	405	CLA	C6-C7-C8	-2.25	108.65	115.92
30	a1	408	PHO	CMC-C2C-C3C	2.25	129.18	124.94
49	S1	621	LUT	C11-C10-C9	-2.25	124.10	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	s	610	CLA	C2D-C1D-ND	2.25	111.76	110.10
29	Y1	603	CLA	CAA-C2A-C3A	-2.25	106.62	112.78
53	r1	626	ERG	C1-C2-C3	2.25	113.35	110.47
29	B	611	CLA	CHA-C1A-NA	-2.25	121.25	126.40
29	g	604	CLA	CHA-C1A-NA	-2.25	121.25	126.40
43	d1	405	PL9	O2-C1-C2	-2.25	116.63	121.78
49	Y	620	LUT	C38-C25-C24	-2.25	118.75	123.56
29	S1	605	CLA	C2A-C1A-CHA	2.25	127.79	123.86
31	c1	514	BCR	C23-C24-C25	-2.25	120.89	127.20
51	y	623	NEX	O24-C25-C38	-2.25	112.36	115.06
49	G1	621	LUT	C31-C32-C33	-2.25	120.10	126.42
49	n	621	LUT	C2-C3-C4	-2.25	107.23	110.30
48	G1	601	CHL	CMA-C3A-C4A	2.25	117.82	111.77
51	R	622	NEX	O24-C25-C24	-2.25	111.69	113.38
49	g1	621	LUT	C11-C12-C13	-2.25	120.10	126.42
29	C	508	CLA	CMD-C2D-C3D	-2.25	122.44	127.61
29	S1	614	CLA	C3D-C2D-C1D	-2.25	102.76	105.83
29	B1	609	CLA	CHD-C1D-ND	-2.25	122.39	124.45
29	n1	611	CLA	C1D-ND-C4D	-2.25	104.74	106.33
50	g	622	XAT	C40-C33-C32	2.25	121.62	118.08
29	b1	602	CLA	O2A-CGA-CBA	2.25	118.96	111.91
48	G1	607	CHL	CHB-C4A-NA	2.25	127.62	124.51
53	R1	626	ERG	C19-C10-C1	-2.25	105.88	109.43
29	B	603	CLA	CHA-C1A-NA	-2.25	121.25	126.40
29	b	610	CLA	C3D-C2D-C1D	-2.25	102.76	105.83
29	n1	602	CLA	C3D-C2D-C1D	-2.25	102.76	105.83
29	n	611	CLA	O2A-CGA-CBA	2.25	118.96	111.91
48	N	609	CHL	CMB-C2B-C1B	-2.25	125.01	128.46
29	s	604	CLA	C2D-C1D-ND	2.25	111.76	110.10
33	H	102	LMG	O8-C28-C29	2.25	118.96	111.91
29	c	506	CLA	C1-C2-C3	-2.25	122.16	126.04
29	b1	614	CLA	O1D-CGD-CBD	-2.25	119.89	124.48
29	r	604	CLA	O2A-CGA-CBA	2.25	118.96	111.91
29	d1	402	CLA	CAC-C3C-C4C	2.25	127.72	124.81
49	N1	621	LUT	C18-C5-C4	2.25	118.52	114.36
29	y1	614	CLA	CMA-C3A-C4A	2.25	117.81	111.77
50	n	622	XAT	O24-C25-C38	-2.25	112.36	115.06
33	c1	521	LMG	C8-O7-C10	-2.25	112.26	117.79
29	B	602	CLA	CMD-C2D-C3D	-2.25	122.45	127.61
29	B1	612	CLA	C1D-ND-C4D	-2.25	104.74	106.33
29	c1	501	CLA	CMD-C2D-C3D	-2.25	122.45	127.61
29	c	505	CLA	CHD-C1D-ND	-2.24	122.39	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	g1	611	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
48	y	609	CHL	CHB-C4A-NA	2.24	127.62	124.51
40	s1	624	LHG	C5-O7-C7	-2.24	112.27	117.79
32	A1	412	SQD	O3-C3-C2	-2.24	105.16	110.35
31	c	517	BCR	C4-C5-C6	-2.24	119.47	122.73
29	C1	501	CLA	C1D-ND-C4D	-2.24	104.74	106.33
29	B1	607	CLA	CGD-CBD-CAD	-2.24	103.47	110.73
29	y	610	CLA	CMB-C2B-C3B	2.24	128.88	124.68
29	A1	405	CLA	CHA-C1A-NA	-2.24	121.26	126.40
29	G	614	CLA	C2D-C1D-ND	2.24	111.76	110.10
31	c1	517	BCR	C29-C30-C25	2.24	113.93	110.48
29	B1	608	CLA	C2A-C1A-CHA	2.24	127.78	123.86
29	N1	611	CLA	CMA-C3A-C4A	2.24	117.80	111.77
37	c1	518	DGD	C6E-C5E-C4E	-2.24	107.75	113.00
29	c1	513	CLA	CHD-C1D-ND	-2.24	122.39	124.45
29	c1	509	CLA	CMB-C2B-C1B	-2.24	125.02	128.46
48	y	601	CHL	CMB-C2B-C1B	-2.24	125.02	128.46
33	A1	413	LMG	O8-C28-C29	2.24	118.94	111.91
29	g1	610	CLA	C3D-C2D-C1D	-2.24	102.77	105.83
29	S1	609	CLA	CHA-C1A-NA	-2.24	121.26	126.40
29	N1	603	CLA	CMD-C2D-C3D	-2.24	122.46	127.61
48	n1	608	CHL	C1B-CHB-C4A	-2.24	125.68	130.12
29	G1	604	CLA	O1D-CGD-CBD	-2.24	119.90	124.48
29	A	406	CLA	C3D-C2D-C1D	-2.24	102.77	105.83
29	C	506	CLA	CAA-C2A-C3A	-2.24	106.64	112.78
37	b	623	DGD	O2G-C1B-O1B	-2.24	118.29	123.70
29	b1	604	CLA	O2A-CGA-CBA	2.24	118.94	111.91
48	S	608	CHL	C1B-CHB-C4A	-2.24	125.68	130.12
48	g1	607	CHL	CHD-C1D-ND	-2.24	122.39	124.45
50	R1	621	XAT	C18-C5-C6	-2.24	118.51	122.26
29	s1	613	CLA	C1C-C2C-C3C	-2.24	104.60	106.96
29	g	613	CLA	CHA-C4D-ND	2.24	137.19	132.50
29	n1	611	CLA	C3D-C2D-C1D	-2.24	102.77	105.83
29	S	610	CLA	CHA-C1A-NA	-2.24	121.27	126.40
48	n1	608	CHL	C1-O2A-CGA	2.24	122.32	116.44
40	S1	624	LHG	O7-C7-O9	-2.24	118.29	123.70
29	B1	606	CLA	CAC-C3C-C4C	2.24	127.72	124.81
29	R1	612	CLA	CHA-C1A-NA	-2.24	121.27	126.40
29	c1	506	CLA	C1-O2A-CGA	2.24	122.32	116.44
29	R1	602	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
29	Y	610	CLA	CMC-C2C-C1C	-2.24	121.63	125.04
29	s	613	CLA	CHA-C4D-ND	2.24	137.18	132.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	405	CLA	C1-O2A-CGA	2.24	122.32	116.44
29	A1	410	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
29	d1	402	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
48	N	606	CHL	CHB-C4A-NA	2.24	127.61	124.51
29	C1	513	CLA	C3D-C2D-C1D	-2.24	102.78	105.83
29	R	612	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
29	b	612	CLA	CHA-C4D-ND	2.24	137.18	132.50
37	C1	518	DGD	C6E-C5E-C4E	-2.24	107.76	113.00
48	Y1	606	CHL	CHD-C4C-C3C	2.24	128.13	124.84
32	B	626	SQD	O3-C3-C2	-2.24	105.18	110.35
29	C	513	CLA	C1D-ND-C4D	-2.24	104.75	106.33
29	n	604	CLA	C1D-ND-C4D	-2.24	104.75	106.33
29	g1	611	CLA	C1D-ND-C4D	-2.24	104.75	106.33
50	R	621	XAT	C20-C13-C12	2.24	121.60	118.08
29	y1	602	CLA	C11-C12-C13	-2.24	108.69	115.92
29	G	614	CLA	C1C-C2C-C3C	-2.24	104.61	106.96
29	y1	608	CLA	C2D-C1D-ND	2.24	111.75	110.10
48	Y1	607	CHL	CHD-C1D-ND	-2.24	122.40	124.45
49	R	620	LUT	C1-C6-C7	2.24	122.10	115.78
30	a	409	PHO	O2A-CGA-O1A	-2.24	117.95	123.59
29	S1	603	CLA	O2A-CGA-CBA	2.24	118.92	111.91
29	D	402	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
29	C1	502	CLA	CMD-C2D-C3D	-2.24	122.47	127.61
48	n1	607	CHL	CMB-C2B-C1B	-2.24	125.03	128.46
48	r	606	CHL	C3C-C4C-NC	-2.24	108.06	110.57
44	f	101	HEM	C1B-NB-C4B	2.23	107.38	105.07
29	c	505	CLA	CMD-C2D-C3D	-2.23	122.47	127.61
29	c1	501	CLA	CHA-C1A-NA	-2.23	121.28	126.40
29	B1	612	CLA	CMD-C2D-C3D	-2.23	122.47	127.61
29	b1	602	CLA	CMD-C2D-C3D	-2.23	122.47	127.61
29	C1	508	CLA	CHA-C4D-ND	2.23	137.17	132.50
29	R1	603	CLA	O2A-CGA-CBA	2.23	118.92	111.91
30	A1	408	PHO	O1D-CGD-CBD	2.23	128.46	124.74
29	Y	614	CLA	C11-C12-C13	-2.23	108.70	115.92
29	d1	402	CLA	CHA-C1A-NA	-2.23	121.28	126.40
30	a	409	PHO	CMA-C3A-C4A	-2.23	109.49	114.38
29	y	611	CLA	CHA-C1A-NA	-2.23	121.28	126.40
29	r1	602	CLA	CMC-C2C-C1C	2.23	128.44	125.04
29	g	611	CLA	C1D-ND-C4D	-2.23	104.75	106.33
37	B	623	DGD	O5D-C6D-C5D	2.23	113.18	109.05
29	s1	611	CLA	CBC-CAC-C3C	-2.23	106.28	112.43
29	c1	501	CLA	C2D-C1D-ND	2.23	111.75	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S	609	CLA	O2D-CGD-O1D	-2.23	119.47	123.84
48	G	601	CHL	C1B-CHB-C4A	-2.23	125.70	130.12
51	s1	623	NEX	C27-C28-C29	-2.23	122.07	125.53
29	S1	602	CLA	CMD-C2D-C3D	-2.23	122.48	127.61
29	c1	505	CLA	CHA-C4D-ND	2.23	137.17	132.50
29	y1	613	CLA	C3D-C2D-C1D	-2.23	102.79	105.83
32	m1	101	SQD	O3-C3-C2	-2.23	105.19	110.35
29	s	602	CLA	C2C-C1C-NC	2.23	112.06	109.97
50	g	622	XAT	C20-C13-C12	2.23	121.59	118.08
29	n1	603	CLA	CHA-C1A-NA	-2.23	121.29	126.40
48	y1	606	CHL	C1-O2A-CGA	2.23	122.30	116.44
49	s1	620	LUT	C37-C21-C26	2.23	112.92	109.55
29	R	610	CLA	CHC-C1C-NC	-2.23	120.82	124.20
49	S1	621	LUT	C1-C6-C7	2.23	122.09	115.78
29	S1	617	CLA	C1D-ND-C4D	-2.23	104.75	106.33
29	b	616	CLA	CHA-C1A-NA	-2.23	121.29	126.40
49	r1	620	LUT	C19-C9-C10	-2.23	119.80	122.92
29	C1	503	CLA	CAA-C2A-C3A	-2.23	106.67	112.78
29	B	602	CLA	O2A-CGA-CBA	2.23	118.90	111.91
29	B	615	CLA	O2A-CGA-CBA	2.23	118.90	111.91
29	B1	611	CLA	CHA-C1A-NA	-2.23	121.29	126.40
29	C1	510	CLA	CHA-C1A-NA	-2.23	121.29	126.40
29	Y1	604	CLA	CMD-C2D-C3D	-2.23	122.49	127.61
29	s1	604	CLA	CHA-C1A-NA	-2.23	121.29	126.40
48	G1	601	CHL	C1-O2A-CGA	2.23	122.29	116.44
48	g1	601	CHL	C1-O2A-CGA	2.23	122.29	116.44
48	Y	605	CHL	CHB-C4A-NA	2.23	127.59	124.51
50	N	622	XAT	C40-C33-C34	-2.23	119.80	122.92
29	G	612	CLA	CHA-C1A-NA	-2.23	121.30	126.40
29	B1	611	CLA	CMA-C3A-C4A	2.23	117.76	111.77
29	c	513	CLA	CHD-C1D-ND	-2.23	122.41	124.45
29	g1	611	CLA	CMB-C2B-C3B	2.23	128.84	124.68
29	B1	608	CLA	CHA-C1A-NA	-2.23	121.30	126.40
29	s1	602	CLA	CHA-C1A-NA	-2.23	121.30	126.40
29	N	610	CLA	O2A-CGA-CBA	2.23	118.90	111.91
29	S	604	CLA	CBC-CAC-C3C	-2.23	106.29	112.43
50	g1	622	XAT	C35-C34-C33	2.23	130.49	127.31
29	b1	615	CLA	CHA-C1A-NA	-2.23	121.30	126.40
29	C1	506	CLA	C1-C2-C3	-2.23	122.19	126.04
29	y1	611	CLA	OBD-CAD-C3D	-2.23	123.16	128.52
31	c	515	BCR	C28-C29-C30	-2.23	106.64	114.60
48	n1	601	CHL	CHA-C1A-NA	-2.23	121.30	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
33	W1	201	LMG	C38-C37-C36	2.23	125.72	114.42
49	n	620	LUT	C20-C13-C12	2.23	121.58	118.08
29	C1	503	CLA	CAC-C3C-C4C	2.23	127.70	124.81
29	y	602	CLA	C1C-C2C-C3C	-2.23	104.62	106.96
29	R1	603	CLA	C1C-C2C-C3C	-2.23	104.62	106.96
29	a1	407	CLA	CAA-C2A-C3A	-2.22	106.69	112.78
29	S1	603	CLA	CHA-C1A-NA	-2.22	121.30	126.40
49	y1	620	LUT	C15-C14-C13	-2.22	124.14	127.31
29	B1	605	CLA	C2A-C1A-CHA	2.22	127.75	123.86
29	Y	614	CLA	O2A-CGA-CBA	2.22	118.89	111.91
29	y1	602	CLA	CHA-C4D-ND	2.22	137.15	132.50
29	B1	615	CLA	C2A-C1A-CHA	2.22	127.75	123.86
31	b	619	BCR	C34-C9-C10	-2.22	119.81	122.92
29	g	602	CLA	O1D-CGD-CBD	-2.22	119.93	124.48
31	c1	517	BCR	C8-C7-C6	-2.22	120.96	127.20
29	C1	512	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
29	N	610	CLA	C1D-ND-C4D	-2.22	104.76	106.33
29	c1	509	CLA	CMA-C3A-C4A	2.22	117.75	111.77
31	b	619	BCR	C39-C30-C25	-2.22	106.69	110.30
49	N	621	LUT	C10-C11-C12	-2.22	116.28	123.22
29	C	505	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
29	d	402	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
29	C1	502	CLA	C1C-C2C-C3C	-2.22	104.62	106.96
49	R1	620	LUT	C8-C7-C6	-2.22	120.96	127.20
48	n	606	CHL	CHD-C4C-C3C	2.22	128.11	124.84
31	c	515	BCR	C34-C9-C8	2.22	121.58	118.08
29	y	608	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
29	C	501	CLA	C1D-ND-C4D	-2.22	104.76	106.33
29	B1	616	CLA	C1D-ND-C4D	-2.22	104.76	106.33
49	n	621	LUT	C1-C6-C5	-2.22	119.48	122.61
48	N1	607	CHL	C4D-CHA-C1A	2.22	123.95	121.25
29	G	604	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
29	Y	612	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
29	s	617	CLA	CMD-C2D-C3D	-2.22	122.50	127.61
29	D1	402	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
29	c1	505	CLA	CMB-C2B-C3B	2.22	128.83	124.68
48	g	607	CHL	C4D-CHA-C1A	2.22	123.95	121.25
29	B1	609	CLA	C2A-C1A-CHA	2.22	127.74	123.86
40	s1	624	LHG	O8-C23-O10	-2.22	117.99	123.59
29	s	603	CLA	C3D-C2D-C1D	-2.22	102.80	105.83
29	G1	613	CLA	O1D-CGD-CBD	-2.22	119.94	124.48
29	a	410	CLA	CMC-C2C-C1C	2.22	128.42	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	y1	607	CHL	CHD-C4C-C3C	2.22	128.10	124.84
29	b1	603	CLA	C1D-ND-C4D	-2.22	104.76	106.33
50	r1	621	XAT	C35-C34-C33	-2.22	124.14	127.31
29	B1	603	CLA	CMD-C2D-C3D	-2.22	122.51	127.61
48	y	601	CHL	C1-O2A-CGA	2.22	122.26	116.44
49	N1	620	LUT	C10-C11-C12	-2.22	116.30	123.22
29	b1	605	CLA	O1D-CGD-CBD	-2.22	119.95	124.48
29	S	613	CLA	C2D-C1D-ND	2.22	111.74	110.10
48	n1	605	CHL	CHD-C4C-C3C	2.22	128.10	124.84
29	g	603	CLA	OBD-CAD-C3D	-2.22	123.19	128.52
43	D	405	PL9	C40-C39-C41	2.22	119.00	115.27
51	n	623	NEX	C19-C9-C10	-2.22	119.82	122.92
49	n	620	LUT	C38-C25-C24	-2.22	118.82	123.56
29	A	410	CLA	CMA-C3A-C4A	2.22	117.73	111.77
48	R1	607	CHL	CHA-C1A-NA	-2.22	121.32	126.40
48	n1	609	CHL	CMB-C2B-C1B	-2.22	125.06	128.46
29	B	611	CLA	C3D-C2D-C1D	-2.22	102.81	105.83
31	d1	404	BCR	C30-C25-C24	2.22	122.05	115.78
29	A1	410	CLA	CAC-C3C-C4C	2.22	127.69	124.81
37	B	623	DGD	O6D-C5D-C6D	2.22	111.14	106.67
29	b1	610	CLA	CMD-C2D-C3D	-2.22	122.52	127.61
48	Y1	607	CHL	C3A-C2A-C1A	2.22	104.66	101.34
50	G	622	XAT	C20-C13-C14	-2.22	119.82	122.92
29	N	614	CLA	CHA-C1A-NA	-2.22	121.33	126.40
44	f	101	HEM	CMB-C2B-C1B	-2.21	121.67	125.04
29	y1	603	CLA	O2A-CGA-CBA	2.21	118.86	111.91
48	y1	605	CHL	CHD-C4C-C3C	2.21	128.09	124.84
50	r	621	XAT	C40-C33-C34	-2.21	119.82	122.92
48	n1	608	CHL	CHB-C4A-NA	2.21	127.57	124.51
29	R	612	CLA	C1D-ND-C4D	-2.21	104.76	106.33
29	g1	614	CLA	C1D-ND-C4D	-2.21	104.76	106.33
50	r	621	XAT	C11-C10-C9	2.21	130.47	127.31
29	C1	512	CLA	O2A-CGA-CBA	2.21	118.86	111.91
29	n	611	CLA	CHA-C1A-NA	-2.21	121.33	126.40
29	r	610	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
48	N1	606	CHL	C1-O2A-CGA	2.21	122.25	116.44
51	y1	623	NEX	C16-C1-C6	-2.21	108.49	110.47
31	C1	517	BCR	C28-C27-C26	-2.21	110.12	114.08
29	c	512	CLA	C2A-C1A-CHA	2.21	127.73	123.86
29	C	513	CLA	C1C-C2C-C3C	-2.21	104.63	106.96
49	Y	621	LUT	C18-C5-C4	2.21	118.45	114.36
48	N	607	CHL	CHD-C4C-C3C	2.21	128.09	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S	603	CLA	C3D-C2D-C1D	-2.21	102.81	105.83
29	c1	508	CLA	O2A-CGA-CBA	2.21	118.85	111.91
29	N1	603	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
29	N1	614	CLA	C2A-C1A-CHA	2.21	127.73	123.86
29	R1	604	CLA	CHA-C1A-NA	-2.21	121.33	126.40
29	s	612	CLA	CMA-C3A-C4A	2.21	117.72	111.77
29	Y1	603	CLA	CMA-C3A-C4A	2.21	117.72	111.77
29	a	405	CLA	CAA-C2A-C3A	-2.21	106.72	112.78
29	g	612	CLA	CHA-C1A-NA	-2.21	121.33	126.40
29	n1	611	CLA	CHA-C1A-NA	-2.21	121.33	126.40
49	G	620	LUT	C20-C13-C12	2.21	121.56	118.08
29	C	508	CLA	C2D-C1D-ND	2.21	111.73	110.10
29	C	505	CLA	CMA-C3A-C4A	2.21	117.71	111.77
29	n1	612	CLA	CMA-C3A-C4A	2.21	117.71	111.77
48	s	607	CHL	CHA-C1A-NA	-2.21	121.34	126.40
32	b1	621	SQD	O3-C3-C2	-2.21	105.24	110.35
49	s	621	LUT	C2-C3-C4	-2.21	107.28	110.30
29	A1	410	CLA	O2A-CGA-CBA	2.21	118.84	111.91
29	S	609	CLA	CMD-C2D-C3D	-2.21	122.53	127.61
29	r1	604	CLA	C3D-C2D-C1D	-2.21	102.82	105.83
51	S	623	NEX	C38-C25-C26	-2.21	118.56	122.26
29	C	509	CLA	O1D-CGD-CBD	-2.21	119.96	124.48
29	C	501	CLA	C1-O2A-CGA	2.21	122.24	116.44
50	y	622	XAT	C11-C10-C9	-2.21	124.16	127.31
48	g1	605	CHL	C1B-CHB-C4A	-2.21	125.74	130.12
31	A1	411	BCR	C34-C9-C10	-2.21	119.83	122.92
29	R	612	CLA	O2D-CGD-O1D	-2.21	119.52	123.84
48	N	601	CHL	C1-O2A-CGA	2.21	122.24	116.44
40	D	409	LHG	O8-C23-O10	-2.21	118.02	123.59
29	N	602	CLA	CHA-C4D-ND	2.21	137.12	132.50
29	s	609	CLA	CMB-C2B-C3B	2.21	128.81	124.68
29	G1	612	CLA	C3D-C2D-C1D	-2.21	102.82	105.83
29	y1	612	CLA	C3D-C2D-C1D	-2.21	102.82	105.83
31	C1	517	BCR	C8-C7-C6	-2.21	121.00	127.20
29	y	613	CLA	CHD-C1D-ND	-2.21	122.43	124.45
29	C	508	CLA	CAA-C2A-C3A	-2.21	106.73	112.78
48	g1	606	CHL	C1-O2A-CGA	2.21	122.23	116.44
29	C1	513	CLA	CHA-C1A-NA	-2.21	121.34	126.40
29	n	610	CLA	C2C-C1C-NC	2.21	112.04	109.97
29	s1	613	CLA	CMD-C2D-C3D	-2.21	122.54	127.61
29	Y	611	CLA	CHA-C1A-NA	-2.21	121.35	126.40
29	d1	403	CLA	CHA-C1A-NA	-2.21	121.35	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	d1	404	BCR	C23-C22-C21	2.21	122.33	118.94
29	y	613	CLA	C1-O2A-CGA	2.21	122.23	116.44
31	B1	618	BCR	C35-C13-C12	2.21	121.55	118.08
33	a	413	LMG	O8-C28-C29	2.20	118.83	111.91
29	G	611	CLA	CAA-C2A-C3A	-2.20	106.74	112.78
29	c	510	CLA	CAA-C2A-C3A	-2.20	106.74	112.78
53	R	626	ERG	C6-C7-C8	-2.20	117.73	122.07
48	g1	608	CHL	CHB-C4A-NA	2.20	127.56	124.51
29	r1	612	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
29	Y1	611	CLA	CHA-C1A-NA	-2.20	121.35	126.40
49	g	620	LUT	C37-C21-C26	2.20	112.88	109.55
29	d1	402	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
29	s1	610	CLA	C3D-C2D-C1D	-2.20	102.82	105.83
29	C1	513	CLA	C1C-C2C-C3C	-2.20	104.64	106.96
31	B	618	BCR	C34-C9-C10	-2.20	119.84	122.92
29	g1	603	CLA	C1D-ND-C4D	-2.20	104.77	106.33
29	C1	501	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
29	N1	603	CLA	CHA-C1A-NA	-2.20	121.35	126.40
48	g1	605	CHL	C4D-CHA-C1A	2.20	123.93	121.25
51	s	623	NEX	C26-C27-C28	-2.20	121.34	125.99
29	S	611	CLA	CHA-C1A-NA	-2.20	121.36	126.40
29	G1	614	CLA	C1-O2A-CGA	2.20	122.22	116.44
29	A1	406	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
30	a	408	PHO	O2D-CGD-O1D	-2.20	119.53	123.84
48	n	607	CHL	C1-C2-C3	-2.20	122.24	126.04
29	y	603	CLA	CAC-C3C-C4C	2.20	127.67	124.81
29	c	509	CLA	CHA-C1A-NA	-2.20	121.36	126.40
29	A	407	CLA	O2A-CGA-CBA	2.20	118.81	111.91
50	g1	622	XAT	C18-C5-C6	-2.20	118.57	122.26
29	r1	604	CLA	CHA-C1A-NA	-2.20	121.36	126.40
29	R	609	CLA	O2A-CGA-CBA	2.20	118.81	111.91
29	Y1	610	CLA	CHA-C1A-NA	-2.20	121.36	126.40
29	c	510	CLA	C1D-ND-C4D	-2.20	104.77	106.33
29	s1	602	CLA	CMD-C2D-C3D	-2.20	122.55	127.61
29	y1	612	CLA	CHA-C1A-NA	-2.20	121.36	126.40
48	Y	601	CHL	C4A-NA-C1A	2.20	107.69	106.71
48	G	606	CHL	CHC-C1C-NC	2.20	127.54	124.20
30	a1	409	PHO	O2A-CGA-O1A	-2.20	118.04	123.59
31	c1	514	BCR	C37-C22-C21	-2.20	119.84	122.92
29	Y	612	CLA	CHA-C1A-NA	-2.20	121.36	126.40
48	r1	606	CHL	CHA-C1A-NA	-2.20	121.36	126.40
29	c	510	CLA	O2A-CGA-CBA	2.20	118.81	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	D1	404	BCR	C12-C13-C14	-2.20	115.57	118.94
29	g1	612	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
29	s1	610	CLA	C2A-C1A-CHA	2.20	127.70	123.86
48	R	607	CHL	C4A-NA-C1A	2.20	107.69	106.71
29	y1	610	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
29	S	609	CLA	C1C-C2C-C3C	-2.20	104.65	106.96
48	N	606	CHL	C1-O2A-CGA	2.20	122.21	116.44
29	s	617	CLA	CMB-C2B-C3B	2.20	128.79	124.68
29	R	612	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
29	A	407	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
29	C	507	CLA	CMB-C2B-C3B	2.20	128.79	124.68
51	g1	623	NEX	O24-C25-C38	-2.20	112.42	115.06
50	r	621	XAT	C19-C9-C8	2.20	121.54	118.08
29	C1	512	CLA	C6-C5-C3	-2.20	107.69	113.45
29	B	604	CLA	CMD-C2D-C3D	-2.20	122.56	127.61
29	N1	604	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
29	Y	612	CLA	O2D-CGD-O1D	-2.20	119.54	123.84
45	h1	101	RRX	C33-C5-C4	2.20	117.83	113.62
29	C	505	CLA	C1-O2A-CGA	2.20	122.21	116.44
29	N	604	CLA	C3D-C2D-C1D	-2.20	102.83	105.83
29	b	605	CLA	C2A-C1A-CHA	2.20	127.70	123.86
29	y1	603	CLA	CMA-C3A-C4A	2.20	117.67	111.77
29	N1	612	CLA	CHA-C1A-NA	-2.20	121.37	126.40
29	b1	617	CLA	CHA-C1A-NA	-2.20	121.37	126.40
30	a1	409	PHO	CMB-C2B-C3B	2.20	128.79	124.68
29	b	605	CLA	O1D-CGD-CBD	-2.20	119.99	124.48
48	g	606	CHL	CMB-C2B-C1B	-2.20	125.09	128.46
29	n	602	CLA	CHC-C1C-NC	-2.19	120.87	124.20
29	B1	606	CLA	OBD-CAD-C3D	-2.19	123.24	128.52
29	Y	603	CLA	O2A-CGA-CBA	2.19	118.80	111.91
31	c	517	BCR	C33-C5-C4	2.19	117.83	113.62
48	Y1	606	CHL	C1B-CHB-C4A	-2.19	125.77	130.12
29	c	508	CLA	CAA-C2A-C3A	-2.19	106.77	112.78
29	N	611	CLA	O2A-CGA-CBA	2.19	118.79	111.91
29	C1	504	CLA	CHA-C1A-NA	-2.19	121.37	126.40
29	c1	509	CLA	CHA-C1A-NA	-2.19	121.37	126.40
29	S	613	CLA	CHA-C1A-NA	-2.19	121.38	126.40
48	y1	607	CHL	CMB-C2B-C1B	-2.19	125.09	128.46
29	c1	503	CLA	CHA-C1A-NA	-2.19	121.38	126.40
29	Y	610	CLA	CHA-C4D-ND	2.19	137.09	132.50
29	d1	403	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
29	y	614	CLA	CMD-C2D-C3D	-2.19	122.57	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
40	D1	410	LHG	C5-O7-C7	-2.19	112.39	117.79
29	C	510	CLA	CHA-C1A-NA	-2.19	121.38	126.40
48	S	608	CHL	C4D-CHA-C1A	2.19	123.92	121.25
29	r	604	CLA	O1D-CGD-CBD	-2.19	120.00	124.48
29	R	610	CLA	C2C-C1C-NC	2.19	112.02	109.97
45	h	101	RRX	C30-C29-C28	-2.19	108.70	113.64
36	B	620	C7Z	C39-C29-C28	2.19	121.53	118.08
51	r1	622	NEX	C5-C4-C3	-2.19	109.15	111.75
29	G	603	CLA	CAA-C2A-C3A	-2.19	106.78	112.78
29	R	604	CLA	CHA-C1A-NA	-2.19	121.38	126.40
29	b1	612	CLA	CHA-C1A-NA	-2.19	121.38	126.40
29	g	602	CLA	C6-C7-C8	-2.19	108.84	115.92
29	R1	610	CLA	CMB-C2B-C3B	2.19	128.78	124.68
48	Y	601	CHL	C1-O2A-CGA	2.19	122.19	116.44
29	C	507	CLA	O2A-CGA-CBA	2.19	118.78	111.91
29	b1	602	CLA	C3D-C2D-C1D	-2.19	102.84	105.83
29	y	602	CLA	C2D-C1D-ND	2.19	111.72	110.10
29	y	612	CLA	C1-C2-C3	-2.19	122.26	126.04
48	N	606	CHL	C1-C2-C3	-2.19	122.26	126.04
50	R1	621	XAT	C15-C35-C34	2.19	127.96	123.47
49	g	620	LUT	C8-C7-C6	-2.19	121.06	127.20
29	y1	613	CLA	CMD-C2D-C3D	-2.19	122.58	127.61
29	G1	602	CLA	CHD-C1D-ND	-2.19	122.44	124.45
29	s1	611	CLA	CHD-C1D-ND	-2.19	122.44	124.45
29	G	610	CLA	CHA-C1A-NA	-2.19	121.39	126.40
29	b	611	CLA	CHA-C1A-NA	-2.19	121.39	126.40
29	r1	602	CLA	CHA-C1A-NA	-2.19	121.39	126.40
31	C1	515	BCR	C1-C6-C7	2.19	121.97	115.78
53	r1	626	ERG	C16-C17-C13	2.19	106.48	103.84
29	Y1	611	CLA	C1D-ND-C4D	-2.19	104.78	106.33
29	s	603	CLA	OBD-CAD-C3D	-2.19	123.26	128.52
29	C	510	CLA	CMB-C2B-C1B	-2.19	125.10	128.46
29	s	610	CLA	CMA-C3A-C4A	2.19	117.65	111.77
29	C1	506	CLA	CAA-C2A-C3A	-2.19	106.79	112.78
29	Y1	614	CLA	O1D-CGD-CBD	-2.19	120.01	124.48
49	Y	620	LUT	C15-C35-C34	-2.19	119.00	123.47
50	G1	622	XAT	C26-C27-C28	-2.19	121.37	125.99
29	g	613	CLA	C1D-ND-C4D	-2.19	104.78	106.33
29	g	604	CLA	C1C-C2C-C3C	-2.19	104.66	106.96
29	N1	610	CLA	C1C-C2C-C3C	-2.19	104.66	106.96
48	G1	605	CHL	CMA-C3A-C2A	2.19	122.65	113.83
48	S	606	CHL	CHD-C4C-C3C	2.19	128.05	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	n	611	CLA	C3D-C2D-C1D	-2.19	102.85	105.83
29	B1	611	CLA	C3D-C2D-C1D	-2.19	102.85	105.83
29	C	506	CLA	CHA-C1A-NA	-2.19	121.39	126.40
29	Y1	612	CLA	C2A-C1A-CHA	2.19	127.68	123.86
29	C1	502	CLA	C2D-C1D-ND	2.18	111.71	110.10
29	S	610	CLA	C2A-C1A-CHA	2.18	127.68	123.86
49	n	620	LUT	C15-C35-C34	-2.18	119.00	123.47
29	S1	609	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
31	c1	515	BCR	C23-C24-C25	-2.18	121.07	127.20
29	C	513	CLA	CHA-C1A-NA	-2.18	121.40	126.40
51	s1	623	NEX	C38-C25-C26	-2.18	118.60	122.26
29	S	610	CLA	CMB-C2B-C1B	-2.18	125.11	128.46
29	s	602	CLA	C1D-ND-C4D	-2.18	104.78	106.33
29	r1	604	CLA	C1D-ND-C4D	-2.18	104.78	106.33
29	r1	609	CLA	C1D-ND-C4D	-2.18	104.78	106.33
49	R	620	LUT	C39-C29-C28	2.18	121.52	118.08
36	B	620	C7Z	C4-C5-C6	-2.18	115.98	120.85
29	g1	603	CLA	O2D-CGD-O1D	-2.18	119.57	123.84
40	d	410	LHG	C5-O7-C7	-2.18	112.42	117.79
29	a1	406	CLA	CHA-C1A-NA	-2.18	121.40	126.40
29	A	407	CLA	CMD-C2D-C3D	-2.18	122.59	127.61
49	n	620	LUT	C10-C11-C12	-2.18	116.41	123.22
49	N	620	LUT	C36-C21-C26	-2.18	106.24	109.55
29	a1	405	CLA	C3D-C2D-C1D	-2.18	102.85	105.83
29	Y	614	CLA	C2D-C1D-ND	2.18	111.71	110.10
29	a1	407	CLA	CHA-C1A-NA	-2.18	121.40	126.40
29	Y	604	CLA	C1D-ND-C4D	-2.18	104.78	106.33
29	n1	603	CLA	C1D-ND-C4D	-2.18	104.78	106.33
48	n	605	CHL	CMB-C2B-C1B	-2.18	125.11	128.46
45	h1	101	RRX	C16-C17-C18	-2.18	124.20	127.31
29	n	604	CLA	O1D-CGD-CBD	-2.18	120.02	124.48
50	r1	621	XAT	C8-C9-C10	2.18	122.29	118.94
29	c	508	CLA	CAC-C3C-C4C	2.18	127.64	124.81
48	g	608	CHL	C3A-C2A-C1A	2.18	104.61	101.34
51	G1	623	NEX	C1-C2-C3	2.18	118.57	113.64
49	Y	621	LUT	C3-C4-C5	-2.18	107.51	111.85
51	s1	623	NEX	C20-C13-C14	-2.18	119.87	122.92
29	Y	602	CLA	CMB-C2B-C3B	2.18	128.76	124.68
29	C	510	CLA	CAA-C2A-C3A	-2.18	106.81	112.78
29	A	406	CLA	CMC-C2C-C3C	2.18	132.03	126.12
29	g1	602	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
29	R	602	CLA	C1-C2-C3	-2.18	122.27	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a1	410	CLA	C1-O2A-CGA	2.18	122.16	116.44
29	y1	603	CLA	CHA-C1A-NA	-2.18	121.41	126.40
29	N1	610	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
29	S1	610	CLA	CMB-C2B-C3B	2.18	128.75	124.68
48	Y1	609	CHL	CMB-C2B-C1B	-2.18	125.11	128.46
29	b	605	CLA	CAC-C3C-C4C	2.18	127.64	124.81
32	c	526	SQD	O3-C3-C2	-2.18	105.31	110.35
29	D1	403	CLA	CHA-C1A-NA	-2.18	121.41	126.40
29	c	511	CLA	CMD-C2D-C3D	-2.18	122.60	127.61
29	C1	509	CLA	C2D-C1D-ND	2.18	111.71	110.10
29	s	613	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
29	C1	512	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
29	c	510	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
48	n1	601	CHL	CMB-C2B-C1B	-2.18	125.12	128.46
29	c1	502	CLA	CHA-C1A-NA	-2.18	121.41	126.40
31	c1	517	BCR	C39-C30-C25	-2.18	106.77	110.30
29	c	505	CLA	O2A-CGA-CBA	2.18	118.74	111.91
29	a1	410	CLA	CAA-CBA-CGA	-2.18	106.89	113.25
29	Y	602	CLA	C16-C15-C13	-2.18	108.88	115.92
31	B1	618	BCR	C23-C22-C21	2.18	122.28	118.94
31	c1	514	BCR	C1-C6-C5	-2.18	119.55	122.61
31	c1	515	BCR	C29-C28-C27	2.18	116.24	111.38
48	S1	607	CHL	CHD-C4C-C3C	2.18	128.04	124.84
48	S1	608	CHL	C1B-CHB-C4A	-2.18	125.81	130.12
37	b	623	DGD	O5D-C1E-C2E	2.18	111.70	108.30
29	G	612	CLA	C3D-C2D-C1D	-2.18	102.86	105.83
29	C1	505	CLA	CHD-C1D-ND	-2.18	122.45	124.45
29	y1	610	CLA	CHA-C1A-NA	-2.18	121.41	126.40
29	r	608	CLA	C1D-ND-C4D	-2.18	104.79	106.33
29	C1	507	CLA	CMA-C3A-C4A	2.18	117.62	111.77
50	R	621	XAT	C6-C7-C8	-2.18	121.39	125.99
49	n1	621	LUT	C2-C3-C4	-2.18	107.33	110.30
29	B	617	CLA	O1D-CGD-CBD	-2.18	120.03	124.48
29	y1	614	CLA	C1-O2A-CGA	2.18	122.15	116.44
29	b1	604	CLA	CHA-C4D-ND	2.18	137.05	132.50
48	g	601	CHL	CMB-C2B-C1B	-2.18	125.12	128.46
50	y1	622	XAT	C11-C10-C9	-2.17	124.21	127.31
33	d	411	LMG	O8-C28-O10	-2.17	118.10	123.59
29	s	610	CLA	CMD-C2D-C3D	-2.17	122.61	127.61
50	n1	622	XAT	C6-C7-C8	-2.17	121.39	125.99
33	a1	413	LMG	C7-O1-C1	-2.17	109.49	113.74
29	N	602	CLA	CMB-C2B-C1B	-2.17	125.12	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	g	621	LUT	C10-C11-C12	-2.17	116.43	123.22
29	s1	614	CLA	C3D-C2D-C1D	-2.17	102.86	105.83
49	y1	621	LUT	C37-C21-C36	2.17	111.10	107.89
49	S	620	LUT	C17-C1-C6	2.17	113.83	110.30
29	B1	615	CLA	CMD-C2D-C3D	-2.17	122.61	127.61
29	y	604	CLA	O2A-CGA-CBA	2.17	118.73	111.91
29	c1	512	CLA	C2A-C1A-CHA	2.17	127.66	123.86
29	b1	605	CLA	CMA-C3A-C4A	2.17	117.61	111.77
55	y	626	PTY	C12-C11-C8	-2.17	105.72	113.62
49	G	620	LUT	C1-C2-C3	2.17	118.55	113.64
29	n1	604	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
29	A	407	CLA	C2D-C1D-ND	2.17	111.70	110.10
48	Y	606	CHL	C1-C2-C3	-2.17	122.29	126.04
48	G1	608	CHL	CMB-C2B-C1B	-2.17	125.13	128.46
36	B1	620	C7Z	C17-C1-C6	-2.17	106.78	110.30
48	s	608	CHL	C1-O2A-CGA	2.17	122.14	116.44
29	G1	603	CLA	O2A-CGA-CBA	2.17	118.72	111.91
29	R1	604	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
29	B	605	CLA	CHA-C1A-NA	-2.17	121.43	126.40
29	B1	602	CLA	CHA-C1A-NA	-2.17	121.43	126.40
48	g	601	CHL	C1B-CHB-C4A	-2.17	125.82	130.12
29	S	612	CLA	C1D-ND-C4D	-2.17	104.79	106.33
29	c1	505	CLA	C1D-ND-C4D	-2.17	104.79	106.33
29	s	609	CLA	CHA-C1A-NA	-2.17	121.43	126.40
29	r	612	CLA	CMD-C2D-C3D	-2.17	122.62	127.61
44	f1	101	HEM	C4D-ND-C1D	2.17	107.31	105.07
48	Y	606	CHL	CMB-C2B-C1B	-2.17	125.13	128.46
48	N1	606	CHL	CHA-C1A-NA	-2.17	121.43	126.40
29	C1	511	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
29	G1	613	CLA	C3D-C2D-C1D	-2.17	102.87	105.83
48	n1	606	CHL	C1-C2-C3	-2.17	122.29	126.04
29	A	405	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
29	R	609	CLA	C1-O2A-CGA	2.17	122.13	116.44
29	B1	604	CLA	C1-O2A-CGA	2.17	122.13	116.44
29	Y1	608	CLA	O1D-CGD-CBD	-2.17	120.05	124.48
29	C	511	CLA	CMD-C2D-C3D	-2.17	122.63	127.61
51	N1	623	NEX	C26-C27-C28	-2.17	121.41	125.99
29	d	402	CLA	C1C-C2C-C3C	-2.17	104.68	106.96
48	g	605	CHL	CMB-C2B-C1B	-2.17	125.13	128.46
29	C1	513	CLA	C11-C12-C13	-2.17	108.92	115.92
29	n	603	CLA	C1D-ND-C4D	-2.17	104.80	106.33
29	b1	608	CLA	C2A-C1A-CHA	2.17	127.65	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S	604	CLA	CAA-C2A-C3A	-2.17	106.85	112.78
29	y	614	CLA	C3D-C2D-C1D	-2.17	102.88	105.83
29	S	610	CLA	C1C-C2C-C3C	-2.17	104.68	106.96
29	C	502	CLA	CHA-C1A-NA	-2.17	121.44	126.40
29	N1	604	CLA	CHA-C1A-NA	-2.17	121.44	126.40
29	b	612	CLA	CAA-C2A-C3A	-2.17	106.85	112.78
48	s	608	CHL	CMB-C2B-C1B	-2.17	125.14	128.46
31	c	517	BCR	C12-C13-C14	-2.16	115.62	118.94
29	a	406	CLA	CMA-C3A-C4A	2.16	117.59	111.77
29	a1	406	CLA	C3D-C2D-C1D	-2.16	102.88	105.83
48	n1	605	CHL	CMB-C2B-C1B	-2.16	125.14	128.46
48	Y	601	CHL	CHC-C1C-NC	2.16	127.49	124.20
29	S	613	CLA	CMC-C2C-C3C	2.16	131.99	126.12
29	g1	611	CLA	CHA-C1A-NA	-2.16	121.44	126.40
29	b	606	CLA	CAA-C2A-C3A	-2.16	106.85	112.78
29	a1	405	CLA	CMA-C3A-C4A	2.16	117.59	111.77
29	Y	610	CLA	OBD-CAD-C3D	-2.16	123.31	128.52
29	B1	607	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
29	Y	603	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
50	R	621	XAT	C24-C23-C22	-2.16	106.59	110.77
29	Y1	610	CLA	C1C-C2C-C3C	-2.16	104.68	106.96
29	n1	602	CLA	CHA-C4D-ND	2.16	137.02	132.50
29	r	610	CLA	CMB-C2B-C3B	2.16	128.72	124.68
31	C	516	BCR	C37-C22-C23	2.16	121.48	118.08
29	n	614	CLA	O2A-CGA-CBA	2.16	118.69	111.91
29	B1	612	CLA	CMA-C3A-C4A	2.16	117.59	111.77
29	a1	407	CLA	CMB-C2B-C1B	-2.16	125.14	128.46
48	S	607	CHL	CMB-C2B-C1B	-2.16	125.14	128.46
48	g1	605	CHL	CMB-C2B-C1B	-2.16	125.14	128.46
29	C	512	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
29	n	614	CLA	O1D-CGD-CBD	-2.16	120.06	124.48
49	Y1	620	LUT	C31-C32-C33	-2.16	120.34	126.42
29	S1	617	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
31	b1	619	BCR	C29-C28-C27	2.16	116.21	111.38
31	c1	517	BCR	C27-C26-C25	-2.16	119.59	122.73
48	N	605	CHL	CMB-C2B-C1B	-2.16	125.14	128.46
29	c	503	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
29	b1	605	CLA	CMA-C3A-C2A	2.16	122.55	113.83
29	C	510	CLA	C2D-C1D-ND	2.16	111.70	110.10
29	R	604	CLA	OBD-CAD-C3D	-2.16	123.32	128.52
48	n	609	CHL	CMB-C2B-C1B	-2.16	125.14	128.46
31	C	516	BCR	C38-C26-C27	2.16	117.77	113.62

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	g	609	CHL	C1C-C2C-C3C	-2.16	105.40	107.11
33	W	201	LMG	O8-C28-O10	-2.16	118.14	123.59
31	a	411	BCR	C23-C22-C21	-2.16	115.62	118.94
29	S1	614	CLA	O2A-CGA-CBA	2.16	118.69	111.91
29	Y	602	CLA	CMD-C2D-C3D	-2.16	122.64	127.61
50	g1	622	XAT	C19-C9-C10	-2.16	119.90	122.92
48	g1	608	CHL	CMB-C2B-C1B	-2.16	125.14	128.46
48	g1	607	CHL	CHC-C1C-NC	2.16	127.48	124.20
36	B1	620	C7Z	C28-C27-C26	-2.16	121.13	127.20
29	y	608	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
29	b	611	CLA	C1D-ND-C4D	-2.16	104.80	106.33
29	D	403	CLA	CMB-C2B-C3B	2.16	128.72	124.68
52	r1	625	LMT	C1'-O5'-C5'	-2.16	109.45	113.69
51	n	623	NEX	O24-C25-C38	-2.16	112.47	115.06
29	n1	612	CLA	C2D-C1D-ND	2.16	111.69	110.10
29	B	616	CLA	C2A-C1A-CHA	2.16	127.63	123.86
29	n	611	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
31	C1	516	BCR	C30-C25-C26	-2.16	119.57	122.61
29	G1	602	CLA	CMA-C3A-C4A	2.16	117.57	111.77
29	c1	503	CLA	C1D-ND-C4D	-2.16	104.80	106.33
29	G	613	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
43	d	405	PL9	C40-C39-C41	2.16	118.90	115.27
29	g1	614	CLA	O2A-CGA-CBA	2.16	118.68	111.91
29	b	614	CLA	CMB-C2B-C3B	2.16	128.72	124.68
29	N	612	CLA	C2D-C1D-ND	2.16	111.69	110.10
52	r1	625	LMT	O5B-C1B-C2B	2.16	114.92	110.35
29	r	602	CLA	CMD-C2D-C3D	-2.16	122.65	127.61
29	b1	602	CLA	O2D-CGD-O1D	-2.16	119.62	123.84
29	B1	603	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
48	s1	601	CHL	CMB-C2B-C1B	-2.16	125.15	128.46
29	G1	604	CLA	O2A-CGA-CBA	2.16	118.68	111.91
43	d	405	PL9	C37-C38-C39	-2.16	122.47	127.66
29	C	507	CLA	OBD-CAD-C3D	-2.16	123.33	128.52
53	r1	626	ERG	C24-C23-C22	-2.16	118.98	125.67
29	g	612	CLA	C1D-ND-C4D	-2.16	104.80	106.33
49	y1	621	LUT	C2-C3-C4	-2.16	107.35	110.30
29	s	604	CLA	CMA-C3A-C4A	2.16	117.57	111.77
31	c1	514	BCR	C31-C1-C6	-2.16	106.80	110.30
29	n1	614	CLA	CHA-C1A-NA	-2.16	121.46	126.40
29	Y	608	CLA	C1D-ND-C4D	-2.16	104.80	106.33
29	S	610	CLA	C3D-C2D-C1D	-2.16	102.89	105.83
29	b	602	CLA	C3D-C2D-C1D	-2.16	102.89	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b1	617	CLA	C1-C2-C3	-2.15	122.32	126.04
29	C1	510	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
31	C1	517	BCR	C33-C5-C4	2.15	117.75	113.62
29	a	405	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
48	Y	609	CHL	CMB-C2B-C1B	-2.15	125.15	128.46
29	a1	405	CLA	CHA-C1A-NA	-2.15	121.47	126.40
29	G1	611	CLA	O2A-CGA-CBA	2.15	118.67	111.91
29	G	603	CLA	CMC-C2C-C1C	2.15	128.32	125.04
36	B1	620	C7Z	C19-C9-C10	-2.15	119.91	122.92
29	r1	603	CLA	C1D-ND-C4D	-2.15	104.81	106.33
29	b	617	CLA	CMA-C3A-C4A	2.15	117.56	111.77
29	b1	608	CLA	C1-C2-C3	-2.15	122.32	126.04
29	R	608	CLA	CMA-C3A-C4A	2.15	117.56	111.77
29	B1	613	CLA	CHA-C1A-NA	-2.15	121.47	126.40
49	s	621	LUT	C19-C9-C10	-2.15	119.91	122.92
29	N	602	CLA	C2C-C1C-NC	2.15	111.99	109.97
29	B1	615	CLA	CMB-C2B-C1B	-2.15	125.16	128.46
29	G1	611	CLA	O2D-CGD-O1D	-2.15	119.63	123.84
49	N1	621	LUT	C15-C14-C13	-2.15	124.24	127.31
49	n1	620	LUT	C18-C5-C6	-2.15	122.11	124.53
51	N	623	NEX	C19-C9-C10	-2.15	119.91	122.92
29	G	603	CLA	CHA-C1A-NA	-2.15	121.47	126.40
33	C1	523	LMG	C9-C8-C7	-2.15	106.70	111.79
29	A1	410	CLA	CGD-CBD-CAD	-2.15	103.76	110.73
29	R1	612	CLA	CAC-C3C-C4C	2.15	127.60	124.81
29	n1	604	CLA	CHA-C1A-NA	-2.15	121.47	126.40
29	c	512	CLA	C1-O2A-CGA	2.15	122.09	116.44
29	R	603	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
29	c1	503	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
48	n	606	CHL	CMB-C2B-C1B	-2.15	125.16	128.46
29	G	613	CLA	C1D-ND-C4D	-2.15	104.81	106.33
29	y1	614	CLA	O1D-CGD-CBD	-2.15	120.08	124.48
29	c1	513	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
31	b1	618	BCR	C33-C5-C6	-2.15	122.11	124.53
48	N	606	CHL	C2C-C3C-C4C	2.15	108.02	106.49
29	G1	602	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
48	r1	606	CHL	CMB-C2B-C1B	-2.15	125.16	128.46
49	S	621	LUT	C30-C31-C32	-2.15	116.51	123.22
29	B	614	CLA	CHA-C1A-NA	-2.15	121.47	126.40
29	g1	602	CLA	CMD-C2D-C3D	-2.15	122.67	127.61
29	C	507	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
29	S1	609	CLA	C3D-C2D-C1D	-2.15	102.90	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	s	611	CLA	CHA-C1A-NA	-2.15	121.47	126.40
29	B	608	CLA	C1D-ND-C4D	-2.15	104.81	106.33
29	S1	610	CLA	C1-O2A-CGA	2.15	122.08	116.44
48	s	608	CHL	C2C-C3C-C4C	2.15	108.02	106.49
29	s1	603	CLA	O2A-CGA-CBA	2.15	118.65	111.91
49	N	621	LUT	C18-C5-C6	-2.15	122.11	124.53
29	C	509	CLA	CHA-C1A-NA	-2.15	121.48	126.40
29	n1	604	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
48	G	601	CHL	C4A-NA-C1A	2.15	107.67	106.71
49	S	621	LUT	C19-C9-C8	2.15	121.46	118.08
48	y	609	CHL	CMB-C2B-C1B	-2.15	125.16	128.46
48	R1	607	CHL	CMB-C2B-C1B	-2.15	125.16	128.46
29	N1	603	CLA	O2D-CGD-O1D	-2.15	119.64	123.84
29	A1	410	CLA	C1D-ND-C4D	-2.15	104.81	106.33
33	w	201	LMG	C4-C3-C2	2.15	114.57	110.82
49	g1	621	LUT	C39-C29-C30	-2.15	119.91	122.92
47	i1	101	4RF	O18-C16-C15	2.15	118.65	111.91
29	b	608	CLA	C3D-C2D-C1D	-2.15	102.90	105.83
48	N1	606	CHL	CMB-C2B-C1B	-2.15	125.16	128.46
29	N1	602	CLA	CMC-C2C-C1C	2.15	128.31	125.04
29	b1	617	CLA	CMA-C3A-C4A	2.15	117.54	111.77
48	S1	608	CHL	CHD-C4C-C3C	2.15	128.00	124.84
48	y	605	CHL	CMB-C2B-C1B	-2.15	125.16	128.46
29	s	612	CLA	CHA-C1A-NA	-2.15	121.48	126.40
48	s1	601	CHL	CHC-C1C-NC	2.15	127.46	124.20
29	N1	604	CLA	C2D-C1D-ND	2.15	111.69	110.10
36	B	620	C7Z	C1-C6-C7	2.15	121.85	115.78
29	b1	617	CLA	CMD-C2D-C3D	-2.15	122.68	127.61
29	D	403	CLA	O1D-CGD-CBD	-2.15	120.09	124.48
29	c	504	CLA	CMD-C2D-C3D	-2.15	122.68	127.61
29	N	612	CLA	CMA-C3A-C4A	2.15	117.54	111.77
31	b	619	BCR	C37-C22-C23	2.15	121.46	118.08
29	B	605	CLA	CHD-C1D-ND	-2.15	122.48	124.45
48	n	601	CHL	CMB-C2B-C1B	-2.15	125.17	128.46
29	r1	603	CLA	CHA-C1A-NA	-2.15	121.48	126.40
29	c1	513	CLA	CMA-C3A-C4A	2.15	117.54	111.77
44	f1	101	HEM	C1B-NB-C4B	2.15	107.29	105.07
31	D	404	BCR	C23-C24-C25	-2.15	121.18	127.20
29	b	611	CLA	CMA-C3A-C4A	2.14	117.54	111.77
49	N1	620	LUT	C35-C34-C33	-2.14	124.25	127.31
29	g	611	CLA	C1-O2A-CGA	2.14	122.07	116.44
29	G	612	CLA	O2D-CGD-O1D	-2.14	119.64	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	N	605	CHL	C1B-CHB-C4A	-2.14	125.87	130.12
29	b	609	CLA	CMA-C3A-C4A	2.14	117.53	111.77
29	S1	617	CLA	CMD-C2D-C3D	-2.14	122.68	127.61
29	g1	610	CLA	CHA-C1A-NA	-2.14	121.49	126.40
48	s	601	CHL	CMA-C3A-C4A	2.14	117.53	111.77
49	S1	621	LUT	C31-C30-C29	-2.14	124.25	127.31
29	y	608	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
31	C	514	BCR	C8-C9-C10	2.14	122.23	118.94
29	R1	610	CLA	C1C-C2C-C3C	-2.14	104.70	106.96
29	s1	605	CLA	CMD-C2D-C3D	-2.14	122.68	127.61
29	n	603	CLA	CHA-C1A-NA	-2.14	121.49	126.40
31	B	619	BCR	C34-C9-C10	-2.14	119.92	122.92
29	N	610	CLA	C2A-C1A-CHA	2.14	127.61	123.86
29	S	602	CLA	C6-C7-C8	-2.14	108.99	115.92
48	g	609	CHL	CHB-C4A-NA	2.14	127.47	124.51
29	B	610	CLA	C1D-ND-C4D	-2.14	104.81	106.33
29	C	512	CLA	C1D-ND-C4D	-2.14	104.81	106.33
29	B	603	CLA	C1-O2A-CGA	2.14	122.06	116.44
48	R1	606	CHL	CHC-C1C-NC	2.14	127.45	124.20
29	n	614	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
29	b1	603	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
29	c	513	CLA	CHA-C1A-NA	-2.14	121.49	126.40
29	G	612	CLA	CMD-C2D-C3D	-2.14	122.69	127.61
51	g	623	NEX	C16-C1-C6	-2.14	108.56	110.47
49	R	620	LUT	C31-C30-C29	-2.14	124.25	127.31
48	S1	607	CHL	CMB-C2B-C1B	-2.14	125.17	128.46
48	n1	606	CHL	C1-O2A-CGA	2.14	122.06	116.44
29	S1	610	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
29	b	602	CLA	C1D-ND-C4D	-2.14	104.81	106.33
29	Y	610	CLA	CMB-C2B-C3B	2.14	128.68	124.68
50	N1	622	XAT	C19-C9-C10	-2.14	119.93	122.92
29	B1	605	CLA	C3D-C2D-C1D	-2.14	102.91	105.83
29	N1	610	CLA	C2A-C1A-CHA	2.14	127.60	123.86
49	N1	620	LUT	C39-C29-C30	-2.14	119.93	122.92
29	B	615	CLA	CMC-C2C-C1C	2.14	128.30	125.04
48	Y1	605	CHL	CMB-C2B-C1B	-2.14	125.18	128.46
37	b	623	DGD	O5D-C6D-C5D	2.14	113.00	109.05
29	C1	509	CLA	CHA-C1A-NA	-2.14	121.50	126.40
29	C1	511	CLA	CHA-C1A-NA	-2.14	121.50	126.40
44	F1	101	HEM	C3D-C4D-ND	-2.14	107.79	110.17
29	c1	501	CLA	C2A-C1A-CHA	2.14	127.60	123.86
29	n1	603	CLA	O1D-CGD-CBD	-2.14	120.11	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	b	611	CLA	O2A-CGA-CBA	2.14	118.62	111.91
29	N1	602	CLA	CHA-C1A-NA	-2.14	121.50	126.40
29	n1	613	CLA	CHA-C1A-NA	-2.14	121.50	126.40
48	r1	607	CHL	CMB-C2B-C1B	-2.14	125.18	128.46
29	r	610	CLA	C1D-ND-C4D	-2.14	104.82	106.33
29	R1	609	CLA	C1D-ND-C4D	-2.14	104.82	106.33
29	g	612	CLA	C3D-C2D-C1D	-2.14	102.92	105.83
29	y	612	CLA	CHA-C1A-NA	-2.14	121.50	126.40
31	C1	517	BCR	C33-C5-C6	-2.14	122.13	124.53
48	r1	607	CHL	CHC-C1C-NC	2.14	127.44	124.20
48	g1	607	CHL	C1B-CHB-C4A	-2.14	125.89	130.12
29	s1	609	CLA	C3D-C2D-C1D	-2.14	102.92	105.83
48	g1	606	CHL	CMB-C2B-C1B	-2.14	125.18	128.46
29	C1	513	CLA	CBA-CAA-C2A	2.14	120.17	113.86
29	Y	613	CLA	C3D-C2D-C1D	-2.14	102.92	105.83
49	s1	620	LUT	C18-C5-C4	2.14	118.31	114.36
33	W1	201	LMG	O8-C28-O10	-2.14	118.20	123.59
50	R1	621	XAT	C40-C33-C34	-2.14	119.93	122.92
30	a1	409	PHO	O1D-CGD-CBD	2.14	128.29	124.74
29	s1	612	CLA	O2D-CGD-O1D	-2.13	119.66	123.84
29	b1	608	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
31	d1	404	BCR	C28-C27-C26	-2.13	110.27	114.08
48	G	606	CHL	C1B-CHB-C4A	-2.13	125.89	130.12
29	B	608	CLA	C3D-C2D-C1D	-2.13	102.92	105.83
29	S	612	CLA	O1D-CGD-CBD	-2.13	120.12	124.48
48	N	601	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
34	Y1	625	SPH	C3-C4-C5	-2.13	120.03	124.79
29	c	510	CLA	C2D-C1D-ND	2.13	111.68	110.10
29	G	613	CLA	CMC-C2C-C1C	2.13	128.29	125.04
48	y1	609	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
48	G1	601	CHL	C4D-CHA-C1A	2.13	123.84	121.25
29	D	403	CLA	CMD-C2D-C3D	-2.13	122.71	127.61
31	b1	618	BCR	C8-C7-C6	-2.13	121.21	127.20
29	c	510	CLA	CBC-CAC-C3C	-2.13	106.55	112.43
48	n1	609	CHL	CHC-C1C-NC	2.13	127.44	124.20
53	r	626	ERG	C11-C12-C13	2.13	116.44	112.78
43	d1	405	PL9	C20-C19-C21	2.13	118.86	115.27
48	g	605	CHL	CHC-C1C-NC	2.13	127.44	124.20
29	N	602	CLA	C1C-C2C-C3C	-2.13	104.72	106.96
29	N	614	CLA	O2A-CGA-CBA	2.13	118.59	111.91
29	s	604	CLA	CHA-C1A-NA	-2.13	121.52	126.40
29	B1	617	CLA	C1-O2A-CGA	2.13	122.03	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
49	S1	621	LUT	C19-C9-C10	-2.13	119.94	122.92
50	R	621	XAT	C39-C29-C30	-2.13	119.94	122.92
31	A1	411	BCR	C38-C26-C25	-2.13	122.14	124.53
49	S	620	LUT	C16-C1-C6	-2.13	106.84	110.30
29	g	602	CLA	CHA-C1A-NA	-2.13	121.52	126.40
29	c1	506	CLA	C6-C5-C3	-2.13	107.87	113.45
31	d	404	BCR	C23-C24-C25	-2.13	121.22	127.20
50	n1	622	XAT	C40-C33-C34	-2.13	119.94	122.92
48	s1	607	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
48	n	601	CHL	CHD-C4C-C3C	2.13	127.97	124.84
29	s	602	CLA	CMA-C3A-C4A	2.13	117.50	111.77
50	R	621	XAT	C19-C9-C8	2.13	121.43	118.08
29	y1	602	CLA	CHA-C1A-NA	-2.13	121.52	126.40
43	d1	405	PL9	C50-C49-C48	-2.13	116.50	122.65
29	D	402	CLA	CAA-C2A-C3A	-2.13	106.95	112.78
49	Y	621	LUT	C30-C31-C32	-2.13	116.58	123.22
31	C1	515	BCR	C35-C13-C12	2.13	121.43	118.08
29	G	603	CLA	C3D-C2D-C1D	-2.13	102.93	105.83
32	b	626	SQD	O8-S-C6	-2.13	102.35	105.74
29	a1	405	CLA	O1D-CGD-CBD	-2.13	120.13	124.48
29	d1	403	CLA	C6-C7-C8	-2.13	109.04	115.92
29	c1	510	CLA	CMB-C2B-C3B	2.13	128.66	124.68
50	Y1	622	XAT	C32-C33-C34	2.13	122.21	118.94
29	n	614	CLA	CHA-C1A-NA	-2.13	121.53	126.40
29	y1	603	CLA	O2D-CGD-O1D	-2.13	119.68	123.84
48	S	601	CHL	C3B-C4B-NB	-2.13	106.46	109.21
29	G1	614	CLA	C1D-ND-C4D	-2.13	104.82	106.33
48	N	606	CHL	CMB-C2B-C1B	-2.13	125.19	128.46
29	n1	610	CLA	CBA-CAA-C2A	2.13	120.14	113.86
29	R	602	CLA	CHA-C1A-NA	-2.13	121.53	126.40
29	c	513	CLA	C1-O2A-CGA	2.13	122.02	116.44
29	Y	611	CLA	CAA-C2A-C3A	-2.13	106.95	112.78
29	y1	602	CLA	CAA-C2A-C3A	-2.13	106.95	112.78
29	b1	605	CLA	C11-C10-C8	-2.13	109.05	115.92
48	y1	605	CHL	CMB-C2B-C1B	-2.13	125.20	128.46
29	b1	615	CLA	O2A-CGA-CBA	2.13	118.58	111.91
53	R	626	ERG	C4-C5-C10	2.13	119.24	116.42
43	D1	405	PL9	C20-C19-C21	2.13	118.85	115.27
49	g	621	LUT	C37-C21-C26	2.13	112.77	109.55
29	C	512	CLA	CHA-C1A-NA	-2.13	121.53	126.40
29	C	501	CLA	O2A-CGA-CBA	2.12	118.58	111.91
29	N1	611	CLA	O2A-CGA-CBA	2.12	118.58	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	G1	609	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
48	g1	601	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
29	D1	403	CLA	O2A-CGA-CBA	2.12	118.57	111.91
48	n1	607	CHL	CHD-C4C-C3C	2.12	127.96	124.84
29	G1	602	CLA	CAA-C2A-C1A	-2.12	105.02	111.97
29	C1	505	CLA	C1-C2-C3	-2.12	122.37	126.04
29	s	604	CLA	CMB-C2B-C1B	-2.12	125.20	128.46
29	B	611	CLA	CAA-C2A-C3A	-2.12	106.96	112.78
31	C	517	BCR	C8-C9-C10	2.12	122.20	118.94
29	C1	510	CLA	C3D-C2D-C1D	-2.12	102.93	105.83
29	n	610	CLA	C1D-ND-C4D	-2.12	104.83	106.33
29	S1	612	CLA	C1D-ND-C4D	-2.12	104.83	106.33
29	g1	614	CLA	CAC-C3C-C4C	2.12	127.56	124.81
48	G	609	CHL	C1-C2-C3	-2.12	122.37	126.04
48	N1	605	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
48	N1	609	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
48	R1	606	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
48	g	608	CHL	C4A-NA-C1A	2.12	107.66	106.71
48	N	609	CHL	CHC-C1C-NC	2.12	127.42	124.20
44	f	101	HEM	C3B-C2B-C1B	2.12	108.06	106.49
29	Y1	614	CLA	CHA-C1A-NA	-2.12	121.54	126.40
51	R	622	NEX	C38-C25-C26	-2.12	118.70	122.26
29	N	602	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
29	g	610	CLA	OBD-CAD-C3D	-2.12	123.42	128.52
29	s1	605	CLA	CHA-C1A-NA	-2.12	121.54	126.40
33	C1	523	LMG	O6-C1-C2	-2.12	105.86	110.35
29	S	613	CLA	C1-O2A-CGA	2.12	122.01	116.44
29	C1	511	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
33	h1	102	LMG	C6-C5-C4	-2.12	108.04	113.00
29	B1	607	CLA	C2D-C1D-ND	2.12	111.67	110.10
29	R1	604	CLA	CMB-C2B-C1B	-2.12	125.20	128.46
48	g	609	CHL	CMB-C2B-C1B	-2.12	125.20	128.46
29	B1	603	CLA	CMC-C2C-C1C	2.12	128.27	125.04
29	G	614	CLA	CAC-C3C-C4C	2.12	127.56	124.81
44	F	101	HEM	C1B-NB-C4B	2.12	107.26	105.07
29	B1	611	CLA	CHD-C1D-ND	-2.12	122.51	124.45
48	G1	605	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
48	s1	608	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
31	c1	516	BCR	C31-C1-C6	-2.12	106.86	110.30
29	n	602	CLA	C2D-C1D-ND	2.12	111.67	110.10
29	r	609	CLA	C1-O2A-CGA	2.12	122.00	116.44
29	g1	604	CLA	C3D-C2D-C1D	-2.12	102.94	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	R	606	CHL	C4D-CHA-C1A	2.12	123.83	121.25
49	S	621	LUT	C1-C6-C5	-2.12	119.63	122.61
29	R	610	CLA	CHA-C1A-NA	-2.12	121.55	126.40
29	G	602	CLA	CHA-C1A-NA	-2.12	121.55	126.40
29	Y	603	CLA	CHA-C1A-NA	-2.12	121.55	126.40
43	D1	405	PL9	C35-C34-C36	2.12	118.83	115.27
29	y	610	CLA	CMD-C2D-C3D	-2.12	122.74	127.61
29	r1	610	CLA	C2C-C1C-NC	2.12	111.96	109.97
48	N1	601	CHL	CHC-C1C-NC	2.12	127.42	124.20
48	G	605	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
48	S1	606	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
48	y1	606	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
29	b	603	CLA	CHA-C1A-NA	-2.12	121.55	126.40
51	S	623	NEX	C17-C1-C6	-2.12	108.58	110.47
29	N	604	CLA	CHA-C1A-NA	-2.12	121.55	126.40
29	R1	610	CLA	CHA-C4D-ND	2.12	136.93	132.50
48	S1	608	CHL	CHC-C1C-NC	2.12	127.42	124.20
48	S1	601	CHL	C3A-C2A-C1A	2.12	104.51	101.34
29	s	602	CLA	CHA-C1A-NA	-2.12	121.55	126.40
51	n1	623	NEX	C24-C23-C22	-2.12	106.69	110.77
51	r	622	NEX	C32-C33-C34	2.12	122.19	118.94
29	c	507	CLA	CMD-C2D-C3D	-2.12	122.75	127.61
48	G	608	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
48	n1	606	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
48	r	606	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
29	S	614	CLA	O2A-CGA-CBA	2.12	118.55	111.91
29	G1	610	CLA	C1C-C2C-C3C	-2.12	104.73	106.96
29	G	613	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
29	n	604	CLA	C3D-C2D-C1D	-2.12	102.94	105.83
29	C1	504	CLA	O2A-CGA-CBA	2.12	118.55	111.91
49	n	620	LUT	C35-C15-C14	-2.12	119.14	123.47
49	R	620	LUT	C11-C12-C13	-2.12	120.47	126.42
48	N1	601	CHL	CMB-C2B-C1B	-2.12	125.21	128.46
29	C1	508	CLA	CHA-C1A-NA	-2.12	121.55	126.40
29	A1	406	CLA	C3D-C2D-C1D	-2.11	102.94	105.83
48	n	606	CHL	CHC-C1C-NC	2.11	127.41	124.20
30	a	409	PHO	C1-C2-C3	-2.11	122.39	126.04
29	B1	606	CLA	O2D-CGD-O1D	-2.11	119.70	123.84
29	r	602	CLA	CHA-C1A-NA	-2.11	121.56	126.40
29	Y1	602	CLA	C2D-C1D-ND	2.11	111.66	110.10
29	c1	505	CLA	O2A-CGA-CBA	2.11	118.54	111.91
29	a	406	CLA	C3D-C2D-C1D	-2.11	102.95	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	c	502	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
29	C	509	CLA	O2A-CGA-CBA	2.11	118.54	111.91
29	S	610	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
36	b1	620	C7Z	C28-C27-C26	-2.11	121.27	127.20
29	C1	509	CLA	O2A-CGA-CBA	2.11	118.54	111.91
29	G	612	CLA	CHA-C4D-ND	2.11	136.92	132.50
29	B1	617	CLA	CHA-C1A-NA	-2.11	121.56	126.40
29	y	604	CLA	CMA-C3A-C4A	2.11	117.45	111.77
29	b	609	CLA	OBD-CAD-C3D	-2.11	123.44	128.52
29	C	510	CLA	C1D-ND-C4D	-2.11	104.83	106.33
45	h1	101	RRX	C28-C27-C26	2.11	116.06	111.85
31	C1	514	BCR	C37-C22-C23	2.11	121.41	118.08
29	b	606	CLA	CMB-C2B-C1B	-2.11	125.22	128.46
29	b	614	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
51	g	623	NEX	C19-C9-C10	-2.11	119.96	122.92
29	n1	611	CLA	CMA-C3A-C4A	2.11	117.45	111.77
29	g1	612	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
29	D1	403	CLA	O1D-CGD-CBD	-2.11	120.16	124.48
50	y	622	XAT	C6-C7-C8	-2.11	121.53	125.99
50	Y	622	XAT	C40-C33-C34	-2.11	119.97	122.92
29	C1	513	CLA	C2C-C1C-NC	2.11	111.95	109.97
29	S	604	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
29	n1	610	CLA	CHA-C4D-ND	2.11	136.91	132.50
29	B	610	CLA	C1C-C2C-C3C	-2.11	104.74	106.96
29	g	613	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
29	n1	612	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
29	c1	502	CLA	CMA-C3A-C4A	2.11	117.45	111.77
48	y	606	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
31	C	515	BCR	C38-C26-C25	-2.11	122.16	124.53
30	A1	408	PHO	CMA-C3A-C4A	-2.11	109.75	114.38
51	s1	623	NEX	C28-C29-C30	2.11	122.18	118.94
48	S	601	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
29	C1	502	CLA	CHD-C1D-ND	-2.11	122.52	124.45
29	R	610	CLA	O2D-CGD-O1D	-2.11	119.71	123.84
29	S1	602	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
50	G1	622	XAT	C32-C33-C34	2.11	122.18	118.94
29	A1	407	CLA	C1-O2A-CGA	2.11	121.98	116.44
29	a	405	CLA	C3D-C2D-C1D	-2.11	102.95	105.83
29	N1	613	CLA	C6-C5-C3	-2.11	107.92	113.45
48	S	608	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
29	S1	614	CLA	C4D-CHA-C1A	2.11	123.81	121.25
29	G1	610	CLA	CMD-C2D-C3D	-2.11	122.76	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	613	CLA	CHA-C1A-NA	-2.11	121.57	126.40
29	n1	603	CLA	O2A-CGA-CBA	2.11	118.52	111.91
29	Y	604	CLA	C1C-C2C-C3C	-2.11	104.74	106.96
48	G	609	CHL	CMB-C2B-C1B	-2.11	125.22	128.46
37	C1	519	DGD	O1G-C1A-O1A	-2.11	118.27	123.59
39	C1	524	DGA	OG2-CB1-OB1	-2.11	118.61	123.70
29	G1	604	CLA	C3D-C2D-C1D	-2.11	102.96	105.83
31	d1	404	BCR	C1-C6-C7	2.11	121.74	115.78
51	n	623	NEX	C40-C33-C34	-2.11	119.97	122.92
29	y	611	CLA	O2A-CGA-CBA	2.11	118.52	111.91
29	b1	604	CLA	O1D-CGD-CBD	-2.11	120.17	124.48
48	g	608	CHL	CMB-C2B-C1B	-2.11	125.23	128.46
48	y	609	CHL	C4D-CHA-C1A	2.11	123.81	121.25
44	F1	101	HEM	CAD-C3D-C4D	2.11	128.34	124.66
29	b	604	CLA	CMB-C2B-C3B	2.11	128.62	124.68
29	B1	609	CLA	CMB-C2B-C3B	2.11	128.62	124.68
49	Y	620	LUT	C7-C8-C9	-2.11	123.05	126.23
29	c	502	CLA	O2A-CGA-CBA	2.11	118.52	111.91
29	B	605	CLA	OBD-CAD-C3D	-2.11	123.45	128.52
49	y1	620	LUT	C19-C9-C10	-2.11	119.97	122.92
29	s1	612	CLA	C2A-C1A-CHA	2.11	127.54	123.86
42	D	401	BCT	O3-C-O1	-2.10	114.09	119.55
29	N1	613	CLA	O2D-CGD-O1D	-2.10	119.72	123.84
31	D1	404	BCR	C24-C25-C26	-2.10	116.36	121.46
29	b1	612	CLA	CAA-CBA-CGA	-2.10	107.10	113.25
52	R1	625	LMT	O1'-C1'-C2'	2.10	111.59	108.30
29	g	610	CLA	C2A-C1A-CHA	2.10	127.54	123.86
29	g	613	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
29	s1	602	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
32	M	101	SQD	O8-S-C6	-2.10	102.39	105.74
48	G	607	CHL	C3C-C4C-NC	-2.10	108.21	110.57
29	S	617	CLA	CHA-C1A-NA	-2.10	121.58	126.40
49	Y	620	LUT	C19-C9-C8	2.10	121.39	118.08
48	r	606	CHL	CHC-C1C-NC	2.10	127.39	124.20
29	G	604	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
29	Y	614	CLA	CMC-C2C-C1C	2.10	128.24	125.04
29	b	602	CLA	CMC-C2C-C1C	2.10	128.24	125.04
29	C1	503	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
48	Y	605	CHL	CMB-C2B-C1B	-2.10	125.23	128.46
29	S	610	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
49	n1	620	LUT	C11-C10-C9	-2.10	124.31	127.31
48	N1	608	CHL	CHA-C1A-NA	-2.10	121.58	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	n	607	CHL	C4A-NA-C1A	2.10	107.65	106.71
49	S1	621	LUT	C40-C33-C34	-2.10	119.98	122.92
29	Y1	612	CLA	C1-O2A-CGA	2.10	121.96	116.44
29	c	506	CLA	CHA-C1A-NA	-2.10	121.58	126.40
48	R1	606	CHL	CHA-C1A-NA	-2.10	121.58	126.40
48	S1	608	CHL	CMB-C2B-C1B	-2.10	125.23	128.46
29	C	504	CLA	C1C-C2C-C3C	-2.10	104.75	106.96
29	S1	612	CLA	C1C-C2C-C3C	-2.10	104.75	106.96
48	G1	601	CHL	CHC-C1C-NC	2.10	127.39	124.20
31	C	516	BCR	C12-C13-C14	-2.10	115.72	118.94
29	n	612	CLA	CMD-C2D-C3D	-2.10	122.78	127.61
29	B	610	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
29	C1	504	CLA	C3D-C2D-C1D	-2.10	102.96	105.83
29	s1	610	CLA	CMB-C2B-C1B	-2.10	125.23	128.46
48	Y	605	CHL	CHD-C4C-C3C	2.10	127.93	124.84
29	B	612	CLA	CMA-C3A-C4A	2.10	117.42	111.77
29	G	602	CLA	C1-O2A-CGA	2.10	121.95	116.44
37	B1	623	DGD	O2G-C1B-O1B	-2.10	118.63	123.70
48	s	608	CHL	CHC-C1C-NC	2.10	127.39	124.20
29	b	608	CLA	C2A-C1A-CHA	2.10	127.53	123.86
29	b	602	CLA	CHA-C1A-NA	-2.10	121.59	126.40
50	R	621	XAT	O4-C5-C18	-2.10	112.54	115.06
29	Y	613	CLA	CHA-C1A-NA	-2.10	121.59	126.40
29	s	613	CLA	O2D-CGD-O1D	-2.10	119.73	123.84
32	m1	101	SQD	O5-C1-O6	-2.10	105.00	109.97
49	y1	621	LUT	C20-C13-C12	2.10	121.38	118.08
29	B1	605	CLA	C1D-ND-C4D	-2.10	104.84	106.33
29	r1	602	CLA	CMB-C2B-C3B	2.10	128.60	124.68
48	G	606	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
48	s	607	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
29	B	608	CLA	CMD-C2D-C3D	-2.10	122.79	127.61
29	C	506	CLA	C1-C2-C3	-2.10	122.42	126.04
29	b	615	CLA	C1D-ND-C4D	-2.10	104.84	106.33
29	S1	612	CLA	OBD-CAD-C3D	-2.10	123.47	128.52
29	r1	609	CLA	CHA-C1A-NA	-2.10	121.59	126.40
29	a	410	CLA	O1D-CGD-CBD	-2.10	120.19	124.48
31	C1	515	BCR	C8-C7-C6	-2.10	121.31	127.20
48	N	605	CHL	CHD-C4C-C3C	2.10	127.92	124.84
49	y	620	LUT	C15-C35-C34	-2.10	119.18	123.47
49	G1	621	LUT	C39-C29-C30	-2.10	119.99	122.92
48	G	601	CHL	CMB-C2B-C1B	-2.10	125.24	128.46
44	F1	101	HEM	C1B-NB-C4B	2.10	107.24	105.07

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a1	406	CLA	C11-C10-C8	-2.10	109.14	115.92
29	G1	611	CLA	CHA-C1A-NA	-2.10	121.60	126.40
29	N1	610	CLA	CHA-C1A-NA	-2.10	121.60	126.40
51	r1	622	NEX	C38-C25-C26	-2.10	118.75	122.26
48	G	605	CHL	C4A-NA-C1A	2.10	107.65	106.71
50	R1	621	XAT	C6-C7-C8	-2.10	121.56	125.99
48	g1	609	CHL	CMB-C2B-C1B	-2.09	125.24	128.46
37	C1	518	DGD	O5D-C6D-C5D	-2.09	105.17	109.05
29	y	604	CLA	C1D-ND-C4D	-2.09	104.85	106.33
49	G	621	LUT	C18-C5-C6	-2.09	122.18	124.53
29	c1	507	CLA	OBD-CAD-C3D	-2.09	123.48	128.52
31	B1	618	BCR	C1-C6-C7	2.09	121.70	115.78
29	g1	602	CLA	CAA-C2A-C3A	-2.09	107.04	112.78
33	D1	411	LMG	O8-C28-O10	-2.09	118.31	123.59
29	y1	602	CLA	CMD-C2D-C3D	-2.09	122.80	127.61
29	S	603	CLA	O2D-CGD-O1D	-2.09	119.74	123.84
31	a	411	BCR	C37-C22-C23	2.09	121.38	118.08
31	C	516	BCR	C34-C9-C10	-2.09	119.99	122.92
48	r	607	CHL	CMB-C2B-C1B	-2.09	125.25	128.46
29	b	617	CLA	C1D-ND-C4D	-2.09	104.85	106.33
31	c	514	BCR	C37-C22-C21	-2.09	119.99	122.92
48	R	607	CHL	CMB-C2B-C1B	-2.09	125.25	128.46
49	n1	621	LUT	C15-C14-C13	-2.09	124.32	127.31
48	n	607	CHL	C4D-CHA-C1A	2.09	123.80	121.25
29	g1	614	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
37	c1	519	DGD	O6D-C5D-C6D	2.09	110.89	106.67
33	c	521	LMG	O8-C28-O10	-2.09	118.31	123.59
29	b1	614	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
29	b	611	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
29	Y1	602	CLA	CHA-C1A-NA	-2.09	121.61	126.40
29	C1	502	CLA	O2A-CGA-CBA	2.09	118.47	111.91
29	S1	617	CLA	CAA-C2A-C3A	-2.09	107.05	112.78
29	C	508	CLA	O2A-CGA-CBA	2.09	118.47	111.91
48	g1	601	CHL	CHC-C1C-NC	2.09	127.38	124.20
48	G	606	CHL	CHD-C4C-C3C	2.09	127.91	124.84
48	s	601	CHL	CMB-C2B-C1B	-2.09	125.25	128.46
48	S1	601	CHL	CMB-C2B-C1B	-2.09	125.25	128.46
29	s	604	CLA	CMB-C2B-C3B	2.09	128.59	124.68
29	N	602	CLA	CMC-C2C-C1C	2.09	128.22	125.04
29	c	502	CLA	C1C-C2C-C3C	-2.09	104.76	106.96
29	A	410	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
29	G	610	CLA	C3D-C2D-C1D	-2.09	102.98	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	G1	602	CLA	C1-O2A-CGA	2.09	121.93	116.44
29	b1	611	CLA	C4D-CHA-C1A	2.09	123.79	121.25
29	a	405	CLA	O2A-CGA-CBA	2.09	118.47	111.91
29	c	503	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
29	n	613	CLA	CHD-C1D-ND	-2.09	122.53	124.45
29	C1	501	CLA	CMD-C2D-C3D	-2.09	122.81	127.61
29	s	612	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
29	G1	613	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
29	R1	612	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
29	S1	613	CLA	C3D-C2D-C1D	-2.09	102.98	105.83
29	c1	502	CLA	CHD-C1D-ND	-2.09	122.53	124.45
48	s1	607	CHL	CHA-C1A-NA	-2.09	121.62	126.40
29	b1	609	CLA	O1D-CGD-CBD	-2.09	120.21	124.48
29	b1	604	CLA	CHA-C1A-NA	-2.09	121.62	126.40
29	n	603	CLA	C2A-C1A-CHA	2.09	127.51	123.86
29	n1	602	CLA	CHA-C1A-NA	-2.09	121.62	126.40
29	c1	504	CLA	CAC-C3C-C4C	2.09	127.52	124.81
29	n1	602	CLA	C1C-C2C-C3C	-2.09	104.76	106.96
48	n1	606	CHL	CHD-C4C-C3C	2.09	127.91	124.84
48	G	601	CHL	C1-O2A-CGA	2.09	121.92	116.44
29	b1	603	CLA	O1D-CGD-CBD	-2.09	120.22	124.48
29	b1	603	CLA	CHA-C1A-NA	-2.09	121.62	126.40
31	A1	411	BCR	C37-C22-C23	2.09	121.36	118.08
29	y1	612	CLA	C1D-ND-C4D	-2.09	104.85	106.33
29	b1	607	CLA	O2A-CGA-CBA	2.09	118.45	111.91
29	G1	614	CLA	CHA-C1A-NA	-2.09	121.62	126.40
29	b1	613	CLA	O2A-CGA-CBA	2.09	118.45	111.91
29	N	610	CLA	CMD-C2D-C3D	-2.09	122.82	127.61
29	c	502	CLA	CHA-C1A-NA	-2.08	121.62	126.40
29	g	614	CLA	C1-O2A-CGA	2.08	121.91	116.44
29	y	612	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
48	N1	607	CHL	C1B-CHB-C4A	-2.08	125.99	130.12
36	b1	620	C7Z	C39-C29-C30	-2.08	120.00	122.92
29	c	504	CLA	O2A-CGA-CBA	2.08	118.45	111.91
34	a1	414	SPH	C3-C4-C5	-2.08	120.14	124.79
29	y1	610	CLA	C1C-C2C-C3C	-2.08	104.77	106.96
29	b1	607	CLA	C1-O2A-CGA	2.08	121.91	116.44
29	c1	503	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
29	n1	604	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
30	A	408	PHO	CMC-C2C-C3C	2.08	128.87	124.94
31	c1	517	BCR	C1-C6-C5	-2.08	119.68	122.61
29	C1	504	CLA	C16-C15-C13	-2.08	109.19	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	s1	608	CHL	C2C-C3C-C4C	2.08	107.97	106.49
48	N	606	CHL	CHD-C4C-C3C	2.08	127.90	124.84
29	B1	607	CLA	C7-C6-C5	-2.08	107.70	113.36
29	c1	507	CLA	CHA-C1A-NA	-2.08	121.63	126.40
29	A1	405	CLA	CMD-C2D-C3D	-2.08	122.82	127.61
29	g	612	CLA	O2D-CGD-O1D	-2.08	119.77	123.84
29	S	610	CLA	C1D-ND-C4D	-2.08	104.86	106.33
29	Y1	603	CLA	C2D-C1D-ND	2.08	111.64	110.10
29	b	612	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
29	N1	603	CLA	O2A-CGA-CBA	2.08	118.44	111.91
31	d1	404	BCR	C33-C5-C6	-2.08	122.19	124.53
29	C	502	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
29	y1	614	CLA	C3D-C2D-C1D	-2.08	102.99	105.83
48	s	608	CHL	C1B-CHB-C4A	-2.08	126.00	130.12
29	R	612	CLA	O2A-CGA-CBA	2.08	118.44	111.91
29	s	617	CLA	C1D-ND-C4D	-2.08	104.86	106.33
29	B1	617	CLA	O1D-CGD-CBD	-2.08	120.23	124.48
32	B	621	SQD	O5-C5-C4	-2.08	105.92	109.69
29	r	608	CLA	C2D-C1D-ND	2.08	111.64	110.10
51	N1	623	NEX	C12-C13-C14	2.08	122.13	118.94
29	R1	609	CLA	CHA-C1A-NA	-2.08	121.64	126.40
29	b	610	CLA	C1C-C2C-C3C	-2.08	104.77	106.96
29	S1	617	CLA	CMB-C2B-C1B	-2.08	125.27	128.46
29	c	503	CLA	CMD-C2D-C3D	-2.08	122.83	127.61
29	y1	608	CLA	C1D-ND-C4D	-2.08	104.86	106.33
29	C	503	CLA	CHA-C1A-NA	-2.08	121.64	126.40
48	R	606	CHL	CMB-C2B-C1B	-2.08	125.27	128.46
29	a	410	CLA	C1-O2A-CGA	2.08	121.90	116.44
29	C1	506	CLA	CHA-C1A-NA	-2.08	121.64	126.40
29	Y	613	CLA	C11-C10-C8	-2.08	109.20	115.92
30	a	409	PHO	C1A-C2A-C3A	-2.08	100.86	102.84
48	N	609	CHL	C1-C2-C3	-2.08	122.45	126.04
31	C	517	BCR	C2-C3-C4	-2.08	106.73	111.38
29	B1	608	CLA	C11-C12-C13	-2.08	109.21	115.92
29	Y1	610	CLA	C1-O2A-CGA	2.08	121.89	116.44
29	r1	608	CLA	C1D-ND-C4D	-2.08	104.86	106.33
44	f1	101	HEM	CMB-C2B-C1B	-2.08	121.88	125.04
29	g	613	CLA	CHA-C1A-NA	-2.08	121.64	126.40
29	N	603	CLA	O2A-CGA-CBA	2.08	118.42	111.91
29	c1	502	CLA	CMD-C2D-C3D	-2.08	122.84	127.61
29	c	509	CLA	O1D-CGD-CBD	-2.08	120.24	124.48
29	y1	602	CLA	CMC-C2C-C1C	2.08	128.20	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	A	410	CLA	O1D-CGD-CBD	-2.08	120.24	124.48
48	y1	605	CHL	CHC-C1C-NC	2.08	127.35	124.20
49	g1	620	LUT	C18-C5-C4	2.08	118.20	114.36
29	s1	604	CLA	C3D-C2D-C1D	-2.08	103.00	105.83
31	B	619	BCR	C1-C6-C5	-2.07	119.69	122.61
31	c1	515	BCR	C38-C26-C25	-2.07	122.20	124.53
48	G1	601	CHL	CMB-C2B-C1B	-2.07	125.28	128.46
29	y	613	CLA	C2D-C1D-ND	2.07	111.63	110.10
31	a	411	BCR	C36-C18-C17	-2.07	120.02	122.92
50	y	622	XAT	C39-C29-C30	-2.07	120.02	122.92
29	C	503	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
29	N1	603	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
29	B1	614	CLA	O2A-CGA-CBA	2.07	118.42	111.91
40	D1	410	LHG	O8-C23-C24	2.07	118.42	111.91
29	N1	603	CLA	C1D-ND-C4D	-2.07	104.86	106.33
29	s1	603	CLA	C1D-ND-C4D	-2.07	104.86	106.33
31	B	619	BCR	C31-C1-C6	-2.07	106.94	110.30
49	S1	621	LUT	C8-C7-C6	-2.07	121.38	127.20
29	b	612	CLA	O2D-CGD-O1D	-2.07	119.78	123.84
29	n1	611	CLA	O2D-CGD-O1D	-2.07	119.78	123.84
29	n	602	CLA	CAC-C3C-C4C	2.07	127.50	124.81
51	s	623	NEX	C38-C25-C26	-2.07	118.79	122.26
29	S	603	CLA	O2A-CGA-CBA	2.07	118.41	111.91
36	b	620	C7Z	C20-C13-C14	-2.07	120.02	122.92
29	S	617	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
29	y1	604	CLA	C3D-C2D-C1D	-2.07	103.00	105.83
49	y1	621	LUT	C19-C9-C10	-2.07	120.02	122.92
29	n	610	CLA	CMB-C2B-C1B	-2.07	125.28	128.46
33	W1	201	LMG	C37-C36-C35	2.07	124.94	114.42
48	S	608	CHL	C1-C2-C3	-2.07	122.46	126.04
29	R	612	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
29	c	512	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
29	g1	604	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
29	n	603	CLA	C1-O2A-CGA	2.07	121.88	116.44
29	s	602	CLA	C1C-C2C-C3C	-2.07	104.78	106.96
29	C	508	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
53	r1	626	ERG	C20-C22-C23	-2.07	119.25	125.67
29	n	610	CLA	CHA-C1A-NA	-2.07	121.66	126.40
33	w1	201	LMG	O8-C28-O10	-2.07	118.37	123.59
29	s	613	CLA	CMD-C2D-C3D	-2.07	122.85	127.61
48	N	605	CHL	C4D-CHA-C1A	2.07	123.77	121.25
30	a1	408	PHO	O1D-CGD-CBD	2.07	128.19	124.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
32	A	412	SQD	O8-S-C6	-2.07	102.44	105.74
29	g	602	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
29	B1	615	CLA	O2D-CGD-O1D	-2.07	119.79	123.84
31	D1	404	BCR	C34-C9-C10	-2.07	120.03	122.92
29	N1	602	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
48	n	605	CHL	CHA-C1A-NA	-2.07	121.66	126.40
49	s	620	LUT	C15-C35-C34	-2.07	119.24	123.47
29	y1	610	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
29	b	603	CLA	OBD-CAD-C3D	-2.07	123.54	128.52
31	c1	515	BCR	C37-C22-C21	-2.07	120.03	122.92
29	D1	403	CLA	C2D-C1D-ND	2.07	111.63	110.10
29	b	610	CLA	CAA-CBA-CGA	-2.07	107.21	113.25
29	Y	610	CLA	CMD-C2D-C3D	-2.07	122.86	127.61
29	b1	617	CLA	C1D-ND-C4D	-2.07	104.87	106.33
29	c1	503	CLA	OBD-CAD-C3D	-2.07	123.54	128.52
29	R1	602	CLA	O1D-CGD-CBD	-2.07	120.25	124.48
33	A	413	LMG	O7-C10-O9	-2.07	118.71	123.70
29	D	403	CLA	C3D-C2D-C1D	-2.07	103.01	105.83
29	R1	608	CLA	C11-C10-C8	-2.07	109.24	115.92
29	C	508	CLA	CHA-C1A-NA	-2.07	121.67	126.40
29	b1	613	CLA	C11-C12-C13	-2.07	109.24	115.92
48	g	605	CHL	C1B-CHB-C4A	-2.07	126.02	130.12
29	B	607	CLA	CHA-C1A-NA	-2.07	121.67	126.40
29	c	502	CLA	CMB-C2B-C3B	2.07	128.54	124.68
29	A1	405	CLA	C1C-C2C-C3C	-2.07	104.78	106.96
49	S	621	LUT	C1-C2-C3	-2.07	108.98	113.64
29	n	603	CLA	C3D-C2D-C1D	-2.06	103.01	105.83
43	d	405	PL9	O1-C4-C3	-2.06	118.45	120.72
49	r	620	LUT	C11-C12-C13	-2.06	120.62	126.42
29	Y1	604	CLA	CHA-C1A-NA	-2.06	121.67	126.40
29	c	501	CLA	C3D-C2D-C1D	-2.06	103.01	105.83
29	d	402	CLA	OBD-CAD-C3D	-2.06	123.55	128.52
29	y1	604	CLA	CMD-C2D-C3D	-2.06	122.87	127.61
29	c	512	CLA	CAA-C2A-C3A	-2.06	107.13	112.78
29	G1	610	CLA	CMB-C2B-C1B	-2.06	125.29	128.46
29	C1	502	CLA	OBD-CAD-C3D	-2.06	123.55	128.52
29	y	602	CLA	CMD-C2D-C3D	-2.06	122.87	127.61
29	s1	617	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
29	r	612	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
49	N	621	LUT	C8-C7-C6	-2.06	121.41	127.20
29	N1	612	CLA	CMD-C2D-C3D	-2.06	122.87	127.61
29	B1	615	CLA	O2A-CGA-CBA	2.06	118.38	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	d1	402	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
29	C	501	CLA	CHA-C1A-NA	-2.06	121.67	126.40
33	h	102	LMG	O7-C10-O9	-2.06	118.72	123.70
29	g	603	CLA	CMC-C2C-C1C	2.06	128.18	125.04
29	Y	604	CLA	O2A-CGA-CBA	2.06	118.38	111.91
29	Y	603	CLA	O1D-CGD-CBD	-2.06	120.26	124.48
33	A1	413	LMG	C3-C4-C5	2.06	113.92	110.24
29	d	403	CLA	CHA-C1A-NA	-2.06	121.68	126.40
29	B	616	CLA	O1D-CGD-CBD	-2.06	120.27	124.48
29	s1	611	CLA	CMD-C2D-C3D	-2.06	122.87	127.61
29	c	509	CLA	C6-C5-C3	-2.06	108.05	113.45
51	Y1	623	NEX	C28-C29-C30	2.06	122.10	118.94
31	c	517	BCR	C37-C22-C21	-2.06	120.04	122.92
50	R1	621	XAT	C26-C27-C28	-2.06	121.64	125.99
29	N	611	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
41	C	527	LMK	C9-C8-C7	-2.06	106.92	111.79
29	n1	602	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
29	S1	603	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
29	a	406	CLA	C5-C3-C2	2.06	125.28	121.12
29	n1	614	CLA	CMD-C2D-C3D	-2.06	122.88	127.61
32	b	621	SQD	O8-S-C6	-2.06	102.46	105.74
29	N1	610	CLA	O2A-CGA-CBA	2.06	118.37	111.91
51	S1	623	NEX	C40-C33-C34	-2.06	120.04	122.92
48	G	606	CHL	CHB-C4A-NA	2.06	127.36	124.51
29	s	610	CLA	C6-C5-C3	-2.06	108.06	113.45
30	a1	408	PHO	C1-C2-C3	-2.06	122.48	126.04
50	Y1	622	XAT	C38-C25-C26	-2.06	118.81	122.26
33	w	201	LMG	O1-C1-C2	2.06	111.52	108.30
29	g	614	CLA	CAC-C3C-C4C	2.06	127.48	124.81
48	n	609	CHL	C4A-NA-C1A	2.06	107.63	106.71
31	D	404	BCR	C8-C9-C10	2.06	122.10	118.94
33	a	413	LMG	C8-O7-C10	-2.06	112.73	117.79
29	S	605	CLA	C2D-C1D-ND	2.06	111.62	110.10
29	N1	613	CLA	C3D-C2D-C1D	-2.06	103.02	105.83
31	b	618	BCR	C35-C13-C14	-2.06	120.04	122.92
29	c1	510	CLA	O2D-CGD-O1D	-2.06	119.82	123.84
29	N1	614	CLA	CMB-C2B-C1B	-2.06	125.30	128.46
37	b1	623	DGD	C1E-C2E-C3E	2.06	114.28	110.00
55	Y	627	PTY	O4-C30-C31	2.06	121.35	112.38
29	r1	612	CLA	C2A-C1A-CHA	2.06	127.45	123.86
29	B	617	CLA	CHA-C1A-NA	-2.06	121.69	126.40
29	N	603	CLA	CHA-C1A-NA	-2.06	121.69	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	g1	602	CLA	CHA-C1A-NA	-2.06	121.69	126.40
48	N1	607	CHL	CHA-C1A-NA	-2.06	121.69	126.40
29	n	604	CLA	CMB-C2B-C3B	2.06	128.52	124.68
29	B	603	CLA	C3D-C2D-C1D	-2.06	103.03	105.83
29	s1	613	CLA	C3D-C2D-C1D	-2.06	103.03	105.83
29	B	614	CLA	C2A-C1A-CHA	2.06	127.45	123.86
29	r	603	CLA	CMB-C2B-C1B	-2.06	125.31	128.46
48	y1	606	CHL	CHA-C1A-NA	-2.05	121.69	126.40
29	S	611	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
29	c	507	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
29	G	603	CLA	O1D-CGD-CBD	-2.05	120.28	124.48
29	c1	508	CLA	C2D-C1D-ND	2.05	111.62	110.10
29	a1	406	CLA	C6-C5-C3	-2.05	108.07	113.45
31	b1	619	BCR	C23-C24-C25	-2.05	121.43	127.20
33	C1	523	LMG	C3-C4-C5	2.05	113.90	110.24
29	b1	613	CLA	C6-C5-C3	-2.05	108.07	113.45
29	y	608	CLA	O2A-CGA-CBA	2.05	118.35	111.91
29	a1	410	CLA	CHA-C1A-NA	-2.05	121.69	126.40
29	y	608	CLA	CMB-C2B-C3B	2.05	128.52	124.68
29	B	617	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
29	c1	511	CLA	C3D-C2D-C1D	-2.05	103.03	105.83
50	g1	622	XAT	C28-C29-C30	2.05	122.09	118.94
29	s	602	CLA	CMC-C2C-C1C	2.05	128.16	125.04
29	a	406	CLA	CHA-C1A-NA	-2.05	121.70	126.40
29	Y	602	CLA	C6-C5-C3	-2.05	108.07	113.45
29	B1	603	CLA	CMB-C2B-C3B	2.05	128.52	124.68
51	g	623	NEX	C31-C32-C33	2.05	132.18	126.42
29	n	611	CLA	C2A-C1A-CHA	2.05	127.45	123.86
29	a1	407	CLA	C2A-C1A-CHA	2.05	127.45	123.86
29	Y	613	CLA	CAA-C2A-C3A	-2.05	107.16	112.78
29	B	611	CLA	CMB-C2B-C1B	-2.05	125.31	128.46
31	c	516	BCR	C35-C13-C12	2.05	121.31	118.08
29	S1	610	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
33	a	413	LMG	C6-C5-C4	-2.05	108.20	113.00
31	c1	514	BCR	C4-C5-C6	-2.05	119.75	122.73
33	W	201	LMG	O7-C10-O9	-2.05	118.75	123.70
29	c	509	CLA	C11-C10-C8	-2.05	109.29	115.92
29	c1	510	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
29	B	606	CLA	CHA-C1A-NA	-2.05	121.70	126.40
29	Y1	612	CLA	O1D-CGD-CBD	-2.05	120.29	124.48
43	d1	405	PL9	C31-C32-C33	-2.05	105.14	111.88
29	n	613	CLA	C11-C12-C13	-2.05	109.29	115.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	S1	614	CLA	C1D-ND-C4D	-2.05	104.88	106.33
40	D	410	LHG	C5-O7-C7	-2.05	112.75	117.79
29	B	613	CLA	O2A-CGA-CBA	2.05	118.34	111.91
43	D	405	PL9	C32-C33-C34	-2.05	122.73	127.66
40	D	410	LHG	C6-C5-C4	-2.05	106.94	111.79
29	G	602	CLA	C1D-ND-C4D	-2.05	104.88	106.33
49	g	621	LUT	C11-C10-C9	-2.05	124.39	127.31
29	b	614	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
29	b	616	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
31	B1	619	BCR	C35-C13-C14	-2.05	120.06	122.92
29	a1	406	CLA	O1D-CGD-CBD	-2.05	120.30	124.48
51	y	623	NEX	C26-C27-C28	-2.05	121.67	125.99
48	S	607	CHL	CHD-C4C-C3C	2.05	127.85	124.84
29	B1	605	CLA	CMA-C3A-C2A	2.05	122.08	113.83
29	c1	506	CLA	CHA-C1A-NA	-2.05	121.71	126.40
29	c1	505	CLA	C3D-C2D-C1D	-2.05	103.04	105.83
48	N	607	CHL	CMA-C3A-C2A	2.05	122.08	113.83
49	N1	620	LUT	C39-C29-C28	2.05	121.30	118.08
29	G1	603	CLA	CMD-C2D-C3D	-2.05	122.91	127.61
29	b1	610	CLA	CHA-C1A-NA	-2.05	121.71	126.40
48	s1	606	CHL	CHD-C4C-C3C	2.05	127.85	124.84
29	s	609	CLA	C1-O2A-CGA	2.04	121.81	116.44
51	N	623	NEX	O24-C25-C24	2.04	114.92	113.38
36	B1	620	C7Z	C31-C30-C29	-2.04	124.39	127.31
29	N1	604	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
29	a	407	CLA	CMB-C2B-C3B	2.04	128.50	124.68
29	g1	602	CLA	C1C-C2C-C3C	-2.04	104.81	106.96
29	N1	611	CLA	OBD-CAD-C3D	-2.04	123.60	128.52
29	b1	614	CLA	CMD-C2D-C3D	-2.04	122.91	127.61
48	R	606	CHL	CHC-C1C-NC	2.04	127.30	124.20
48	g1	606	CHL	CHC-C1C-NC	2.04	127.30	124.20
48	N1	605	CHL	C2C-C3C-C4C	2.04	107.95	106.49
29	C1	512	CLA	C1D-ND-C4D	-2.04	104.88	106.33
29	R1	612	CLA	C1D-ND-C4D	-2.04	104.88	106.33
29	y1	603	CLA	O1D-CGD-CBD	-2.04	120.30	124.48
29	Y1	612	CLA	C3D-C2D-C1D	-2.04	103.04	105.83
37	c1	520	DGD	C3B-C2B-C1B	-2.04	106.19	113.62
48	S	606	CHL	CMB-C2B-C1B	-2.04	125.32	128.46
29	G	611	CLA	CHA-C1A-NA	-2.04	121.72	126.40
29	c	507	CLA	C2A-C1A-CHA	2.04	127.43	123.86
29	R1	610	CLA	C6-C5-C3	-2.04	108.10	113.45
48	s	601	CHL	CHC-C1C-NC	2.04	127.30	124.20

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	A	408	PHO	C1B-NB-C4B	2.04	111.29	107.09
31	C1	514	BCR	C37-C22-C21	-2.04	120.06	122.92
29	D1	403	CLA	CAA-C2A-C3A	-2.04	107.18	112.78
29	n	613	CLA	C2A-C1A-CHA	2.04	127.43	123.86
29	C	503	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
29	A1	405	CLA	CAC-C3C-C4C	2.04	127.46	124.81
29	g	610	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
29	R1	602	CLA	C2D-C1D-ND	2.04	111.61	110.10
29	N	602	CLA	C6-C7-C8	-2.04	109.32	115.92
29	G1	613	CLA	C1-O2A-CGA	2.04	121.80	116.44
31	C1	517	BCR	C35-C13-C12	2.04	121.29	118.08
29	C	506	CLA	CAC-C3C-C4C	2.04	127.46	124.81
29	B	603	CLA	CAA-C2A-C3A	-2.04	107.19	112.78
29	c1	507	CLA	O2A-CGA-CBA	2.04	118.31	111.91
51	y	623	NEX	C16-C1-C6	-2.04	108.64	110.47
48	N	608	CHL	C1B-CHB-C4A	-2.04	126.07	130.12
29	c1	508	CLA	O1D-CGD-CBD	-2.04	120.31	124.48
31	B1	619	BCR	C4-C5-C6	-2.04	119.77	122.73
36	B	620	C7Z	C31-C32-C33	-2.04	120.68	126.42
29	G	614	CLA	C3D-C2D-C1D	-2.04	103.05	105.83
53	R1	626	ERG	C6-C7-C8	-2.04	118.05	122.07
43	D1	405	PL9	C20-C19-C18	-2.04	118.44	123.68
48	Y1	601	CHL	CMB-C2B-C3B	2.04	128.50	124.68
37	C1	518	DGD	C3G-C2G-C1G	-2.04	106.96	111.79
48	Y1	606	CHL	CMB-C2B-C1B	-2.04	125.33	128.46
49	n	621	LUT	C37-C21-C22	-2.04	105.57	109.44
48	n	608	CHL	C1-O2A-CGA	2.04	121.80	116.44
49	n	621	LUT	C19-C9-C8	2.04	121.29	118.08
29	B1	617	CLA	CMD-C2D-C3D	-2.04	122.92	127.61
29	b1	613	CLA	C2D-C1D-ND	2.04	111.61	110.10
49	G	620	LUT	C8-C7-C6	-2.04	121.47	127.20
36	b1	620	C7Z	C8-C7-C6	-2.04	121.48	127.20
29	B	602	CLA	CHA-C1A-NA	-2.04	121.73	126.40
31	c	514	BCR	C19-C18-C17	2.04	122.07	118.94
49	s	620	LUT	C31-C30-C29	-2.04	124.40	127.31
29	N	610	CLA	CHA-C1A-NA	-2.04	121.73	126.40
29	B1	617	CLA	CHD-C1D-ND	-2.04	122.58	124.45
49	R	620	LUT	C31-C32-C33	-2.04	120.69	126.42
40	C1	525	LHG	C6-C5-C4	-2.04	106.97	111.79
29	Y	604	CLA	CMD-C2D-C3D	-2.04	122.93	127.61
51	y1	623	NEX	C28-C29-C30	2.04	122.07	118.94
49	s1	620	LUT	C31-C30-C29	-2.04	124.40	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Y1	608	CLA	CBC-CAC-C3C	-2.04	106.81	112.43
49	G	620	LUT	C38-C25-C24	-2.04	119.20	123.56
50	R1	621	XAT	C5-C4-C3	-2.04	108.72	112.75
29	B	616	CLA	CMA-C3A-C2A	2.04	122.05	113.83
43	D	405	PL9	O2-C1-C2	-2.04	117.11	121.78
48	y	607	CHL	CHA-C1A-NA	-2.04	121.73	126.40
50	R	621	XAT	C20-C13-C14	-2.04	120.07	122.92
29	c	505	CLA	CMB-C2B-C3B	2.04	128.49	124.68
29	b1	605	CLA	C11-C12-C13	-2.04	109.34	115.92
49	g	620	LUT	C3-C4-C5	-2.04	107.80	111.85
29	b1	611	CLA	CHD-C1D-ND	-2.04	122.58	124.45
31	D	404	BCR	C3-C4-C5	-2.04	110.44	114.08
29	N1	603	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
43	D	405	PL9	C50-C49-C48	-2.04	116.76	122.65
31	b	618	BCR	C30-C25-C26	-2.04	119.75	122.61
29	n	603	CLA	O1D-CGD-CBD	-2.04	120.32	124.48
40	d	408	LHG	O8-C23-O10	-2.04	118.46	123.59
29	s	602	CLA	C3D-C2D-C1D	-2.03	103.05	105.83
43	D	405	PL9	C11-C12-C13	-2.03	105.19	111.88
29	r	602	CLA	O1D-CGD-CBD	-2.03	120.32	124.48
49	S	621	LUT	C28-C29-C30	-2.03	115.82	118.94
29	g	610	CLA	CHA-C1A-NA	-2.03	121.74	126.40
29	B	605	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
29	g1	614	CLA	CAA-C2A-C3A	-2.03	107.21	112.78
29	r	612	CLA	CMA-C3A-C4A	2.03	117.24	111.77
29	g1	604	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
51	N	623	NEX	C26-C27-C28	-2.03	121.69	125.99
48	g1	601	CHL	C1-C2-C3	-2.03	122.53	126.04
48	N1	605	CHL	CHC-C1C-NC	2.03	127.29	124.20
29	g	611	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
49	s	620	LUT	C36-C21-C26	-2.03	106.47	109.55
29	Y	602	CLA	CAC-C3C-C4C	2.03	127.45	124.81
29	D1	402	CLA	CMC-C2C-C1C	2.03	128.13	125.04
29	Y1	613	CLA	CMB-C2B-C3B	2.03	128.48	124.68
29	Y	608	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
29	b	604	CLA	CMA-C3A-C4A	2.03	117.23	111.77
29	B1	602	CLA	C1-C2-C3	-2.03	122.53	126.04
29	B1	606	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
49	S1	621	LUT	C16-C1-C6	-2.03	107.00	110.30
29	b	609	CLA	C2A-C1A-CHA	2.03	127.41	123.86
48	n1	609	CHL	CHB-C4A-NA	2.03	127.32	124.51
48	s1	601	CHL	C1D-CHD-C4C	-2.03	121.68	126.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B1	612	CLA	CHA-C1A-NA	-2.03	121.75	126.40
29	G1	612	CLA	CHA-C1A-NA	-2.03	121.75	126.40
29	b	615	CLA	O2A-CGA-CBA	2.03	118.28	111.91
29	y1	613	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
29	R	603	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
29	G1	614	CLA	CMD-C2D-C3D	-2.03	122.94	127.61
29	G1	610	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
29	b1	606	CLA	CAC-C3C-C2C	-2.03	124.06	127.53
29	r1	612	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
50	R1	621	XAT	O4-C5-C18	-2.03	112.62	115.06
50	g1	622	XAT	O24-C25-C38	-2.03	112.62	115.06
29	B	605	CLA	C16-C15-C13	-2.03	109.36	115.92
31	c1	516	BCR	C23-C24-C25	-2.03	121.50	127.20
51	y1	623	NEX	C40-C33-C32	2.03	121.27	118.08
31	d1	404	BCR	C31-C1-C6	-2.03	107.01	110.30
29	N1	603	CLA	C6-C5-C3	-2.03	108.14	113.45
29	c	506	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
53	R1	626	ERG	C4-C5-C10	2.03	119.11	116.42
48	n	608	CHL	C3A-C2A-C1A	2.03	104.38	101.34
29	c	504	CLA	C1C-C2C-C3C	-2.03	104.82	106.96
29	N1	604	CLA	O2A-CGA-CBA	2.03	118.27	111.91
48	y1	606	CHL	CHD-C4C-C3C	2.03	127.82	124.84
29	y1	614	CLA	O2D-CGD-O1D	-2.03	119.87	123.84
43	d1	405	PL9	C37-C38-C39	-2.03	122.78	127.66
29	y1	612	CLA	CMA-C3A-C2A	2.03	122.01	113.83
49	Y	620	LUT	C30-C31-C32	-2.03	116.89	123.22
29	b	603	CLA	CAA-C2A-C3A	-2.03	107.22	112.78
29	b	616	CLA	O1D-CGD-CBD	-2.03	120.33	124.48
48	s1	601	CHL	CHB-C4A-NA	2.03	127.32	124.51
29	B	613	CLA	C6-C5-C3	-2.03	108.14	113.45
29	R	602	CLA	C3D-C2D-C1D	-2.03	103.06	105.83
29	s1	605	CLA	C2A-C1A-CHA	2.03	127.40	123.86
29	r1	608	CLA	CHA-C1A-NA	-2.03	121.75	126.40
29	g	603	CLA	O1D-CGD-CBD	-2.03	120.34	124.48
33	c	523	LMG	C1-C2-C3	-2.03	105.77	110.00
29	S1	604	CLA	C1D-ND-C4D	-2.03	104.89	106.33
29	B1	612	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
29	a	405	CLA	CAC-C3C-C4C	2.03	127.44	124.81
49	y	620	LUT	C30-C31-C32	-2.03	116.89	123.22
29	C	503	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
29	S1	605	CLA	C3D-C2D-C1D	-2.03	103.07	105.83
29	G1	610	CLA	CHA-C1A-NA	-2.03	121.76	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	C1	507	CLA	C2D-C1D-ND	2.03	111.60	110.10
29	d1	402	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
48	N1	601	CHL	C1-O2A-CGA	2.03	121.76	116.44
29	C1	502	CLA	C11-C12-C13	-2.03	109.37	115.92
52	r1	625	LMT	C3B-C4B-C5B	-2.03	106.63	110.24
29	d1	403	CLA	O2D-CGD-O1D	-2.03	119.88	123.84
50	y1	622	XAT	C12-C13-C14	2.03	122.05	118.94
51	g1	623	NEX	C19-C9-C10	-2.03	120.09	122.92
51	S1	623	NEX	C4-C3-C2	2.03	114.68	110.77
49	y1	620	LUT	C2-C3-C4	-2.02	107.53	110.30
29	N	603	CLA	CAA-C2A-C3A	-2.02	107.23	112.78
29	g	613	CLA	O1D-CGD-CBD	-2.02	120.34	124.48
29	r	608	CLA	CHA-C1A-NA	-2.02	121.76	126.40
29	b1	607	CLA	CHA-C1A-NA	-2.02	121.76	126.40
31	C	515	BCR	C35-C13-C12	2.02	121.27	118.08
29	D1	403	CLA	C6-C7-C8	-2.02	109.38	115.92
48	n1	609	CHL	C4A-NA-C1A	2.02	107.62	106.71
29	c	504	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
29	B	610	CLA	CHA-C1A-NA	-2.02	121.76	126.40
48	s1	608	CHL	CHB-C4A-NA	2.02	127.31	124.51
31	c	514	BCR	C38-C26-C27	2.02	117.50	113.62
29	N1	603	CLA	CBC-CAC-C3C	-2.02	106.85	112.43
31	b1	618	BCR	C1-C6-C7	2.02	121.50	115.78
29	b	604	CLA	C2D-C1D-ND	2.02	111.59	110.10
29	y	604	CLA	C3D-C2D-C1D	-2.02	103.07	105.83
29	c1	506	CLA	CAA-CBA-CGA	-2.02	107.34	113.25
48	N	606	CHL	C3A-C2A-C1A	2.02	104.37	101.34
49	s1	620	LUT	C30-C31-C32	-2.02	116.90	123.22
29	g	611	CLA	CMD-C2D-C3D	-2.02	122.96	127.61
43	D1	405	PL9	C7-C8-C9	-2.02	123.42	126.79
43	D	405	PL9	C20-C19-C21	2.02	118.67	115.27
29	b1	604	CLA	C4D-CHA-C1A	2.02	123.71	121.25
48	N	608	CHL	C4D-CHA-C1A	2.02	123.71	121.25
29	C	509	CLA	C2D-C1D-ND	2.02	111.59	110.10
29	y1	604	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
29	B1	606	CLA	C2A-C1A-CHA	2.02	127.39	123.86
49	N	621	LUT	C31-C30-C29	-2.02	124.42	127.31
29	b1	609	CLA	CMD-C2D-C3D	-2.02	122.96	127.61
31	C1	516	BCR	C23-C24-C25	-2.02	121.53	127.20
29	n	614	CLA	CAC-C3C-C4C	2.02	127.43	124.81
29	b1	612	CLA	C1C-C2C-C3C	-2.02	104.83	106.96
29	g1	603	CLA	CMB-C2B-C3B	2.02	128.46	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
48	n	606	CHL	C3A-C2A-C1A	2.02	104.36	101.34
31	d	404	BCR	C12-C13-C14	-2.02	115.84	118.94
29	s1	613	CLA	C1D-ND-C4D	-2.02	104.90	106.33
29	s1	614	CLA	C1D-ND-C4D	-2.02	104.90	106.33
29	A	407	CLA	CHA-C1A-NA	-2.02	121.77	126.40
38	b	624	3PH	O21-C21-O22	-2.02	118.82	123.70
48	N1	605	CHL	C3A-C2A-C1A	2.02	104.36	101.34
29	Y	603	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
48	n1	601	CHL	C1-O2A-CGA	2.02	121.74	116.44
48	N	606	CHL	CHC-C1C-NC	2.02	127.27	124.20
29	y1	612	CLA	CMD-C2D-C3D	-2.02	122.97	127.61
29	C1	501	CLA	CMA-C3A-C2A	2.02	121.97	113.83
29	b	617	CLA	O2A-CGA-CBA	2.02	118.24	111.91
29	D	402	CLA	O1D-CGD-CBD	-2.02	120.35	124.48
29	b	605	CLA	C11-C10-C8	-2.02	109.39	115.92
29	y1	604	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
55	y	627	PTY	C6-O7-C8	-2.02	114.14	117.90
51	S	623	NEX	O24-C25-C24	-2.02	111.87	113.38
51	Y	623	NEX	C11-C10-C9	2.02	130.19	127.31
29	B	615	CLA	CHA-C1A-NA	-2.02	121.78	126.40
29	r	603	CLA	O2A-CGA-CBA	2.02	118.24	111.91
29	s1	605	CLA	CAA-C2A-C3A	-2.02	107.25	112.78
49	s	620	LUT	C37-C21-C26	2.02	112.60	109.55
29	g	602	CLA	C1-O2A-CGA	2.02	121.74	116.44
29	G	613	CLA	CHA-C1A-NA	-2.02	121.78	126.40
29	c1	507	CLA	C1D-ND-C4D	-2.02	104.90	106.33
32	b	626	SQD	O3-C3-C2	-2.02	105.69	110.35
29	c1	502	CLA	C1C-C2C-C3C	-2.02	104.84	106.96
29	B1	613	CLA	O2A-CGA-CBA	2.02	118.24	111.91
29	N1	611	CLA	CHA-C1A-NA	-2.02	121.78	126.40
29	G1	603	CLA	C2A-C1A-CHA	2.02	127.38	123.86
48	g	608	CHL	CHD-C4C-C3C	2.02	127.80	124.84
37	B1	623	DGD	O1G-C1A-O1A	-2.02	118.50	123.59
49	N1	620	LUT	C2-C3-C4	-2.02	107.55	110.30
29	n	603	CLA	O2A-CGA-CBA	2.02	118.23	111.91
29	b1	610	CLA	C3D-C2D-C1D	-2.02	103.08	105.83
29	r	609	CLA	CMB-C2B-C3B	2.01	128.45	124.68
29	y1	611	CLA	CMB-C2B-C3B	2.01	128.45	124.68
29	S	617	CLA	C1D-ND-C4D	-2.01	104.90	106.33
29	B1	615	CLA	C1D-ND-C4D	-2.01	104.90	106.33
29	C	508	CLA	C6-C7-C8	-2.01	109.41	115.92
29	c	508	CLA	CMD-C2D-C3D	-2.01	122.98	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	a1	410	CLA	CMD-C2D-C3D	-2.01	122.98	127.61
29	y1	611	CLA	CMD-C2D-C3D	-2.01	122.98	127.61
29	S	611	CLA	C2A-C1A-CHA	2.01	127.38	123.86
29	a1	407	CLA	O2A-CGA-CBA	2.01	118.23	111.91
49	s1	620	LUT	C15-C35-C34	-2.01	119.35	123.47
29	y1	610	CLA	O2D-CGD-O1D	-2.01	119.90	123.84
32	b1	621	SQD	O8-S-C6	-2.01	102.53	105.74
29	C1	509	CLA	O1D-CGD-CBD	-2.01	120.36	124.48
33	B1	622	LMG	O7-C10-O9	-2.01	118.84	123.70
49	n1	621	LUT	C12-C13-C14	-2.01	115.85	118.94
31	B1	619	BCR	C1-C6-C7	2.01	121.47	115.78
48	S	606	CHL	C4A-NA-C1A	2.01	107.61	106.71
29	C	513	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
32	A1	412	SQD	C1-C2-C3	-2.01	105.80	110.00
47	k	101	4RF	O18-C16-C15	2.01	118.22	111.91
31	b	618	BCR	C37-C22-C23	2.01	121.25	118.08
50	N	622	XAT	C19-C9-C10	-2.01	120.10	122.92
29	N	614	CLA	C3D-C2D-C1D	-2.01	103.08	105.83
29	D	402	CLA	C2C-C1C-NC	2.01	111.86	109.97
29	c1	508	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
29	c1	509	CLA	C11-C10-C8	-2.01	109.42	115.92
32	C	526	SQD	O8-S-C6	-2.01	102.53	105.74
49	y	621	LUT	C16-C1-C6	-2.01	107.04	110.30
50	n	622	XAT	C39-C29-C30	-2.01	120.11	122.92
50	y	622	XAT	C40-C33-C34	-2.01	120.11	122.92
29	G	611	CLA	C1-O2A-CGA	2.01	121.72	116.44
29	n	602	CLA	CHA-C1A-NA	-2.01	121.79	126.40
29	c	506	CLA	CMA-C3A-C4A	2.01	117.18	111.77
48	n1	607	CHL	C1B-CHB-C4A	-2.01	126.13	130.12
29	c1	507	CLA	CMB-C2B-C1B	-2.01	125.37	128.46
31	B1	618	BCR	C30-C25-C26	-2.01	119.78	122.61
29	Y	602	CLA	C2D-C1D-ND	2.01	111.59	110.10
48	g	608	CHL	CHC-C1C-NC	2.01	127.25	124.20
31	B1	619	BCR	C37-C22-C21	-2.01	120.11	122.92
29	c	503	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
30	a1	409	PHO	C1-C2-C3	-2.01	122.57	126.04
29	Y	614	CLA	C11-C10-C8	-2.01	109.42	115.92
29	y	613	CLA	C6-C7-C8	-2.01	109.42	115.92
49	y	620	LUT	C35-C15-C14	-2.01	119.36	123.47
49	N1	620	LUT	C19-C9-C10	-2.01	120.11	122.92
29	R	602	CLA	C1D-ND-C4D	-2.01	104.91	106.33
29	B	615	CLA	C3D-C2D-C1D	-2.01	103.09	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	n	612	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
29	S	612	CLA	CHA-C1A-NA	-2.01	121.80	126.40
29	Y	613	CLA	C16-C15-C13	-2.01	109.42	115.92
50	Y1	622	XAT	C4-C3-C2	-2.01	106.89	110.77
29	y	603	CLA	CHA-C1A-NA	-2.01	121.80	126.40
31	B1	618	BCR	C2-C1-C6	2.01	113.57	110.48
31	B	619	BCR	C39-C30-C25	-2.01	107.04	110.30
51	y	623	NEX	C5-C4-C3	2.01	114.12	111.75
29	b	607	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
50	G1	622	XAT	C25-C24-C23	2.01	116.72	112.75
29	g	602	CLA	CBC-CAC-C3C	-2.01	106.90	112.43
49	n1	621	LUT	C31-C30-C29	-2.01	124.45	127.31
29	g1	602	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
29	N1	602	CLA	CMB-C2B-C1B	-2.01	125.38	128.46
33	a1	413	LMG	O7-C10-O9	-2.01	118.85	123.70
49	r	620	LUT	C35-C15-C14	-2.01	119.36	123.47
29	C	512	CLA	C1-C2-C3	-2.01	122.57	126.04
29	G	602	CLA	C16-C15-C13	-2.01	109.43	115.92
29	B1	602	CLA	O1D-CGD-CBD	-2.01	120.38	124.48
29	G1	604	CLA	C2A-C1A-CHA	2.01	127.37	123.86
29	B1	608	CLA	O2A-CGA-CBA	2.01	118.20	111.91
29	C	509	CLA	C11-C10-C8	-2.01	109.44	115.92
49	y	620	LUT	C8-C7-C6	-2.01	121.57	127.20
29	N1	614	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
29	c1	506	CLA	C3D-C2D-C1D	-2.01	103.09	105.83
29	Y1	614	CLA	O2D-CGD-O1D	-2.01	119.92	123.84
54	s1	625	LPX	C3-C4-C5	-2.01	106.89	112.79
31	c	517	BCR	C31-C1-C6	-2.00	107.05	110.30
29	N	614	CLA	O1D-CGD-CBD	-2.00	120.38	124.48
37	b	623	DGD	O6D-C5D-C6D	2.00	110.71	106.67
53	r1	626	ERG	C13-C14-C8	2.00	117.37	113.48
33	d1	411	LMG	C1-O6-C5	2.00	117.62	113.69
29	G	613	CLA	CAA-C2A-C3A	-2.00	107.29	112.78
29	b	607	CLA	CHA-C1A-NA	-2.00	121.81	126.40
29	s	605	CLA	CHA-C1A-NA	-2.00	121.81	126.40
32	m	101	SQD	O8-S-C6	-2.00	102.55	105.74
31	b	619	BCR	C4-C5-C6	-2.00	119.82	122.73
29	B1	607	CLA	CMC-C2C-C1C	2.00	128.09	125.04
48	g	601	CHL	C4D-CHA-C1A	2.00	123.69	121.25
29	B	607	CLA	OBD-CAD-C3D	-2.00	123.70	128.52
29	r	608	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
29	r1	610	CLA	CHD-C1D-ND	-2.00	122.61	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	B	612	CLA	CHA-C1A-NA	-2.00	121.81	126.40
48	Y	605	CHL	CHD-C1D-C2D	2.00	129.68	125.48
29	b	607	CLA	CMD-C2D-C3D	-2.00	123.01	127.61
31	b1	619	BCR	C1-C6-C7	2.00	121.44	115.78
29	S	603	CLA	C2A-C1A-CHA	2.00	127.36	123.86
31	D	404	BCR	C34-C9-C10	-2.00	120.12	122.92
29	s1	617	CLA	CMD-C2D-C3D	-2.00	123.01	127.61
29	a	405	CLA	OBD-CAD-C3D	-2.00	123.70	128.52
29	D1	403	CLA	CAC-C3C-C4C	2.00	127.41	124.81
31	c	514	BCR	C40-C30-C25	-2.00	107.05	110.30
33	h	102	LMG	C8-O7-C10	-2.00	112.87	117.79
29	B1	608	CLA	O1D-CGD-CBD	-2.00	120.39	124.48
29	r	612	CLA	O2A-CGA-CBA	2.00	118.19	111.91
29	y1	610	CLA	C1D-ND-C4D	-2.00	104.91	106.33
29	D1	402	CLA	CAC-C3C-C4C	2.00	127.41	124.81

All (696) chirality outliers are listed below:

Mol	Chain	Res	Type	Atom
29	A	405	CLA	ND
29	A	406	CLA	ND
29	A	407	CLA	ND
29	A	410	CLA	ND
29	B	602	CLA	ND
29	B	603	CLA	ND
29	B	604	CLA	ND
29	B	605	CLA	ND
29	B	606	CLA	ND
29	B	607	CLA	ND
29	B	608	CLA	ND
29	B	609	CLA	ND
29	B	610	CLA	ND
29	B	611	CLA	ND
29	B	612	CLA	ND
29	B	613	CLA	ND
29	B	614	CLA	ND
29	B	615	CLA	ND
29	B	616	CLA	ND
29	B	617	CLA	ND
29	C	501	CLA	ND
29	C	502	CLA	ND
29	C	503	CLA	ND

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Mol	Chain	Res	Type	Atom
29	C	504	CLA	ND
29	C	505	CLA	ND
29	C	506	CLA	ND
29	C	507	CLA	ND
29	C	508	CLA	ND
29	C	509	CLA	ND
29	C	510	CLA	ND
29	C	511	CLA	ND
29	C	512	CLA	ND
29	C	513	CLA	ND
29	D	402	CLA	ND
29	D	403	CLA	ND
29	N	602	CLA	ND
29	N	603	CLA	ND
29	N	604	CLA	ND
29	N	610	CLA	ND
29	N	611	CLA	ND
29	N	612	CLA	ND
29	N	613	CLA	ND
29	N	614	CLA	ND
29	G	602	CLA	ND
29	G	603	CLA	ND
29	G	604	CLA	ND
29	G	610	CLA	ND
29	G	611	CLA	ND
29	G	612	CLA	ND
29	G	613	CLA	ND
29	G	614	CLA	ND
29	R	602	CLA	ND
29	R	603	CLA	ND
29	R	604	CLA	ND
29	R	608	CLA	ND
29	R	609	CLA	ND
29	R	610	CLA	ND
29	R	612	CLA	ND
29	S	602	CLA	ND
29	S	603	CLA	ND
29	S	604	CLA	ND
29	S	605	CLA	ND
29	S	609	CLA	ND
29	S	610	CLA	ND
29	S	611	CLA	ND

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Mol	Chain	Res	Type	Atom
29	S	612	CLA	ND
29	S	613	CLA	ND
29	S	614	CLA	ND
29	S	617	CLA	ND
29	Y	602	CLA	ND
29	Y	603	CLA	ND
29	Y	604	CLA	ND
29	Y	608	CLA	ND
29	Y	610	CLA	ND
29	Y	611	CLA	ND
29	Y	612	CLA	ND
29	Y	613	CLA	ND
29	Y	614	CLA	ND
29	a	405	CLA	ND
29	a	406	CLA	ND
29	a	407	CLA	ND
29	a	410	CLA	ND
29	b	602	CLA	ND
29	b	603	CLA	ND
29	b	604	CLA	ND
29	b	605	CLA	ND
29	b	606	CLA	ND
29	b	607	CLA	ND
29	b	608	CLA	ND
29	b	609	CLA	ND
29	b	610	CLA	ND
29	b	611	CLA	ND
29	b	612	CLA	ND
29	b	613	CLA	ND
29	b	614	CLA	ND
29	b	615	CLA	ND
29	b	616	CLA	ND
29	b	617	CLA	ND
29	c	501	CLA	ND
29	c	502	CLA	ND
29	c	503	CLA	ND
29	c	504	CLA	ND
29	c	505	CLA	ND
29	c	506	CLA	ND
29	c	507	CLA	ND
29	c	508	CLA	ND
29	c	509	CLA	ND

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Mol	Chain	Res	Type	Atom
29	c	510	CLA	ND
29	c	511	CLA	ND
29	c	512	CLA	ND
29	c	513	CLA	ND
29	d	402	CLA	ND
29	d	403	CLA	ND
29	n	602	CLA	ND
29	n	603	CLA	ND
29	n	604	CLA	ND
29	n	610	CLA	ND
29	n	611	CLA	ND
29	n	612	CLA	ND
29	n	613	CLA	ND
29	n	614	CLA	ND
29	g	602	CLA	ND
29	g	603	CLA	ND
29	g	604	CLA	ND
29	g	610	CLA	ND
29	g	611	CLA	ND
29	g	612	CLA	ND
29	g	613	CLA	ND
29	g	614	CLA	ND
29	r	602	CLA	ND
29	r	603	CLA	ND
29	r	604	CLA	ND
29	r	608	CLA	ND
29	r	609	CLA	ND
29	r	610	CLA	ND
29	r	612	CLA	ND
29	s	602	CLA	ND
29	s	603	CLA	ND
29	s	604	CLA	ND
29	s	605	CLA	ND
29	s	609	CLA	ND
29	s	610	CLA	ND
29	s	611	CLA	ND
29	s	612	CLA	ND
29	s	613	CLA	ND
29	s	614	CLA	ND
29	s	617	CLA	ND
29	y	602	CLA	ND
29	y	603	CLA	ND

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Mol	Chain	Res	Type	Atom
29	y	604	CLA	ND
29	y	608	CLA	ND
29	y	610	CLA	ND
29	y	611	CLA	ND
29	y	612	CLA	ND
29	y	613	CLA	ND
29	y	614	CLA	ND
29	A1	405	CLA	ND
29	A1	406	CLA	ND
29	A1	407	CLA	ND
29	A1	410	CLA	ND
29	B1	602	CLA	ND
29	B1	603	CLA	ND
29	B1	604	CLA	ND
29	B1	605	CLA	ND
29	B1	606	CLA	ND
29	B1	607	CLA	ND
29	B1	608	CLA	ND
29	B1	609	CLA	ND
29	B1	610	CLA	ND
29	B1	611	CLA	ND
29	B1	612	CLA	ND
29	B1	613	CLA	ND
29	B1	614	CLA	ND
29	B1	615	CLA	ND
29	B1	616	CLA	ND
29	B1	617	CLA	ND
29	C1	501	CLA	ND
29	C1	502	CLA	ND
29	C1	503	CLA	ND
29	C1	504	CLA	ND
29	C1	505	CLA	ND
29	C1	506	CLA	ND
29	C1	507	CLA	ND
29	C1	508	CLA	ND
29	C1	509	CLA	ND
29	C1	510	CLA	ND
29	C1	511	CLA	ND
29	C1	512	CLA	ND
29	C1	513	CLA	ND
29	D1	402	CLA	ND
29	D1	403	CLA	ND

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Mol	Chain	Res	Type	Atom
29	N1	602	CLA	ND
29	N1	603	CLA	ND
29	N1	604	CLA	ND
29	N1	610	CLA	ND
29	N1	611	CLA	ND
29	N1	612	CLA	ND
29	N1	613	CLA	ND
29	N1	614	CLA	ND
29	G1	602	CLA	ND
29	G1	603	CLA	ND
29	G1	604	CLA	ND
29	G1	610	CLA	ND
29	G1	611	CLA	ND
29	G1	612	CLA	ND
29	G1	613	CLA	ND
29	G1	614	CLA	ND
29	R1	602	CLA	ND
29	R1	603	CLA	ND
29	R1	604	CLA	ND
29	R1	608	CLA	ND
29	R1	609	CLA	ND
29	R1	610	CLA	ND
29	R1	612	CLA	ND
29	S1	602	CLA	ND
29	S1	603	CLA	ND
29	S1	604	CLA	ND
29	S1	605	CLA	ND
29	S1	609	CLA	ND
29	S1	610	CLA	ND
29	S1	611	CLA	ND
29	S1	612	CLA	ND
29	S1	613	CLA	ND
29	S1	614	CLA	ND
29	S1	617	CLA	ND
29	Y1	602	CLA	ND
29	Y1	603	CLA	ND
29	Y1	604	CLA	ND
29	Y1	608	CLA	ND
29	Y1	610	CLA	ND
29	Y1	611	CLA	ND
29	Y1	612	CLA	ND
29	Y1	613	CLA	ND

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

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Mol	Chain	Res	Type	Atom
29	n1	613	CLA	ND
29	n1	614	CLA	ND
29	g1	602	CLA	ND
29	g1	603	CLA	ND
29	g1	604	CLA	ND
29	g1	610	CLA	ND
29	g1	611	CLA	ND
29	g1	612	CLA	ND
29	g1	613	CLA	ND
29	g1	614	CLA	ND
29	r1	602	CLA	ND
29	r1	603	CLA	ND
29	r1	604	CLA	ND
29	r1	608	CLA	ND
29	r1	609	CLA	ND
29	r1	610	CLA	ND
29	r1	612	CLA	ND
29	s1	602	CLA	ND
29	s1	603	CLA	ND
29	s1	604	CLA	ND
29	s1	605	CLA	ND
29	s1	609	CLA	ND
29	s1	610	CLA	ND
29	s1	611	CLA	ND
29	s1	612	CLA	ND
29	s1	613	CLA	ND
29	s1	614	CLA	ND
29	s1	617	CLA	ND
29	y1	602	CLA	ND
29	y1	603	CLA	ND
29	y1	604	CLA	ND
29	y1	608	CLA	ND
29	y1	610	CLA	ND
29	y1	611	CLA	ND
29	y1	612	CLA	ND
29	y1	613	CLA	ND
29	y1	614	CLA	ND
36	B	620	C7Z	C3
36	b	620	C7Z	C3
36	B1	620	C7Z	C3
36	b1	620	C7Z	C3
41	C	527	LMK	C8

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Mol	Chain	Res	Type	Atom
41	C	527	LMK	C3
41	c	527	LMK	C8
41	c	527	LMK	C3
41	C1	527	LMK	C8
41	C1	527	LMK	C3
41	c1	527	LMK	C8
41	c1	527	LMK	C3
45	H	101	RRX	C28
45	h	101	RRX	C28
45	H1	101	RRX	C28
45	h1	101	RRX	C28
48	N	601	CHL	NA
48	N	601	CHL	ND
48	N	601	CHL	C8
48	N	601	CHL	NC
48	N	605	CHL	NA
48	N	605	CHL	ND
48	N	605	CHL	C8
48	N	605	CHL	NC
48	N	606	CHL	NA
48	N	606	CHL	ND
48	N	606	CHL	C8
48	N	606	CHL	NC
48	N	607	CHL	NA
48	N	607	CHL	ND
48	N	607	CHL	C8
48	N	607	CHL	NC
48	N	608	CHL	NA
48	N	608	CHL	ND
48	N	608	CHL	NC
48	N	609	CHL	NA
48	N	609	CHL	ND
48	N	609	CHL	C8
48	N	609	CHL	NC
48	G	601	CHL	NA
48	G	601	CHL	ND
48	G	601	CHL	C8
48	G	601	CHL	NC
48	G	605	CHL	C3A
48	G	605	CHL	NA
48	G	605	CHL	ND
48	G	605	CHL	NC

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

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Mol	Chain	Res	Type	Atom
48	Y	606	CHL	C8
48	Y	606	CHL	NC
48	Y	607	CHL	NA
48	Y	607	CHL	ND
48	Y	607	CHL	C8
48	Y	607	CHL	NC
48	Y	609	CHL	NA
48	Y	609	CHL	ND
48	Y	609	CHL	C8
48	Y	609	CHL	NC
48	n	601	CHL	NA
48	n	601	CHL	ND
48	n	601	CHL	C8
48	n	601	CHL	NC
48	n	605	CHL	NA
48	n	605	CHL	ND
48	n	605	CHL	C8
48	n	605	CHL	NC
48	n	606	CHL	NA
48	n	606	CHL	ND
48	n	606	CHL	C8
48	n	606	CHL	NC
48	n	607	CHL	NA
48	n	607	CHL	ND
48	n	607	CHL	C8
48	n	607	CHL	NC
48	n	608	CHL	NA
48	n	608	CHL	ND
48	n	608	CHL	NC
48	n	609	CHL	NA
48	n	609	CHL	ND
48	n	609	CHL	C8
48	n	609	CHL	NC
48	g	601	CHL	NA
48	g	601	CHL	ND
48	g	601	CHL	C8
48	g	601	CHL	NC
48	g	605	CHL	C3A
48	g	605	CHL	NA
48	g	605	CHL	ND
48	g	605	CHL	NC
48	g	606	CHL	NA

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

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

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

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

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

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Mol	Chain	Res	Type	Atom
48	y1	607	CHL	C8
48	y1	607	CHL	NC
48	y1	609	CHL	NA
48	y1	609	CHL	ND
48	y1	609	CHL	C8
48	y1	609	CHL	NC
49	G	621	LUT	C26
49	R	620	LUT	C26
49	n1	621	LUT	C26
50	N	622	XAT	C6
50	G	622	XAT	C26
50	n	622	XAT	C6
50	g	622	XAT	C26
50	g	622	XAT	C6
50	r	621	XAT	C26
50	r	621	XAT	C6
50	N1	622	XAT	C6
50	G1	622	XAT	C26
50	Y1	622	XAT	C26
50	g1	622	XAT	C26
50	r1	621	XAT	C26
51	g	623	NEX	C26
51	g1	623	NEX	C26
53	R	626	ERG	C20
53	R	626	ERG	C24
53	R	626	ERG	C9
53	R	626	ERG	C10
53	R	626	ERG	C14
53	r	626	ERG	C20
53	r	626	ERG	C24
53	r	626	ERG	C9
53	r	626	ERG	C10
53	r	626	ERG	C14
53	R1	626	ERG	C20
53	R1	626	ERG	C24
53	R1	626	ERG	C9
53	R1	626	ERG	C10
53	R1	626	ERG	C14
53	r1	626	ERG	C20
53	r1	626	ERG	C24
53	r1	626	ERG	C9
53	r1	626	ERG	C10

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Mol	Chain	Res	Type	Atom
53	r1	626	ERG	C14

All (9527) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
29	A	405	CLA	O2A-C1-C2-C3
29	A	406	CLA	C1A-C2A-CAA-CBA
29	A	406	CLA	C3A-C2A-CAA-CBA
29	A	406	CLA	C2-C1-O2A-CGA
29	A	407	CLA	C2-C1-O2A-CGA
29	A	407	CLA	CHA-CBD-CGD-O1D
29	A	407	CLA	CHA-CBD-CGD-O2D
29	A	410	CLA	C2-C3-C5-C6
29	A	410	CLA	C4-C3-C5-C6
29	B	602	CLA	C3A-C2A-CAA-CBA
29	B	602	CLA	CHA-CBD-CGD-O1D
29	B	602	CLA	CHA-CBD-CGD-O2D
29	B	602	CLA	CAD-CBD-CGD-O1D
29	B	602	CLA	CAD-CBD-CGD-O2D
29	B	603	CLA	CHA-CBD-CGD-O1D
29	B	603	CLA	CHA-CBD-CGD-O2D
29	B	603	CLA	CBD-CGD-O2D-CED
29	B	604	CLA	CBD-CGD-O2D-CED
29	B	604	CLA	C14-C13-C15-C16
29	B	606	CLA	CHA-CBD-CGD-O1D
29	B	606	CLA	CHA-CBD-CGD-O2D
29	B	606	CLA	CAD-CBD-CGD-O1D
29	B	607	CLA	C1A-C2A-CAA-CBA
29	B	607	CLA	CHA-CBD-CGD-O1D
29	B	607	CLA	CHA-CBD-CGD-O2D
29	B	607	CLA	CBD-CGD-O2D-CED
29	B	607	CLA	C4-C3-C5-C6
29	B	608	CLA	C1A-C2A-CAA-CBA
29	B	608	CLA	C3A-C2A-CAA-CBA
29	B	608	CLA	CBD-CGD-O2D-CED
29	B	608	CLA	C2-C3-C5-C6
29	B	608	CLA	C4-C3-C5-C6
29	B	609	CLA	C1A-C2A-CAA-CBA
29	B	610	CLA	C3A-C2A-CAA-CBA
29	B	610	CLA	CHA-CBD-CGD-O1D
29	B	610	CLA	CHA-CBD-CGD-O2D
29	B	610	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
29	B	610	CLA	CAD-CBD-CGD-O2D
29	B	610	CLA	CBD-CGD-O2D-CED
29	B	611	CLA	C1A-C2A-CAA-CBA
29	B	611	CLA	C3A-C2A-CAA-CBA
29	B	612	CLA	CHA-CBD-CGD-O1D
29	B	612	CLA	CHA-CBD-CGD-O2D
29	B	612	CLA	CBD-CGD-O2D-CED
29	B	613	CLA	C1A-C2A-CAA-CBA
29	B	613	CLA	C3A-C2A-CAA-CBA
29	B	614	CLA	CBD-CGD-O2D-CED
29	C	501	CLA	C1A-C2A-CAA-CBA
29	C	502	CLA	CHA-CBD-CGD-O1D
29	C	502	CLA	CHA-CBD-CGD-O2D
29	C	502	CLA	CAD-CBD-CGD-O1D
29	C	503	CLA	CHA-CBD-CGD-O1D
29	C	503	CLA	CHA-CBD-CGD-O2D
29	C	503	CLA	CAD-CBD-CGD-O1D
29	C	503	CLA	CBD-CGD-O2D-CED
29	C	503	CLA	C2-C3-C5-C6
29	C	503	CLA	C4-C3-C5-C6
29	C	504	CLA	CHA-CBD-CGD-O1D
29	C	504	CLA	CHA-CBD-CGD-O2D
29	C	504	CLA	CAD-CBD-CGD-O1D
29	C	505	CLA	CHA-CBD-CGD-O1D
29	C	506	CLA	C2-C1-O2A-CGA
29	C	508	CLA	CHA-CBD-CGD-O1D
29	C	508	CLA	CHA-CBD-CGD-O2D
29	C	509	CLA	C2-C1-O2A-CGA
29	C	509	CLA	C6-C7-C8-C9
29	C	513	CLA	C1A-C2A-CAA-CBA
29	D	403	CLA	C2-C3-C5-C6
29	D	403	CLA	C4-C3-C5-C6
29	N	602	CLA	CBD-CGD-O2D-CED
29	N	603	CLA	C2-C1-O2A-CGA
29	N	604	CLA	C1A-C2A-CAA-CBA
29	N	604	CLA	C3A-C2A-CAA-CBA
29	N	610	CLA	C1A-C2A-CAA-CBA
29	N	610	CLA	C3A-C2A-CAA-CBA
29	N	612	CLA	CHA-CBD-CGD-O2D
29	N	613	CLA	CHA-CBD-CGD-O1D
29	N	613	CLA	CHA-CBD-CGD-O2D
29	N	614	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	G	602	CLA	C1A-C2A-CAA-CBA
29	G	602	CLA	C3A-C2A-CAA-CBA
29	G	603	CLA	CBD-CGD-O2D-CED
29	G	603	CLA	C11-C10-C8-C9
29	G	610	CLA	CBD-CGD-O2D-CED
29	G	611	CLA	CHA-CBD-CGD-O1D
29	G	611	CLA	CHA-CBD-CGD-O2D
29	G	611	CLA	CBD-CGD-O2D-CED
29	G	613	CLA	CHA-CBD-CGD-O1D
29	G	613	CLA	CHA-CBD-CGD-O2D
29	G	613	CLA	CBD-CGD-O2D-CED
29	R	603	CLA	C3A-C2A-CAA-CBA
29	R	608	CLA	C1A-C2A-CAA-CBA
29	R	608	CLA	C3A-C2A-CAA-CBA
29	R	608	CLA	CHA-CBD-CGD-O1D
29	R	608	CLA	CBD-CGD-O2D-CED
29	R	610	CLA	CHA-CBD-CGD-O1D
29	R	610	CLA	CHA-CBD-CGD-O2D
29	R	610	CLA	CBD-CGD-O2D-CED
29	R	612	CLA	C2-C1-O2A-CGA
29	S	602	CLA	C2-C1-O2A-CGA
29	S	602	CLA	CHA-CBD-CGD-O2D
29	S	603	CLA	C1A-C2A-CAA-CBA
29	S	603	CLA	C3A-C2A-CAA-CBA
29	S	603	CLA	CHA-CBD-CGD-O1D
29	S	603	CLA	CHA-CBD-CGD-O2D
29	S	603	CLA	CBD-CGD-O2D-CED
29	S	605	CLA	C1A-C2A-CAA-CBA
29	S	609	CLA	CBD-CGD-O2D-CED
29	S	610	CLA	C3A-C2A-CAA-CBA
29	S	610	CLA	CBD-CGD-O2D-CED
29	S	611	CLA	C1A-C2A-CAA-CBA
29	S	611	CLA	C3A-C2A-CAA-CBA
29	S	611	CLA	CHA-CBD-CGD-O1D
29	S	611	CLA	CHA-CBD-CGD-O2D
29	S	617	CLA	CHA-CBD-CGD-O1D
29	S	617	CLA	CHA-CBD-CGD-O2D
29	S	617	CLA	CBD-CGD-O2D-CED
29	Y	604	CLA	CHA-CBD-CGD-O1D
29	Y	604	CLA	CHA-CBD-CGD-O2D
29	Y	608	CLA	C1A-C2A-CAA-CBA
29	Y	610	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	Y	611	CLA	C2-C3-C5-C6
29	Y	611	CLA	C4-C3-C5-C6
29	Y	613	CLA	CHA-CBD-CGD-O1D
29	Y	613	CLA	CHA-CBD-CGD-O2D
29	a	405	CLA	C2-C1-O2A-CGA
29	a	405	CLA	CHA-CBD-CGD-O1D
29	a	405	CLA	CHA-CBD-CGD-O2D
29	a	405	CLA	CBD-CGD-O2D-CED
29	a	405	CLA	O2A-C1-C2-C3
29	a	406	CLA	C1A-C2A-CAA-CBA
29	a	406	CLA	C3A-C2A-CAA-CBA
29	a	406	CLA	C2-C1-O2A-CGA
29	a	407	CLA	C1A-C2A-CAA-CBA
29	a	407	CLA	C2-C1-O2A-CGA
29	a	410	CLA	C2-C3-C5-C6
29	a	410	CLA	C4-C3-C5-C6
29	b	602	CLA	CHA-CBD-CGD-O1D
29	b	602	CLA	CHA-CBD-CGD-O2D
29	b	603	CLA	CHA-CBD-CGD-O1D
29	b	603	CLA	CHA-CBD-CGD-O2D
29	b	604	CLA	CBD-CGD-O2D-CED
29	b	605	CLA	C1A-C2A-CAA-CBA
29	b	605	CLA	CHA-CBD-CGD-O1D
29	b	605	CLA	CHA-CBD-CGD-O2D
29	b	605	CLA	CAD-CBD-CGD-O1D
29	b	608	CLA	C1A-C2A-CAA-CBA
29	b	608	CLA	C3A-C2A-CAA-CBA
29	b	608	CLA	CHA-CBD-CGD-O1D
29	b	608	CLA	CHA-CBD-CGD-O2D
29	b	608	CLA	CAD-CBD-CGD-O1D
29	b	608	CLA	CAD-CBD-CGD-O2D
29	b	608	CLA	C2-C3-C5-C6
29	b	608	CLA	C4-C3-C5-C6
29	b	608	CLA	C11-C10-C8-C9
29	b	609	CLA	C2-C3-C5-C6
29	b	609	CLA	C4-C3-C5-C6
29	b	610	CLA	CBD-CGD-O2D-CED
29	b	611	CLA	CBD-CGD-O2D-CED
29	b	612	CLA	CHA-CBD-CGD-O1D
29	b	612	CLA	CHA-CBD-CGD-O2D
29	b	613	CLA	C1A-C2A-CAA-CBA
29	b	613	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	b	613	CLA	CHA-CBD-CGD-O1D
29	b	613	CLA	CHA-CBD-CGD-O2D
29	b	613	CLA	CAD-CBD-CGD-O1D
29	b	613	CLA	CAD-CBD-CGD-O2D
29	b	616	CLA	CHA-CBD-CGD-O1D
29	b	616	CLA	CHA-CBD-CGD-O2D
29	b	617	CLA	CBD-CGD-O2D-CED
29	c	501	CLA	CHA-CBD-CGD-O1D
29	c	501	CLA	CHA-CBD-CGD-O2D
29	c	502	CLA	CHA-CBD-CGD-O1D
29	c	502	CLA	CHA-CBD-CGD-O2D
29	c	502	CLA	CAD-CBD-CGD-O1D
29	c	504	CLA	CHA-CBD-CGD-O1D
29	c	504	CLA	CHA-CBD-CGD-O2D
29	c	504	CLA	CAD-CBD-CGD-O1D
29	c	504	CLA	CAD-CBD-CGD-O2D
29	c	505	CLA	CHA-CBD-CGD-O1D
29	c	505	CLA	CHA-CBD-CGD-O2D
29	c	506	CLA	C2-C1-O2A-CGA
29	c	508	CLA	CHA-CBD-CGD-O1D
29	c	508	CLA	CHA-CBD-CGD-O2D
29	c	509	CLA	C2-C1-O2A-CGA
29	c	511	CLA	CBD-CGD-O2D-CED
29	c	512	CLA	C1A-C2A-CAA-CBA
29	c	512	CLA	CBA-CGA-O2A-C1
29	c	512	CLA	O1A-CGA-O2A-C1
29	c	513	CLA	C1A-C2A-CAA-CBA
29	d	402	CLA	CBD-CGD-O2D-CED
29	d	403	CLA	CBD-CGD-O2D-CED
29	d	403	CLA	C4-C3-C5-C6
29	n	610	CLA	C1A-C2A-CAA-CBA
29	n	610	CLA	CBD-CGD-O2D-CED
29	n	611	CLA	CBD-CGD-O2D-CED
29	n	612	CLA	CBD-CGD-O2D-CED
29	n	613	CLA	C1A-C2A-CAA-CBA
29	n	613	CLA	CBD-CGD-O2D-CED
29	n	614	CLA	C1A-C2A-CAA-CBA
29	n	614	CLA	CBD-CGD-O2D-CED
29	g	602	CLA	C3A-C2A-CAA-CBA
29	g	604	CLA	C2-C1-O2A-CGA
29	g	610	CLA	CHA-CBD-CGD-O1D
29	g	610	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
29	g	610	CLA	CBD-CGD-O2D-CED
29	g	611	CLA	CBD-CGD-O2D-CED
29	r	602	CLA	C6-C7-C8-C9
29	r	603	CLA	C1A-C2A-CAA-CBA
29	r	603	CLA	C3A-C2A-CAA-CBA
29	r	603	CLA	CBD-CGD-O2D-CED
29	r	604	CLA	C1A-C2A-CAA-CBA
29	r	604	CLA	CHA-CBD-CGD-O1D
29	r	604	CLA	CHA-CBD-CGD-O2D
29	r	604	CLA	CBD-CGD-O2D-CED
29	r	608	CLA	C1A-C2A-CAA-CBA
29	r	608	CLA	C3A-C2A-CAA-CBA
29	r	608	CLA	CHA-CBD-CGD-O1D
29	r	608	CLA	CHA-CBD-CGD-O2D
29	r	609	CLA	O1A-CGA-O2A-C1
29	r	609	CLA	CHA-CBD-CGD-O1D
29	r	609	CLA	CHA-CBD-CGD-O2D
29	r	609	CLA	CBD-CGD-O2D-CED
29	s	602	CLA	C2-C1-O2A-CGA
29	s	603	CLA	C1A-C2A-CAA-CBA
29	s	603	CLA	C3A-C2A-CAA-CBA
29	s	605	CLA	C1A-C2A-CAA-CBA
29	s	605	CLA	CBA-CGA-O2A-C1
29	s	605	CLA	O1A-CGA-O2A-C1
29	s	605	CLA	CHA-CBD-CGD-O2D
29	s	609	CLA	C1A-C2A-CAA-CBA
29	s	609	CLA	C3A-C2A-CAA-CBA
29	s	609	CLA	C2A-CAA-CBA-CGA
29	s	609	CLA	CHA-CBD-CGD-O1D
29	s	609	CLA	CHA-CBD-CGD-O2D
29	s	610	CLA	C1A-C2A-CAA-CBA
29	s	610	CLA	C3A-C2A-CAA-CBA
29	s	611	CLA	C1A-C2A-CAA-CBA
29	s	611	CLA	C3A-C2A-CAA-CBA
29	s	611	CLA	CHA-CBD-CGD-O1D
29	s	611	CLA	CHA-CBD-CGD-O2D
29	s	613	CLA	CHA-CBD-CGD-O1D
29	s	613	CLA	CHA-CBD-CGD-O2D
29	s	613	CLA	CBD-CGD-O2D-CED
29	s	614	CLA	CBD-CGD-O2D-CED
29	s	617	CLA	C1A-C2A-CAA-CBA
29	s	617	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
29	s	617	CLA	C2-C1-O2A-CGA
29	s	617	CLA	CBD-CGD-O2D-CED
29	y	603	CLA	C2-C1-O2A-CGA
29	y	603	CLA	CBD-CGD-O2D-CED
29	y	608	CLA	C1A-C2A-CAA-CBA
29	y	608	CLA	CHA-CBD-CGD-O1D
29	y	608	CLA	CHA-CBD-CGD-O2D
29	y	608	CLA	CBD-CGD-O2D-CED
29	y	610	CLA	CHA-CBD-CGD-O1D
29	y	610	CLA	CHA-CBD-CGD-O2D
29	y	610	CLA	CBD-CGD-O2D-CED
29	y	613	CLA	CHA-CBD-CGD-O1D
29	y	613	CLA	CHA-CBD-CGD-O2D
29	y	613	CLA	CBD-CGD-O2D-CED
29	A1	405	CLA	C1A-C2A-CAA-CBA
29	A1	405	CLA	C3A-C2A-CAA-CBA
29	A1	405	CLA	C2A-CAA-CBA-CGA
29	A1	405	CLA	CBD-CGD-O2D-CED
29	A1	406	CLA	C1A-C2A-CAA-CBA
29	A1	406	CLA	C3A-C2A-CAA-CBA
29	A1	406	CLA	C2-C1-O2A-CGA
29	A1	407	CLA	C2-C1-O2A-CGA
29	A1	407	CLA	CHA-CBD-CGD-O1D
29	A1	407	CLA	CHA-CBD-CGD-O2D
29	B1	602	CLA	C3A-C2A-CAA-CBA
29	B1	603	CLA	CHA-CBD-CGD-O1D
29	B1	603	CLA	CHA-CBD-CGD-O2D
29	B1	603	CLA	CBD-CGD-O2D-CED
29	B1	604	CLA	CBD-CGD-O2D-CED
29	B1	604	CLA	C2-C3-C5-C6
29	B1	604	CLA	C4-C3-C5-C6
29	B1	607	CLA	C1A-C2A-CAA-CBA
29	B1	608	CLA	C1A-C2A-CAA-CBA
29	B1	608	CLA	C3A-C2A-CAA-CBA
29	B1	608	CLA	CHA-CBD-CGD-O1D
29	B1	608	CLA	CHA-CBD-CGD-O2D
29	B1	608	CLA	CAD-CBD-CGD-O1D
29	B1	608	CLA	C4-C3-C5-C6
29	B1	609	CLA	C1A-C2A-CAA-CBA
29	B1	609	CLA	CHA-CBD-CGD-O2D
29	B1	610	CLA	C3A-C2A-CAA-CBA
29	B1	610	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
29	B1	610	CLA	CAD-CBD-CGD-O2D
29	B1	612	CLA	CHA-CBD-CGD-O1D
29	B1	612	CLA	CHA-CBD-CGD-O2D
29	B1	613	CLA	C2-C1-O2A-CGA
29	B1	613	CLA	CHA-CBD-CGD-O1D
29	B1	613	CLA	CHA-CBD-CGD-O2D
29	B1	613	CLA	CAD-CBD-CGD-O1D
29	B1	613	CLA	CAD-CBD-CGD-O2D
29	B1	613	CLA	CBD-CGD-O2D-CED
29	B1	614	CLA	C2-C1-O2A-CGA
29	B1	614	CLA	CHA-CBD-CGD-O1D
29	B1	614	CLA	CHA-CBD-CGD-O2D
29	B1	614	CLA	CBD-CGD-O2D-CED
29	B1	616	CLA	CHA-CBD-CGD-O1D
29	B1	616	CLA	CBD-CGD-O2D-CED
29	B1	617	CLA	CBD-CGD-O2D-CED
29	C1	501	CLA	C1A-C2A-CAA-CBA
29	C1	501	CLA	CBD-CGD-O2D-CED
29	C1	502	CLA	CBD-CGD-O2D-CED
29	C1	503	CLA	C2-C3-C5-C6
29	C1	503	CLA	C4-C3-C5-C6
29	C1	504	CLA	CHA-CBD-CGD-O1D
29	C1	504	CLA	CHA-CBD-CGD-O2D
29	C1	504	CLA	CAD-CBD-CGD-O1D
29	C1	504	CLA	CAD-CBD-CGD-O2D
29	C1	504	CLA	CBD-CGD-O2D-CED
29	C1	504	CLA	C4-C3-C5-C6
29	C1	506	CLA	C2-C1-O2A-CGA
29	C1	506	CLA	CHA-CBD-CGD-O1D
29	C1	506	CLA	CHA-CBD-CGD-O2D
29	C1	506	CLA	CAD-CBD-CGD-O1D
29	C1	507	CLA	CHA-CBD-CGD-O1D
29	C1	507	CLA	CHA-CBD-CGD-O2D
29	C1	508	CLA	CHA-CBD-CGD-O1D
29	C1	508	CLA	CHA-CBD-CGD-O2D
29	C1	510	CLA	CBD-CGD-O2D-CED
29	C1	513	CLA	C1A-C2A-CAA-CBA
29	C1	513	CLA	CBD-CGD-O2D-CED
29	D1	402	CLA	C3A-C2A-CAA-CBA
29	D1	402	CLA	CHA-CBD-CGD-O1D
29	D1	402	CLA	CHA-CBD-CGD-O2D
29	N1	602	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	N1	602	CLA	C4-C3-C5-C6
29	N1	603	CLA	C2-C1-O2A-CGA
29	N1	603	CLA	CBD-CGD-O2D-CED
29	N1	604	CLA	C1A-C2A-CAA-CBA
29	N1	604	CLA	C3A-C2A-CAA-CBA
29	N1	610	CLA	C1A-C2A-CAA-CBA
29	N1	610	CLA	C3A-C2A-CAA-CBA
29	N1	612	CLA	CBD-CGD-O2D-CED
29	N1	613	CLA	CHA-CBD-CGD-O1D
29	N1	613	CLA	CHA-CBD-CGD-O2D
29	N1	614	CLA	C1A-C2A-CAA-CBA
29	G1	602	CLA	C1A-C2A-CAA-CBA
29	G1	602	CLA	C3A-C2A-CAA-CBA
29	G1	603	CLA	CBD-CGD-O2D-CED
29	G1	610	CLA	CHA-CBD-CGD-O1D
29	G1	610	CLA	CHA-CBD-CGD-O2D
29	G1	613	CLA	CBD-CGD-O2D-CED
29	R1	602	CLA	CBD-CGD-O2D-CED
29	R1	603	CLA	C3A-C2A-CAA-CBA
29	R1	603	CLA	CHA-CBD-CGD-O1D
29	R1	603	CLA	CHA-CBD-CGD-O2D
29	R1	603	CLA	CBD-CGD-O2D-CED
29	R1	604	CLA	CHA-CBD-CGD-O1D
29	R1	604	CLA	CHA-CBD-CGD-O2D
29	R1	608	CLA	C3A-C2A-CAA-CBA
29	R1	610	CLA	CHA-CBD-CGD-O1D
29	R1	610	CLA	CHA-CBD-CGD-O2D
29	R1	610	CLA	CBD-CGD-O2D-CED
29	R1	612	CLA	C3A-C2A-CAA-CBA
29	S1	602	CLA	C2-C1-O2A-CGA
29	S1	602	CLA	C4-C3-C5-C6
29	S1	602	CLA	C11-C10-C8-C9
29	S1	603	CLA	C1A-C2A-CAA-CBA
29	S1	603	CLA	CHA-CBD-CGD-O1D
29	S1	603	CLA	CHA-CBD-CGD-O2D
29	S1	605	CLA	C1A-C2A-CAA-CBA
29	S1	605	CLA	CHA-CBD-CGD-O1D
29	S1	605	CLA	CHA-CBD-CGD-O2D
29	S1	609	CLA	CBD-CGD-O2D-CED
29	S1	610	CLA	C3A-C2A-CAA-CBA
29	S1	610	CLA	CHA-CBD-CGD-O1D
29	S1	610	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
29	S1	610	CLA	CBD-CGD-O2D-CED
29	S1	610	CLA	O1D-CGD-O2D-CED
29	S1	611	CLA	C1A-C2A-CAA-CBA
29	S1	611	CLA	C3A-C2A-CAA-CBA
29	S1	611	CLA	CBD-CGD-O2D-CED
29	S1	611	CLA	C2-C3-C5-C6
29	S1	611	CLA	C4-C3-C5-C6
29	S1	612	CLA	CBD-CGD-O2D-CED
29	S1	614	CLA	C2-C1-O2A-CGA
29	S1	614	CLA	CBD-CGD-O2D-CED
29	Y1	603	CLA	CBD-CGD-O2D-CED
29	Y1	604	CLA	C2-C1-O2A-CGA
29	Y1	604	CLA	CHA-CBD-CGD-O2D
29	Y1	611	CLA	C2-C3-C5-C6
29	Y1	611	CLA	C4-C3-C5-C6
29	Y1	613	CLA	CBD-CGD-O2D-CED
29	Y1	614	CLA	CBD-CGD-O2D-CED
29	a1	405	CLA	CHA-CBD-CGD-O1D
29	a1	405	CLA	CHA-CBD-CGD-O2D
29	a1	405	CLA	CBD-CGD-O2D-CED
29	a1	406	CLA	CBA-CGA-O2A-C1
29	a1	406	CLA	O1A-CGA-O2A-C1
29	a1	406	CLA	CHA-CBD-CGD-O1D
29	a1	406	CLA	CHA-CBD-CGD-O2D
29	a1	407	CLA	C2A-CAA-CBA-CGA
29	a1	410	CLA	CBA-CGA-O2A-C1
29	a1	410	CLA	C4-C3-C5-C6
29	b1	602	CLA	CBD-CGD-O2D-CED
29	b1	603	CLA	CBA-CGA-O2A-C1
29	b1	603	CLA	O1A-CGA-O2A-C1
29	b1	603	CLA	CHA-CBD-CGD-O1D
29	b1	603	CLA	CHA-CBD-CGD-O2D
29	b1	604	CLA	CBD-CGD-O2D-CED
29	b1	604	CLA	C2-C3-C5-C6
29	b1	604	CLA	C4-C3-C5-C6
29	b1	605	CLA	C1A-C2A-CAA-CBA
29	b1	605	CLA	C2-C1-O2A-CGA
29	b1	606	CLA	CBD-CGD-O2D-CED
29	b1	606	CLA	C4-C3-C5-C6
29	b1	607	CLA	C1A-C2A-CAA-CBA
29	b1	607	CLA	CHA-CBD-CGD-O1D
29	b1	607	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
29	b1	607	CLA	CBD-CGD-O2D-CED
29	b1	608	CLA	C1A-C2A-CAA-CBA
29	b1	608	CLA	C3A-C2A-CAA-CBA
29	b1	608	CLA	CHA-CBD-CGD-O1D
29	b1	608	CLA	CAD-CBD-CGD-O1D
29	b1	608	CLA	CAD-CBD-CGD-O2D
29	b1	609	CLA	C1A-C2A-CAA-CBA
29	b1	609	CLA	C3A-C2A-CAA-CBA
29	b1	609	CLA	CHA-CBD-CGD-O1D
29	b1	609	CLA	CHA-CBD-CGD-O2D
29	b1	609	CLA	CBD-CGD-O2D-CED
29	b1	609	CLA	C4-C3-C5-C6
29	b1	612	CLA	CHA-CBD-CGD-O2D
29	b1	613	CLA	C2-C1-O2A-CGA
29	b1	615	CLA	C1A-C2A-CAA-CBA
29	b1	615	CLA	C2-C3-C5-C6
29	b1	615	CLA	C4-C3-C5-C6
29	b1	616	CLA	C11-C10-C8-C9
29	c1	501	CLA	CBD-CGD-O2D-CED
29	c1	502	CLA	CAD-CBD-CGD-O1D
29	c1	502	CLA	CAD-CBD-CGD-O2D
29	c1	504	CLA	CHA-CBD-CGD-O1D
29	c1	504	CLA	CHA-CBD-CGD-O2D
29	c1	504	CLA	CAD-CBD-CGD-O1D
29	c1	505	CLA	C1A-C2A-CAA-CBA
29	c1	505	CLA	C3A-C2A-CAA-CBA
29	c1	506	CLA	C2-C1-O2A-CGA
29	c1	506	CLA	CBD-CGD-O2D-CED
29	c1	509	CLA	C6-C7-C8-C9
29	c1	511	CLA	C1A-C2A-CAA-CBA
29	c1	511	CLA	CHA-CBD-CGD-O1D
29	c1	511	CLA	CHA-CBD-CGD-O2D
29	c1	512	CLA	CBA-CGA-O2A-C1
29	c1	512	CLA	O1A-CGA-O2A-C1
29	c1	512	CLA	CAD-CBD-CGD-O1D
29	c1	512	CLA	CAD-CBD-CGD-O2D
29	c1	513	CLA	C1A-C2A-CAA-CBA
29	c1	513	CLA	C3A-C2A-CAA-CBA
29	c1	513	CLA	C11-C10-C8-C9
29	d1	402	CLA	C2-C3-C5-C6
29	d1	402	CLA	C4-C3-C5-C6
29	n1	604	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	n1	610	CLA	C1A-C2A-CAA-CBA
29	n1	610	CLA	CBD-CGD-O2D-CED
29	n1	611	CLA	CBD-CGD-O2D-CED
29	n1	612	CLA	CBD-CGD-O2D-CED
29	n1	613	CLA	CHA-CBD-CGD-O1D
29	n1	613	CLA	CHA-CBD-CGD-O2D
29	n1	613	CLA	C11-C12-C13-C14
29	n1	614	CLA	C1A-C2A-CAA-CBA
29	g1	602	CLA	C1A-C2A-CAA-CBA
29	g1	602	CLA	C3A-C2A-CAA-CBA
29	g1	602	CLA	CBD-CGD-O2D-CED
29	g1	603	CLA	CBD-CGD-O2D-CED
29	g1	604	CLA	C2-C1-O2A-CGA
29	g1	610	CLA	C1A-C2A-CAA-CBA
29	g1	610	CLA	CHA-CBD-CGD-O1D
29	g1	610	CLA	CHA-CBD-CGD-O2D
29	g1	611	CLA	CHA-CBD-CGD-O1D
29	g1	611	CLA	CHA-CBD-CGD-O2D
29	g1	611	CLA	CBD-CGD-O2D-CED
29	g1	611	CLA	C11-C10-C8-C7
29	g1	612	CLA	CHA-CBD-CGD-O2D
29	g1	612	CLA	CBD-CGD-O2D-CED
29	r1	602	CLA	C6-C7-C8-C9
29	r1	603	CLA	C1A-C2A-CAA-CBA
29	r1	603	CLA	C3A-C2A-CAA-CBA
29	r1	603	CLA	CBA-CGA-O2A-C1
29	r1	603	CLA	O1A-CGA-O2A-C1
29	r1	603	CLA	CBD-CGD-O2D-CED
29	r1	604	CLA	CHA-CBD-CGD-O1D
29	r1	604	CLA	CHA-CBD-CGD-O2D
29	r1	608	CLA	C1A-C2A-CAA-CBA
29	r1	608	CLA	C3A-C2A-CAA-CBA
29	r1	608	CLA	CHA-CBD-CGD-O1D
29	r1	608	CLA	CBD-CGD-O2D-CED
29	r1	609	CLA	CBD-CGD-O2D-CED
29	r1	610	CLA	CHA-CBD-CGD-O1D
29	r1	610	CLA	CHA-CBD-CGD-O2D
29	r1	610	CLA	CBD-CGD-O2D-CED
29	r1	612	CLA	CBD-CGD-O2D-CED
29	s1	602	CLA	C2-C1-O2A-CGA
29	s1	602	CLA	CHA-CBD-CGD-O1D
29	s1	602	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
29	s1	603	CLA	C1A-C2A-CAA-CBA
29	s1	603	CLA	C3A-C2A-CAA-CBA
29	s1	603	CLA	CBD-CGD-O2D-CED
29	s1	605	CLA	CBA-CGA-O2A-C1
29	s1	605	CLA	O1A-CGA-O2A-C1
29	s1	609	CLA	CBD-CGD-O2D-CED
29	s1	610	CLA	C1A-C2A-CAA-CBA
29	s1	610	CLA	C3A-C2A-CAA-CBA
29	s1	610	CLA	C2-C3-C5-C6
29	s1	610	CLA	C4-C3-C5-C6
29	s1	611	CLA	C1A-C2A-CAA-CBA
29	s1	611	CLA	C3A-C2A-CAA-CBA
29	s1	611	CLA	CHA-CBD-CGD-O1D
29	s1	611	CLA	CHA-CBD-CGD-O2D
29	s1	611	CLA	CBD-CGD-O2D-CED
29	s1	613	CLA	CBD-CGD-O2D-CED
29	s1	614	CLA	C3A-C2A-CAA-CBA
29	s1	617	CLA	C1A-C2A-CAA-CBA
29	s1	617	CLA	C2-C1-O2A-CGA
29	s1	617	CLA	CHA-CBD-CGD-O1D
29	s1	617	CLA	CHA-CBD-CGD-O2D
29	y1	603	CLA	CHA-CBD-CGD-O1D
29	y1	603	CLA	CHA-CBD-CGD-O2D
29	y1	604	CLA	CHA-CBD-CGD-O1D
29	y1	604	CLA	CHA-CBD-CGD-O2D
29	y1	608	CLA	C2-C1-O2A-CGA
29	y1	608	CLA	CHA-CBD-CGD-O1D
29	y1	608	CLA	CHA-CBD-CGD-O2D
29	y1	608	CLA	CBD-CGD-O2D-CED
29	y1	610	CLA	CBD-CGD-O2D-CED
29	y1	611	CLA	C1A-C2A-CAA-CBA
29	y1	611	CLA	CHA-CBD-CGD-O1D
29	y1	611	CLA	CHA-CBD-CGD-O2D
30	A	409	PHO	C3A-C2A-CAA-CBA
30	a	408	PHO	C1A-C2A-CAA-CBA
30	a	409	PHO	C3A-C2A-CAA-CBA
31	A	411	BCR	C11-C12-C13-C35
31	A	411	BCR	C17-C18-C19-C20
31	A	411	BCR	C36-C18-C19-C20
31	B	618	BCR	C11-C10-C9-C8
31	B	618	BCR	C11-C10-C9-C34
31	B	618	BCR	C10-C11-C12-C13

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

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

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

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Mol	Chain	Res	Type	Atoms
31	D1	404	BCR	C36-C18-C19-C20
31	D1	404	BCR	C23-C24-C25-C26
31	D1	404	BCR	C23-C24-C25-C30
31	a1	411	BCR	C11-C10-C9-C8
31	a1	411	BCR	C11-C10-C9-C34
31	a1	411	BCR	C10-C11-C12-C13
31	a1	411	BCR	C19-C20-C21-C22
31	b1	618	BCR	C11-C10-C9-C8
31	b1	618	BCR	C11-C10-C9-C34
31	b1	618	BCR	C10-C11-C12-C13
31	b1	618	BCR	C11-C12-C13-C14
31	b1	618	BCR	C11-C12-C13-C35
31	b1	619	BCR	C7-C8-C9-C10
31	b1	619	BCR	C7-C8-C9-C34
31	b1	619	BCR	C11-C10-C9-C8
31	b1	619	BCR	C11-C10-C9-C34
31	b1	619	BCR	C10-C11-C12-C13
31	c1	514	BCR	C11-C10-C9-C8
31	c1	514	BCR	C11-C10-C9-C34
31	c1	514	BCR	C9-C10-C11-C12
31	c1	514	BCR	C10-C11-C12-C13
31	c1	515	BCR	C11-C10-C9-C8
31	c1	515	BCR	C11-C10-C9-C34
31	c1	515	BCR	C10-C11-C12-C13
31	c1	516	BCR	C5-C6-C7-C8
31	c1	516	BCR	C7-C8-C9-C10
31	c1	516	BCR	C7-C8-C9-C34
31	c1	516	BCR	C11-C10-C9-C8
31	c1	516	BCR	C11-C10-C9-C34
31	c1	516	BCR	C10-C11-C12-C13
31	c1	516	BCR	C17-C18-C19-C20
31	c1	516	BCR	C36-C18-C19-C20
31	c1	516	BCR	C21-C22-C23-C24
31	c1	516	BCR	C37-C22-C23-C24
31	c1	517	BCR	C11-C10-C9-C8
31	c1	517	BCR	C11-C10-C9-C34
31	c1	517	BCR	C10-C11-C12-C13
31	c1	517	BCR	C17-C18-C19-C20
31	c1	517	BCR	C36-C18-C19-C20
31	c1	517	BCR	C21-C22-C23-C24
31	c1	517	BCR	C37-C22-C23-C24
31	d1	404	BCR	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
31	d1	404	BCR	C11-C10-C9-C34
31	d1	404	BCR	C10-C11-C12-C13
31	d1	404	BCR	C11-C12-C13-C14
31	d1	404	BCR	C11-C12-C13-C35
31	d1	404	BCR	C13-C14-C15-C16
31	d1	404	BCR	C21-C22-C23-C24
31	d1	404	BCR	C37-C22-C23-C24
31	d1	404	BCR	C23-C24-C25-C26
31	d1	404	BCR	C23-C24-C25-C30
32	A	412	SQD	C5-C6-S-O7
32	A	412	SQD	C5-C6-S-O8
32	A	412	SQD	C5-C6-S-O9
32	B	621	SQD	C2-C1-O6-C44
32	B	621	SQD	O5-C1-O6-C44
32	B	621	SQD	O5-C5-C6-S
32	B	621	SQD	C5-C6-S-O7
32	B	621	SQD	C5-C6-S-O8
32	B	621	SQD	C5-C6-S-O9
32	B	626	SQD	C2-C1-O6-C44
32	B	626	SQD	O5-C1-O6-C44
32	B	626	SQD	C5-C6-S-O7
32	B	626	SQD	C5-C6-S-O8
32	B	626	SQD	C5-C6-S-O9
32	C	526	SQD	O5-C5-C6-S
32	C	526	SQD	C5-C6-S-O7
32	C	526	SQD	C5-C6-S-O8
32	C	526	SQD	C5-C6-S-O9
32	M	101	SQD	C5-C6-S-O7
32	M	101	SQD	C5-C6-S-O8
32	M	101	SQD	C5-C6-S-O9
32	a	412	SQD	O47-C45-C46-O48
32	a	412	SQD	O5-C5-C6-S
32	b	621	SQD	O5-C1-O6-C44
32	b	621	SQD	O5-C5-C6-S
32	b	626	SQD	C2-C1-O6-C44
32	b	626	SQD	O5-C1-O6-C44
32	m	101	SQD	C5-C6-S-O7
32	m	101	SQD	C5-C6-S-O8
32	m	101	SQD	C5-C6-S-O9
32	B1	621	SQD	C2-C1-O6-C44
32	B1	621	SQD	O5-C1-O6-C44
32	B1	621	SQD	O5-C5-C6-S

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Mol	Chain	Res	Type	Atoms
32	B1	626	SQD	C2-C1-O6-C44
32	B1	626	SQD	O5-C1-O6-C44
32	B1	626	SQD	C5-C6-S-O7
32	B1	626	SQD	C5-C6-S-O8
32	B1	626	SQD	C5-C6-S-O9
32	C1	526	SQD	O5-C5-C6-S
32	C1	526	SQD	C5-C6-S-O7
32	C1	526	SQD	C5-C6-S-O8
32	C1	526	SQD	C5-C6-S-O9
32	M1	101	SQD	C5-C6-S-O7
32	M1	101	SQD	C5-C6-S-O8
32	M1	101	SQD	C5-C6-S-O9
32	a1	412	SQD	O47-C45-C46-O48
32	a1	412	SQD	O5-C5-C6-S
32	b1	621	SQD	C2-C1-O6-C44
32	b1	621	SQD	O5-C1-O6-C44
32	c1	526	SQD	O5-C5-C6-S
32	m1	101	SQD	O5-C5-C6-S
32	m1	101	SQD	C5-C6-S-O8
33	A	413	LMG	O6-C1-O1-C7
33	B	622	LMG	O9-C10-O7-C8
33	B	622	LMG	C11-C10-O7-C8
33	W	201	LMG	O6-C1-O1-C7
33	W	201	LMG	C7-C8-O7-C10
33	W	201	LMG	C11-C10-O7-C8
33	a	413	LMG	O6-C1-O1-C7
33	b	622	LMG	O6-C1-O1-C7
33	b	622	LMG	O9-C10-O7-C8
33	b	622	LMG	C11-C10-O7-C8
33	B1	622	LMG	O6-C1-O1-C7
33	B1	622	LMG	O9-C10-O7-C8
33	W1	201	LMG	C11-C10-O7-C8
33	b1	622	LMG	O9-C10-O7-C8
33	c1	521	LMG	O10-C28-O8-C9
33	c1	523	LMG	C2-C1-O1-C7
33	c1	523	LMG	O6-C1-O1-C7
34	A	414	SPH	C1-C2-C3-O3
34	A	414	SPH	C1-C2-C3-C4
34	A	414	SPH	N2-C2-C3-O3
34	A	414	SPH	N2-C2-C3-C4
34	A	414	SPH	C2-C3-C4-C5
34	A	414	SPH	O3-C3-C4-C5

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Mol	Chain	Res	Type	Atoms
34	Y	625	SPH	C1-C2-C3-O3
34	Y	625	SPH	C1-C2-C3-C4
34	Y	625	SPH	N2-C2-C3-O3
34	Y	625	SPH	N2-C2-C3-C4
34	Y	625	SPH	C2-C3-C4-C5
34	a	414	SPH	O1-C1-C2-N2
34	a	414	SPH	O1-C1-C2-C3
34	a	414	SPH	C1-C2-C3-O3
34	a	414	SPH	C1-C2-C3-C4
34	a	414	SPH	N2-C2-C3-O3
34	a	414	SPH	N2-C2-C3-C4
34	y	625	SPH	C2-C3-C4-C5
34	y	625	SPH	O3-C3-C4-C5
34	A1	414	SPH	O1-C1-C2-N2
34	A1	414	SPH	O1-C1-C2-C3
34	A1	414	SPH	C1-C2-C3-O3
34	A1	414	SPH	C1-C2-C3-C4
34	A1	414	SPH	N2-C2-C3-O3
34	A1	414	SPH	N2-C2-C3-C4
34	Y1	625	SPH	O1-C1-C2-N2
34	Y1	625	SPH	O1-C1-C2-C3
34	Y1	625	SPH	C2-C3-C4-C5
34	Y1	625	SPH	O3-C3-C4-C5
34	a1	414	SPH	O1-C1-C2-N2
34	a1	414	SPH	C1-C2-C3-O3
34	y1	625	SPH	C1-C2-C3-O3
34	y1	625	SPH	C1-C2-C3-C4
34	y1	625	SPH	N2-C2-C3-C4
36	B	620	C7Z	C21-C26-C27-C28
36	B	620	C7Z	C27-C28-C29-C30
36	B	620	C7Z	C27-C28-C29-C39
36	b	620	C7Z	C5-C6-C7-C8
36	b	620	C7Z	C27-C28-C29-C30
36	b	620	C7Z	C27-C28-C29-C39
36	B1	620	C7Z	C27-C28-C29-C30
36	B1	620	C7Z	C27-C28-C29-C39
36	b1	620	C7Z	C11-C12-C13-C20
36	b1	620	C7Z	C11-C12-C13-C14
36	b1	620	C7Z	C27-C28-C29-C30
36	b1	620	C7Z	C27-C28-C29-C39
37	B	623	DGD	C2B-C1B-O2G-C2G
37	B	623	DGD	O1B-C1B-O2G-C2G

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Mol	Chain	Res	Type	Atoms
37	B	623	DGD	O6D-C1D-O3G-C3G
37	B	623	DGD	C2E-C1E-O5D-C6D
37	B	623	DGD	O6E-C1E-O5D-C6D
37	b	623	DGD	O1B-C1B-O2G-C2G
37	b	623	DGD	O6D-C1D-O3G-C3G
37	b	623	DGD	C2E-C1E-O5D-C6D
37	b	623	DGD	O6E-C1E-O5D-C6D
37	B1	623	DGD	O1B-C1B-O2G-C2G
37	B1	623	DGD	C2D-C1D-O3G-C3G
37	B1	623	DGD	O6D-C1D-O3G-C3G
37	B1	623	DGD	C2E-C1E-O5D-C6D
37	B1	623	DGD	O6E-C1E-O5D-C6D
37	b1	623	DGD	O1B-C1B-O2G-C2G
37	b1	623	DGD	O6D-C1D-O3G-C3G
37	b1	623	DGD	O6E-C1E-O5D-C6D
38	B	624	3PH	C1-O11-P-O13
38	B	624	3PH	C1-O11-P-O14
38	B	624	3PH	C1-O11-P-O12
38	T	101	3PH	C1-O11-P-O14
38	T	101	3PH	C1-O11-P-O12
38	T	101	3PH	C22-C21-O21-C2
38	S	626	3PH	C1-C2-O21-C21
38	S	626	3PH	O22-C21-O21-C2
38	b	624	3PH	C1-O11-P-O14
38	b	624	3PH	O22-C21-O21-C2
38	b	624	3PH	C22-C21-O21-C2
38	t	101	3PH	C1-O11-P-O13
38	t	101	3PH	C1-O11-P-O14
38	t	101	3PH	O22-C21-O21-C2
38	t	101	3PH	C22-C21-O21-C2
38	s	626	3PH	O22-C21-O21-C2
38	T1	101	3PH	C1-O11-P-O13
38	T1	101	3PH	C1-O11-P-O14
38	T1	101	3PH	C1-O11-P-O12
38	T1	101	3PH	C22-C21-O21-C2
38	S1	626	3PH	C1-O11-P-O13
38	S1	626	3PH	C1-O11-P-O14
38	S1	626	3PH	C1-O11-P-O12
38	S1	626	3PH	O22-C21-O21-C2
38	b1	624	3PH	C1-O11-P-O13
38	b1	624	3PH	C1-O11-P-O14
38	b1	624	3PH	O21-C2-C3-O31

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Mol	Chain	Res	Type	Atoms
38	b1	624	3PH	C22-C21-O21-C2
38	b1	624	3PH	O32-C31-O31-C3
38	b1	624	3PH	C32-C31-O31-C3
38	t1	101	3PH	O22-C21-O21-C2
38	s1	626	3PH	C1-O11-P-O13
38	s1	626	3PH	C1-O11-P-O14
38	s1	626	3PH	O22-C21-O21-C2
39	B	625	DGA	CG1-CG2-OG2-CB1
39	B	625	DGA	CG1-CG2-CG3-OXT
39	B	625	DGA	OG2-CG2-CG3-OXT
39	J	101	DGA	CG1-CG2-CG3-OXT
39	J	101	DGA	OG2-CG2-CG3-OXT
39	b	625	DGA	CG1-CG2-CG3-OXT
39	b	625	DGA	OG2-CG2-CG3-OXT
39	j	101	DGA	CG1-CG2-CG3-OXT
39	j	101	DGA	OG2-CG2-CG3-OXT
39	B1	625	DGA	OB1-CB1-OG2-CG2
39	b1	625	DGA	CB2-CB1-OG2-CG2
39	b1	625	DGA	OB1-CB1-OG2-CG2
39	c1	524	DGA	OG2-CG2-CG3-OXT
40	C	525	LHG	C3-O3-P-O4
40	C	525	LHG	C4-O6-P-O3
40	C	525	LHG	C4-O6-P-O4
40	C	525	LHG	C4-O6-P-O5
40	D	408	LHG	O1-C1-C2-C3
40	D	408	LHG	O2-C2-C3-O3
40	D	408	LHG	C3-O3-P-O4
40	D	408	LHG	C4-O6-P-O5
40	D	409	LHG	O1-C1-C2-C3
40	D	409	LHG	C1-C2-C3-O3
40	D	409	LHG	C3-O3-P-O5
40	D	410	LHG	O1-C1-C2-O2
40	D	410	LHG	O1-C1-C2-C3
40	D	410	LHG	C3-O3-P-O5
40	D	410	LHG	C4-O6-P-O5
40	D	410	LHG	O7-C5-C6-O8
40	L	101	LHG	C3-O3-P-O4
40	L	101	LHG	C3-O3-P-O5
40	L	101	LHG	C4-O6-P-O5
40	L	101	LHG	C8-C7-O7-C5
40	N	624	LHG	C1-C2-C3-O3
40	N	624	LHG	C3-O3-P-O5

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

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Mol	Chain	Res	Type	Atoms
40	s	624	LHG	C3-O3-P-O5
40	y	624	LHG	O1-C1-C2-C3
40	y	624	LHG	C3-O3-P-O5
40	D1	408	LHG	O1-C1-C2-C3
40	D1	408	LHG	C3-O3-P-O4
40	D1	408	LHG	C3-O3-P-O5
40	D1	408	LHG	C3-O3-P-O6
40	D1	409	LHG	O1-C1-C2-C3
40	D1	409	LHG	O2-C2-C3-O3
40	D1	409	LHG	C3-O3-P-O4
40	D1	409	LHG	C4-O6-P-O5
40	D1	410	LHG	O1-C1-C2-O2
40	D1	410	LHG	O1-C1-C2-C3
40	D1	410	LHG	C3-O3-P-O4
40	D1	410	LHG	C3-O3-P-O5
40	D1	410	LHG	C3-O3-P-O6
40	D1	410	LHG	C4-O6-P-O5
40	L1	101	LHG	O1-C1-C2-C3
40	L1	101	LHG	C4-O6-P-O4
40	L1	101	LHG	C5-C6-O8-C23
40	L1	101	LHG	O9-C7-O7-C5
40	L1	101	LHG	C8-C7-O7-C5
40	N1	624	LHG	O1-C1-C2-C3
40	N1	624	LHG	O2-C2-C3-O3
40	N1	624	LHG	C3-O3-P-O5
40	N1	624	LHG	C4-O6-P-O5
40	G1	624	LHG	O1-C1-C2-O2
40	G1	624	LHG	C4-O6-P-O5
40	G1	624	LHG	O7-C5-C6-O8
40	S1	624	LHG	C3-O3-P-O5
40	S1	624	LHG	C4-O6-P-O3
40	S1	624	LHG	C4-O6-P-O4
40	S1	624	LHG	C4-O6-P-O5
40	Y1	624	LHG	O1-C1-C2-C3
40	Y1	624	LHG	C1-C2-C3-O3
40	Y1	624	LHG	O2-C2-C3-O3
40	Y1	624	LHG	C3-O3-P-O5
40	c1	525	LHG	O1-C1-C2-O2
40	c1	525	LHG	C4-O6-P-O4
40	d1	408	LHG	O1-C1-C2-C3
40	d1	408	LHG	C1-C2-C3-O3
40	d1	408	LHG	C3-O3-P-O4

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Mol	Chain	Res	Type	Atoms
40	d1	408	LHG	C3-O3-P-O5
40	d1	408	LHG	C4-O6-P-O5
40	d1	409	LHG	O1-C1-C2-O2
40	d1	409	LHG	O1-C1-C2-C3
40	d1	409	LHG	C1-C2-C3-O3
40	d1	409	LHG	C4-O6-P-O3
40	d1	410	LHG	O1-C1-C2-C3
40	d1	410	LHG	C3-O3-P-O4
40	d1	410	LHG	C3-O3-P-O5
40	d1	410	LHG	C3-O3-P-O6
40	d1	410	LHG	C4-O6-P-O5
40	d1	410	LHG	O7-C5-C6-O8
40	n1	624	LHG	O1-C1-C2-C3
40	n1	624	LHG	C4-O6-P-O4
40	n1	624	LHG	O7-C5-C6-O8
40	g1	624	LHG	O1-C1-C2-C3
40	g1	624	LHG	O2-C2-C3-O3
40	g1	624	LHG	C4-O6-P-O3
40	g1	624	LHG	C4-O6-P-O4
40	g1	624	LHG	C4-O6-P-O5
40	g1	624	LHG	O7-C5-C6-O8
40	g1	624	LHG	C8-C7-O7-C5
40	s1	624	LHG	O1-C1-C2-C3
40	s1	624	LHG	C1-C2-C3-O3
40	s1	624	LHG	C4-O6-P-O3
40	s1	624	LHG	C4-O6-P-O4
40	s1	624	LHG	C4-O6-P-O5
40	y1	624	LHG	O1-C1-C2-C3
40	y1	624	LHG	C4-O6-P-O5
41	C	527	LMK	C7-C8-O7-C10
41	C	527	LMK	C1-C2-C3-C4
41	C	527	LMK	C1-C2-C3-N4
41	C	527	LMK	C2-C3-N4-C5
41	C	527	LMK	C2-C3-N4-C6
41	C	527	LMK	C2-C3-N4-C46
41	C1	527	LMK	O9-C10-O7-C8
41	C1	527	LMK	C1-C2-C3-C4
41	C1	527	LMK	C1-C2-C3-N4
41	C1	527	LMK	C2-C3-N4-C5
41	C1	527	LMK	C2-C3-N4-C6
41	C1	527	LMK	C2-C3-N4-C46
43	D	405	PL9	C37-C38-C39-C41

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Mol	Chain	Res	Type	Atoms
43	d	405	PL9	C37-C38-C39-C40
43	D1	405	PL9	C7-C8-C9-C10
43	D1	405	PL9	C12-C11-C9-C8
43	D1	405	PL9	C18-C19-C21-C22
43	D1	405	PL9	C22-C23-C24-C26
43	D1	405	PL9	C27-C28-C29-C31
43	d1	405	PL9	C37-C38-C39-C40
43	d1	405	PL9	C37-C38-C39-C41
43	d1	405	PL9	C42-C43-C44-C46
45	H	101	RRX	C23-C24-C25-C26
45	h	101	RRX	C23-C24-C25-C26
45	h	101	RRX	C5-C6-C7-C8
45	H1	101	RRX	C23-C24-C25-C26
45	H1	101	RRX	C37-C22-C23-C24
45	H1	101	RRX	C21-C22-C23-C24
45	H1	101	RRX	C19-C20-C21-C22
45	h1	101	RRX	C23-C24-C25-C26
45	h1	101	RRX	C5-C6-C7-C8
46	I	101	GOL	C1-C2-C3-O3
47	I	102	4RF	O18-C19-C20-O21
47	I	102	4RF	C24-C22-O21-C20
47	K	101	4RF	O21-C20-C39-O40
47	i	101	4RF	O18-C19-C20-O21
47	i	101	4RF	O21-C20-C39-O40
47	i	101	4RF	C24-C22-O21-C20
47	i	101	4RF	C15-C16-O18-C19
47	I1	102	4RF	C24-C22-O21-C20
47	I1	102	4RF	C15-C16-O18-C19
47	I1	102	4RF	O17-C16-O18-C19
47	K1	101	4RF	O21-C20-C39-O40
47	i1	101	4RF	C24-C22-O21-C20
48	N	605	CHL	C2A-CAA-CBA-CGA
48	N	609	CHL	CHA-CBD-CGD-O1D
48	N	609	CHL	CHA-CBD-CGD-O2D
48	G	601	CHL	CHA-CBD-CGD-O1D
48	G	601	CHL	CHA-CBD-CGD-O2D
48	G	605	CHL	C1A-C2A-CAA-CBA
48	G	605	CHL	C3A-C2A-CAA-CBA
48	G	609	CHL	CHA-CBD-CGD-O1D
48	G	609	CHL	CHA-CBD-CGD-O2D
48	G	609	CHL	C4-C3-C5-C6
48	R	607	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
48	R	607	CHL	CHA-CBD-CGD-O2D
48	Y	601	CHL	CHA-CBD-CGD-O1D
48	Y	601	CHL	CHA-CBD-CGD-O2D
48	n	601	CHL	CHA-CBD-CGD-O1D
48	n	601	CHL	CHA-CBD-CGD-O2D
48	n	608	CHL	CHA-CBD-CGD-O1D
48	n	608	CHL	CHA-CBD-CGD-O2D
48	g	601	CHL	CHA-CBD-CGD-O1D
48	g	601	CHL	CHA-CBD-CGD-O2D
48	g	605	CHL	C1A-C2A-CAA-CBA
48	g	605	CHL	CHA-CBD-CGD-O1D
48	g	605	CHL	CHA-CBD-CGD-O2D
48	g	609	CHL	C2-C3-C5-C6
48	g	609	CHL	C4-C3-C5-C6
48	r	606	CHL	CHA-CBD-CGD-O1D
48	s	601	CHL	CHA-CBD-CGD-O1D
48	s	601	CHL	CHA-CBD-CGD-O2D
48	s	606	CHL	CHA-CBD-CGD-O1D
48	s	606	CHL	CHA-CBD-CGD-O2D
48	y	606	CHL	C2-C3-C5-C6
48	y	606	CHL	C4-C3-C5-C6
48	y	607	CHL	C14-C13-C15-C16
48	N1	608	CHL	CHA-CBD-CGD-O1D
48	N1	608	CHL	CHA-CBD-CGD-O2D
48	N1	609	CHL	CHA-CBD-CGD-O1D
48	N1	609	CHL	CHA-CBD-CGD-O2D
48	N1	609	CHL	CAD-CBD-CGD-O1D
48	N1	609	CHL	CAD-CBD-CGD-O2D
48	G1	601	CHL	CHA-CBD-CGD-O1D
48	G1	601	CHL	CHA-CBD-CGD-O2D
48	G1	605	CHL	CHA-CBD-CGD-O1D
48	G1	605	CHL	CHA-CBD-CGD-O2D
48	G1	607	CHL	C1A-C2A-CAA-CBA
48	G1	609	CHL	CHA-CBD-CGD-O1D
48	G1	609	CHL	CHA-CBD-CGD-O2D
48	G1	609	CHL	C2-C3-C5-C6
48	G1	609	CHL	C4-C3-C5-C6
48	R1	606	CHL	CHA-CBD-CGD-O1D
48	R1	606	CHL	CHA-CBD-CGD-O2D
48	S1	601	CHL	CHA-CBD-CGD-O1D
48	S1	601	CHL	CHA-CBD-CGD-O2D
48	S1	608	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
48	S1	608	CHL	CHA-CBD-CGD-O2D
48	Y1	601	CHL	CHA-CBD-CGD-O1D
48	Y1	601	CHL	CHA-CBD-CGD-O2D
48	Y1	609	CHL	CHA-CBD-CGD-O1D
48	Y1	609	CHL	CHA-CBD-CGD-O2D
48	n1	601	CHL	CHA-CBD-CGD-O1D
48	n1	601	CHL	C2-C3-C5-C6
48	n1	601	CHL	C4-C3-C5-C6
48	n1	606	CHL	C2A-CAA-CBA-CGA
48	g1	601	CHL	CHA-CBD-CGD-O1D
48	g1	601	CHL	CHA-CBD-CGD-O2D
48	g1	605	CHL	C1A-C2A-CAA-CBA
48	g1	605	CHL	CHA-CBD-CGD-O1D
48	g1	605	CHL	CHA-CBD-CGD-O2D
48	g1	607	CHL	C1A-C2A-CAA-CBA
48	g1	607	CHL	C3A-C2A-CAA-CBA
48	g1	609	CHL	CHA-CBD-CGD-O1D
48	g1	609	CHL	CHA-CBD-CGD-O2D
48	g1	609	CHL	C2-C3-C5-C6
48	g1	609	CHL	C4-C3-C5-C6
48	r1	606	CHL	CHA-CBD-CGD-O1D
48	r1	607	CHL	CHA-CBD-CGD-O1D
48	r1	607	CHL	CHA-CBD-CGD-O2D
48	s1	601	CHL	CHA-CBD-CGD-O1D
48	s1	601	CHL	CHA-CBD-CGD-O2D
48	s1	608	CHL	CHA-CBD-CGD-O1D
48	s1	608	CHL	CHA-CBD-CGD-O2D
48	y1	601	CHL	C3A-C2A-CAA-CBA
48	y1	601	CHL	CHA-CBD-CGD-O1D
48	y1	601	CHL	CHA-CBD-CGD-O2D
48	y1	607	CHL	C11-C10-C8-C9
49	N	621	LUT	C21-C26-C27-C28
49	G	621	LUT	C21-C26-C27-C28
49	S	621	LUT	C25-C26-C27-C28
49	Y	621	LUT	C21-C26-C27-C28
49	n	620	LUT	C31-C32-C33-C34
49	n	620	LUT	C31-C32-C33-C40
49	g	620	LUT	C25-C26-C27-C28
49	g	620	LUT	C31-C32-C33-C34
49	g	620	LUT	C31-C32-C33-C40
49	r	620	LUT	C11-C12-C13-C14
49	r	620	LUT	C11-C12-C13-C20

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Mol	Chain	Res	Type	Atoms
49	s	621	LUT	C31-C32-C33-C34
49	s	621	LUT	C31-C32-C33-C40
49	y	621	LUT	C21-C26-C27-C28
49	N1	620	LUT	C27-C28-C29-C39
49	N1	621	LUT	C7-C8-C9-C10
49	N1	621	LUT	C7-C8-C9-C19
49	G1	620	LUT	C1-C6-C7-C8
49	R1	620	LUT	C7-C8-C9-C10
49	R1	620	LUT	C7-C8-C9-C19
49	R1	620	LUT	C31-C32-C33-C34
49	R1	620	LUT	C31-C32-C33-C40
49	S1	620	LUT	C25-C26-C27-C28
49	S1	621	LUT	C11-C12-C13-C20
49	S1	621	LUT	C27-C28-C29-C39
49	Y1	620	LUT	C25-C26-C27-C28
49	Y1	620	LUT	C27-C28-C29-C30
49	Y1	620	LUT	C27-C28-C29-C39
49	Y1	620	LUT	C31-C32-C33-C34
49	Y1	620	LUT	C31-C32-C33-C40
49	Y1	621	LUT	C21-C26-C27-C28
49	n1	621	LUT	C1-C6-C7-C8
49	n1	621	LUT	C21-C26-C27-C28
49	g1	620	LUT	C27-C28-C29-C30
49	g1	620	LUT	C27-C28-C29-C39
49	g1	621	LUT	C21-C26-C27-C28
49	r1	620	LUT	C27-C28-C29-C30
49	r1	620	LUT	C27-C28-C29-C39
49	s1	620	LUT	C27-C28-C29-C30
49	s1	620	LUT	C27-C28-C29-C39
49	s1	621	LUT	C1-C6-C7-C8
49	s1	621	LUT	C11-C12-C13-C14
49	s1	621	LUT	C11-C12-C13-C20
49	y1	621	LUT	C21-C26-C27-C28
50	N	622	XAT	C27-C28-C29-C30
50	N	622	XAT	C27-C28-C29-C39
50	n	622	XAT	C11-C12-C13-C20
50	y	622	XAT	C20-C13-C14-C15
50	y	622	XAT	C14-C15-C35-C34
50	y	622	XAT	O24-C26-C27-C28
50	y	622	XAT	C31-C32-C33-C34
50	y	622	XAT	C31-C32-C33-C40
50	G1	622	XAT	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
50	R1	621	XAT	C31-C32-C33-C34
50	R1	621	XAT	C31-C32-C33-C40
50	Y1	622	XAT	C26-C27-C28-C29
50	n1	622	XAT	C27-C28-C29-C39
50	r1	621	XAT	C30-C31-C32-C33
50	y1	622	XAT	C31-C32-C33-C34
50	y1	622	XAT	C31-C32-C33-C40
51	R	622	NEX	C12-C13-C14-C15
51	R	622	NEX	C20-C13-C14-C15
51	R	622	NEX	C14-C15-C35-C34
51	R	622	NEX	C30-C31-C32-C33
51	Y	623	NEX	C11-C12-C13-C14
51	Y	623	NEX	C11-C12-C13-C20
51	g	623	NEX	C30-C31-C32-C33
51	g	623	NEX	C31-C32-C33-C34
51	g	623	NEX	C31-C32-C33-C40
51	r	622	NEX	C10-C11-C12-C13
51	r	622	NEX	C12-C13-C14-C15
51	r	622	NEX	C20-C13-C14-C15
51	r	622	NEX	C14-C15-C35-C34
51	s	623	NEX	C7-C8-C9-C19
51	G1	623	NEX	C10-C11-C12-C13
51	R1	622	NEX	C7-C8-C9-C19
51	R1	622	NEX	C10-C11-C12-C13
51	R1	622	NEX	C20-C13-C14-C15
51	R1	622	NEX	C14-C15-C35-C34
51	R1	622	NEX	C30-C31-C32-C33
51	S1	623	NEX	C28-C29-C30-C31
51	S1	623	NEX	C39-C29-C30-C31
51	Y1	623	NEX	C11-C12-C13-C20
51	Y1	623	NEX	C14-C15-C35-C34
51	r1	622	NEX	C12-C13-C14-C15
51	r1	622	NEX	C20-C13-C14-C15
51	r1	622	NEX	C28-C29-C30-C31
51	r1	622	NEX	C39-C29-C30-C31
51	r1	622	NEX	C30-C31-C32-C33
51	r1	622	NEX	C32-C33-C34-C35
51	r1	622	NEX	C40-C33-C34-C35
51	y1	623	NEX	C10-C11-C12-C13
51	y1	623	NEX	C11-C12-C13-C20
52	r	625	LMT	O5'-C1'-O1'-C1
53	R	626	ERG	C16-C17-C20-C21

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Mol	Chain	Res	Type	Atoms
53	r	626	ERG	C13-C17-C20-C21
53	r	626	ERG	C16-C17-C20-C21
53	R1	626	ERG	C13-C17-C20-C21
53	R1	626	ERG	C16-C17-C20-C21
53	R1	626	ERG	C16-C17-C20-C22
53	r1	626	ERG	C13-C17-C20-C21
53	r1	626	ERG	C13-C17-C20-C22
53	r1	626	ERG	C16-C17-C20-C21
53	r1	626	ERG	C16-C17-C20-C22
53	r1	626	ERG	C22-C23-C24-C25
54	S	625	LPX	O1-C3-C4-C5
54	S	625	LPX	C3-O1-P1-O3
54	S	625	LPX	C3-O1-P1-O2
54	S	625	LPX	C3-O1-P1-O4
54	S	625	LPX	C1-O2-P1-O4
54	S	625	LPX	O2-C1-C2-N1
54	s	625	LPX	C3-C4-C5-O6
54	s	625	LPX	C1-O2-P1-O4
54	S1	625	LPX	O1-C3-C4-C5
54	S1	625	LPX	O1-C3-C4-O5
54	S1	625	LPX	C3-O1-P1-O2
54	S1	625	LPX	O2-C1-C2-N1
54	s1	625	LPX	O5-C4-C5-O6
54	s1	625	LPX	C3-C4-C5-O6
54	s1	625	LPX	C3-O1-P1-O4
54	s1	625	LPX	C1-O2-P1-O3
54	s1	625	LPX	O2-C1-C2-N1
55	Y	626	PTY	C3-O11-P1-O12
55	Y	626	PTY	C3-O11-P1-O14
55	Y	627	PTY	N1-C2-C3-O11
55	Y	627	PTY	C5-O14-P1-O11
55	y	626	PTY	C3-O11-P1-O12
55	y	626	PTY	C3-O11-P1-O13
55	y	626	PTY	C3-O11-P1-O14
55	y	626	PTY	C5-O14-P1-O13
55	y	627	PTY	N1-C2-C3-O11
55	y	627	PTY	O10-C8-O7-C6
55	y	627	PTY	C11-C8-O7-C6
55	y	627	PTY	C5-O14-P1-O11
55	y	627	PTY	C5-O14-P1-O12
55	y	627	PTY	C5-O14-P1-O13
55	Y1	626	PTY	N1-C2-C3-O11

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Mol	Chain	Res	Type	Atoms
55	Y1	626	PTY	C2-C3-O11-P1
55	Y1	627	PTY	N1-C2-C3-O11
55	Y1	627	PTY	C5-O14-P1-O12
55	Y1	627	PTY	C5-O14-P1-O13
55	y1	626	PTY	C11-C8-O7-C6
55	y1	626	PTY	C5-O14-P1-O11
55	y1	626	PTY	C5-O14-P1-O12
55	y1	627	PTY	C5-O14-P1-O13
55	Y1	627	PTY	C11-C8-O7-C6
55	y1	627	PTY	C11-C8-O7-C6
29	A	405	CLA	O1D-CGD-O2D-CED
29	R	603	CLA	O1D-CGD-O2D-CED
29	S	603	CLA	O1D-CGD-O2D-CED
29	S	613	CLA	O1D-CGD-O2D-CED
29	a	405	CLA	O1D-CGD-O2D-CED
29	b	602	CLA	O1D-CGD-O2D-CED
29	r	609	CLA	O1D-CGD-O2D-CED
29	B1	612	CLA	O1D-CGD-O2D-CED
29	B1	615	CLA	O1D-CGD-O2D-CED
29	N1	613	CLA	O1D-CGD-O2D-CED
29	R1	609	CLA	O1D-CGD-O2D-CED
29	S1	605	CLA	O1D-CGD-O2D-CED
29	Y1	608	CLA	O1D-CGD-O2D-CED
29	b1	608	CLA	O1D-CGD-O2D-CED
29	g1	610	CLA	O1D-CGD-O2D-CED
29	r1	609	CLA	O1D-CGD-O2D-CED
55	Y	627	PTY	C11-C8-O7-C6
55	Y1	627	PTY	O10-C8-O7-C6
29	B	612	CLA	O1D-CGD-O2D-CED
29	c	503	CLA	O1D-CGD-O2D-CED
29	r	603	CLA	O1D-CGD-O2D-CED
29	s	613	CLA	O1D-CGD-O2D-CED
29	A1	405	CLA	O1D-CGD-O2D-CED
29	B1	616	CLA	O1D-CGD-O2D-CED
29	C1	503	CLA	O1D-CGD-O2D-CED
29	N1	610	CLA	O1D-CGD-O2D-CED
29	R1	603	CLA	O1D-CGD-O2D-CED
29	R1	608	CLA	O1D-CGD-O2D-CED
29	R1	610	CLA	O1D-CGD-O2D-CED
29	S1	611	CLA	O1D-CGD-O2D-CED
29	S1	617	CLA	O1D-CGD-O2D-CED
29	n1	610	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	n1	613	CLA	O1D-CGD-O2D-CED
29	r1	608	CLA	O1D-CGD-O2D-CED
29	s1	613	CLA	O1D-CGD-O2D-CED
29	y1	608	CLA	O1D-CGD-O2D-CED
55	Y	627	PTY	C31-C30-O4-C1
29	A	405	CLA	CBD-CGD-O2D-CED
29	B	606	CLA	CBD-CGD-O2D-CED
29	B	611	CLA	CBD-CGD-O2D-CED
29	B	613	CLA	CBD-CGD-O2D-CED
29	B	615	CLA	CBD-CGD-O2D-CED
29	B	617	CLA	CBD-CGD-O2D-CED
29	C	501	CLA	CBD-CGD-O2D-CED
29	C	502	CLA	CBD-CGD-O2D-CED
29	C	506	CLA	CBD-CGD-O2D-CED
29	C	511	CLA	CBD-CGD-O2D-CED
29	C	513	CLA	CBD-CGD-O2D-CED
29	D	402	CLA	CBD-CGD-O2D-CED
29	N	611	CLA	CBD-CGD-O2D-CED
29	N	614	CLA	CBD-CGD-O2D-CED
29	G	602	CLA	CBD-CGD-O2D-CED
29	G	604	CLA	CBD-CGD-O2D-CED
29	G	612	CLA	CBD-CGD-O2D-CED
29	G	614	CLA	CBD-CGD-O2D-CED
29	R	603	CLA	CBD-CGD-O2D-CED
29	R	609	CLA	CBD-CGD-O2D-CED
29	R	612	CLA	CBD-CGD-O2D-CED
29	S	613	CLA	CBD-CGD-O2D-CED
29	S	614	CLA	CBD-CGD-O2D-CED
29	Y	603	CLA	CBD-CGD-O2D-CED
29	Y	608	CLA	CBD-CGD-O2D-CED
29	Y	612	CLA	CBD-CGD-O2D-CED
29	Y	613	CLA	CBD-CGD-O2D-CED
29	Y	614	CLA	CBD-CGD-O2D-CED
29	a	410	CLA	CBD-CGD-O2D-CED
29	b	602	CLA	CBD-CGD-O2D-CED
29	b	606	CLA	CBD-CGD-O2D-CED
29	b	607	CLA	CBD-CGD-O2D-CED
29	b	608	CLA	CBD-CGD-O2D-CED
29	b	612	CLA	CBD-CGD-O2D-CED
29	b	615	CLA	CBD-CGD-O2D-CED
29	c	502	CLA	CBD-CGD-O2D-CED
29	c	503	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	c	509	CLA	CBD-CGD-O2D-CED
29	c	510	CLA	CBD-CGD-O2D-CED
29	n	602	CLA	CBD-CGD-O2D-CED
29	g	603	CLA	CBD-CGD-O2D-CED
29	g	604	CLA	CBD-CGD-O2D-CED
29	g	613	CLA	CBD-CGD-O2D-CED
29	g	614	CLA	CBD-CGD-O2D-CED
29	r	602	CLA	CBD-CGD-O2D-CED
29	r	608	CLA	CBD-CGD-O2D-CED
29	r	612	CLA	CBD-CGD-O2D-CED
29	s	604	CLA	CBD-CGD-O2D-CED
29	s	612	CLA	CBD-CGD-O2D-CED
29	y	602	CLA	CBD-CGD-O2D-CED
29	y	604	CLA	CBD-CGD-O2D-CED
29	y	612	CLA	CBD-CGD-O2D-CED
29	y	614	CLA	CBD-CGD-O2D-CED
29	A1	410	CLA	CBD-CGD-O2D-CED
29	B1	606	CLA	CBD-CGD-O2D-CED
29	B1	610	CLA	CBD-CGD-O2D-CED
29	B1	611	CLA	CBD-CGD-O2D-CED
29	B1	612	CLA	CBD-CGD-O2D-CED
29	B1	615	CLA	CBD-CGD-O2D-CED
29	C1	503	CLA	CBD-CGD-O2D-CED
29	C1	507	CLA	CBD-CGD-O2D-CED
29	C1	511	CLA	CBD-CGD-O2D-CED
29	D1	402	CLA	CBD-CGD-O2D-CED
29	D1	403	CLA	CBD-CGD-O2D-CED
29	N1	602	CLA	CBD-CGD-O2D-CED
29	N1	610	CLA	CBD-CGD-O2D-CED
29	N1	611	CLA	CBD-CGD-O2D-CED
29	N1	613	CLA	CBD-CGD-O2D-CED
29	N1	614	CLA	CBD-CGD-O2D-CED
29	G1	602	CLA	CBD-CGD-O2D-CED
29	G1	604	CLA	CBD-CGD-O2D-CED
29	G1	610	CLA	CBD-CGD-O2D-CED
29	R1	608	CLA	CBD-CGD-O2D-CED
29	R1	609	CLA	CBD-CGD-O2D-CED
29	R1	612	CLA	CBD-CGD-O2D-CED
29	S1	605	CLA	CBD-CGD-O2D-CED
29	S1	613	CLA	CBD-CGD-O2D-CED
29	S1	617	CLA	CBD-CGD-O2D-CED
29	Y1	604	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	Y1	608	CLA	CBD-CGD-O2D-CED
29	Y1	612	CLA	CBD-CGD-O2D-CED
29	b1	603	CLA	CBD-CGD-O2D-CED
29	b1	608	CLA	CBD-CGD-O2D-CED
29	b1	611	CLA	CBD-CGD-O2D-CED
29	b1	617	CLA	CBD-CGD-O2D-CED
29	c1	502	CLA	CBD-CGD-O2D-CED
29	c1	503	CLA	CBD-CGD-O2D-CED
29	c1	509	CLA	CBD-CGD-O2D-CED
29	c1	511	CLA	CBD-CGD-O2D-CED
29	c1	513	CLA	CBD-CGD-O2D-CED
29	d1	403	CLA	CBD-CGD-O2D-CED
29	n1	602	CLA	CBD-CGD-O2D-CED
29	n1	604	CLA	CBD-CGD-O2D-CED
29	n1	613	CLA	CBD-CGD-O2D-CED
29	g1	604	CLA	CBD-CGD-O2D-CED
29	g1	610	CLA	CBD-CGD-O2D-CED
29	r1	602	CLA	CBD-CGD-O2D-CED
29	s1	602	CLA	CBD-CGD-O2D-CED
29	s1	604	CLA	CBD-CGD-O2D-CED
29	s1	605	CLA	CBD-CGD-O2D-CED
29	s1	612	CLA	CBD-CGD-O2D-CED
29	s1	614	CLA	CBD-CGD-O2D-CED
29	s1	617	CLA	CBD-CGD-O2D-CED
29	y1	602	CLA	CBD-CGD-O2D-CED
29	y1	603	CLA	CBD-CGD-O2D-CED
29	y1	604	CLA	CBD-CGD-O2D-CED
29	y1	613	CLA	CBD-CGD-O2D-CED
29	y1	614	CLA	CBD-CGD-O2D-CED
30	a	409	PHO	CBD-CGD-O2D-CED
30	A1	408	PHO	CBD-CGD-O2D-CED
30	a1	408	PHO	CBD-CGD-O2D-CED
30	a1	409	PHO	CBD-CGD-O2D-CED
29	A	406	CLA	O1A-CGA-O2A-C1
29	C	505	CLA	O1A-CGA-O2A-C1
29	C	512	CLA	O1A-CGA-O2A-C1
29	N	611	CLA	O1A-CGA-O2A-C1
29	G	602	CLA	O1A-CGA-O2A-C1
29	G	611	CLA	O1A-CGA-O2A-C1
29	S	604	CLA	O1A-CGA-O2A-C1
29	Y	608	CLA	O1A-CGA-O2A-C1
29	b	603	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	g	614	CLA	O1A-CGA-O2A-C1
29	r	603	CLA	O1A-CGA-O2A-C1
29	y	604	CLA	O1A-CGA-O2A-C1
29	D1	403	CLA	O1A-CGA-O2A-C1
29	N1	611	CLA	O1A-CGA-O2A-C1
29	G1	614	CLA	O1A-CGA-O2A-C1
29	R1	603	CLA	O1A-CGA-O2A-C1
29	S1	604	CLA	O1A-CGA-O2A-C1
29	S1	605	CLA	O1A-CGA-O2A-C1
29	a1	410	CLA	O1A-CGA-O2A-C1
29	g1	604	CLA	O1A-CGA-O2A-C1
29	r1	609	CLA	O1A-CGA-O2A-C1
29	y1	604	CLA	O1A-CGA-O2A-C1
29	y1	611	CLA	O1A-CGA-O2A-C1
29	y1	612	CLA	O1A-CGA-O2A-C1
32	c1	526	SQD	O10-C23-O48-C46
33	C1	521	LMG	O10-C28-O8-C9
33	W1	201	LMG	O10-C28-O8-C9
33	c1	523	LMG	O10-C28-O8-C9
40	L1	101	LHG	O10-C23-O8-C6
47	I	102	4RF	O17-C16-O18-C19
47	i	101	4RF	O17-C16-O18-C19
55	y	626	PTY	O30-C30-O4-C1
29	B	606	CLA	O1D-CGD-O2D-CED
29	B	617	CLA	O1D-CGD-O2D-CED
29	N	614	CLA	O1D-CGD-O2D-CED
29	R	609	CLA	O1D-CGD-O2D-CED
29	R	612	CLA	O1D-CGD-O2D-CED
29	Y	608	CLA	O1D-CGD-O2D-CED
29	b	606	CLA	O1D-CGD-O2D-CED
29	B1	610	CLA	O1D-CGD-O2D-CED
29	G1	610	CLA	O1D-CGD-O2D-CED
29	S1	613	CLA	O1D-CGD-O2D-CED
29	S1	614	CLA	O1D-CGD-O2D-CED
29	Y1	614	CLA	O1D-CGD-O2D-CED
29	b1	603	CLA	O1D-CGD-O2D-CED
29	c1	511	CLA	O1D-CGD-O2D-CED
29	n1	604	CLA	O1D-CGD-O2D-CED
29	g1	604	CLA	O1D-CGD-O2D-CED
29	r1	603	CLA	O1D-CGD-O2D-CED
29	s1	612	CLA	O1D-CGD-O2D-CED
29	s1	614	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	y1	613	CLA	O1D-CGD-O2D-CED
29	y1	614	CLA	O1D-CGD-O2D-CED
29	B	603	CLA	O1D-CGD-O2D-CED
29	B	607	CLA	O1D-CGD-O2D-CED
29	B	608	CLA	O1D-CGD-O2D-CED
29	C	503	CLA	O1D-CGD-O2D-CED
29	G	610	CLA	O1D-CGD-O2D-CED
29	G	614	CLA	O1D-CGD-O2D-CED
29	R	608	CLA	O1D-CGD-O2D-CED
29	R	610	CLA	O1D-CGD-O2D-CED
29	S	610	CLA	O1D-CGD-O2D-CED
29	S	617	CLA	O1D-CGD-O2D-CED
29	Y	610	CLA	O1D-CGD-O2D-CED
29	b	610	CLA	O1D-CGD-O2D-CED
29	b	611	CLA	O1D-CGD-O2D-CED
29	c	511	CLA	O1D-CGD-O2D-CED
29	d	403	CLA	O1D-CGD-O2D-CED
29	n	610	CLA	O1D-CGD-O2D-CED
29	n	613	CLA	O1D-CGD-O2D-CED
29	n	614	CLA	O1D-CGD-O2D-CED
29	g	610	CLA	O1D-CGD-O2D-CED
29	g	611	CLA	O1D-CGD-O2D-CED
29	g	613	CLA	O1D-CGD-O2D-CED
29	r	604	CLA	O1D-CGD-O2D-CED
29	s	614	CLA	O1D-CGD-O2D-CED
29	y	610	CLA	O1D-CGD-O2D-CED
29	A1	410	CLA	O1D-CGD-O2D-CED
29	B1	613	CLA	O1D-CGD-O2D-CED
29	B1	614	CLA	O1D-CGD-O2D-CED
29	C1	502	CLA	O1D-CGD-O2D-CED
29	C1	504	CLA	O1D-CGD-O2D-CED
29	C1	510	CLA	O1D-CGD-O2D-CED
29	C1	513	CLA	O1D-CGD-O2D-CED
29	N1	603	CLA	O1D-CGD-O2D-CED
29	G1	603	CLA	O1D-CGD-O2D-CED
29	G1	613	CLA	O1D-CGD-O2D-CED
29	R1	612	CLA	O1D-CGD-O2D-CED
29	S1	609	CLA	O1D-CGD-O2D-CED
29	a1	405	CLA	O1D-CGD-O2D-CED
29	c1	501	CLA	O1D-CGD-O2D-CED
29	c1	503	CLA	O1D-CGD-O2D-CED
29	c1	506	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	n1	611	CLA	O1D-CGD-O2D-CED
29	n1	612	CLA	O1D-CGD-O2D-CED
29	g1	611	CLA	O1D-CGD-O2D-CED
29	r1	610	CLA	O1D-CGD-O2D-CED
29	s1	603	CLA	O1D-CGD-O2D-CED
29	s1	609	CLA	O1D-CGD-O2D-CED
29	y1	610	CLA	O1D-CGD-O2D-CED
29	C	512	CLA	CBA-CGA-O2A-C1
29	G	611	CLA	CBA-CGA-O2A-C1
29	S	604	CLA	CBA-CGA-O2A-C1
29	Y	611	CLA	CBA-CGA-O2A-C1
29	b	603	CLA	CBA-CGA-O2A-C1
29	r	603	CLA	CBA-CGA-O2A-C1
29	y	604	CLA	CBA-CGA-O2A-C1
29	D1	403	CLA	CBA-CGA-O2A-C1
29	G1	614	CLA	CBA-CGA-O2A-C1
29	R1	603	CLA	CBA-CGA-O2A-C1
29	S1	604	CLA	CBA-CGA-O2A-C1
29	g1	602	CLA	CBA-CGA-O2A-C1
29	r1	609	CLA	CBA-CGA-O2A-C1
29	y1	611	CLA	CBA-CGA-O2A-C1
33	c1	523	LMG	C29-C28-O8-C9
40	L1	101	LHG	C24-C23-O8-C6
55	Y	627	PTY	O30-C30-O4-C1
33	c1	521	LMG	C4-C5-C6-O5
29	C	507	CLA	CBD-CGD-O2D-CED
29	C	510	CLA	CBD-CGD-O2D-CED
29	C	512	CLA	CBD-CGD-O2D-CED
29	D	403	CLA	CBD-CGD-O2D-CED
29	N	603	CLA	CBD-CGD-O2D-CED
29	N	604	CLA	CBD-CGD-O2D-CED
29	N	612	CLA	CBD-CGD-O2D-CED
29	N	613	CLA	CBD-CGD-O2D-CED
29	R	602	CLA	CBD-CGD-O2D-CED
29	R	604	CLA	CBD-CGD-O2D-CED
29	S	602	CLA	CBD-CGD-O2D-CED
29	S	604	CLA	CBD-CGD-O2D-CED
29	S	605	CLA	CBD-CGD-O2D-CED
29	S	612	CLA	CBD-CGD-O2D-CED
29	Y	604	CLA	CBD-CGD-O2D-CED
29	b	603	CLA	CBD-CGD-O2D-CED
29	b	613	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	b	614	CLA	CBD-CGD-O2D-CED
29	b	616	CLA	CBD-CGD-O2D-CED
29	c	512	CLA	CBD-CGD-O2D-CED
29	c	513	CLA	CBD-CGD-O2D-CED
29	n	603	CLA	CBD-CGD-O2D-CED
29	g	602	CLA	CBD-CGD-O2D-CED
29	g	612	CLA	CBD-CGD-O2D-CED
29	s	602	CLA	CBD-CGD-O2D-CED
29	s	605	CLA	CBD-CGD-O2D-CED
29	s	609	CLA	CBD-CGD-O2D-CED
29	A1	407	CLA	CBD-CGD-O2D-CED
29	B1	607	CLA	CBD-CGD-O2D-CED
29	B1	608	CLA	CBD-CGD-O2D-CED
29	B1	609	CLA	CBD-CGD-O2D-CED
29	C1	512	CLA	CBD-CGD-O2D-CED
29	G1	612	CLA	CBD-CGD-O2D-CED
29	G1	614	CLA	CBD-CGD-O2D-CED
29	R1	604	CLA	CBD-CGD-O2D-CED
29	S1	602	CLA	CBD-CGD-O2D-CED
29	S1	603	CLA	CBD-CGD-O2D-CED
29	S1	604	CLA	CBD-CGD-O2D-CED
29	Y1	602	CLA	CBD-CGD-O2D-CED
29	b1	613	CLA	CBD-CGD-O2D-CED
29	c1	507	CLA	CBD-CGD-O2D-CED
29	n1	614	CLA	CBD-CGD-O2D-CED
29	g1	613	CLA	CBD-CGD-O2D-CED
29	y1	612	CLA	CBD-CGD-O2D-CED
55	y1	627	PTY	O10-C8-O7-C6
29	B	603	CLA	O1A-CGA-O2A-C1
29	B	611	CLA	O1A-CGA-O2A-C1
29	D	403	CLA	O1A-CGA-O2A-C1
29	G	604	CLA	O1A-CGA-O2A-C1
29	G	614	CLA	O1A-CGA-O2A-C1
29	R	603	CLA	O1A-CGA-O2A-C1
29	R	608	CLA	O1A-CGA-O2A-C1
29	S	605	CLA	O1A-CGA-O2A-C1
29	S	613	CLA	O1A-CGA-O2A-C1
29	S	617	CLA	O1A-CGA-O2A-C1
29	Y	604	CLA	O1A-CGA-O2A-C1
29	Y	611	CLA	O1A-CGA-O2A-C1
29	a	406	CLA	O1A-CGA-O2A-C1
29	c	506	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	n	603	CLA	O1A-CGA-O2A-C1
29	g	604	CLA	O1A-CGA-O2A-C1
29	g	613	CLA	O1A-CGA-O2A-C1
29	r	608	CLA	O1A-CGA-O2A-C1
29	s	613	CLA	O1A-CGA-O2A-C1
29	y	611	CLA	O1A-CGA-O2A-C1
29	A1	406	CLA	O1A-CGA-O2A-C1
29	B1	603	CLA	O1A-CGA-O2A-C1
29	B1	611	CLA	O1A-CGA-O2A-C1
29	C1	505	CLA	O1A-CGA-O2A-C1
29	C1	512	CLA	O1A-CGA-O2A-C1
29	C1	513	CLA	O1A-CGA-O2A-C1
29	G1	604	CLA	O1A-CGA-O2A-C1
29	G1	611	CLA	O1A-CGA-O2A-C1
29	S1	613	CLA	O1A-CGA-O2A-C1
29	Y1	604	CLA	O1A-CGA-O2A-C1
29	Y1	608	CLA	O1A-CGA-O2A-C1
29	Y1	611	CLA	O1A-CGA-O2A-C1
29	Y1	612	CLA	O1A-CGA-O2A-C1
29	b1	611	CLA	O1A-CGA-O2A-C1
29	c1	506	CLA	O1A-CGA-O2A-C1
29	g1	602	CLA	O1A-CGA-O2A-C1
29	g1	611	CLA	O1A-CGA-O2A-C1
29	g1	613	CLA	O1A-CGA-O2A-C1
29	g1	614	CLA	O1A-CGA-O2A-C1
29	s1	613	CLA	O1A-CGA-O2A-C1
32	c	526	SQD	O10-C23-O48-C46
33	C	521	LMG	O10-C28-O8-C9
33	W	201	LMG	O10-C28-O8-C9
33	c	521	LMG	O10-C28-O8-C9
33	C1	523	LMG	O10-C28-O8-C9
33	w1	201	LMG	O10-C28-O8-C9
47	i1	101	4RF	O17-C16-O18-C19
29	B	614	CLA	O1D-CGD-O2D-CED
29	G	613	CLA	O1D-CGD-O2D-CED
29	d	402	CLA	O1D-CGD-O2D-CED
29	n	611	CLA	O1D-CGD-O2D-CED
29	s	617	CLA	O1D-CGD-O2D-CED
29	B1	603	CLA	O1D-CGD-O2D-CED
29	B1	604	CLA	O1D-CGD-O2D-CED
29	C1	501	CLA	O1D-CGD-O2D-CED
29	R1	602	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	Y1	613	CLA	O1D-CGD-O2D-CED
29	b1	602	CLA	O1D-CGD-O2D-CED
29	b1	604	CLA	O1D-CGD-O2D-CED
29	b1	606	CLA	O1D-CGD-O2D-CED
29	g1	602	CLA	O1D-CGD-O2D-CED
29	g1	603	CLA	O1D-CGD-O2D-CED
29	r1	612	CLA	O1D-CGD-O2D-CED
29	B	604	CLA	O1D-CGD-O2D-CED
29	B	610	CLA	O1D-CGD-O2D-CED
29	N	602	CLA	O1D-CGD-O2D-CED
29	G	611	CLA	O1D-CGD-O2D-CED
29	S	609	CLA	O1D-CGD-O2D-CED
29	b	617	CLA	O1D-CGD-O2D-CED
29	n	612	CLA	O1D-CGD-O2D-CED
29	g	603	CLA	O1D-CGD-O2D-CED
29	y	603	CLA	O1D-CGD-O2D-CED
29	y	613	CLA	O1D-CGD-O2D-CED
29	B1	617	CLA	O1D-CGD-O2D-CED
29	N1	612	CLA	O1D-CGD-O2D-CED
29	S1	612	CLA	O1D-CGD-O2D-CED
29	Y1	603	CLA	O1D-CGD-O2D-CED
29	b1	607	CLA	O1D-CGD-O2D-CED
29	g1	612	CLA	O1D-CGD-O2D-CED
29	s1	611	CLA	O1D-CGD-O2D-CED
55	y	627	PTY	C31-C30-O4-C1
29	A	410	CLA	CBD-CGD-O2D-CED
29	Y	602	CLA	CBD-CGD-O2D-CED
29	G1	611	CLA	CBD-CGD-O2D-CED
29	n1	603	CLA	CBD-CGD-O2D-CED
29	B	615	CLA	O1D-CGD-O2D-CED
29	G	603	CLA	O1D-CGD-O2D-CED
29	b	604	CLA	O1D-CGD-O2D-CED
29	r	608	CLA	O1D-CGD-O2D-CED
29	y	608	CLA	O1D-CGD-O2D-CED
29	C1	511	CLA	O1D-CGD-O2D-CED
29	b1	609	CLA	O1D-CGD-O2D-CED
29	n1	602	CLA	O1D-CGD-O2D-CED
32	B1	626	SQD	O49-C7-O47-C45
32	M1	101	SQD	O49-C7-O47-C45
33	W	201	LMG	O9-C10-O7-C8
33	W1	201	LMG	O9-C10-O7-C8
38	T	101	3PH	O22-C21-O21-C2

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Mol	Chain	Res	Type	Atoms
38	T1	101	3PH	O22-C21-O21-C2
38	b1	624	3PH	O22-C21-O21-C2
39	B	625	DGA	OB1-CB1-OG2-CG2
39	b	625	DGA	OB1-CB1-OG2-CG2
40	L	101	LHG	O9-C7-O7-C5
40	G	624	LHG	O9-C7-O7-C5
40	n	624	LHG	O9-C7-O7-C5
40	d1	410	LHG	O9-C7-O7-C5
40	n1	624	LHG	O9-C7-O7-C5
40	g1	624	LHG	O9-C7-O7-C5
40	y1	624	LHG	O9-C7-O7-C5
47	I	102	4RF	O23-C22-O21-C20
47	i	101	4RF	O23-C22-O21-C20
47	I1	102	4RF	O23-C22-O21-C20
47	i1	101	4RF	O23-C22-O21-C20
55	y1	626	PTY	O10-C8-O7-C6
29	B1	606	CLA	O1D-CGD-O2D-CED
29	D1	403	CLA	O1D-CGD-O2D-CED
29	B	605	CLA	C3-C5-C6-C7
29	C	505	CLA	C3-C5-C6-C7
29	C	506	CLA	C3-C5-C6-C7
29	S	603	CLA	C3-C5-C6-C7
29	S	604	CLA	C3-C5-C6-C7
29	Y	602	CLA	C3-C5-C6-C7
29	b	602	CLA	C3-C5-C6-C7
29	b	605	CLA	C3-C5-C6-C7
29	b	608	CLA	C3-C5-C6-C7
29	c	506	CLA	C3-C5-C6-C7
29	n	602	CLA	C3-C5-C6-C7
29	n	604	CLA	C3-C5-C6-C7
29	r	602	CLA	C3-C5-C6-C7
29	A1	410	CLA	C3-C5-C6-C7
29	N1	610	CLA	C3-C5-C6-C7
29	G1	603	CLA	C3-C5-C6-C7
29	R1	612	CLA	C3-C5-C6-C7
29	S1	602	CLA	C3-C5-C6-C7
29	S1	613	CLA	C3-C5-C6-C7
29	a1	410	CLA	C3-C5-C6-C7
29	b1	602	CLA	C3-C5-C6-C7
29	b1	605	CLA	C3-C5-C6-C7
29	b1	609	CLA	C3-C5-C6-C7
29	n1	610	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
29	s1	603	CLA	C3-C5-C6-C7
29	s1	604	CLA	C3-C5-C6-C7
29	s1	614	CLA	C3-C5-C6-C7
30	A	409	PHO	C3-C5-C6-C7
30	a	409	PHO	C3-C5-C6-C7
30	a1	409	PHO	C3-C5-C6-C7
48	g1	601	CHL	C3-C5-C6-C7
29	A	406	CLA	CBA-CGA-O2A-C1
29	B	603	CLA	CBA-CGA-O2A-C1
29	C	505	CLA	CBA-CGA-O2A-C1
29	N	611	CLA	CBA-CGA-O2A-C1
29	G	602	CLA	CBA-CGA-O2A-C1
29	G	614	CLA	CBA-CGA-O2A-C1
29	R	603	CLA	CBA-CGA-O2A-C1
29	S	617	CLA	CBA-CGA-O2A-C1
29	Y	603	CLA	CBA-CGA-O2A-C1
29	Y	608	CLA	CBA-CGA-O2A-C1
29	a	406	CLA	CBA-CGA-O2A-C1
29	n	603	CLA	CBA-CGA-O2A-C1
29	g	604	CLA	CBA-CGA-O2A-C1
29	g	614	CLA	CBA-CGA-O2A-C1
29	r	609	CLA	CBA-CGA-O2A-C1
29	s	613	CLA	CBA-CGA-O2A-C1
29	y	611	CLA	CBA-CGA-O2A-C1
29	y	612	CLA	CBA-CGA-O2A-C1
29	A1	406	CLA	CBA-CGA-O2A-C1
29	B1	603	CLA	CBA-CGA-O2A-C1
29	B1	610	CLA	CBA-CGA-O2A-C1
29	B1	614	CLA	CBA-CGA-O2A-C1
29	C1	505	CLA	CBA-CGA-O2A-C1
29	C1	512	CLA	CBA-CGA-O2A-C1
29	N1	611	CLA	CBA-CGA-O2A-C1
29	G1	604	CLA	CBA-CGA-O2A-C1
29	G1	611	CLA	CBA-CGA-O2A-C1
29	R1	602	CLA	CBA-CGA-O2A-C1
29	R1	608	CLA	CBA-CGA-O2A-C1
29	S1	605	CLA	CBA-CGA-O2A-C1
29	S1	613	CLA	CBA-CGA-O2A-C1
29	Y1	604	CLA	CBA-CGA-O2A-C1
29	Y1	608	CLA	CBA-CGA-O2A-C1
29	Y1	611	CLA	CBA-CGA-O2A-C1
29	n1	603	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	n1	611	CLA	CBA-CGA-O2A-C1
29	g1	604	CLA	CBA-CGA-O2A-C1
29	g1	611	CLA	CBA-CGA-O2A-C1
29	s1	613	CLA	CBA-CGA-O2A-C1
29	s1	614	CLA	CBA-CGA-O2A-C1
29	y1	604	CLA	CBA-CGA-O2A-C1
32	c	526	SQD	C24-C23-O48-C46
32	c1	526	SQD	C24-C23-O48-C46
33	C	521	LMG	C29-C28-O8-C9
33	W	201	LMG	C29-C28-O8-C9
33	C1	521	LMG	C29-C28-O8-C9
33	C1	523	LMG	C29-C28-O8-C9
33	W1	201	LMG	C29-C28-O8-C9
33	c1	521	LMG	C29-C28-O8-C9
33	w1	201	LMG	C29-C28-O8-C9
37	B	623	DGD	C2A-C1A-O1G-C1G
38	t	101	3PH	C32-C31-O31-C3
47	I	102	4RF	C15-C16-O18-C19
55	y	626	PTY	C31-C30-O4-C1
52	r1	625	LMT	O5B-C5B-C6B-O6B
29	n	602	CLA	C15-C16-C17-C18
33	B1	622	LMG	C11-C10-O7-C8
33	b1	622	LMG	C11-C10-O7-C8
37	b	623	DGD	C2B-C1B-O2G-C2G
37	B1	623	DGD	C2B-C1B-O2G-C2G
37	b1	623	DGD	C2B-C1B-O2G-C2G
38	t1	101	3PH	C22-C21-O21-C2
39	B1	625	DGA	CB2-CB1-OG2-CG2
40	G	624	LHG	C8-C7-O7-C5
40	n	624	LHG	C8-C7-O7-C5
40	d1	410	LHG	C8-C7-O7-C5
40	n1	624	LHG	C8-C7-O7-C5
40	y1	624	LHG	C8-C7-O7-C5
29	G	612	CLA	O1D-CGD-O2D-CED
29	b	612	CLA	O1D-CGD-O2D-CED
29	g	604	CLA	O1D-CGD-O2D-CED
29	s	612	CLA	O1D-CGD-O2D-CED
29	N1	614	CLA	O1D-CGD-O2D-CED
29	G1	604	CLA	O1D-CGD-O2D-CED
29	d1	403	CLA	O1D-CGD-O2D-CED
29	y1	602	CLA	O1D-CGD-O2D-CED
29	C	509	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	a	407	CLA	CBD-CGD-O2D-CED
29	b	609	CLA	CBD-CGD-O2D-CED
29	c	506	CLA	CBD-CGD-O2D-CED
29	a1	406	CLA	CBD-CGD-O2D-CED
29	a1	407	CLA	CBD-CGD-O2D-CED
29	b1	605	CLA	CBD-CGD-O2D-CED
29	b1	612	CLA	CBD-CGD-O2D-CED
30	A1	409	PHO	CBD-CGD-O2D-CED
55	Y1	627	PTY	O30-C30-O4-C1
29	B	606	CLA	C4-C3-C5-C6
29	C	501	CLA	C4-C3-C5-C6
29	D	402	CLA	C4-C3-C5-C6
29	b	603	CLA	C4-C3-C5-C6
29	b	615	CLA	C4-C3-C5-C6
29	g	602	CLA	C4-C3-C5-C6
29	r	608	CLA	C4-C3-C5-C6
29	Y1	612	CLA	C4-C3-C5-C6
48	N	601	CHL	C4-C3-C5-C6
48	N1	601	CHL	C4-C3-C5-C6
48	N1	606	CHL	C4-C3-C5-C6
29	C	501	CLA	C2-C3-C5-C6
29	d	403	CLA	C2-C3-C5-C6
29	C1	504	CLA	C2-C3-C5-C6
29	b1	606	CLA	C2-C3-C5-C6
29	b1	609	CLA	C2-C3-C5-C6
48	N	601	CHL	C2-C3-C5-C6
48	G	609	CHL	C2-C3-C5-C6
48	N1	606	CHL	C2-C3-C5-C6
29	c	507	CLA	CBD-CGD-O2D-CED
29	s	611	CLA	CBD-CGD-O2D-CED
29	y	611	CLA	CBD-CGD-O2D-CED
29	B1	605	CLA	CBD-CGD-O2D-CED
29	r1	604	CLA	CBD-CGD-O2D-CED
30	A	409	PHO	CBD-CGD-O2D-CED
29	R	603	CLA	C2A-CAA-CBA-CGA
29	R	608	CLA	C2A-CAA-CBA-CGA
29	R	609	CLA	C2A-CAA-CBA-CGA
29	S	614	CLA	C2A-CAA-CBA-CGA
29	Y	608	CLA	C2A-CAA-CBA-CGA
29	c	507	CLA	C2A-CAA-CBA-CGA
29	g	613	CLA	C2A-CAA-CBA-CGA
29	g	614	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
29	s	602	CLA	C2A-CAA-CBA-CGA
29	s	603	CLA	C2A-CAA-CBA-CGA
29	s	614	CLA	C2A-CAA-CBA-CGA
29	N1	604	CLA	C2A-CAA-CBA-CGA
29	G1	613	CLA	C2A-CAA-CBA-CGA
29	R1	609	CLA	C2A-CAA-CBA-CGA
29	R1	612	CLA	C2A-CAA-CBA-CGA
29	b1	613	CLA	C2A-CAA-CBA-CGA
29	b1	617	CLA	C2A-CAA-CBA-CGA
29	c1	507	CLA	C2A-CAA-CBA-CGA
29	n1	602	CLA	C2A-CAA-CBA-CGA
29	n1	611	CLA	C2A-CAA-CBA-CGA
29	g1	613	CLA	C2A-CAA-CBA-CGA
29	g1	614	CLA	C2A-CAA-CBA-CGA
29	r1	609	CLA	C2A-CAA-CBA-CGA
29	s1	602	CLA	C2A-CAA-CBA-CGA
29	s1	609	CLA	C2A-CAA-CBA-CGA
29	s1	612	CLA	C2A-CAA-CBA-CGA
29	s1	617	CLA	C2A-CAA-CBA-CGA
30	A	409	PHO	C2A-CAA-CBA-CGA
48	N	608	CHL	C2A-CAA-CBA-CGA
48	S	608	CHL	C2A-CAA-CBA-CGA
48	n	608	CHL	C2A-CAA-CBA-CGA
48	Y1	607	CHL	C2A-CAA-CBA-CGA
29	B1	604	CLA	O1A-CGA-O2A-C1
29	b	615	CLA	O1D-CGD-O2D-CED
33	A	413	LMG	C17-C18-C19-C20
33	A	413	LMG	C35-C36-C37-C38
33	A	413	LMG	C38-C39-C40-C41
33	B	622	LMG	C17-C18-C19-C20
33	C	521	LMG	C17-C18-C19-C20
33	C	521	LMG	C35-C36-C37-C38
33	C	523	LMG	C17-C18-C19-C20
33	C	523	LMG	C41-C42-C43-C44
33	D	411	LMG	C17-C18-C19-C20
33	D	411	LMG	C20-C21-C22-C23
33	H	102	LMG	C38-C39-C40-C41
33	W	201	LMG	C35-C36-C37-C38
33	W	201	LMG	C38-C39-C40-C41
33	a	413	LMG	C17-C18-C19-C20
33	a	413	LMG	C35-C36-C37-C38
33	a	413	LMG	C38-C39-C40-C41

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Mol	Chain	Res	Type	Atoms
33	b	622	LMG	C17-C18-C19-C20
33	c	521	LMG	C17-C18-C19-C20
33	c	521	LMG	C35-C36-C37-C38
33	c	523	LMG	C41-C42-C43-C44
33	d	411	LMG	C17-C18-C19-C20
33	d	411	LMG	C20-C21-C22-C23
33	h	102	LMG	C38-C39-C40-C41
33	w	201	LMG	C35-C36-C37-C38
33	A1	413	LMG	C17-C18-C19-C20
33	A1	413	LMG	C35-C36-C37-C38
33	A1	413	LMG	C38-C39-C40-C41
33	B1	622	LMG	C17-C18-C19-C20
33	C1	521	LMG	C17-C18-C19-C20
33	C1	521	LMG	C35-C36-C37-C38
33	C1	523	LMG	C17-C18-C19-C20
33	C1	523	LMG	C41-C42-C43-C44
33	D1	411	LMG	C17-C18-C19-C20
33	D1	411	LMG	C20-C21-C22-C23
33	H1	102	LMG	C38-C39-C40-C41
33	W1	201	LMG	C35-C36-C37-C38
33	W1	201	LMG	C38-C39-C40-C41
33	a1	413	LMG	C17-C18-C19-C20
33	a1	413	LMG	C35-C36-C37-C38
33	a1	413	LMG	C38-C39-C40-C41
33	b1	622	LMG	C17-C18-C19-C20
33	c1	521	LMG	C17-C18-C19-C20
33	c1	521	LMG	C35-C36-C37-C38
33	c1	523	LMG	C17-C18-C19-C20
33	c1	523	LMG	C41-C42-C43-C44
33	d1	411	LMG	C17-C18-C19-C20
33	d1	411	LMG	C20-C21-C22-C23
33	h1	102	LMG	C38-C39-C40-C41
33	w1	201	LMG	C35-C36-C37-C38
33	w1	201	LMG	C38-C39-C40-C41
37	C	518	DGD	C8B-C9B-CAB-CBB
37	C	519	DGD	C8A-C9A-CAA-CBA
37	C	519	DGD	CBB-CCB-CDB-CEB
37	C	520	DGD	CBB-CCB-CDB-CEB
37	c	518	DGD	C8B-C9B-CAB-CBB
37	c	519	DGD	C8A-C9A-CAA-CBA
37	c	519	DGD	CBB-CCB-CDB-CEB
37	c	520	DGD	CBB-CCB-CDB-CEB

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Mol	Chain	Res	Type	Atoms
37	C1	518	DGD	C8B-C9B-CAB-CBB
37	C1	519	DGD	C8A-C9A-CAA-CBA
37	C1	520	DGD	CBB-CCB-CDB-CEB
37	c1	518	DGD	C8B-C9B-CAB-CBB
37	c1	519	DGD	C8A-C9A-CAA-CBA
37	c1	519	DGD	CBB-CCB-CDB-CEB
37	c1	520	DGD	CBB-CCB-CDB-CEB
40	c	525	LHG	C11-C12-C13-C14
47	K1	101	4RF	C29-C30-C31-C32
29	R	602	CLA	C3-C5-C6-C7
29	R	612	CLA	C3-C5-C6-C7
29	S	610	CLA	C3-C5-C6-C7
29	c	504	CLA	C3-C5-C6-C7
29	c	511	CLA	C3-C5-C6-C7
29	n	603	CLA	C3-C5-C6-C7
29	r	608	CLA	C3-C5-C6-C7
29	s	609	CLA	C3-C5-C6-C7
29	y	603	CLA	C3-C5-C6-C7
29	B1	610	CLA	C3-C5-C6-C7
29	C1	511	CLA	C3-C5-C6-C7
29	c1	504	CLA	C3-C5-C6-C7
29	c1	505	CLA	C3-C5-C6-C7
29	c1	506	CLA	C3-C5-C6-C7
29	c1	507	CLA	C3-C5-C6-C7
29	r1	609	CLA	C3-C5-C6-C7
29	s1	610	CLA	C3-C5-C6-C7
29	y1	604	CLA	C3-C5-C6-C7
29	y1	613	CLA	C3-C5-C6-C7
29	B	611	CLA	CBA-CGA-O2A-C1
29	B	613	CLA	CBA-CGA-O2A-C1
29	C	506	CLA	CBA-CGA-O2A-C1
29	C	509	CLA	CBA-CGA-O2A-C1
29	D	403	CLA	CBA-CGA-O2A-C1
29	N	603	CLA	CBA-CGA-O2A-C1
29	G	604	CLA	CBA-CGA-O2A-C1
29	R	604	CLA	CBA-CGA-O2A-C1
29	R	608	CLA	CBA-CGA-O2A-C1
29	S	602	CLA	CBA-CGA-O2A-C1
29	S	605	CLA	CBA-CGA-O2A-C1
29	S	613	CLA	CBA-CGA-O2A-C1
29	Y	604	CLA	CBA-CGA-O2A-C1
29	Y	613	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	b	608	CLA	CBA-CGA-O2A-C1
29	c	506	CLA	CBA-CGA-O2A-C1
29	c	509	CLA	CBA-CGA-O2A-C1
29	n	611	CLA	CBA-CGA-O2A-C1
29	g	611	CLA	CBA-CGA-O2A-C1
29	g	613	CLA	CBA-CGA-O2A-C1
29	r	608	CLA	CBA-CGA-O2A-C1
29	y	603	CLA	CBA-CGA-O2A-C1
29	y	608	CLA	CBA-CGA-O2A-C1
29	B1	604	CLA	CBA-CGA-O2A-C1
29	B1	611	CLA	CBA-CGA-O2A-C1
29	C1	504	CLA	CBA-CGA-O2A-C1
29	C1	511	CLA	CBA-CGA-O2A-C1
29	C1	513	CLA	CBA-CGA-O2A-C1
29	N1	610	CLA	CBA-CGA-O2A-C1
29	R1	604	CLA	CBA-CGA-O2A-C1
29	R1	609	CLA	CBA-CGA-O2A-C1
29	S1	602	CLA	CBA-CGA-O2A-C1
29	S1	617	CLA	CBA-CGA-O2A-C1
29	Y1	603	CLA	CBA-CGA-O2A-C1
29	Y1	612	CLA	CBA-CGA-O2A-C1
29	Y1	613	CLA	CBA-CGA-O2A-C1
29	a1	407	CLA	CBA-CGA-O2A-C1
29	b1	604	CLA	CBA-CGA-O2A-C1
29	b1	611	CLA	CBA-CGA-O2A-C1
29	c1	506	CLA	CBA-CGA-O2A-C1
29	c1	509	CLA	CBA-CGA-O2A-C1
29	d1	403	CLA	CBA-CGA-O2A-C1
29	n1	602	CLA	CBA-CGA-O2A-C1
29	g1	613	CLA	CBA-CGA-O2A-C1
29	g1	614	CLA	CBA-CGA-O2A-C1
29	r1	608	CLA	CBA-CGA-O2A-C1
29	s1	610	CLA	CBA-CGA-O2A-C1
29	y1	603	CLA	CBA-CGA-O2A-C1
29	y1	612	CLA	CBA-CGA-O2A-C1
32	M	101	SQD	C24-C23-O48-C46
33	c	521	LMG	C29-C28-O8-C9
38	T1	101	3PH	C32-C31-O31-C3
38	t1	101	3PH	C32-C31-O31-C3
47	i1	101	4RF	C15-C16-O18-C19
55	Y1	627	PTY	C31-C30-O4-C1
33	c1	521	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
33	c	523	LMG	C17-C18-C19-C20
33	w	201	LMG	C38-C39-C40-C41
37	C1	519	DGD	CBB-CCB-CDB-CEB
29	C	511	CLA	O1D-CGD-O2D-CED
29	D	402	CLA	O1D-CGD-O2D-CED
29	N	611	CLA	O1D-CGD-O2D-CED
29	G	602	CLA	O1D-CGD-O2D-CED
29	G	604	CLA	O1D-CGD-O2D-CED
29	b	608	CLA	O1D-CGD-O2D-CED
37	c1	520	DGD	C4D-C5D-C6D-O5D
43	d1	405	PL9	C47-C48-C49-C51
29	N	610	CLA	CBD-CGD-O2D-CED
29	c	504	CLA	CBD-CGD-O2D-CED
29	C	501	CLA	O1D-CGD-O2D-CED
29	S	614	CLA	O1D-CGD-O2D-CED
29	Y	603	CLA	O1D-CGD-O2D-CED
29	Y	613	CLA	O1D-CGD-O2D-CED
29	Y	614	CLA	O1D-CGD-O2D-CED
29	n	602	CLA	O1D-CGD-O2D-CED
29	r	602	CLA	O1D-CGD-O2D-CED
29	D1	402	CLA	O1D-CGD-O2D-CED
29	G1	602	CLA	O1D-CGD-O2D-CED
29	Y1	604	CLA	O1D-CGD-O2D-CED
29	b1	617	CLA	O1D-CGD-O2D-CED
29	c1	502	CLA	O1D-CGD-O2D-CED
29	c1	509	CLA	O1D-CGD-O2D-CED
29	s1	605	CLA	O1D-CGD-O2D-CED
29	y1	604	CLA	O1D-CGD-O2D-CED
30	a1	409	PHO	O1D-CGD-O2D-CED
32	m	101	SQD	O49-C7-O47-C45
43	d	405	PL9	C37-C38-C39-C41
43	D1	405	PL9	C7-C8-C9-C11
29	C	509	CLA	O1A-CGA-O2A-C1
29	R	609	CLA	O1A-CGA-O2A-C1
29	S	609	CLA	O1A-CGA-O2A-C1
29	Y	603	CLA	O1A-CGA-O2A-C1
29	Y	612	CLA	O1A-CGA-O2A-C1
29	b	606	CLA	O1A-CGA-O2A-C1
29	c	509	CLA	O1A-CGA-O2A-C1
29	n	611	CLA	O1A-CGA-O2A-C1
29	g	611	CLA	O1A-CGA-O2A-C1
29	s	617	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	y	608	CLA	O1A-CGA-O2A-C1
29	y	612	CLA	O1A-CGA-O2A-C1
29	B1	610	CLA	O1A-CGA-O2A-C1
29	B1	614	CLA	O1A-CGA-O2A-C1
29	C1	509	CLA	O1A-CGA-O2A-C1
29	N1	610	CLA	O1A-CGA-O2A-C1
29	R1	602	CLA	O1A-CGA-O2A-C1
29	R1	604	CLA	O1A-CGA-O2A-C1
29	S1	609	CLA	O1A-CGA-O2A-C1
29	S1	617	CLA	O1A-CGA-O2A-C1
29	Y1	603	CLA	O1A-CGA-O2A-C1
29	c1	509	CLA	O1A-CGA-O2A-C1
29	n1	602	CLA	O1A-CGA-O2A-C1
29	n1	603	CLA	O1A-CGA-O2A-C1
29	n1	611	CLA	O1A-CGA-O2A-C1
29	r1	608	CLA	O1A-CGA-O2A-C1
29	s1	617	CLA	O1A-CGA-O2A-C1
29	y1	603	CLA	O1A-CGA-O2A-C1
32	M	101	SQD	O10-C23-O48-C46
38	b	624	3PH	O32-C31-O31-C3
38	t1	101	3PH	O32-C31-O31-C3
29	r	612	CLA	O1D-CGD-O2D-CED
29	y	602	CLA	O1D-CGD-O2D-CED
29	N1	602	CLA	O1D-CGD-O2D-CED
29	y1	603	CLA	O1D-CGD-O2D-CED
31	B	618	BCR	C9-C10-C11-C12
31	C	514	BCR	C13-C14-C15-C16
31	B1	618	BCR	C9-C10-C11-C12
31	D1	404	BCR	C9-C10-C11-C12
31	c1	514	BCR	C13-C14-C15-C16
31	c1	515	BCR	C9-C10-C11-C12
45	h1	101	RRX	C19-C20-C21-C22
45	h1	101	RRX	C15-C16-C17-C18
51	S	623	NEX	C9-C10-C11-C12
52	r	625	LMT	O5B-C5B-C6B-O6B
33	D1	411	LMG	C4-C5-C6-O5
29	a	406	CLA	CBD-CGD-O2D-CED
29	c	501	CLA	CBD-CGD-O2D-CED
29	n	604	CLA	CBD-CGD-O2D-CED
29	N1	604	CLA	CBD-CGD-O2D-CED
29	B	613	CLA	O1D-CGD-O2D-CED
29	C	506	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	C	513	CLA	O1D-CGD-O2D-CED
29	a	410	CLA	O1D-CGD-O2D-CED
29	c	502	CLA	O1D-CGD-O2D-CED
29	c	509	CLA	O1D-CGD-O2D-CED
29	s	604	CLA	O1D-CGD-O2D-CED
29	N1	611	CLA	O1D-CGD-O2D-CED
30	a1	408	PHO	O1D-CGD-O2D-CED
40	D	409	LHG	O2-C2-C3-O3
40	N	624	LHG	O2-C2-C3-O3
40	S	624	LHG	O2-C2-C3-O3
40	c	525	LHG	O2-C2-C3-O3
40	d	409	LHG	O2-C2-C3-O3
40	d	410	LHG	O2-C2-C3-O3
40	g	624	LHG	O2-C2-C3-O3
40	y	624	LHG	O2-C2-C3-O3
40	D1	408	LHG	O2-C2-C3-O3
40	G1	624	LHG	O2-C2-C3-O3
40	S1	624	LHG	O2-C2-C3-O3
40	d1	408	LHG	O2-C2-C3-O3
40	d1	409	LHG	O2-C2-C3-O3
40	n1	624	LHG	O2-C2-C3-O3
40	s1	624	LHG	O2-C2-C3-O3
54	S	625	LPX	O1-C3-C4-O5
54	s	625	LPX	O1-C3-C4-O5
54	s1	625	LPX	O1-C3-C4-O5
29	B	608	CLA	C3-C5-C6-C7
29	R	610	CLA	C3-C5-C6-C7
29	S	613	CLA	C3-C5-C6-C7
29	n	610	CLA	C3-C5-C6-C7
29	r	603	CLA	C3-C5-C6-C7
29	s	613	CLA	C3-C5-C6-C7
29	A1	406	CLA	C3-C5-C6-C7
29	C1	509	CLA	C3-C5-C6-C7
29	S1	610	CLA	C3-C5-C6-C7
29	Y1	614	CLA	C3-C5-C6-C7
29	r1	602	CLA	C3-C5-C6-C7
30	A1	409	PHO	C3-C5-C6-C7
29	B	608	CLA	CBA-CGA-O2A-C1
29	N	610	CLA	CBA-CGA-O2A-C1
29	R	610	CLA	CBA-CGA-O2A-C1
29	S	610	CLA	CBA-CGA-O2A-C1
29	b	610	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	s	602	CLA	CBA-CGA-O2A-C1
29	s	610	CLA	CBA-CGA-O2A-C1
29	s	617	CLA	CBA-CGA-O2A-C1
29	y	602	CLA	CBA-CGA-O2A-C1
29	A1	407	CLA	CBA-CGA-O2A-C1
29	C1	509	CLA	CBA-CGA-O2A-C1
29	c1	508	CLA	CBA-CGA-O2A-C1
29	s1	602	CLA	CBA-CGA-O2A-C1
29	s1	603	CLA	CBA-CGA-O2A-C1
29	s1	604	CLA	CBA-CGA-O2A-C1
29	s1	617	CLA	CBA-CGA-O2A-C1
29	y1	608	CLA	CBA-CGA-O2A-C1
29	y1	614	CLA	CBA-CGA-O2A-C1
32	m	101	SQD	C24-C23-O48-C46
32	M1	101	SQD	C24-C23-O48-C46
29	B	613	CLA	O1A-CGA-O2A-C1
29	C	506	CLA	O1A-CGA-O2A-C1
29	Y	613	CLA	O1A-CGA-O2A-C1
29	b	608	CLA	O1A-CGA-O2A-C1
29	s	602	CLA	O1A-CGA-O2A-C1
29	R1	608	CLA	O1A-CGA-O2A-C1
29	s1	614	CLA	O1A-CGA-O2A-C1
37	B	623	DGD	O1A-C1A-O1G-C1G
38	T	101	3PH	O32-C31-O31-C3
38	t	101	3PH	O32-C31-O31-C3
29	B	611	CLA	O1D-CGD-O2D-CED
29	C	502	CLA	O1D-CGD-O2D-CED
29	Y	612	CLA	O1D-CGD-O2D-CED
29	b	607	CLA	O1D-CGD-O2D-CED
29	y	604	CLA	O1D-CGD-O2D-CED
29	y	612	CLA	O1D-CGD-O2D-CED
29	C1	507	CLA	O1D-CGD-O2D-CED
29	b1	611	CLA	O1D-CGD-O2D-CED
54	s	625	LPX	O5-C4-C5-O6
32	m	101	SQD	C8-C7-O47-C45
32	B1	621	SQD	C8-C7-O47-C45
32	B1	626	SQD	C8-C7-O47-C45
32	M1	101	SQD	C8-C7-O47-C45
33	C	521	LMG	C11-C10-O7-C8
33	C1	523	LMG	C11-C10-O7-C8
39	B	625	DGA	CB2-CB1-OG2-CG2
39	b	625	DGA	CB2-CB1-OG2-CG2

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Mol	Chain	Res	Type	Atoms
43	d1	405	PL9	C47-C48-C49-C50
29	s	603	CLA	CBD-CGD-O2D-CED
29	B1	602	CLA	CBD-CGD-O2D-CED
29	b1	610	CLA	CBD-CGD-O2D-CED
29	g1	614	CLA	CBD-CGD-O2D-CED
29	s1	610	CLA	CBD-CGD-O2D-CED
33	H	102	LMG	O6-C5-C6-O5
37	c1	519	DGD	O6E-C5E-C6E-O5E
32	M1	101	SQD	C11-C10-C9-C8
40	C1	525	LHG	C11-C12-C13-C14
40	L1	101	LHG	C11-C12-C13-C14
47	I1	102	4RF	C33-C34-C35-C36
30	a	409	PHO	O1D-CGD-O2D-CED
29	S	602	CLA	O1A-CGA-O2A-C1
29	R1	609	CLA	O1A-CGA-O2A-C1
33	H1	102	LMG	C11-C12-C13-C14
40	C	525	LHG	C11-C12-C13-C14
52	r1	625	LMT	C4B-C5B-C6B-O6B
29	s1	604	CLA	O1D-CGD-O2D-CED
40	L	101	LHG	C7-C8-C9-C10
39	C	524	DGA	CCB-CDB-CEB-CFB
47	k1	101	4RF	C48-C49-C50-C51
29	N1	610	CLA	C5-C6-C7-C8
29	C	512	CLA	C3-C5-C6-C7
29	B1	617	CLA	C3-C5-C6-C7
29	c1	508	CLA	C3-C5-C6-C7
29	c1	512	CLA	C3-C5-C6-C7
48	S	608	CHL	C3-C5-C6-C7
29	R	609	CLA	CBA-CGA-O2A-C1
29	S	609	CLA	CBA-CGA-O2A-C1
29	Y	612	CLA	CBA-CGA-O2A-C1
29	b	606	CLA	CBA-CGA-O2A-C1
29	S1	609	CLA	CBA-CGA-O2A-C1
38	T	101	3PH	C32-C31-O31-C3
38	b	624	3PH	C32-C31-O31-C3
29	c	510	CLA	O1D-CGD-O2D-CED
29	y	614	CLA	O1D-CGD-O2D-CED
29	B1	611	CLA	O1D-CGD-O2D-CED
37	B1	623	DGD	O6E-C5E-C6E-O5E
52	R	625	LMT	O5'-C5'-C6'-O6'
32	B1	621	SQD	O49-C7-O47-C45
33	C1	523	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
40	s1	624	LHG	C9-C10-C11-C12
40	D1	410	LHG	C2-C3-O3-P
29	B	608	CLA	O1A-CGA-O2A-C1
29	R	604	CLA	O1A-CGA-O2A-C1
29	R	610	CLA	O1A-CGA-O2A-C1
29	b	610	CLA	O1A-CGA-O2A-C1
29	y	603	CLA	O1A-CGA-O2A-C1
29	A1	407	CLA	O1A-CGA-O2A-C1
29	C1	504	CLA	O1A-CGA-O2A-C1
29	C1	511	CLA	O1A-CGA-O2A-C1
29	S1	602	CLA	O1A-CGA-O2A-C1
29	Y1	613	CLA	O1A-CGA-O2A-C1
29	b1	604	CLA	O1A-CGA-O2A-C1
29	c1	508	CLA	O1A-CGA-O2A-C1
29	d1	403	CLA	O1A-CGA-O2A-C1
29	s1	602	CLA	O1A-CGA-O2A-C1
29	s1	610	CLA	O1A-CGA-O2A-C1
32	m	101	SQD	O10-C23-O48-C46
32	M1	101	SQD	O10-C23-O48-C46
38	T1	101	3PH	O32-C31-O31-C3
44	F	101	HEM	C3D-CAD-CBD-CGD
44	f	101	HEM	C3D-CAD-CBD-CGD
44	F1	101	HEM	C3D-CAD-CBD-CGD
29	r1	608	CLA	C5-C6-C7-C8
29	B	604	CLA	C4-C3-C5-C6
29	C	504	CLA	C4-C3-C5-C6
29	N	610	CLA	C4-C3-C5-C6
29	b	606	CLA	C4-C3-C5-C6
29	c	503	CLA	C4-C3-C5-C6
29	B1	606	CLA	C4-C3-C5-C6
29	N1	610	CLA	C4-C3-C5-C6
29	G1	602	CLA	C4-C3-C5-C6
29	Y1	602	CLA	C4-C3-C5-C6
29	b1	603	CLA	C4-C3-C5-C6
29	c1	503	CLA	C4-C3-C5-C6
29	g1	611	CLA	C4-C3-C5-C6
29	s1	614	CLA	C4-C3-C5-C6
43	D1	405	PL9	C20-C19-C21-C22
52	R	625	LMT	C4B-C5B-C6B-O6B
29	B	604	CLA	C2-C3-C5-C6
29	B	607	CLA	C2-C3-C5-C6
29	C	504	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	N	610	CLA	C2-C3-C5-C6
29	b	606	CLA	C2-C3-C5-C6
29	b	615	CLA	C2-C3-C5-C6
29	c	503	CLA	C2-C3-C5-C6
29	r	608	CLA	C2-C3-C5-C6
29	B1	606	CLA	C2-C3-C5-C6
29	B1	608	CLA	C2-C3-C5-C6
29	N1	610	CLA	C2-C3-C5-C6
29	G1	602	CLA	C2-C3-C5-C6
29	S1	602	CLA	C2-C3-C5-C6
29	Y1	602	CLA	C2-C3-C5-C6
29	a1	410	CLA	C2-C3-C5-C6
29	b1	603	CLA	C2-C3-C5-C6
29	c1	503	CLA	C2-C3-C5-C6
29	g1	611	CLA	C2-C3-C5-C6
29	s1	614	CLA	C2-C3-C5-C6
39	c1	524	DGA	CA1-CA2-CA3-CA4
55	y	627	PTY	O30-C30-O4-C1
29	A	407	CLA	C2A-CAA-CBA-CGA
29	S	602	CLA	C2A-CAA-CBA-CGA
29	a	407	CLA	C2A-CAA-CBA-CGA
29	G1	614	CLA	C2A-CAA-CBA-CGA
29	S1	602	CLA	C2A-CAA-CBA-CGA
29	Y1	610	CLA	C2A-CAA-CBA-CGA
29	b1	605	CLA	C2A-CAA-CBA-CGA
48	n	605	CHL	C2A-CAA-CBA-CGA
48	y	607	CHL	C2A-CAA-CBA-CGA
48	Y1	605	CHL	C2A-CAA-CBA-CGA
48	Y1	606	CHL	C2A-CAA-CBA-CGA
29	g	602	CLA	O1D-CGD-O2D-CED
29	B1	608	CLA	O1D-CGD-O2D-CED
29	Y1	612	CLA	O1D-CGD-O2D-CED
29	c1	513	CLA	O1D-CGD-O2D-CED
29	r1	602	CLA	O1D-CGD-O2D-CED
29	s1	617	CLA	O1D-CGD-O2D-CED
47	k	101	4RF	C48-C49-C50-C51
47	k1	101	4RF	C12-C13-C14-C15
33	D1	411	LMG	O6-C5-C6-O5
52	R1	625	LMT	O5'-C5'-C6'-O6'
29	N	603	CLA	O1A-CGA-O2A-C1
29	y	602	CLA	O1A-CGA-O2A-C1
29	C1	506	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	a1	407	CLA	O1A-CGA-O2A-C1
29	s1	603	CLA	O1A-CGA-O2A-C1
29	s1	604	CLA	O1A-CGA-O2A-C1
29	y1	608	CLA	O1A-CGA-O2A-C1
32	c	526	SQD	O5-C1-O6-C44
33	B	622	LMG	O6-C1-O1-C7
33	W1	201	LMG	O6-C1-O1-C7
33	a1	413	LMG	O6-C1-O1-C7
52	R	625	LMT	O5'-C1'-O1'-C1
43	d	405	PL9	C39-C41-C42-C43
43	D1	405	PL9	C14-C16-C17-C18
43	d1	405	PL9	C39-C41-C42-C43
29	A	405	CLA	CBA-CGA-O2A-C1
29	C	511	CLA	CBA-CGA-O2A-C1
29	g	602	CLA	CBA-CGA-O2A-C1
29	r	604	CLA	CBA-CGA-O2A-C1
29	C1	506	CLA	CBA-CGA-O2A-C1
29	b1	606	CLA	CBA-CGA-O2A-C1
33	c	523	LMG	C29-C28-O8-C9
38	s1	626	3PH	C32-C31-O31-C3
40	D1	410	LHG	C24-C23-O8-C6
47	K	101	4RF	C31-C32-C33-C34
47	k	101	4RF	C12-C13-C14-C15
29	c	512	CLA	O1D-CGD-O2D-CED
29	g	614	CLA	O1D-CGD-O2D-CED
29	s1	602	CLA	O1D-CGD-O2D-CED
40	L1	101	LHG	C7-C8-C9-C10
29	N	603	CLA	O1D-CGD-O2D-CED
29	S	612	CLA	O1D-CGD-O2D-CED
29	b	614	CLA	O1D-CGD-O2D-CED
29	G1	614	CLA	O1D-CGD-O2D-CED
29	R1	604	CLA	O1D-CGD-O2D-CED
29	S1	603	CLA	O1D-CGD-O2D-CED
29	Y1	602	CLA	O1D-CGD-O2D-CED
29	b1	613	CLA	O1D-CGD-O2D-CED
30	A1	408	PHO	O1D-CGD-O2D-CED
29	S	610	CLA	O1A-CGA-O2A-C1
29	y1	614	CLA	O1A-CGA-O2A-C1
39	j1	101	DGA	CB2-CB1-OG2-CG2
40	S1	624	LHG	C8-C7-O7-C5
55	Y	627	PTY	O10-C8-O7-C6
43	D1	405	PL9	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
29	C	507	CLA	O1D-CGD-O2D-CED
29	C	512	CLA	O1D-CGD-O2D-CED
29	b	613	CLA	O1D-CGD-O2D-CED
29	B1	609	CLA	O1D-CGD-O2D-CED
29	S1	602	CLA	O1D-CGD-O2D-CED
29	c1	507	CLA	O1D-CGD-O2D-CED
29	n1	614	CLA	O1D-CGD-O2D-CED
29	s	609	CLA	O1D-CGD-O2D-CED
40	L	101	LHG	C1-C2-C3-O3
40	S	624	LHG	C1-C2-C3-O3
40	d	409	LHG	C1-C2-C3-O3
40	g	624	LHG	C1-C2-C3-O3
40	s	624	LHG	C1-C2-C3-O3
40	D1	408	LHG	C1-C2-C3-O3
40	D1	409	LHG	C1-C2-C3-O3
40	N1	624	LHG	C1-C2-C3-O3
40	G1	624	LHG	C1-C2-C3-O3
40	c1	525	LHG	C1-C2-C3-O3
40	g1	624	LHG	C1-C2-C3-O3
33	C	521	LMG	O9-C10-O7-C8
29	C	511	CLA	O1A-CGA-O2A-C1
29	N	610	CLA	O1A-CGA-O2A-C1
29	G	613	CLA	O1A-CGA-O2A-C1
29	r	604	CLA	O1A-CGA-O2A-C1
29	s	603	CLA	O1A-CGA-O2A-C1
29	s	610	CLA	O1A-CGA-O2A-C1
29	b1	612	CLA	O1A-CGA-O2A-C1
40	D1	410	LHG	O10-C23-O8-C6
29	R1	610	CLA	C3-C5-C6-C7
29	b1	610	CLA	C3-C5-C6-C7
29	n1	604	CLA	C3-C5-C6-C7
29	r1	603	CLA	C3-C5-C6-C7
29	s1	609	CLA	C3-C5-C6-C7
29	R	604	CLA	O1D-CGD-O2D-CED
29	S	604	CLA	O1D-CGD-O2D-CED
29	Y	604	CLA	O1D-CGD-O2D-CED
29	S1	604	CLA	O1D-CGD-O2D-CED
29	B	606	CLA	CBA-CGA-O2A-C1
29	C	513	CLA	CBA-CGA-O2A-C1
29	N	602	CLA	CBA-CGA-O2A-C1
29	G	613	CLA	CBA-CGA-O2A-C1
29	S	603	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	a	407	CLA	CBA-CGA-O2A-C1
29	a	410	CLA	CBA-CGA-O2A-C1
29	b	613	CLA	CBA-CGA-O2A-C1
29	c	511	CLA	CBA-CGA-O2A-C1
29	r	602	CLA	CBA-CGA-O2A-C1
29	s	603	CLA	CBA-CGA-O2A-C1
29	y	614	CLA	CBA-CGA-O2A-C1
29	B1	606	CLA	CBA-CGA-O2A-C1
29	B1	612	CLA	CBA-CGA-O2A-C1
29	B1	617	CLA	CBA-CGA-O2A-C1
29	N1	602	CLA	CBA-CGA-O2A-C1
29	N1	603	CLA	CBA-CGA-O2A-C1
29	G1	602	CLA	CBA-CGA-O2A-C1
29	G1	613	CLA	CBA-CGA-O2A-C1
29	R1	612	CLA	CBA-CGA-O2A-C1
29	S1	610	CLA	CBA-CGA-O2A-C1
29	b1	605	CLA	CBA-CGA-O2A-C1
29	b1	608	CLA	CBA-CGA-O2A-C1
29	b1	612	CLA	CBA-CGA-O2A-C1
29	b1	613	CLA	CBA-CGA-O2A-C1
29	c1	510	CLA	CBA-CGA-O2A-C1
29	c1	511	CLA	CBA-CGA-O2A-C1
29	r1	602	CLA	CBA-CGA-O2A-C1
29	r1	604	CLA	CBA-CGA-O2A-C1
30	A1	409	PHO	CBA-CGA-O2A-C1
32	A1	412	SQD	C24-C23-O48-C46
32	m1	101	SQD	C24-C23-O48-C46
37	C	520	DGD	C2A-C1A-O1G-C1G
37	c	520	DGD	C2A-C1A-O1G-C1G
37	C1	520	DGD	C2A-C1A-O1G-C1G
37	c1	520	DGD	C2A-C1A-O1G-C1G
38	S	626	3PH	C32-C31-O31-C3
38	s	626	3PH	C32-C31-O31-C3
40	L	101	LHG	C24-C23-O8-C6
40	d	410	LHG	C24-C23-O8-C6
40	C1	525	LHG	C24-C23-O8-C6
40	d1	408	LHG	C24-C23-O8-C6
47	k	101	4RF	C43-C41-O40-C39
55	y1	626	PTY	C31-C30-O4-C1
29	A1	406	CLA	CBD-CGD-O2D-CED
29	c1	512	CLA	CBD-CGD-O2D-CED
52	R1	625	LMT	C4'-C5'-C6'-O6'

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Mol	Chain	Res	Type	Atoms
39	C1	524	DGA	CAA-CBA-CCA-CDA
29	S	602	CLA	O1D-CGD-O2D-CED
31	C	515	BCR	C19-C20-C21-C22
49	N	621	LUT	C29-C30-C31-C32
49	r1	620	LUT	C29-C30-C31-C32
47	i1	101	4RF	C13-C14-C15-C16
40	D1	409	LHG	C9-C10-C11-C12
29	b	609	CLA	C5-C6-C7-C8
29	b	615	CLA	C10-C11-C12-C13
29	B1	604	CLA	C13-C15-C16-C17
29	S1	609	CLA	C10-C11-C12-C13
33	H1	102	LMG	O6-C5-C6-O5
33	a1	413	LMG	O6-C5-C6-O5
32	m1	101	SQD	O10-C23-O48-C46
33	c	523	LMG	O10-C28-O8-C9
37	B1	623	DGD	C4E-C5E-C6E-O5E
52	r	625	LMT	C4B-C5B-C6B-O6B
32	b1	626	SQD	C11-C12-C13-C14
40	L1	101	LHG	O6-C4-C5-O7
33	a	413	LMG	O6-C5-C6-O5
52	R	625	LMT	C4'-C5'-C6'-O6'
37	c1	520	DGD	O6D-C5D-C6D-O5D
29	B	608	CLA	C10-C11-C12-C13
29	C	507	CLA	C13-C15-C16-C17
29	C	512	CLA	C5-C6-C7-C8
29	b	608	CLA	C5-C6-C7-C8
29	r	610	CLA	C10-C11-C12-C13
29	y	612	CLA	C5-C6-C7-C8
29	B1	602	CLA	C13-C15-C16-C17
29	B1	612	CLA	C8-C10-C11-C12
29	B1	613	CLA	C10-C11-C12-C13
29	B1	616	CLA	C8-C10-C11-C12
29	C1	503	CLA	C8-C10-C11-C12
29	Y1	602	CLA	C5-C6-C7-C8
29	Y1	613	CLA	C5-C6-C7-C8
29	c1	511	CLA	C8-C10-C11-C12
29	c1	513	CLA	C15-C16-C17-C18
29	d1	402	CLA	C10-C11-C12-C13
40	d	408	LHG	O2-C2-C3-O3
40	c1	525	LHG	O2-C2-C3-O3
29	N1	602	CLA	C3-C5-C6-C7
29	R1	602	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
37	C1	518	DGD	C1B-C2B-C3B-C4B
39	J1	101	DGA	CB1-CB2-CB3-CB4
40	D	410	LHG	C23-C24-C25-C26
40	G1	624	LHG	C7-C8-C9-C10
40	d1	410	LHG	C23-C24-C25-C26
32	a	412	SQD	C2-C1-O6-C44
32	c	526	SQD	C2-C1-O6-C44
33	B	622	LMG	C2-C1-O1-C7
33	b	622	LMG	C2-C1-O1-C7
37	B	623	DGD	C2D-C1D-O3G-C3G
37	b	623	DGD	C2D-C1D-O3G-C3G
37	C1	519	DGD	C2E-C1E-O5D-C6D
37	b1	623	DGD	C2D-C1D-O3G-C3G
37	b1	623	DGD	C2E-C1E-O5D-C6D
33	a1	413	LMG	O1-C7-C8-O7
33	d1	411	LMG	O1-C7-C8-O7
47	i1	101	4RF	O21-C20-C39-O40
39	c	524	DGA	CB9-CAB-CBB-CCB
47	I	102	4RF	C33-C34-C35-C36
47	i	101	4RF	C33-C34-C35-C36
29	S	603	CLA	O1A-CGA-O2A-C1
29	g	602	CLA	O1A-CGA-O2A-C1
29	B1	617	CLA	O1A-CGA-O2A-C1
29	N1	603	CLA	O1A-CGA-O2A-C1
29	r1	602	CLA	O1A-CGA-O2A-C1
52	R	625	LMT	O5B-C5B-C6B-O6B
29	s	603	CLA	C4-C3-C5-C6
48	s	608	CHL	C4-C3-C5-C6
29	D	402	CLA	C2-C3-C5-C6
29	Y1	612	CLA	C2-C3-C5-C6
48	N1	601	CHL	C2-C3-C5-C6
29	B	602	CLA	C11-C12-C13-C14
29	B	603	CLA	C14-C13-C15-C16
29	B	605	CLA	C6-C7-C8-C9
29	B	617	CLA	C14-C13-C15-C16
29	C	501	CLA	C11-C12-C13-C14
29	C	513	CLA	C11-C10-C8-C9
29	D	402	CLA	C6-C7-C8-C9
29	D	402	CLA	C14-C13-C15-C16
29	N	604	CLA	C11-C12-C13-C14
29	N	610	CLA	C11-C10-C8-C9
29	G	613	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	R	602	CLA	C6-C7-C8-C9
29	R	608	CLA	C11-C10-C8-C9
29	R	610	CLA	C6-C7-C8-C9
29	Y	603	CLA	C6-C7-C8-C9
29	Y	604	CLA	C11-C10-C8-C9
29	Y	614	CLA	C14-C13-C15-C16
29	b	603	CLA	C14-C13-C15-C16
29	b	605	CLA	C6-C7-C8-C9
29	b	606	CLA	C11-C10-C8-C9
29	b	607	CLA	C6-C7-C8-C9
29	b	616	CLA	C11-C10-C8-C9
29	c	501	CLA	C11-C12-C13-C14
29	c	504	CLA	C6-C7-C8-C9
29	c	505	CLA	C11-C10-C8-C9
29	c	513	CLA	C11-C10-C8-C9
29	g	611	CLA	C14-C13-C15-C16
29	r	610	CLA	C6-C7-C8-C9
29	s	603	CLA	C14-C13-C15-C16
29	s	609	CLA	C11-C10-C8-C9
29	y	604	CLA	C6-C7-C8-C9
29	A1	410	CLA	C6-C7-C8-C9
29	B1	602	CLA	C11-C12-C13-C14
29	B1	604	CLA	C11-C10-C8-C9
29	B1	606	CLA	C11-C10-C8-C9
29	B1	607	CLA	C6-C7-C8-C9
29	B1	610	CLA	C14-C13-C15-C16
29	B1	617	CLA	C14-C13-C15-C16
29	C1	508	CLA	C6-C7-C8-C9
29	C1	513	CLA	C11-C10-C8-C9
29	N1	604	CLA	C11-C12-C13-C14
29	R1	602	CLA	C6-C7-C8-C9
29	R1	612	CLA	C11-C10-C8-C9
29	S1	609	CLA	C11-C10-C8-C9
29	Y1	604	CLA	C11-C10-C8-C9
29	Y1	614	CLA	C6-C7-C8-C9
29	b1	602	CLA	C11-C12-C13-C14
29	b1	604	CLA	C11-C10-C8-C9
29	b1	608	CLA	C11-C10-C8-C9
29	b1	610	CLA	C14-C13-C15-C16
29	c1	501	CLA	C11-C12-C13-C14
29	c1	502	CLA	C6-C7-C8-C9
29	c1	504	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
29	c1	511	CLA	C11-C10-C8-C9
29	g1	602	CLA	C11-C12-C13-C14
29	g1	613	CLA	C11-C10-C8-C9
29	r1	612	CLA	C6-C7-C8-C9
29	r1	612	CLA	C11-C10-C8-C9
29	s1	609	CLA	C11-C10-C8-C9
29	s1	611	CLA	C6-C7-C8-C9
29	y1	612	CLA	C11-C12-C13-C14
30	a1	408	PHO	C6-C7-C8-C9
30	a1	409	PHO	C6-C7-C8-C9
48	N	605	CHL	C14-C13-C15-C16
48	N	609	CHL	C11-C12-C13-C14
48	G	607	CHL	C14-C13-C15-C16
48	Y	607	CHL	C6-C7-C8-C9
48	Y	607	CHL	C14-C13-C15-C16
48	Y	609	CHL	C11-C12-C13-C14
48	g	601	CHL	C14-C13-C15-C16
48	g	609	CHL	C14-C13-C15-C16
48	y	601	CHL	C11-C10-C8-C9
48	y	606	CHL	C11-C10-C8-C9
48	y	607	CHL	C6-C7-C8-C9
48	y	609	CHL	C11-C12-C13-C14
48	N1	606	CHL	C14-C13-C15-C16
48	G1	607	CHL	C11-C10-C8-C9
48	G1	607	CHL	C14-C13-C15-C16
48	Y1	607	CHL	C11-C10-C8-C9
48	Y1	609	CHL	C11-C12-C13-C14
48	g1	601	CHL	C14-C13-C15-C16
48	g1	609	CHL	C14-C13-C15-C16
48	s1	608	CHL	C11-C10-C8-C9
48	y1	609	CHL	C11-C12-C13-C14
29	N	612	CLA	O1D-CGD-O2D-CED
29	R	602	CLA	O1D-CGD-O2D-CED
29	c	513	CLA	O1D-CGD-O2D-CED
29	n	603	CLA	O1D-CGD-O2D-CED
29	s	605	CLA	O1D-CGD-O2D-CED
29	A1	407	CLA	O1D-CGD-O2D-CED
29	B1	607	CLA	O1D-CGD-O2D-CED
29	G1	612	CLA	O1D-CGD-O2D-CED
29	Y	610	CLA	C5-C6-C7-C8
29	Y	611	CLA	C10-C11-C12-C13
29	Y	613	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
29	a	405	CLA	C2A-CAA-CBA-CGA
29	y	608	CLA	C2A-CAA-CBA-CGA
29	B1	604	CLA	C2A-CAA-CBA-CGA
29	Y1	613	CLA	C2A-CAA-CBA-CGA
29	b1	604	CLA	C2A-CAA-CBA-CGA
48	n	606	CHL	C2A-CAA-CBA-CGA
48	S1	601	CHL	C2A-CAA-CBA-CGA
48	n1	605	CHL	C2A-CAA-CBA-CGA
31	C	514	BCR	C36-C18-C19-C20
31	C	517	BCR	C37-C22-C23-C24
31	D	404	BCR	C36-C18-C19-C20
31	B1	618	BCR	C37-C22-C23-C24
31	C1	515	BCR	C7-C8-C9-C34
31	C1	515	BCR	C11-C12-C13-C35
31	C1	517	BCR	C37-C22-C23-C24
31	D1	404	BCR	C7-C8-C9-C34
31	D1	404	BCR	C37-C22-C23-C24
31	c1	514	BCR	C36-C18-C19-C20
31	c1	515	BCR	C7-C8-C9-C34
36	b	620	C7Z	C11-C12-C13-C20
36	B1	620	C7Z	C7-C8-C9-C19
36	b1	620	C7Z	C7-C8-C9-C19
45	H	101	RRX	C7-C8-C9-C34
45	h1	101	RRX	C36-C18-C19-C20
45	h1	101	RRX	C11-C12-C13-C35
49	Y	620	LUT	C27-C28-C29-C39
49	r	620	LUT	C7-C8-C9-C19
49	S1	621	LUT	C7-C8-C9-C19
49	n1	620	LUT	C27-C28-C29-C39
49	g1	621	LUT	C31-C32-C33-C40
49	s1	620	LUT	C31-C32-C33-C40
49	y1	620	LUT	C27-C28-C29-C39
50	R	621	XAT	C27-C28-C29-C39
50	r	621	XAT	C27-C28-C29-C39
51	y	623	NEX	C11-C12-C13-C20
31	C	516	BCR	C7-C8-C9-C10
31	C	516	BCR	C21-C22-C23-C24
31	C	517	BCR	C21-C22-C23-C24
31	B1	618	BCR	C11-C12-C13-C14
31	B1	618	BCR	C21-C22-C23-C24
31	C1	515	BCR	C7-C8-C9-C10
31	C1	515	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	C1	517	BCR	C21-C22-C23-C24
31	D1	404	BCR	C21-C22-C23-C24
31	c1	515	BCR	C7-C8-C9-C10
36	B	620	C7Z	C7-C8-C9-C10
36	B1	620	C7Z	C7-C8-C9-C10
36	b1	620	C7Z	C7-C8-C9-C10
45	H	101	RRX	C7-C8-C9-C10
45	h1	101	RRX	C17-C18-C19-C20
49	r	620	LUT	C7-C8-C9-C10
49	S1	621	LUT	C7-C8-C9-C10
49	g1	621	LUT	C31-C32-C33-C34
51	y1	623	NEX	C11-C12-C13-C14
29	D	403	CLA	O1D-CGD-O2D-CED
32	b	621	SQD	C8-C7-O47-C45
32	m1	101	SQD	C8-C7-O47-C45
33	c1	521	LMG	C11-C10-O7-C8
40	L1	101	LHG	C17-C18-C19-C20
40	c1	525	LHG	C33-C34-C35-C36
33	b1	622	LMG	C4-C5-C6-O5
32	B	626	SQD	C23-C24-C25-C26
33	D	411	LMG	C10-C11-C12-C13
39	j	101	DGA	CA1-CA2-CA3-CA4
40	D	408	LHG	C23-C24-C25-C26
40	D	410	LHG	C7-C8-C9-C10
40	d	410	LHG	C23-C24-C25-C26
29	a	410	CLA	O1A-CGA-O2A-C1
29	y	614	CLA	O1A-CGA-O2A-C1
29	G1	602	CLA	O1A-CGA-O2A-C1
29	R1	612	CLA	O1A-CGA-O2A-C1
29	S1	610	CLA	O1A-CGA-O2A-C1
29	b1	613	CLA	O1A-CGA-O2A-C1
29	c1	510	CLA	O1A-CGA-O2A-C1
29	c1	511	CLA	O1A-CGA-O2A-C1
29	r1	604	CLA	O1A-CGA-O2A-C1
38	S	626	3PH	O32-C31-O31-C3
47	k	101	4RF	O42-C41-O40-C39
29	N	610	CLA	C15-C16-C17-C18
29	G	603	CLA	C5-C6-C7-C8
29	Y	614	CLA	C8-C10-C11-C12
29	b	604	CLA	C15-C16-C17-C18
29	c	503	CLA	C15-C16-C17-C18
29	c	504	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	c	512	CLA	C13-C15-C16-C17
29	c	513	CLA	C10-C11-C12-C13
29	n	610	CLA	C15-C16-C17-C18
29	g	603	CLA	C8-C10-C11-C12
29	g	603	CLA	C10-C11-C12-C13
29	r	603	CLA	C5-C6-C7-C8
29	B1	614	CLA	C13-C15-C16-C17
29	R1	603	CLA	C5-C6-C7-C8
29	S1	611	CLA	C8-C10-C11-C12
29	Y1	610	CLA	C5-C6-C7-C8
29	b1	612	CLA	C15-C16-C17-C18
29	c1	506	CLA	C5-C6-C7-C8
29	g1	613	CLA	C10-C11-C12-C13
29	r1	603	CLA	C10-C11-C12-C13
29	y1	603	CLA	C13-C15-C16-C17
30	A	408	PHO	C15-C16-C17-C18
29	b	616	CLA	O1D-CGD-O2D-CED
29	s	602	CLA	O1D-CGD-O2D-CED
29	g1	613	CLA	O1D-CGD-O2D-CED
40	d1	409	LHG	C9-C10-C11-C12
47	k	101	4RF	C05-C06-C07-C08
37	B	623	DGD	C4D-C5D-C6D-O5D
52	r	625	LMT	O5'-C5'-C6'-O6'
52	r1	625	LMT	O5'-C5'-C6'-O6'
29	g	612	CLA	O1D-CGD-O2D-CED
29	S	609	CLA	C3-C5-C6-C7
29	S1	609	CLA	C3-C5-C6-C7
48	N	605	CHL	C3-C5-C6-C7
29	C	504	CLA	CBA-CGA-O2A-C1
29	a	405	CLA	CBA-CGA-O2A-C1
29	s	604	CLA	CBA-CGA-O2A-C1
29	y	610	CLA	CBA-CGA-O2A-C1
29	C1	503	CLA	CBA-CGA-O2A-C1
29	a1	405	CLA	CBA-CGA-O2A-C1
29	c1	513	CLA	CBA-CGA-O2A-C1
32	C1	526	SQD	C24-C23-O48-C46
38	B1	624	3PH	C32-C31-O31-C3
29	B	603	CLA	C8-C10-C11-C12
29	B	603	CLA	C15-C16-C17-C18
29	B	608	CLA	C13-C15-C16-C17
29	C	503	CLA	C15-C16-C17-C18
29	C	506	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	N	613	CLA	C5-C6-C7-C8
29	G	602	CLA	C15-C16-C17-C18
29	R	608	CLA	C10-C11-C12-C13
29	S	610	CLA	C13-C15-C16-C17
29	S	611	CLA	C8-C10-C11-C12
29	S	611	CLA	C15-C16-C17-C18
29	Y	614	CLA	C5-C6-C7-C8
29	b	606	CLA	C15-C16-C17-C18
29	b	610	CLA	C10-C11-C12-C13
29	b	615	CLA	C13-C15-C16-C17
29	c	509	CLA	C15-C16-C17-C18
29	n	604	CLA	C8-C10-C11-C12
29	g	613	CLA	C15-C16-C17-C18
29	s	609	CLA	C10-C11-C12-C13
29	s	611	CLA	C8-C10-C11-C12
29	y	602	CLA	C13-C15-C16-C17
29	y	603	CLA	C13-C15-C16-C17
29	B1	607	CLA	C13-C15-C16-C17
29	B1	609	CLA	C5-C6-C7-C8
29	C1	504	CLA	C15-C16-C17-C18
29	C1	508	CLA	C15-C16-C17-C18
29	C1	511	CLA	C10-C11-C12-C13
29	C1	511	CLA	C15-C16-C17-C18
29	N1	613	CLA	C5-C6-C7-C8
29	G1	602	CLA	C5-C6-C7-C8
29	G1	602	CLA	C8-C10-C11-C12
29	G1	603	CLA	C13-C15-C16-C17
29	S1	609	CLA	C8-C10-C11-C12
29	Y1	611	CLA	C10-C11-C12-C13
29	Y1	613	CLA	C15-C16-C17-C18
29	b1	604	CLA	C15-C16-C17-C18
29	b1	606	CLA	C15-C16-C17-C18
29	b1	614	CLA	C8-C10-C11-C12
29	c1	501	CLA	C10-C11-C12-C13
29	c1	508	CLA	C15-C16-C17-C18
29	n1	610	CLA	C8-C10-C11-C12
29	g1	611	CLA	C13-C15-C16-C17
29	r1	609	CLA	C10-C11-C12-C13
29	y1	602	CLA	C8-C10-C11-C12
29	y1	612	CLA	C13-C15-C16-C17
48	N	609	CHL	C13-C15-C16-C17
48	Y1	607	CHL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
48	y1	607	CHL	C8-C10-C11-C12
33	d1	411	LMG	O6-C5-C6-O5
33	h1	102	LMG	C15-C16-C17-C18
32	a1	412	SQD	C23-C24-C25-C26
33	B	622	LMG	C10-C11-C12-C13
33	H1	102	LMG	C28-C29-C30-C31
37	c	519	DGD	C1A-C2A-C3A-C4A
38	S	626	3PH	C31-C32-C33-C34
38	s1	626	3PH	C31-C32-C33-C34
39	C1	524	DGA	CA1-CA2-CA3-CA4
39	j1	101	DGA	CA1-CA2-CA3-CA4
40	C	525	LHG	C23-C24-C25-C26
40	c	525	LHG	C7-C8-C9-C10
40	c	525	LHG	C23-C24-C25-C26
40	y	624	LHG	C7-C8-C9-C10
47	i1	101	4RF	C22-C24-C25-C26
55	y1	626	PTY	C30-C31-C32-C33
29	C	510	CLA	O1D-CGD-O2D-CED
29	A	407	CLA	CBD-CGD-O2D-CED
53	r	626	ERG	C17-C20-C22-C23
53	r1	626	ERG	C17-C20-C22-C23
51	N1	623	NEX	C14-C15-C35-C34
29	N	613	CLA	O1D-CGD-O2D-CED
29	B	608	CLA	C5-C6-C7-C8
29	B	610	CLA	C8-C10-C11-C12
29	B	612	CLA	C15-C16-C17-C18
29	C	501	CLA	C10-C11-C12-C13
29	C	502	CLA	C13-C15-C16-C17
29	N	603	CLA	C8-C10-C11-C12
29	N	613	CLA	C8-C10-C11-C12
29	S	603	CLA	C13-C15-C16-C17
29	S	609	CLA	C10-C11-C12-C13
29	Y	602	CLA	C10-C11-C12-C13
29	Y	603	CLA	C15-C16-C17-C18
29	Y	604	CLA	C13-C15-C16-C17
29	a	410	CLA	C8-C10-C11-C12
29	b	603	CLA	C10-C11-C12-C13
29	b	603	CLA	C13-C15-C16-C17
29	b	608	CLA	C10-C11-C12-C13
29	b	612	CLA	C13-C15-C16-C17
29	b	617	CLA	C5-C6-C7-C8
29	c	506	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	c	512	CLA	C10-C11-C12-C13
29	n	604	CLA	C10-C11-C12-C13
29	s	609	CLA	C8-C10-C11-C12
29	s	611	CLA	C13-C15-C16-C17
29	s	611	CLA	C15-C16-C17-C18
29	y	613	CLA	C5-C6-C7-C8
29	y	613	CLA	C15-C16-C17-C18
29	B1	603	CLA	C5-C6-C7-C8
29	B1	607	CLA	C5-C6-C7-C8
29	B1	607	CLA	C10-C11-C12-C13
29	B1	608	CLA	C5-C6-C7-C8
29	B1	609	CLA	C8-C10-C11-C12
29	B1	610	CLA	C8-C10-C11-C12
29	C1	512	CLA	C13-C15-C16-C17
29	C1	513	CLA	C8-C10-C11-C12
29	D1	403	CLA	C10-C11-C12-C13
29	N1	610	CLA	C13-C15-C16-C17
29	N1	613	CLA	C8-C10-C11-C12
29	G1	603	CLA	C15-C16-C17-C18
29	G1	611	CLA	C15-C16-C17-C18
29	R1	603	CLA	C10-C11-C12-C13
29	S1	610	CLA	C5-C6-C7-C8
29	S1	614	CLA	C5-C6-C7-C8
29	Y1	602	CLA	C15-C16-C17-C18
29	Y1	611	CLA	C5-C6-C7-C8
29	Y1	613	CLA	C10-C11-C12-C13
29	b1	602	CLA	C15-C16-C17-C18
29	b1	603	CLA	C15-C16-C17-C18
29	b1	604	CLA	C8-C10-C11-C12
29	b1	610	CLA	C5-C6-C7-C8
29	b1	610	CLA	C13-C15-C16-C17
29	b1	611	CLA	C15-C16-C17-C18
29	b1	613	CLA	C10-C11-C12-C13
29	b1	614	CLA	C13-C15-C16-C17
29	b1	615	CLA	C10-C11-C12-C13
29	c1	504	CLA	C15-C16-C17-C18
29	c1	506	CLA	C15-C16-C17-C18
29	c1	509	CLA	C15-C16-C17-C18
29	d1	403	CLA	C10-C11-C12-C13
29	g1	610	CLA	C10-C11-C12-C13
29	r1	610	CLA	C10-C11-C12-C13
29	s1	603	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	s1	611	CLA	C13-C15-C16-C17
29	s1	613	CLA	C5-C6-C7-C8
33	b	622	LMG	C19-C20-C21-C22
29	b	603	CLA	O1D-CGD-O2D-CED
29	C1	512	CLA	O1D-CGD-O2D-CED
40	C	525	LHG	O1-C1-C2-O2
40	D	409	LHG	O1-C1-C2-O2
40	G	624	LHG	O1-C1-C2-O2
40	d	408	LHG	O1-C1-C2-O2
40	D1	408	LHG	O1-C1-C2-O2
40	L1	101	LHG	O1-C1-C2-O2
40	d1	408	LHG	O1-C1-C2-O2
46	I	101	GOL	O2-C2-C3-O3
29	C	513	CLA	O1A-CGA-O2A-C1
29	G1	613	CLA	O1A-CGA-O2A-C1
37	c1	520	DGD	O1A-C1A-O1G-C1G
32	A	412	SQD	C7-C8-C9-C10
32	m	101	SQD	C7-C8-C9-C10
32	M1	101	SQD	C7-C8-C9-C10
33	C	523	LMG	C28-C29-C30-C31
33	H	102	LMG	C28-C29-C30-C31
33	b	622	LMG	C28-C29-C30-C31
33	c	523	LMG	C10-C11-C12-C13
33	d	411	LMG	C28-C29-C30-C31
37	c1	519	DGD	C1B-C2B-C3B-C4B
38	b	624	3PH	C31-C32-C33-C34
38	B1	624	3PH	C31-C32-C33-C34
38	T1	101	3PH	C31-C32-C33-C34
38	s1	626	3PH	C21-C22-C23-C24
39	C	524	DGA	CB1-CB2-CB3-CB4
39	c	524	DGA	CB1-CB2-CB3-CB4
39	j1	101	DGA	CB1-CB2-CB3-CB4
40	N	624	LHG	C7-C8-C9-C10
40	d	409	LHG	C7-C8-C9-C10
40	d	410	LHG	C7-C8-C9-C10
40	n	624	LHG	C7-C8-C9-C10
40	C1	525	LHG	C23-C24-C25-C26
40	D1	408	LHG	C7-C8-C9-C10
40	D1	409	LHG	C23-C24-C25-C26
40	D1	410	LHG	C23-C24-C25-C26
40	c1	525	LHG	C7-C8-C9-C10
40	d1	408	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
40	d1	408	LHG	C23-C24-C25-C26
40	d1	410	LHG	C7-C8-C9-C10
40	y1	624	LHG	C7-C8-C9-C10
47	i	101	4RF	C13-C14-C15-C16
47	i	101	4RF	C41-C43-C44-C45
47	k	101	4RF	C41-C43-C44-C45
47	I1	102	4RF	C13-C14-C15-C16
47	i1	101	4RF	C41-C43-C44-C45
55	y	626	PTY	C8-C11-C12-C13
33	C	521	LMG	O6-C5-C6-O5
40	C1	525	LHG	C33-C34-C35-C36
40	D1	410	LHG	C24-C25-C26-C27
47	k1	101	4RF	C05-C06-C07-C08
29	B	608	CLA	C8-C10-C11-C12
29	B	608	CLA	C15-C16-C17-C18
29	B	614	CLA	C13-C15-C16-C17
29	B	617	CLA	C8-C10-C11-C12
29	C	507	CLA	C8-C10-C11-C12
29	C	507	CLA	C15-C16-C17-C18
29	C	508	CLA	C10-C11-C12-C13
29	C	512	CLA	C13-C15-C16-C17
29	N	602	CLA	C8-C10-C11-C12
29	b	604	CLA	C8-C10-C11-C12
29	b	614	CLA	C5-C6-C7-C8
29	c	507	CLA	C8-C10-C11-C12
29	n	604	CLA	C15-C16-C17-C18
29	r	602	CLA	C8-C10-C11-C12
29	r	612	CLA	C10-C11-C12-C13
29	s	604	CLA	C5-C6-C7-C8
29	y	611	CLA	C5-C6-C7-C8
29	B1	603	CLA	C10-C11-C12-C13
29	C1	502	CLA	C13-C15-C16-C17
29	N1	604	CLA	C10-C11-C12-C13
29	G1	602	CLA	C13-C15-C16-C17
29	S1	611	CLA	C15-C16-C17-C18
29	S1	613	CLA	C5-C6-C7-C8
29	b1	607	CLA	C8-C10-C11-C12
29	b1	612	CLA	C5-C6-C7-C8
29	b1	617	CLA	C8-C10-C11-C12
29	b1	617	CLA	C13-C15-C16-C17
29	c1	513	CLA	C10-C11-C12-C13
29	g1	602	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	s1	602	CLA	C5-C6-C7-C8
29	s1	614	CLA	C5-C6-C7-C8
29	y1	613	CLA	C15-C16-C17-C18
48	n1	606	CHL	C5-C6-C7-C8
48	n1	609	CHL	C15-C16-C17-C18
29	c	504	CLA	CBA-CGA-O2A-C1
29	g	610	CLA	CBA-CGA-O2A-C1
33	d	411	LMG	C31-C32-C33-C34
37	C1	519	DGD	C5B-C6B-C7B-C8B
39	B1	625	DGA	CA3-CA4-CA5-CA6
40	C	525	LHG	C16-C17-C18-C19
40	S1	624	LHG	C9-C10-C11-C12
29	n1	603	CLA	O1D-CGD-O2D-CED
33	h	102	LMG	O6-C5-C6-O5
32	b	621	SQD	O49-C7-O47-C45
32	m1	101	SQD	O49-C7-O47-C45
29	B	602	CLA	C2-C1-O2A-CGA
29	B	613	CLA	C2-C1-O2A-CGA
29	B	614	CLA	C2-C1-O2A-CGA
29	G	614	CLA	C2-C1-O2A-CGA
29	Y	603	CLA	C2-C1-O2A-CGA
29	Y	614	CLA	C2-C1-O2A-CGA
29	b	605	CLA	C2-C1-O2A-CGA
29	b	613	CLA	C2-C1-O2A-CGA
29	b	614	CLA	C2-C1-O2A-CGA
29	n	610	CLA	C2-C1-O2A-CGA
29	g	602	CLA	C2-C1-O2A-CGA
29	g	614	CLA	C2-C1-O2A-CGA
29	y	604	CLA	C2-C1-O2A-CGA
29	y	608	CLA	C2-C1-O2A-CGA
29	B1	606	CLA	C2-C1-O2A-CGA
29	B1	607	CLA	C2-C1-O2A-CGA
29	C1	509	CLA	C2-C1-O2A-CGA
29	C1	512	CLA	C2-C1-O2A-CGA
29	N1	611	CLA	C2-C1-O2A-CGA
29	N1	613	CLA	C2-C1-O2A-CGA
29	G1	602	CLA	C2-C1-O2A-CGA
29	G1	604	CLA	C2-C1-O2A-CGA
29	R1	603	CLA	C2-C1-O2A-CGA
29	Y1	603	CLA	C2-C1-O2A-CGA
29	Y1	608	CLA	C2-C1-O2A-CGA
29	Y1	614	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
29	b1	602	CLA	C2-C1-O2A-CGA
29	b1	608	CLA	C2-C1-O2A-CGA
29	b1	611	CLA	C2-C1-O2A-CGA
29	b1	617	CLA	C2-C1-O2A-CGA
29	c1	510	CLA	C2-C1-O2A-CGA
29	n1	603	CLA	C2-C1-O2A-CGA
29	n1	611	CLA	C2-C1-O2A-CGA
29	g1	614	CLA	C2-C1-O2A-CGA
29	r1	604	CLA	C2-C1-O2A-CGA
29	s1	610	CLA	C2-C1-O2A-CGA
29	y1	603	CLA	C2-C1-O2A-CGA
30	A1	409	PHO	C2-C1-O2A-CGA
29	C	501	CLA	C15-C16-C17-C18
29	D	403	CLA	C13-C15-C16-C17
29	G	611	CLA	C5-C6-C7-C8
29	R	603	CLA	C10-C11-C12-C13
29	n	603	CLA	C15-C16-C17-C18
29	s	613	CLA	C5-C6-C7-C8
29	y	612	CLA	C13-C15-C16-C17
29	B1	614	CLA	C5-C6-C7-C8
29	C1	510	CLA	C5-C6-C7-C8
29	C1	510	CLA	C13-C15-C16-C17
29	S1	602	CLA	C8-C10-C11-C12
29	S1	603	CLA	C13-C15-C16-C17
29	a1	405	CLA	C5-C6-C7-C8
29	b1	606	CLA	C13-C15-C16-C17
29	b1	609	CLA	C13-C15-C16-C17
29	d1	402	CLA	C8-C10-C11-C12
48	g	607	CHL	C5-C6-C7-C8
37	b1	623	DGD	C4D-C5D-C6D-O5D
33	B	622	LMG	C28-C29-C30-C31
38	S1	626	3PH	C31-C32-C33-C34
39	c	524	DGA	CA1-CA2-CA3-CA4
39	j	101	DGA	CB1-CB2-CB3-CB4
40	S1	624	LHG	C23-C24-C25-C26
40	n1	624	LHG	C7-C8-C9-C10
48	G1	608	CHL	C2A-CAA-CBA-CGA
48	R1	606	CHL	C2A-CAA-CBA-CGA
32	b	626	SQD	C8-C7-O47-C45
33	h1	102	LMG	C11-C10-O7-C8
29	c	502	CLA	C13-C15-C16-C17
29	c	510	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	g	611	CLA	C15-C16-C17-C18
29	s	610	CLA	C10-C11-C12-C13
29	s	610	CLA	C13-C15-C16-C17
29	B1	602	CLA	C10-C11-C12-C13
29	S1	604	CLA	C5-C6-C7-C8
29	a1	406	CLA	C5-C6-C7-C8
29	a1	406	CLA	C13-C15-C16-C17
29	b1	604	CLA	C10-C11-C12-C13
29	b1	607	CLA	C13-C15-C16-C17
29	b1	616	CLA	C13-C15-C16-C17
29	n1	603	CLA	C8-C10-C11-C12
30	a	408	PHO	C8-C10-C11-C12
29	A	410	CLA	O1D-CGD-O2D-CED
29	C	501	CLA	C11-C10-C8-C7
29	C	505	CLA	C12-C13-C15-C16
29	C	509	CLA	C12-C13-C15-C16
29	C	513	CLA	C12-C13-C15-C16
29	b	608	CLA	C11-C12-C13-C15
29	g	603	CLA	C11-C12-C13-C15
29	s	603	CLA	C12-C13-C15-C16
29	B1	602	CLA	C11-C10-C8-C7
29	G1	603	CLA	C11-C12-C13-C15
29	Y1	613	CLA	C12-C13-C15-C16
29	b1	610	CLA	C11-C12-C13-C15
29	b1	610	CLA	C12-C13-C15-C16
29	g1	602	CLA	C11-C12-C13-C15
29	r1	609	CLA	C6-C7-C8-C10
29	y1	602	CLA	C11-C12-C13-C15
30	a1	408	PHO	C11-C12-C13-C15
48	N	609	CHL	C11-C12-C13-C15
48	Y	606	CHL	C12-C13-C15-C16
48	g	601	CHL	C11-C12-C13-C15
48	y	601	CHL	C11-C10-C8-C7
48	y	607	CHL	C6-C7-C8-C10
29	a	405	CLA	O1A-CGA-O2A-C1
29	b	613	CLA	O1A-CGA-O2A-C1
29	r	602	CLA	O1A-CGA-O2A-C1
29	B1	612	CLA	O1A-CGA-O2A-C1
29	N1	602	CLA	O1A-CGA-O2A-C1
32	A1	412	SQD	O10-C23-O48-C46
37	C	520	DGD	O1A-C1A-O1G-C1G
38	s	626	3PH	O32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
40	L	101	LHG	O10-C23-O8-C6
40	d1	408	LHG	O10-C23-O8-C6
55	y1	626	PTY	O30-C30-O4-C1
31	C	514	BCR	C9-C10-C11-C12
31	a	411	BCR	C9-C10-C11-C12
31	b	618	BCR	C9-C10-C11-C12
31	b1	619	BCR	C19-C20-C21-C22
36	b1	620	C7Z	C29-C30-C31-C32
49	N1	620	LUT	C29-C30-C31-C32
49	G1	621	LUT	C29-C30-C31-C32
55	Y	626	PTY	C8-C11-C12-C13
29	b	615	CLA	C2A-CAA-CBA-CGA
29	g	610	CLA	C2A-CAA-CBA-CGA
29	s	613	CLA	C2A-CAA-CBA-CGA
29	A1	410	CLA	C2A-CAA-CBA-CGA
29	C1	507	CLA	C2A-CAA-CBA-CGA
29	R1	602	CLA	C2A-CAA-CBA-CGA
29	R1	604	CLA	C2A-CAA-CBA-CGA
29	c1	504	CLA	C2A-CAA-CBA-CGA
29	s1	613	CLA	C2A-CAA-CBA-CGA
48	N	606	CHL	C2A-CAA-CBA-CGA
48	Y	607	CHL	C2A-CAA-CBA-CGA
48	g	606	CHL	C2A-CAA-CBA-CGA
48	y	605	CHL	C2A-CAA-CBA-CGA
48	N1	608	CHL	C2A-CAA-CBA-CGA
29	N	604	CLA	O1D-CGD-O2D-CED
29	S	605	CLA	O1D-CGD-O2D-CED
29	Y	602	CLA	O1D-CGD-O2D-CED
29	a1	406	CLA	O1D-CGD-O2D-CED
29	b1	612	CLA	O1D-CGD-O2D-CED
29	y1	612	CLA	O1D-CGD-O2D-CED
29	B	607	CLA	C10-C11-C12-C13
29	D	403	CLA	C15-C16-C17-C18
29	G	602	CLA	C8-C10-C11-C12
29	Y	604	CLA	C15-C16-C17-C18
29	Y	611	CLA	C13-C15-C16-C17
29	b	602	CLA	C15-C16-C17-C18
29	d	403	CLA	C8-C10-C11-C12
29	g	611	CLA	C10-C11-C12-C13
29	r	610	CLA	C5-C6-C7-C8
29	r	612	CLA	C8-C10-C11-C12
29	y	610	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	B1	608	CLA	C8-C10-C11-C12
29	B1	608	CLA	C15-C16-C17-C18
29	B1	617	CLA	C8-C10-C11-C12
29	R1	612	CLA	C8-C10-C11-C12
29	S1	610	CLA	C13-C15-C16-C17
29	a1	410	CLA	C8-C10-C11-C12
29	b1	607	CLA	C5-C6-C7-C8
29	b1	614	CLA	C15-C16-C17-C18
29	c1	505	CLA	C10-C11-C12-C13
29	c1	512	CLA	C10-C11-C12-C13
29	n1	603	CLA	C5-C6-C7-C8
29	g1	611	CLA	C10-C11-C12-C13
29	y1	603	CLA	C15-C16-C17-C18
47	K1	101	4RF	C27-C28-C29-C30
40	C	525	LHG	C33-C34-C35-C36
29	B	606	CLA	O1A-CGA-O2A-C1
29	c	511	CLA	O1A-CGA-O2A-C1
29	b1	605	CLA	O1A-CGA-O2A-C1
30	A1	409	PHO	O1A-CGA-O2A-C1
37	c	520	DGD	O1A-C1A-O1G-C1G
32	b1	626	SQD	O5-C1-O6-C44
33	b1	622	LMG	O6-C1-O1-C7
37	C	519	DGD	O6E-C1E-O5D-C6D
37	c	519	DGD	O6E-C1E-O5D-C6D
37	C1	519	DGD	O6E-C1E-O5D-C6D
52	r1	625	LMT	O5'-C1'-O1'-C1
29	c	501	CLA	C10-C11-C12-C13
29	r	603	CLA	C8-C10-C11-C12
29	C1	512	CLA	C5-C6-C7-C8
29	N1	603	CLA	C8-C10-C11-C12
29	R1	603	CLA	C8-C10-C11-C12
29	Y1	604	CLA	C8-C10-C11-C12
29	c1	510	CLA	C15-C16-C17-C18
48	N	606	CHL	C5-C6-C7-C8
29	y	611	CLA	O1D-CGD-O2D-CED
29	G1	611	CLA	O1D-CGD-O2D-CED
37	c	518	DGD	C1B-C2B-C3B-C4B
47	I	102	4RF	C41-C43-C44-C45
31	C	517	BCR	C10-C11-C12-C13
31	b	619	BCR	C10-C11-C12-C13
31	c	515	BCR	C10-C11-C12-C13
31	B1	619	BCR	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
50	N1	622	XAT	C10-C11-C12-C13
50	Y1	622	XAT	C30-C31-C32-C33
51	N	623	NEX	C10-C11-C12-C13
51	G	623	NEX	C30-C31-C32-C33
51	R	622	NEX	C10-C11-C12-C13
51	S	623	NEX	C10-C11-C12-C13
51	y	623	NEX	C30-C31-C32-C33
51	G1	623	NEX	C30-C31-C32-C33
51	S1	623	NEX	C10-C11-C12-C13
51	g1	623	NEX	C10-C11-C12-C13
51	g1	623	NEX	C30-C31-C32-C33
37	c1	518	DGD	O6E-C5E-C6E-O5E
40	C	525	LHG	O2-C2-C3-O3
40	L	101	LHG	O2-C2-C3-O3
40	G	624	LHG	O2-C2-C3-O3
40	C1	525	LHG	O2-C2-C3-O3
33	c1	521	LMG	O9-C10-O7-C8
40	S1	624	LHG	O9-C7-O7-C5
29	R	603	CLA	C3-C5-C6-C7
29	y	611	CLA	C3-C5-C6-C7
29	S1	603	CLA	C3-C5-C6-C7
48	G1	601	CHL	C3-C5-C6-C7
29	G1	612	CLA	C2A-CAA-CBA-CGA
48	S1	606	CHL	C2A-CAA-CBA-CGA
29	B	602	CLA	C13-C15-C16-C17
29	C	501	CLA	C8-C10-C11-C12
29	C	513	CLA	C15-C16-C17-C18
29	D	403	CLA	C8-C10-C11-C12
29	N	604	CLA	C15-C16-C17-C18
29	G	611	CLA	C10-C11-C12-C13
29	R	608	CLA	C8-C10-C11-C12
29	S	610	CLA	C15-C16-C17-C18
29	S	611	CLA	C13-C15-C16-C17
29	Y	603	CLA	C13-C15-C16-C17
29	Y	611	CLA	C5-C6-C7-C8
29	Y	612	CLA	C10-C11-C12-C13
29	a	410	CLA	C5-C6-C7-C8
29	b	602	CLA	C10-C11-C12-C13
29	b	605	CLA	C8-C10-C11-C12
29	c	504	CLA	C10-C11-C12-C13
29	c	506	CLA	C15-C16-C17-C18
29	n	603	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	g	602	CLA	C8-C10-C11-C12
29	s	611	CLA	C5-C6-C7-C8
29	y	612	CLA	C15-C16-C17-C18
29	C1	506	CLA	C5-C6-C7-C8
29	C1	508	CLA	C13-C15-C16-C17
29	D1	403	CLA	C5-C6-C7-C8
29	G1	603	CLA	C10-C11-C12-C13
29	S1	610	CLA	C10-C11-C12-C13
29	Y1	602	CLA	C8-C10-C11-C12
29	b1	615	CLA	C5-C6-C7-C8
29	y1	602	CLA	C15-C16-C17-C18
29	y1	612	CLA	C8-C10-C11-C12
29	y1	614	CLA	C8-C10-C11-C12
48	N	609	CHL	C15-C16-C17-C18
48	g1	607	CHL	C5-C6-C7-C8
29	A	405	CLA	O1A-CGA-O2A-C1
29	N	602	CLA	O1A-CGA-O2A-C1
29	a	407	CLA	O1A-CGA-O2A-C1
29	s	604	CLA	O1A-CGA-O2A-C1
29	B1	606	CLA	O1A-CGA-O2A-C1
29	C1	503	CLA	O1A-CGA-O2A-C1
29	a1	405	CLA	O1A-CGA-O2A-C1
29	b1	608	CLA	O1A-CGA-O2A-C1
37	C1	520	DGD	O1A-C1A-O1G-C1G
38	s1	626	3PH	O32-C31-O31-C3
40	d	410	LHG	O10-C23-O8-C6
40	C1	525	LHG	O10-C23-O8-C6
39	b	625	DGA	CA1-CA2-CA3-CA4
47	k1	101	4RF	C41-C43-C44-C45
32	b	626	SQD	C11-C12-C13-C14
29	B	604	CLA	C13-C15-C16-C17
29	B	616	CLA	C8-C10-C11-C12
29	C	510	CLA	C13-C15-C16-C17
29	Y	613	CLA	C10-C11-C12-C13
29	b	602	CLA	C13-C15-C16-C17
29	b	607	CLA	C5-C6-C7-C8
29	b	610	CLA	C15-C16-C17-C18
29	c	501	CLA	C15-C16-C17-C18
29	n	602	CLA	C10-C11-C12-C13
29	n	603	CLA	C8-C10-C11-C12
29	n	613	CLA	C13-C15-C16-C17
29	y	614	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	B1	602	CLA	C5-C6-C7-C8
29	C1	507	CLA	C13-C15-C16-C17
29	C1	507	CLA	C15-C16-C17-C18
29	C1	508	CLA	C10-C11-C12-C13
29	S1	610	CLA	C8-C10-C11-C12
29	Y1	613	CLA	C8-C10-C11-C12
29	b1	602	CLA	C13-C15-C16-C17
29	b1	616	CLA	C8-C10-C11-C12
29	c1	506	CLA	C13-C15-C16-C17
29	c1	508	CLA	C5-C6-C7-C8
29	n1	613	CLA	C13-C15-C16-C17
29	g1	613	CLA	C15-C16-C17-C18
29	y1	603	CLA	C8-C10-C11-C12
48	n	609	CHL	C15-C16-C17-C18
32	M	101	SQD	C12-C13-C14-C15
32	a1	412	SQD	C15-C16-C17-C18
29	C	504	CLA	O1A-CGA-O2A-C1
29	g	610	CLA	O1A-CGA-O2A-C1
29	y	610	CLA	O1A-CGA-O2A-C1
29	b1	606	CLA	O1A-CGA-O2A-C1
29	c1	513	CLA	O1A-CGA-O2A-C1
32	C1	526	SQD	O10-C23-O48-C46
54	S1	625	LPX	O5-C4-C5-O6
32	c	526	SQD	C8-C7-O47-C45
33	C	523	LMG	C11-C10-O7-C8
33	a1	413	LMG	C11-C10-O7-C8
39	C1	524	DGA	CA3-CA4-CA5-CA6
40	y	624	LHG	C30-C31-C32-C33
29	a1	407	CLA	O1D-CGD-O2D-CED
29	B	602	CLA	C15-C16-C17-C18
29	D	403	CLA	C10-C11-C12-C13
29	N	602	CLA	C10-C11-C12-C13
29	G	611	CLA	C15-C16-C17-C18
29	R	608	CLA	C5-C6-C7-C8
29	S	611	CLA	C5-C6-C7-C8
29	Y	602	CLA	C8-C10-C11-C12
29	Y	604	CLA	C8-C10-C11-C12
29	Y	612	CLA	C5-C6-C7-C8
29	Y	612	CLA	C8-C10-C11-C12
29	b	608	CLA	C8-C10-C11-C12
29	b	610	CLA	C13-C15-C16-C17
29	b	615	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	c	505	CLA	C8-C10-C11-C12
29	c	507	CLA	C13-C15-C16-C17
29	d	403	CLA	C10-C11-C12-C13
29	s	602	CLA	C10-C11-C12-C13
29	y	612	CLA	C10-C11-C12-C13
29	B1	608	CLA	C10-C11-C12-C13
29	B1	614	CLA	C10-C11-C12-C13
29	C1	510	CLA	C15-C16-C17-C18
29	S1	602	CLA	C5-C6-C7-C8
29	Y1	611	CLA	C13-C15-C16-C17
29	b1	608	CLA	C10-C11-C12-C13
29	b1	617	CLA	C5-C6-C7-C8
29	c1	505	CLA	C5-C6-C7-C8
29	s1	609	CLA	C5-C6-C7-C8
29	s1	610	CLA	C10-C11-C12-C13
29	s1	611	CLA	C15-C16-C17-C18
29	y1	614	CLA	C5-C6-C7-C8
48	n	606	CHL	C5-C6-C7-C8
48	S1	608	CHL	C10-C11-C12-C13
40	C	525	LHG	C3-O3-P-O6
40	D	408	LHG	C3-O3-P-O6
40	D	408	LHG	C4-O6-P-O3
40	D	409	LHG	C3-O3-P-O6
40	D	410	LHG	C3-O3-P-O6
40	L	101	LHG	C3-O3-P-O6
40	G	624	LHG	C4-O6-P-O3
40	S	624	LHG	C4-O6-P-O3
40	Y	624	LHG	C4-O6-P-O3
40	c	525	LHG	C4-O6-P-O3
40	d	408	LHG	C3-O3-P-O6
40	d	408	LHG	C4-O6-P-O3
40	n	624	LHG	C4-O6-P-O3
40	s	624	LHG	C4-O6-P-O3
40	C1	525	LHG	C4-O6-P-O3
40	D1	409	LHG	C3-O3-P-O6
40	D1	409	LHG	C4-O6-P-O3
40	D1	410	LHG	C4-O6-P-O3
40	L1	101	LHG	C3-O3-P-O6
40	N1	624	LHG	C4-O6-P-O3
40	G1	624	LHG	C4-O6-P-O3
40	c1	525	LHG	C4-O6-P-O3
40	d1	408	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
40	d1	408	LHG	C4-O6-P-O3
40	d1	409	LHG	C3-O3-P-O6
40	d1	410	LHG	C4-O6-P-O3
40	n1	624	LHG	C4-O6-P-O3
54	s	625	LPX	C1-O2-P1-O1
54	s1	625	LPX	C3-O1-P1-O2
55	y	627	PTY	C3-O11-P1-O14
55	Y1	626	PTY	C3-O11-P1-O14
55	Y1	627	PTY	C5-O14-P1-O11
55	y1	626	PTY	C3-O11-P1-O14
55	y1	627	PTY	C3-O11-P1-O14
55	y1	627	PTY	C5-O14-P1-O11
33	b1	622	LMG	C28-C29-C30-C31
40	d	408	LHG	C23-C24-C25-C26
40	g	624	LHG	C7-C8-C9-C10
29	B	609	CLA	C3-C5-C6-C7
29	N	610	CLA	C3-C5-C6-C7
29	c1	503	CLA	C3-C5-C6-C7
40	d1	410	LHG	C29-C30-C31-C32
29	C	503	CLA	CBA-CGA-O2A-C1
29	G	603	CLA	CBA-CGA-O2A-C1
29	R	602	CLA	CBA-CGA-O2A-C1
29	c	513	CLA	CBA-CGA-O2A-C1
29	C1	510	CLA	CBA-CGA-O2A-C1
29	R1	610	CLA	CBA-CGA-O2A-C1
29	Y1	602	CLA	CBA-CGA-O2A-C1
29	c1	504	CLA	CBA-CGA-O2A-C1
29	r1	612	CLA	CBA-CGA-O2A-C1
39	C1	524	DGA	CA2-CA1-OG1-CG1
40	l	101	LHG	C24-C23-O8-C6
40	d1	409	LHG	C24-C23-O8-C6
47	k1	101	4RF	C15-C16-O18-C19
43	d1	405	PL9	C42-C43-C44-C45
29	C	509	CLA	O1D-CGD-O2D-CED
29	B	612	CLA	C8-C10-C11-C12
29	Y	613	CLA	C5-C6-C7-C8
29	Y	613	CLA	C15-C16-C17-C18
29	c	505	CLA	C10-C11-C12-C13
29	Y1	614	CLA	C8-C10-C11-C12
29	b1	608	CLA	C5-C6-C7-C8
29	s1	609	CLA	C10-C11-C12-C13
48	Y	606	CHL	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
48	N1	606	CHL	C5-C6-C7-C8
38	B1	624	3PH	O32-C31-O31-C3
33	a	413	LMG	C4-C5-C6-O5
29	c	506	CLA	O1D-CGD-O2D-CED
48	g	608	CHL	C2A-CAA-CBA-CGA
33	h1	102	LMG	C28-C29-C30-C31
37	c1	519	DGD	C1A-C2A-C3A-C4A
40	s	624	LHG	C7-C8-C9-C10
40	d1	409	LHG	C7-C8-C9-C10
47	I	102	4RF	C13-C14-C15-C16
29	b	609	CLA	O1D-CGD-O2D-CED
29	r1	604	CLA	O1D-CGD-O2D-CED
30	A	409	PHO	O1D-CGD-O2D-CED
40	C	525	LHG	C1-C2-C3-O3
40	D	408	LHG	C1-C2-C3-O3
40	l	101	LHG	C1-C2-C3-O3
40	y	624	LHG	C1-C2-C3-O3
40	C1	525	LHG	C1-C2-C3-O3
40	n1	624	LHG	C1-C2-C3-O3
54	s	625	LPX	O1-C3-C4-C5
32	M	101	SQD	O49-C7-O47-C45
32	b	626	SQD	O49-C7-O47-C45
32	c	526	SQD	O49-C7-O47-C45
33	C	523	LMG	O9-C10-O7-C8
33	A1	413	LMG	O9-C10-O7-C8
33	a1	413	LMG	O9-C10-O7-C8
33	h1	102	LMG	O9-C10-O7-C8
39	j1	101	DGA	OB1-CB1-OG2-CG2
29	S	602	CLA	C4-C3-C5-C6
29	S	611	CLA	C4-C3-C5-C6
29	b	614	CLA	C4-C3-C5-C6
29	N1	613	CLA	C4-C3-C5-C6
29	B	606	CLA	C2-C3-C5-C6
29	g	602	CLA	C2-C3-C5-C6
29	Y	602	CLA	C15-C16-C17-C18
29	Y	614	CLA	C13-C15-C16-C17
29	c	509	CLA	C10-C11-C12-C13
29	s	603	CLA	C8-C10-C11-C12
29	A1	406	CLA	C15-C16-C17-C18
29	B1	608	CLA	C13-C15-C16-C17
29	a1	406	CLA	C8-C10-C11-C12
29	r1	610	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
37	c1	518	DGD	C4A-C5A-C6A-C7A
29	C	501	CLA	C2A-CAA-CBA-CGA
29	C	505	CLA	C2A-CAA-CBA-CGA
29	G	613	CLA	C2A-CAA-CBA-CGA
29	S	613	CLA	C2A-CAA-CBA-CGA
29	Y	602	CLA	C2A-CAA-CBA-CGA
29	b	611	CLA	C2A-CAA-CBA-CGA
29	y	602	CLA	C2A-CAA-CBA-CGA
29	B1	614	CLA	C2A-CAA-CBA-CGA
29	C1	505	CLA	C2A-CAA-CBA-CGA
29	N1	602	CLA	C2A-CAA-CBA-CGA
29	S1	610	CLA	C2A-CAA-CBA-CGA
29	S1	614	CLA	C2A-CAA-CBA-CGA
29	Y1	602	CLA	C2A-CAA-CBA-CGA
29	Y1	608	CLA	C2A-CAA-CBA-CGA
29	a1	406	CLA	C2A-CAA-CBA-CGA
29	y1	608	CLA	C2A-CAA-CBA-CGA
48	S1	608	CHL	C2A-CAA-CBA-CGA
48	y1	607	CHL	C2A-CAA-CBA-CGA
29	N	610	CLA	C16-C17-C18-C20
29	b	607	CLA	C16-C17-C18-C20
29	B1	605	CLA	C16-C17-C18-C20
29	B1	611	CLA	C16-C17-C18-C20
29	b1	612	CLA	C16-C17-C18-C20
29	c1	501	CLA	C16-C17-C18-C19
29	c1	512	CLA	C16-C17-C18-C20
37	C1	518	DGD	O6E-C5E-C6E-O5E
48	G	601	CHL	C3-C5-C6-C7
30	A1	409	PHO	O1D-CGD-O2D-CED
29	A	407	CLA	CBA-CGA-O2A-C1
29	c	505	CLA	CBA-CGA-O2A-C1
29	d	403	CLA	CBA-CGA-O2A-C1
29	g	603	CLA	CBA-CGA-O2A-C1
29	r	610	CLA	CBA-CGA-O2A-C1
29	B1	608	CLA	CBA-CGA-O2A-C1
29	S1	614	CLA	CBA-CGA-O2A-C1
29	Y1	614	CLA	CBA-CGA-O2A-C1
29	b1	602	CLA	CBA-CGA-O2A-C1
29	c1	503	CLA	CBA-CGA-O2A-C1
32	b	626	SQD	C24-C23-O48-C46
32	b1	621	SQD	C24-C23-O48-C46
38	B	624	3PH	C32-C31-O31-C3

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Mol	Chain	Res	Type	Atoms
47	K1	101	4RF	C43-C41-O40-C39
29	N	604	CLA	C13-C15-C16-C17
29	b	603	CLA	C15-C16-C17-C18
29	s	610	CLA	C15-C16-C17-C18
29	B1	606	CLA	C15-C16-C17-C18
29	C1	508	CLA	C8-C10-C11-C12
29	c1	512	CLA	C15-C16-C17-C18
39	c	524	DGA	CB7-CB8-CB9-CAB
31	C	514	BCR	C15-C16-C17-C18
31	c1	515	BCR	C19-C20-C21-C22
40	L	101	LHG	C23-C24-C25-C26
40	G1	624	LHG	C23-C24-C25-C26
32	B	626	SQD	C34-C35-C36-C37
38	S	626	3PH	C25-C26-C27-C28
39	J1	101	DGA	CB3-CB4-CB5-CB6
40	D	408	LHG	C28-C29-C30-C31
40	N	624	LHG	C25-C26-C27-C28
40	d	409	LHG	C24-C25-C26-C27
40	G1	624	LHG	C28-C29-C30-C31
40	c1	525	LHG	C13-C14-C15-C16
40	c1	525	LHG	C29-C30-C31-C32
41	c	527	LMK	C13-C14-C15-C27
52	R1	625	LMT	C4-C5-C6-C7
55	Y	626	PTY	C39-C40-C41-C42
32	M	101	SQD	C8-C7-O47-C45
33	A1	413	LMG	C11-C10-O7-C8
33	H1	102	LMG	C11-C10-O7-C8
33	w1	201	LMG	C11-C10-O7-C8
40	N	624	LHG	C8-C7-O7-C5
55	Y1	626	PTY	C11-C8-O7-C6
29	n1	602	CLA	C10-C11-C12-C13
29	n1	610	CLA	C5-C6-C7-C8
31	A	411	BCR	C11-C10-C9-C34
31	b	619	BCR	C11-C10-C9-C34
50	G	622	XAT	C20-C13-C14-C15
50	n	622	XAT	C40-C33-C34-C35
50	R1	621	XAT	C20-C13-C14-C15
50	n1	622	XAT	C20-C13-C14-C15
51	R	622	NEX	C39-C29-C30-C31
51	Y	623	NEX	C39-C29-C30-C31
51	n	623	NEX	C11-C10-C9-C19
51	g	623	NEX	C11-C10-C9-C19

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Mol	Chain	Res	Type	Atoms
51	g	623	NEX	C39-C29-C30-C31
51	s	623	NEX	C39-C29-C30-C31
51	N1	623	NEX	C20-C13-C14-C15
51	G1	623	NEX	C20-C13-C14-C15
51	G1	623	NEX	C39-C29-C30-C31
51	R1	622	NEX	C39-C29-C30-C31
51	R1	622	NEX	C40-C33-C34-C35
51	Y1	623	NEX	C39-C29-C30-C31
51	n1	623	NEX	C11-C10-C9-C19
51	n1	623	NEX	C39-C29-C30-C31
51	g1	623	NEX	C40-C33-C34-C35
51	y1	623	NEX	C40-C33-C34-C35
29	B	617	CLA	C3-C5-C6-C7
29	d	403	CLA	C3-C5-C6-C7
29	c1	511	CLA	C3-C5-C6-C7
32	M	101	SQD	C26-C27-C28-C29
32	c	526	SQD	C15-C16-C17-C18
32	A1	412	SQD	C15-C16-C17-C18
32	C1	526	SQD	C11-C10-C9-C8
32	m1	101	SQD	C12-C13-C14-C15
33	B	622	LMG	C31-C32-C33-C34
33	d1	411	LMG	C19-C20-C21-C22
37	C	519	DGD	C3A-C4A-C5A-C6A
37	c	519	DGD	CCB-CDB-CEB-CFB
37	c1	519	DGD	CCB-CDB-CEB-CFB
38	B	624	3PH	C3C-C3D-C3E-C3F
38	B1	624	3PH	C3C-C3D-C3E-C3F
38	T1	101	3PH	C2C-C2D-C2E-C2F
38	S1	626	3PH	C2B-C2C-C2D-C2E
38	s1	626	3PH	C2B-C2C-C2D-C2E
39	B	625	DGA	CA6-CA7-CA8-CA9
39	b	625	DGA	CA4-CA5-CA6-CA7
39	B1	625	DGA	CA4-CA5-CA6-CA7
39	C1	524	DGA	CA4-CA5-CA6-CA7
39	C1	524	DGA	CA9-CAA-CBA-CCA
40	D	408	LHG	C31-C32-C33-C34
40	D	409	LHG	C10-C11-C12-C13
40	G	624	LHG	C9-C10-C11-C12
40	G	624	LHG	C13-C14-C15-C16
40	y	624	LHG	C13-C14-C15-C16
40	y	624	LHG	C33-C34-C35-C36
40	C1	525	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
40	D1	408	LHG	C13-C14-C15-C16
40	N1	624	LHG	C13-C14-C15-C16
40	S1	624	LHG	C26-C27-C28-C29
40	Y1	624	LHG	C16-C17-C18-C19
40	d1	408	LHG	C30-C31-C32-C33
40	d1	409	LHG	C32-C33-C34-C35
47	K	101	4RF	C43-C44-C45-C46
47	k	101	4RF	C27-C28-C29-C30
52	r1	625	LMT	C11-C10-C9-C8
55	Y1	626	PTY	C40-C41-C42-C43
55	y1	626	PTY	C35-C36-C37-C38
29	c	504	CLA	O1D-CGD-O2D-CED
29	B1	605	CLA	O1D-CGD-O2D-CED
29	B	611	CLA	C16-C17-C18-C20
29	G	613	CLA	C16-C17-C18-C20
29	Y	604	CLA	C16-C17-C18-C19
29	b	617	CLA	C16-C17-C18-C20
29	c	513	CLA	C16-C17-C18-C19
29	d	403	CLA	C16-C17-C18-C20
29	B1	603	CLA	C16-C17-C18-C19
29	C1	505	CLA	C16-C17-C18-C19
29	S1	613	CLA	C6-C7-C8-C9
29	b1	602	CLA	C16-C17-C18-C19
29	c1	509	CLA	C16-C17-C18-C19
29	c1	510	CLA	C16-C17-C18-C20
29	n1	602	CLA	C16-C17-C18-C20
29	g1	602	CLA	C16-C17-C18-C19
29	b	612	CLA	CBA-CGA-O2A-C1
34	Y1	625	SPH	C14-C15-C16-C17
37	C	518	DGD	C3B-C4B-C5B-C6B
37	C1	520	DGD	C2A-C3A-C4A-C5A
37	C1	520	DGD	C9B-CAB-CBB-CCB
38	B	624	3PH	C28-C29-C2A-C2B
38	B	624	3PH	C3B-C3C-C3D-C3E
38	b	624	3PH	C23-C24-C25-C26
38	B1	624	3PH	C26-C27-C28-C29
39	b1	625	DGA	CA8-CA9-CAA-CBA
40	D	408	LHG	C25-C26-C27-C28
40	Y	624	LHG	C13-C14-C15-C16
40	g	624	LHG	C13-C14-C15-C16
40	y	624	LHG	C16-C17-C18-C19
40	N1	624	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
41	C	527	LMK	C12-C13-C14-C15
41	C	527	LMK	C31-C32-C33-C34
47	K	101	4RF	C10-C11-C12-C13
47	k	101	4RF	C46-C47-C48-C49
47	K1	101	4RF	C26-C27-C28-C29
52	R	625	LMT	C11-C10-C9-C8
54	S	625	LPX	C11-C12-C13-C14
54	S1	625	LPX	C10-C11-C12-C13
34	Y	625	SPH	O3-C3-C4-C5
34	A1	414	SPH	O3-C3-C4-C5
29	N	610	CLA	O1D-CGD-O2D-CED
29	c	507	CLA	O1D-CGD-O2D-CED
37	C	518	DGD	O6E-C5E-C6E-O5E
32	B	621	SQD	O49-C7-O47-C45
32	b1	621	SQD	O49-C7-O47-C45
33	w1	201	LMG	O9-C10-O7-C8
40	N	624	LHG	O9-C7-O7-C5
55	Y1	626	PTY	O10-C8-O7-C6
29	C	513	CLA	C8-C10-C11-C12
29	N	604	CLA	C10-C11-C12-C13
29	b	610	CLA	C5-C6-C7-C8
29	c	513	CLA	C8-C10-C11-C12
29	C1	508	CLA	C5-C6-C7-C8
29	C1	510	CLA	C8-C10-C11-C12
29	D1	403	CLA	C8-C10-C11-C12
29	R1	610	CLA	C5-C6-C7-C8
29	n1	604	CLA	C10-C11-C12-C13
29	y1	613	CLA	C5-C6-C7-C8
40	l	101	LHG	C23-C24-C25-C26
29	B	609	CLA	CBD-CGD-O2D-CED
29	y1	611	CLA	CBD-CGD-O2D-CED
38	B	624	3PH	C29-C2A-C2B-C2C
38	B1	624	3PH	C24-C25-C26-C27
39	B	625	DGA	CA4-CA5-CA6-CA7
39	C	524	DGA	CBB-CAB-CB9-CB8
39	C	524	DGA	CB9-CAB-CBB-CCB
39	b	625	DGA	CB9-CAB-CBB-CCB
40	C	525	LHG	C29-C30-C31-C32
40	c	525	LHG	C28-C29-C30-C31
40	d	408	LHG	C33-C34-C35-C36
40	l	101	LHG	C10-C11-C12-C13
40	g	624	LHG	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
40	D1	408	LHG	C11-C12-C13-C14
40	D1	408	LHG	C25-C26-C27-C28
40	N1	624	LHG	C9-C10-C11-C12
40	s1	624	LHG	C30-C31-C32-C33
47	I	102	4RF	C03-C04-C05-C06
29	s	611	CLA	O1D-CGD-O2D-CED
38	T1	101	3PH	C2-C1-O11-P
40	D1	409	LHG	C2-C3-O3-P
40	d1	410	LHG	C2-C3-O3-P
29	c	505	CLA	O1A-CGA-O2A-C1
32	B	626	SQD	C12-C13-C14-C15
32	A1	412	SQD	C24-C25-C26-C27
37	c	519	DGD	C3B-C4B-C5B-C6B
37	c	520	DGD	C9B-CAB-CBB-CCB
38	T	101	3PH	C22-C23-C24-C25
38	t1	101	3PH	C2A-C2B-C2C-C2D
39	b	625	DGA	CB2-CB3-CB4-CB5
39	b	625	DGA	CCB-CDB-CEB-CFB
39	c	524	DGA	CAB-CBB-CCB-CDB
40	N	624	LHG	C13-C14-C15-C16
40	Y1	624	LHG	C11-C10-C9-C8
40	n1	624	LHG	C11-C12-C13-C14
40	n1	624	LHG	C13-C14-C15-C16
40	n1	624	LHG	C33-C34-C35-C36
40	y1	624	LHG	C16-C17-C18-C19
41	c	527	LMK	C11-C12-C13-C14
41	c	527	LMK	C29-C30-C31-C32
55	Y1	626	PTY	C15-C16-C17-C18
32	b	621	SQD	C26-C27-C28-C29
33	d	411	LMG	C18-C19-C20-C21
33	B1	622	LMG	C31-C32-C33-C34
37	C	518	DGD	C3A-C4A-C5A-C6A
38	b1	624	3PH	C27-C28-C29-C2A
39	b	625	DGA	CB5-CB6-CB7-CB8
39	C1	524	DGA	CB6-CB7-CB8-CB9
40	D	409	LHG	C13-C14-C15-C16
40	D	410	LHG	C29-C30-C31-C32
40	N	624	LHG	C14-C15-C16-C17
40	G	624	LHG	C28-C29-C30-C31
40	N1	624	LHG	C14-C15-C16-C17
55	Y	626	PTY	C14-C15-C16-C17
55	Y1	626	PTY	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
29	s	610	CLA	C3-C5-C6-C7
29	C1	507	CLA	C3-C5-C6-C7
29	r1	608	CLA	C3-C5-C6-C7
32	B	621	SQD	C23-C24-C25-C26
32	C1	526	SQD	C7-C8-C9-C10
33	c1	523	LMG	C10-C11-C12-C13
39	J1	101	DGA	CA1-CA2-CA3-CA4
39	b1	625	DGA	CB1-CB2-CB3-CB4
40	D1	409	LHG	C7-C8-C9-C10
40	y1	624	LHG	C23-C24-C25-C26
47	I1	102	4RF	C41-C43-C44-C45
31	b	619	BCR	C11-C10-C9-C8
32	a1	412	SQD	C2-C1-O6-C44
32	b1	626	SQD	C2-C1-O6-C44
37	C	519	DGD	C2E-C1E-O5D-C6D
37	c	519	DGD	C2E-C1E-O5D-C6D
50	G	622	XAT	C12-C13-C14-C15
50	n	622	XAT	C32-C33-C34-C35
50	y	622	XAT	C12-C13-C14-C15
50	R1	621	XAT	C12-C13-C14-C15
50	n1	622	XAT	C12-C13-C14-C15
51	R	622	NEX	C28-C29-C30-C31
51	Y	623	NEX	C28-C29-C30-C31
51	n	623	NEX	C11-C10-C9-C8
51	g	623	NEX	C11-C10-C9-C8
51	g	623	NEX	C28-C29-C30-C31
51	s	623	NEX	C28-C29-C30-C31
51	N1	623	NEX	C12-C13-C14-C15
51	N1	623	NEX	C28-C29-C30-C31
51	G1	623	NEX	C12-C13-C14-C15
51	G1	623	NEX	C28-C29-C30-C31
51	R1	622	NEX	C12-C13-C14-C15
51	R1	622	NEX	C28-C29-C30-C31
51	R1	622	NEX	C32-C33-C34-C35
51	Y1	623	NEX	C28-C29-C30-C31
51	n1	623	NEX	C11-C10-C9-C8
51	n1	623	NEX	C28-C29-C30-C31
51	g1	623	NEX	C32-C33-C34-C35
51	y1	623	NEX	C32-C33-C34-C35
29	Y1	610	CLA	CBA-CGA-O2A-C1
32	b	621	SQD	C25-C26-C27-C28
32	A1	412	SQD	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
33	H	102	LMG	C12-C13-C14-C15
33	h	102	LMG	C31-C32-C33-C34
33	H1	102	LMG	C30-C31-C32-C33
37	C1	519	DGD	C4B-C5B-C6B-C7B
38	s	626	3PH	C26-C27-C28-C29
39	b	625	DGA	CEB-CFB-CGB-CHB
39	b1	625	DGA	CA2-CA3-CA4-CA5
39	b1	625	DGA	CB5-CB6-CB7-CB8
40	C	525	LHG	C30-C31-C32-C33
40	D	409	LHG	C25-C26-C27-C28
40	G	624	LHG	C11-C10-C9-C8
40	S	624	LHG	C12-C13-C14-C15
40	c	525	LHG	C26-C27-C28-C29
40	d	408	LHG	C25-C26-C27-C28
40	l	101	LHG	C34-C35-C36-C37
40	y	624	LHG	C11-C10-C9-C8
40	C1	525	LHG	C30-C31-C32-C33
40	D1	408	LHG	C30-C31-C32-C33
40	S1	624	LHG	C31-C32-C33-C34
40	Y1	624	LHG	C15-C16-C17-C18
40	d1	409	LHG	C34-C35-C36-C37
40	y1	624	LHG	C28-C29-C30-C31
40	y1	624	LHG	C29-C30-C31-C32
47	K1	101	4RF	C10-C11-C12-C13
47	i1	101	4RF	C07-C08-C09-C10
55	Y1	626	PTY	C39-C40-C41-C42
55	y1	626	PTY	C31-C32-C33-C34
29	B	603	CLA	C5-C6-C7-C8
29	B	604	CLA	C15-C16-C17-C18
29	C	511	CLA	C5-C6-C7-C8
29	y	604	CLA	C5-C6-C7-C8
29	B1	611	CLA	C8-C10-C11-C12
29	B1	612	CLA	C13-C15-C16-C17
29	N1	602	CLA	C15-C16-C17-C18
29	R1	602	CLA	C10-C11-C12-C13
29	a1	410	CLA	C10-C11-C12-C13
29	c1	503	CLA	C15-C16-C17-C18
29	c1	510	CLA	C13-C15-C16-C17
29	g1	613	CLA	C8-C10-C11-C12
29	b1	602	CLA	O1A-CGA-O2A-C1
29	r1	612	CLA	O1A-CGA-O2A-C1
40	l	101	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
29	C	501	CLA	C16-C17-C18-C20
29	C	509	CLA	C16-C17-C18-C20
29	G	602	CLA	C16-C17-C18-C20
29	G	610	CLA	C16-C17-C18-C19
29	Y	604	CLA	C16-C17-C18-C20
29	Y	614	CLA	C16-C17-C18-C19
29	b	605	CLA	C16-C17-C18-C20
29	c	509	CLA	C16-C17-C18-C19
29	c	510	CLA	C16-C17-C18-C20
29	n	602	CLA	C16-C17-C18-C20
29	s	604	CLA	C6-C7-C8-C9
29	B1	610	CLA	C16-C17-C18-C20
29	R1	608	CLA	C11-C12-C13-C14
29	R1	610	CLA	C11-C12-C13-C14
29	Y1	613	CLA	C16-C17-C18-C19
29	Y1	613	CLA	C16-C17-C18-C20
29	Y1	614	CLA	C16-C17-C18-C19
29	b1	610	CLA	C16-C17-C18-C20
29	g1	610	CLA	C16-C17-C18-C20
29	r1	608	CLA	C11-C12-C13-C15
29	y1	614	CLA	C16-C17-C18-C19
29	a	407	CLA	O1D-CGD-O2D-CED
29	n	604	CLA	O1D-CGD-O2D-CED
29	b1	605	CLA	O1D-CGD-O2D-CED
29	Y	604	CLA	C4-C3-C5-C6
29	c	510	CLA	C4-C3-C5-C6
29	c1	505	CLA	C4-C3-C5-C6
29	y1	613	CLA	C4-C3-C5-C6
43	d1	405	PL9	C40-C39-C41-C42
32	a1	412	SQD	C26-C27-C28-C29
33	w	201	LMG	C37-C38-C39-C40
33	B1	622	LMG	C18-C19-C20-C21
33	D1	411	LMG	C32-C33-C34-C35
33	c1	521	LMG	C12-C13-C14-C15
34	Y	625	SPH	C14-C15-C16-C17
38	S	626	3PH	C2A-C2B-C2C-C2D
38	s	626	3PH	C2C-C2D-C2E-C2F
38	s	626	3PH	C39-C3A-C3B-C3C
38	B1	624	3PH	C2B-C2C-C2D-C2E
38	B1	624	3PH	C32-C33-C34-C35
39	C	524	DGA	CA6-CA7-CA8-CA9
39	j	101	DGA	CA4-CA5-CA6-CA7

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Mol	Chain	Res	Type	Atoms
39	B1	625	DGA	CDB-CEB-CFB-CGB
40	Y	624	LHG	C26-C27-C28-C29
40	c	525	LHG	C29-C30-C31-C32
40	C1	525	LHG	C29-C30-C31-C32
41	c1	527	LMK	C31-C32-C33-C34
47	K	101	4RF	C05-C06-C07-C08
47	I1	102	4RF	C05-C06-C07-C08
52	r	625	LMT	C11-C10-C9-C8
55	Y	626	PTY	C40-C41-C42-C43
29	y	614	CLA	C2-C3-C5-C6
29	N1	613	CLA	C2-C3-C5-C6
29	y1	613	CLA	C2-C3-C5-C6
30	A	408	PHO	C2-C3-C5-C6
29	C	505	CLA	C11-C10-C8-C9
29	C	507	CLA	C6-C7-C8-C9
29	D	403	CLA	C11-C12-C13-C14
29	G	613	CLA	C6-C7-C8-C9
29	S	603	CLA	C6-C7-C8-C9
29	S	603	CLA	C11-C10-C8-C9
29	S	610	CLA	C14-C13-C15-C16
29	Y	602	CLA	C11-C10-C8-C9
29	b	602	CLA	C6-C7-C8-C9
29	b	616	CLA	C14-C13-C15-C16
29	c	503	CLA	C14-C13-C15-C16
29	c	509	CLA	C6-C7-C8-C9
29	c	512	CLA	C14-C13-C15-C16
29	d	403	CLA	C11-C10-C8-C9
29	n	610	CLA	C6-C7-C8-C9
29	n	610	CLA	C14-C13-C15-C16
29	n	613	CLA	C14-C13-C15-C16
29	g	611	CLA	C6-C7-C8-C9
29	r	603	CLA	C11-C10-C8-C9
29	r	610	CLA	C11-C10-C8-C9
29	B1	604	CLA	C14-C13-C15-C16
29	B1	605	CLA	C11-C12-C13-C14
29	B1	606	CLA	C11-C12-C13-C14
29	C1	503	CLA	C6-C7-C8-C9
29	C1	505	CLA	C14-C13-C15-C16
29	G1	610	CLA	C11-C10-C8-C9
29	G1	613	CLA	C6-C7-C8-C9
29	R1	610	CLA	C6-C7-C8-C9
29	Y1	610	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	b1	604	CLA	C6-C7-C8-C9
29	c1	509	CLA	C14-C13-C15-C16
29	c1	510	CLA	C14-C13-C15-C16
29	g1	602	CLA	C6-C7-C8-C9
29	g1	603	CLA	C6-C7-C8-C9
30	a1	408	PHO	C11-C12-C13-C14
30	a1	409	PHO	C11-C10-C8-C9
48	G	601	CHL	C11-C12-C13-C14
48	n	606	CHL	C14-C13-C15-C16
48	n	607	CHL	C11-C10-C8-C9
48	r1	606	CHL	C2A-CAA-CBA-CGA
37	c	519	DGD	C1B-C2B-C3B-C4B
38	t1	101	3PH	C31-C32-C33-C34
32	B	621	SQD	C24-C25-C26-C27
32	a	412	SQD	C33-C34-C35-C36
32	a1	412	SQD	C34-C35-C36-C37
32	b1	621	SQD	C11-C12-C13-C14
33	D	411	LMG	C15-C16-C17-C18
33	H1	102	LMG	C34-C35-C36-C37
34	y	625	SPH	C6-C7-C8-C9
34	y	625	SPH	C11-C12-C13-C14
34	y1	625	SPH	C7-C8-C9-C10
37	C1	520	DGD	C4A-C5A-C6A-C7A
38	B	624	3PH	C25-C26-C27-C28
38	t	101	3PH	C2E-C2F-C2G-C2H
38	s	626	3PH	C3B-C3C-C3D-C3E
38	b1	624	3PH	C24-C25-C26-C27
38	b1	624	3PH	C3E-C3F-C3G-C3H
38	t1	101	3PH	C2B-C2C-C2D-C2E
38	s1	626	3PH	C27-C28-C29-C2A
39	C	524	DGA	CA4-CA5-CA6-CA7
39	c1	524	DGA	CAA-CBA-CCA-CDA
39	c1	524	DGA	CB3-CB4-CB5-CB6
40	L	101	LHG	C9-C10-C11-C12
40	L	101	LHG	C31-C32-C33-C34
40	N	624	LHG	C28-C29-C30-C31
40	N	624	LHG	C33-C34-C35-C36
40	s	624	LHG	C11-C12-C13-C14
40	y	624	LHG	C29-C30-C31-C32
40	L1	101	LHG	C11-C10-C9-C8
40	G1	624	LHG	C16-C17-C18-C19
40	d1	408	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
40	g1	624	LHG	C11-C10-C9-C8
40	y1	624	LHG	C31-C32-C33-C34
47	I	102	4RF	C51-C52-C53-C54
47	I1	102	4RF	C49-C50-C51-C52
47	K1	101	4RF	C12-C13-C14-C15
52	R	625	LMT	C4-C5-C6-C7
55	y	626	PTY	C19-C20-C21-C22
29	B	615	CLA	C10-C11-C12-C13
29	b	607	CLA	C8-C10-C11-C12
29	B1	615	CLA	C15-C16-C17-C18
29	B1	617	CLA	C5-C6-C7-C8
29	N1	604	CLA	C15-C16-C17-C18
29	c1	510	CLA	C8-C10-C11-C12
29	s1	611	CLA	C8-C10-C11-C12
29	N	602	CLA	C2A-CAA-CBA-CGA
29	r	604	CLA	C2A-CAA-CBA-CGA
29	s	612	CLA	C2A-CAA-CBA-CGA
29	C1	502	CLA	C2A-CAA-CBA-CGA
29	S1	603	CLA	C2A-CAA-CBA-CGA
29	r1	610	CLA	C2A-CAA-CBA-CGA
30	a	409	PHO	C2A-CAA-CBA-CGA
48	N1	606	CHL	C2A-CAA-CBA-CGA
29	A	407	CLA	O1A-CGA-O2A-C1
29	c	504	CLA	O1A-CGA-O2A-C1
29	C1	510	CLA	O1A-CGA-O2A-C1
31	C	516	BCR	C37-C22-C23-C24
31	B1	618	BCR	C11-C12-C13-C35
36	B	620	C7Z	C7-C8-C9-C19
36	b	620	C7Z	C7-C8-C9-C19
45	H1	101	RRX	C7-C8-C9-C34
32	B	621	SQD	C11-C10-C9-C8
32	b	626	SQD	C17-C18-C19-C20
37	c1	520	DGD	C9B-CAB-CBB-CCB
38	B1	624	3PH	C3D-C3E-C3F-C3G
38	S1	626	3PH	C25-C26-C27-C28
39	B	625	DGA	CB3-CB4-CB5-CB6
39	C	524	DGA	CA2-CA3-CA4-CA5
40	S	624	LHG	C28-C29-C30-C31
40	c	525	LHG	C13-C14-C15-C16
40	d	409	LHG	C10-C11-C12-C13
40	D1	409	LHG	C11-C12-C13-C14
40	Y1	624	LHG	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
40	s1	624	LHG	C26-C27-C28-C29
41	c	527	LMK	C12-C13-C14-C15
47	I	102	4RF	C31-C32-C33-C34
47	k	101	4RF	C47-C48-C49-C50
47	K1	101	4RF	C46-C47-C48-C49
40	C	525	LHG	O1-C1-C2-C3
40	L	101	LHG	O1-C1-C2-C3
40	Y	624	LHG	O1-C1-C2-C3
40	d	409	LHG	O1-C1-C2-C3
40	n	624	LHG	O1-C1-C2-C3
40	g	624	LHG	O1-C1-C2-C3
40	C1	525	LHG	O1-C1-C2-C3
40	G1	624	LHG	O1-C1-C2-C3
40	c1	525	LHG	O1-C1-C2-C3
31	c	516	BCR	C17-C18-C19-C20
31	d	404	BCR	C17-C18-C19-C20
36	b	620	C7Z	C7-C8-C9-C10
45	H1	101	RRX	C7-C8-C9-C10
45	h1	101	RRX	C11-C12-C13-C14
51	Y1	623	NEX	C11-C12-C13-C14
29	B1	608	CLA	C3-C5-C6-C7
29	c	501	CLA	O1D-CGD-O2D-CED
32	B	626	SQD	O49-C7-O47-C45
29	C	511	CLA	C15-C16-C17-C18
29	S	602	CLA	C10-C11-C12-C13
29	Y	610	CLA	C13-C15-C16-C17
29	y	610	CLA	C13-C15-C16-C17
29	B1	606	CLA	C10-C11-C12-C13
29	a1	406	CLA	C10-C11-C12-C13
29	c1	513	CLA	C8-C10-C11-C12
29	n1	604	CLA	C15-C16-C17-C18
29	g1	603	CLA	C13-C15-C16-C17
29	y1	610	CLA	C5-C6-C7-C8
32	B	621	SQD	C8-C7-O47-C45
32	B	626	SQD	C8-C7-O47-C45
38	s1	626	3PH	C22-C21-O21-C2
40	G1	624	LHG	C8-C7-O7-C5
32	a1	412	SQD	C31-C32-C33-C34
39	C1	524	DGA	CA6-CA7-CA8-CA9
39	J1	101	DGA	CB6-CB7-CB8-CB9
39	c1	524	DGA	CBB-CAB-CB9-CB8
40	c	525	LHG	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
40	d	408	LHG	C11-C12-C13-C14
40	y	624	LHG	C11-C12-C13-C14
40	y	624	LHG	C28-C29-C30-C31
40	G1	624	LHG	C13-C14-C15-C16
40	s1	624	LHG	C24-C25-C26-C27
47	k1	101	4RF	C49-C50-C51-C52
47	k1	101	4RF	C52-C53-C54-C55
54	S1	625	LPX	C15-C16-C17-C18
55	Y1	626	PTY	C19-C20-C21-C22
33	a1	413	LMG	C4-C5-C6-O5
32	M	101	SQD	C7-C8-C9-C10
32	m1	101	SQD	C7-C8-C9-C10
40	d	409	LHG	C23-C24-C25-C26
40	d1	409	LHG	C23-C24-C25-C26
55	y	626	PTY	C30-C31-C32-C33
29	B1	614	CLA	C2C-C3C-CAC-CBC
32	A	412	SQD	C12-C13-C14-C15
32	a	412	SQD	C10-C11-C12-C13
32	c1	526	SQD	C17-C18-C19-C20
33	H	102	LMG	C13-C14-C15-C16
33	c	523	LMG	C18-C19-C20-C21
33	d	411	LMG	C19-C20-C21-C22
33	C1	523	LMG	C34-C35-C36-C37
33	h1	102	LMG	C12-C13-C14-C15
37	c	518	DGD	C3A-C4A-C5A-C6A
37	c	518	DGD	CAB-CBB-CCB-CDB
38	b	624	3PH	C28-C29-C2A-C2B
38	T1	101	3PH	C38-C39-C3A-C3B
38	s1	626	3PH	C29-C2A-C2B-C2C
39	b	625	DGA	CDB-CEB-CFB-CGB
39	j	101	DGA	CB7-CB8-CB9-CAB
39	b1	625	DGA	CB6-CB7-CB8-CB9
40	D	408	LHG	C24-C25-C26-C27
40	D1	408	LHG	C28-C29-C30-C31
40	D1	409	LHG	C17-C18-C19-C20
40	D1	410	LHG	C29-C30-C31-C32
40	G1	624	LHG	C11-C10-C9-C8
40	G1	624	LHG	C11-C12-C13-C14
40	d1	408	LHG	C31-C32-C33-C34
40	g1	624	LHG	C28-C29-C30-C31
40	s1	624	LHG	C11-C12-C13-C14
47	I	102	4RF	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
47	k	101	4RF	C09-C10-C11-C12
47	k1	101	4RF	C30-C31-C32-C33
52	R1	625	LMT	C3-C4-C5-C6
54	s	625	LPX	C11-C12-C13-C14
55	y	626	PTY	C17-C18-C19-C20
29	B	611	CLA	C16-C17-C18-C19
29	G	610	CLA	C16-C17-C18-C20
29	G	613	CLA	C16-C17-C18-C19
29	R	603	CLA	C11-C12-C13-C14
29	S	604	CLA	C6-C7-C8-C9
29	S	604	CLA	C6-C7-C8-C10
29	b	602	CLA	C16-C17-C18-C20
29	b	607	CLA	C16-C17-C18-C19
29	c	501	CLA	C16-C17-C18-C19
29	c	501	CLA	C16-C17-C18-C20
29	d	403	CLA	C16-C17-C18-C19
29	n	603	CLA	C16-C17-C18-C19
29	g	602	CLA	C16-C17-C18-C19
29	y	614	CLA	C16-C17-C18-C19
29	y	614	CLA	C16-C17-C18-C20
29	A1	406	CLA	C16-C17-C18-C19
29	A1	406	CLA	C16-C17-C18-C20
29	B1	602	CLA	C16-C17-C18-C19
29	B1	602	CLA	C16-C17-C18-C20
29	B1	603	CLA	C16-C17-C18-C20
29	B1	608	CLA	C16-C17-C18-C20
29	B1	611	CLA	C16-C17-C18-C19
29	C1	505	CLA	C16-C17-C18-C20
29	C1	513	CLA	C16-C17-C18-C19
29	C1	513	CLA	C16-C17-C18-C20
29	G1	602	CLA	C16-C17-C18-C19
29	G1	602	CLA	C16-C17-C18-C20
29	c1	507	CLA	C16-C17-C18-C19
29	c1	507	CLA	C16-C17-C18-C20
29	c1	512	CLA	C16-C17-C18-C19
29	d1	402	CLA	C16-C17-C18-C20
29	n1	602	CLA	C16-C17-C18-C19
29	s1	613	CLA	C6-C7-C8-C10
48	S	608	CHL	C11-C12-C13-C14
48	s	608	CHL	C11-C12-C13-C15
29	B	604	CLA	C5-C6-C7-C8
29	C	504	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
29	D	402	CLA	C13-C15-C16-C17
29	b	603	CLA	C5-C6-C7-C8
29	c	508	CLA	C15-C16-C17-C18
29	C1	501	CLA	C13-C15-C16-C17
29	N1	602	CLA	C10-C11-C12-C13
29	N1	602	CLA	C13-C15-C16-C17
29	b1	606	CLA	C5-C6-C7-C8
29	b1	612	CLA	C8-C10-C11-C12
29	c1	509	CLA	C13-C15-C16-C17
29	r1	608	CLA	C10-C11-C12-C13
32	C	526	SQD	C29-C30-C31-C32
32	C1	526	SQD	C28-C29-C30-C31
33	d	411	LMG	C12-C13-C14-C15
33	W1	201	LMG	C29-C30-C31-C32
38	B	624	3PH	C2C-C2D-C2E-C2F
38	B	624	3PH	C3D-C3E-C3F-C3G
38	T	101	3PH	C24-C25-C26-C27
38	S	626	3PH	C35-C36-C37-C38
38	B1	624	3PH	C3A-C3B-C3C-C3D
39	B	625	DGA	CA9-CAA-CBA-CCA
39	b	625	DGA	CBB-CCB-CDB-CEB
40	S	624	LHG	C26-C27-C28-C29
40	d	409	LHG	C11-C12-C13-C14
40	l	101	LHG	C11-C10-C9-C8
40	n	624	LHG	C25-C26-C27-C28
40	D1	410	LHG	C31-C32-C33-C34
40	c1	525	LHG	C12-C13-C14-C15
40	d1	410	LHG	C26-C27-C28-C29
40	s1	624	LHG	C28-C29-C30-C31
47	i	101	4RF	C44-C45-C46-C47
47	K1	101	4RF	C07-C08-C09-C10
47	i1	101	4RF	C44-C45-C46-C47
52	r1	625	LMT	C5-C6-C7-C8
55	y	626	PTY	C15-C16-C17-C18
55	Y1	626	PTY	C36-C37-C38-C39
55	Y	626	PTY	N1-C2-C3-O11
29	Y1	610	CLA	CBD-CGD-O2D-CED
53	R	626	ERG	C13-C17-C20-C21
53	r	626	ERG	C13-C17-C20-C22
53	r	626	ERG	C16-C17-C20-C22
53	R1	626	ERG	C13-C17-C20-C22
32	B1	626	SQD	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
33	b1	622	LMG	C12-C13-C14-C15
37	c	520	DGD	C4A-C5A-C6A-C7A
38	T	101	3PH	C33-C34-C35-C36
38	b	624	3PH	C3E-C3F-C3G-C3H
38	t	101	3PH	C34-C35-C36-C37
38	b1	624	3PH	C34-C35-C36-C37
39	B	625	DGA	CB5-CB6-CB7-CB8
39	c	524	DGA	CB3-CB4-CB5-CB6
40	S	624	LHG	C11-C12-C13-C14
40	d	409	LHG	C28-C29-C30-C31
40	s	624	LHG	C31-C32-C33-C34
40	S1	624	LHG	C28-C29-C30-C31
40	d1	408	LHG	C11-C12-C13-C14
40	d1	409	LHG	C13-C14-C15-C16
47	k	101	4RF	C11-C12-C13-C14
47	k	101	4RF	C24-C25-C26-C27
47	k1	101	4RF	C28-C29-C30-C31
52	R	625	LMT	C5-C6-C7-C8
55	y1	626	PTY	C19-C20-C21-C22
32	b	621	SQD	C23-C24-C25-C26
37	C1	519	DGD	C1A-C2A-C3A-C4A
40	y	624	LHG	C23-C24-C25-C26
40	D1	410	LHG	C7-C8-C9-C10
29	y	604	CLA	C8-C10-C11-C12
29	c1	501	CLA	C8-C10-C11-C12
29	R	602	CLA	O1A-CGA-O2A-C1
29	c1	504	CLA	O1A-CGA-O2A-C1
32	b1	621	SQD	O10-C23-O48-C46
38	t	101	3PH	C2D-C2E-C2F-C2G
38	s	626	3PH	C24-C25-C26-C27
38	T1	101	3PH	C3A-C3B-C3C-C3D
39	B	625	DGA	CB9-CAB-CBB-CCB
39	b	625	DGA	CA6-CA7-CA8-CA9
39	c	524	DGA	CEB-CFB-CGB-CHB
39	B1	625	DGA	CA8-CA9-CAA-CBA
39	C1	524	DGA	CB2-CB3-CB4-CB5
39	c1	524	DGA	CA7-CA8-CA9-CAA
40	s	624	LHG	C26-C27-C28-C29
40	N1	624	LHG	C11-C12-C13-C14
40	d1	409	LHG	C31-C32-C33-C34
40	s1	624	LHG	C13-C14-C15-C16
47	i1	101	4RF	C51-C52-C53-C54

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Mol	Chain	Res	Type	Atoms
47	k1	101	4RF	C44-C45-C46-C47
52	r1	625	LMT	C3-C4-C5-C6
29	N1	604	CLA	O1D-CGD-O2D-CED
29	B	603	CLA	C3-C5-C6-C7
29	s	604	CLA	C3-C5-C6-C7
29	S1	611	CLA	C3-C5-C6-C7
37	B	623	DGD	O6E-C5E-C6E-O5E
29	b	614	CLA	CBA-CGA-O2A-C1
29	n	602	CLA	CBA-CGA-O2A-C1
40	D	410	LHG	C24-C23-O8-C6
32	b	621	SQD	C12-C13-C14-C15
33	W	201	LMG	C29-C30-C31-C32
33	h	102	LMG	C12-C13-C14-C15
37	C	519	DGD	C4A-C5A-C6A-C7A
38	b	624	3PH	C2E-C2F-C2G-C2H
38	s1	626	3PH	C37-C38-C39-C3A
39	c	524	DGA	CBB-CCB-CDB-CEB
39	j1	101	DGA	CB2-CB3-CB4-CB5
40	s	624	LHG	C13-C14-C15-C16
55	y1	626	PTY	C23-C24-C25-C26
29	B	609	CLA	C3A-C2A-CAA-CBA
29	C	513	CLA	C3A-C2A-CAA-CBA
29	N	603	CLA	C3A-C2A-CAA-CBA
29	N	614	CLA	C3A-C2A-CAA-CBA
29	G	603	CLA	C3A-C2A-CAA-CBA
29	Y	603	CLA	C3A-C2A-CAA-CBA
29	b	605	CLA	C3A-C2A-CAA-CBA
29	c	512	CLA	C3A-C2A-CAA-CBA
29	c	513	CLA	C3A-C2A-CAA-CBA
29	n	603	CLA	C3A-C2A-CAA-CBA
29	n	613	CLA	C3A-C2A-CAA-CBA
29	g	603	CLA	C3A-C2A-CAA-CBA
29	r	604	CLA	C3A-C2A-CAA-CBA
29	y	603	CLA	C3A-C2A-CAA-CBA
29	C1	501	CLA	C3A-C2A-CAA-CBA
29	C1	507	CLA	C3A-C2A-CAA-CBA
29	C1	512	CLA	C3A-C2A-CAA-CBA
29	C1	513	CLA	C3A-C2A-CAA-CBA
29	N1	603	CLA	C3A-C2A-CAA-CBA
29	N1	614	CLA	C3A-C2A-CAA-CBA
29	G1	603	CLA	C3A-C2A-CAA-CBA
29	Y1	603	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	b1	605	CLA	C3A-C2A-CAA-CBA
29	c1	507	CLA	C3A-C2A-CAA-CBA
29	c1	512	CLA	C3A-C2A-CAA-CBA
29	n1	603	CLA	C3A-C2A-CAA-CBA
29	n1	610	CLA	C3A-C2A-CAA-CBA
29	n1	613	CLA	C3A-C2A-CAA-CBA
29	n1	614	CLA	C3A-C2A-CAA-CBA
29	g1	603	CLA	C3A-C2A-CAA-CBA
29	s1	612	CLA	C3A-C2A-CAA-CBA
29	y1	603	CLA	C3A-C2A-CAA-CBA
30	a	408	PHO	C3A-C2A-CAA-CBA
48	G	606	CHL	C3A-C2A-CAA-CBA
48	g	605	CHL	C3A-C2A-CAA-CBA
48	g	607	CHL	C3A-C2A-CAA-CBA
48	N1	607	CHL	C3A-C2A-CAA-CBA
48	G1	605	CHL	C3A-C2A-CAA-CBA
48	G1	606	CHL	C3A-C2A-CAA-CBA
48	G1	607	CHL	C3A-C2A-CAA-CBA
29	Y	613	CLA	C8-C10-C11-C12
29	c	506	CLA	C13-C15-C16-C17
29	y	613	CLA	C10-C11-C12-C13
29	C1	505	CLA	C13-C15-C16-C17
31	C	514	BCR	C19-C20-C21-C22
32	b1	621	SQD	C25-C26-C27-C28
33	C	523	LMG	C18-C19-C20-C21
33	d	411	LMG	C13-C14-C15-C16
34	y1	625	SPH	C11-C10-C9-C8
38	T1	101	3PH	C2D-C2E-C2F-C2G
38	S1	626	3PH	C24-C25-C26-C27
39	B	625	DGA	CA3-CA4-CA5-CA6
40	D	408	LHG	C11-C12-C13-C14
40	S	624	LHG	C13-C14-C15-C16
40	Y	624	LHG	C11-C10-C9-C8
40	s	624	LHG	C30-C31-C32-C33
40	C1	525	LHG	C24-C25-C26-C27
40	D1	410	LHG	C25-C26-C27-C28
40	c1	525	LHG	C26-C27-C28-C29
40	c1	525	LHG	C28-C29-C30-C31
40	n1	624	LHG	C16-C17-C18-C19
47	k1	101	4RF	C09-C10-C11-C12
54	s	625	LPX	C15-C16-C17-C18
29	g1	614	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
29	c	513	CLA	O1A-CGA-O2A-C1
29	B1	608	CLA	O1A-CGA-O2A-C1
29	Y1	602	CLA	O1A-CGA-O2A-C1
39	C1	524	DGA	OA1-CA1-OG1-CG1
47	k1	101	4RF	O17-C16-O18-C19
29	G	602	CLA	C16-C17-C18-C19
29	R	608	CLA	C11-C12-C13-C14
29	R	608	CLA	C11-C12-C13-C15
29	b	617	CLA	C16-C17-C18-C19
29	n	602	CLA	C16-C17-C18-C19
29	g	602	CLA	C16-C17-C18-C20
29	b1	602	CLA	C16-C17-C18-C20
29	c1	504	CLA	C16-C17-C18-C19
29	c1	509	CLA	C16-C17-C18-C20
29	d1	402	CLA	C16-C17-C18-C19
29	g1	602	CLA	C16-C17-C18-C20
29	g1	613	CLA	C16-C17-C18-C19
29	r1	608	CLA	C11-C12-C13-C14
29	s1	613	CLA	C6-C7-C8-C9
29	y1	612	CLA	C16-C17-C18-C19
29	y1	612	CLA	C16-C17-C18-C20
32	A1	412	SQD	C9-C10-C11-C12
32	B1	626	SQD	C15-C16-C17-C18
33	c1	523	LMG	C33-C34-C35-C36
37	C1	518	DGD	C3A-C4A-C5A-C6A
38	B	624	3PH	C2B-C2C-C2D-C2E
38	S	626	3PH	C24-C25-C26-C27
38	t1	101	3PH	C29-C2A-C2B-C2C
39	B1	625	DGA	CDA-CEA-CFA-CGA
40	Y	624	LHG	C29-C30-C31-C32
40	Y	624	LHG	C31-C32-C33-C34
40	d	410	LHG	C25-C26-C27-C28
40	G1	624	LHG	C9-C10-C11-C12
47	I	102	4RF	C52-C53-C54-C55
47	k1	101	4RF	C24-C25-C26-C27
52	r	625	LMT	C4-C5-C6-C7
52	R1	625	LMT	C6-C7-C8-C9
33	b1	622	LMG	C7-C8-C9-O8
40	g	624	LHG	C4-C5-C6-O8
47	k1	101	4RF	O18-C19-C20-C39
40	G1	624	LHG	O9-C7-O7-C5
32	B	626	SQD	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
32	m	101	SQD	C27-C28-C29-C30
33	c1	523	LMG	C37-C38-C39-C40
39	B1	625	DGA	CB5-CB6-CB7-CB8
40	D1	410	LHG	C33-C34-C35-C36
55	y1	626	PTY	C17-C18-C19-C20
55	y1	626	PTY	C32-C33-C34-C35
53	R1	626	ERG	C17-C20-C22-C23
37	C1	520	DGD	O6D-C5D-C6D-O5D
50	Y	622	XAT	C14-C15-C35-C34
50	Y1	622	XAT	C14-C15-C35-C34
50	g1	622	XAT	C14-C15-C35-C34
51	G1	623	NEX	C14-C15-C35-C34
29	C1	512	CLA	C3-C5-C6-C7
40	g	624	LHG	C23-C24-C25-C26
34	A1	414	SPH	C6-C7-C8-C9
38	t	101	3PH	C32-C33-C34-C35
38	B1	624	3PH	C29-C2A-C2B-C2C
39	b1	625	DGA	CDB-CEB-CFB-CGB
39	c1	524	DGA	CA4-CA5-CA6-CA7
40	L1	101	LHG	C29-C30-C31-C32
40	S1	624	LHG	C14-C15-C16-C17
47	k1	101	4RF	C31-C32-C33-C34
52	R1	625	LMT	C5-C6-C7-C8
29	C	503	CLA	O1A-CGA-O2A-C1
29	R1	610	CLA	O1A-CGA-O2A-C1
47	K1	101	4RF	O42-C41-O40-C39
29	B	607	CLA	C5-C6-C7-C8
29	c	508	CLA	C10-C11-C12-C13
29	b	612	CLA	C4-C3-C5-C6
29	y	614	CLA	C4-C3-C5-C6
29	C1	501	CLA	C4-C3-C5-C6
29	y1	611	CLA	C4-C3-C5-C6
30	A	408	PHO	C4-C3-C5-C6
30	a	408	PHO	C4-C3-C5-C6
43	D	405	PL9	C40-C39-C41-C42
43	d	405	PL9	C40-C39-C41-C42
43	D1	405	PL9	C15-C14-C16-C17
39	J	101	DGA	CA2-CA1-OG1-CG1
29	Y	604	CLA	C2-C3-C5-C6
29	b	603	CLA	C2-C3-C5-C6
29	s	603	CLA	C2-C3-C5-C6
29	y1	611	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
30	a	408	PHO	C2-C3-C5-C6
32	b1	621	SQD	C8-C7-O47-C45
32	b1	626	SQD	C8-C7-O47-C45
33	h	102	LMG	C11-C10-O7-C8
33	C1	521	LMG	C11-C10-O7-C8
40	g	624	LHG	C8-C7-O7-C5
40	y	624	LHG	C8-C7-O7-C5
40	D1	409	LHG	C8-C7-O7-C5
40	N1	624	LHG	C8-C7-O7-C5
32	b1	621	SQD	C26-C27-C28-C29
37	C1	519	DGD	C3A-C4A-C5A-C6A
39	c1	524	DGA	CB5-CB6-CB7-CB8
40	d	409	LHG	C27-C28-C29-C30
40	y	624	LHG	C32-C33-C34-C35
40	N1	624	LHG	C25-C26-C27-C28
29	C	507	CLA	C2A-CAA-CBA-CGA
29	R	602	CLA	C2A-CAA-CBA-CGA
29	y	610	CLA	C2A-CAA-CBA-CGA
40	D	408	LHG	O1-C1-C2-O2
40	L	101	LHG	O1-C1-C2-O2
40	S	624	LHG	O1-C1-C2-O2
40	l	101	LHG	O1-C1-C2-O2
40	y	624	LHG	O1-C1-C2-O2
40	C1	525	LHG	O1-C1-C2-O2
40	D1	409	LHG	O1-C1-C2-O2
40	Y1	624	LHG	O1-C1-C2-O2
40	d1	410	LHG	O1-C1-C2-O2
40	n1	624	LHG	O1-C1-C2-O2
40	g1	624	LHG	O1-C1-C2-O2
40	s1	624	LHG	O1-C1-C2-O2
40	y1	624	LHG	O1-C1-C2-O2
41	C1	527	LMK	O9-C10-C11-C12
32	b	621	SQD	C10-C11-C12-C13
38	b	624	3PH	C24-C25-C26-C27
38	S1	626	3PH	C26-C27-C28-C29
39	c	524	DGA	CA6-CA7-CA8-CA9
39	j1	101	DGA	CB6-CB7-CB8-CB9
40	L	101	LHG	C28-C29-C30-C31
40	G	624	LHG	C26-C27-C28-C29
40	d	408	LHG	C30-C31-C32-C33
40	l	101	LHG	C25-C26-C27-C28
40	S1	624	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
54	s	625	LPX	C9-C10-C11-C12
55	Y1	626	PTY	C22-C23-C24-C25
55	y1	626	PTY	C21-C22-C23-C24
29	s1	610	CLA	O1D-CGD-O2D-CED
29	G	603	CLA	O1A-CGA-O2A-C1
29	d	403	CLA	O1A-CGA-O2A-C1
29	g	603	CLA	O1A-CGA-O2A-C1
29	Y1	614	CLA	O1A-CGA-O2A-C1
33	b1	622	LMG	O6-C5-C6-O5
29	c	512	CLA	C16-C17-C18-C19
29	r	602	CLA	C11-C12-C13-C14
29	s	610	CLA	C16-C17-C18-C19
29	c1	510	CLA	C16-C17-C18-C19
32	b	621	SQD	C13-C14-C15-C16
40	c	525	LHG	C33-C34-C35-C36
29	B	605	CLA	C5-C6-C7-C8
29	Y	612	CLA	C13-C15-C16-C17
29	g	603	CLA	C5-C6-C7-C8
29	G1	603	CLA	C8-C10-C11-C12
29	Y1	612	CLA	C8-C10-C11-C12
29	n1	602	CLA	C5-C6-C7-C8
33	c	523	LMG	C13-C14-C15-C16
40	C	525	LHG	C26-C27-C28-C29
40	n1	624	LHG	C25-C26-C27-C28
47	K1	101	4RF	C08-C09-C10-C11
54	S	625	LPX	C16-C17-C18-C19
29	c	509	CLA	C3-C5-C6-C7
29	a1	406	CLA	C3-C5-C6-C7
48	g	601	CHL	C3-C5-C6-C7
48	N1	607	CHL	C3-C5-C6-C7
29	s	603	CLA	O1D-CGD-O2D-CED
32	b1	626	SQD	C27-C28-C29-C30
34	Y1	625	SPH	C11-C10-C9-C8
39	b	625	DGA	CB4-CB5-CB6-CB7
40	L	101	LHG	C11-C10-C9-C8
40	g1	624	LHG	C31-C32-C33-C34
41	C1	527	LMK	C12-C13-C14-C15
52	R1	625	LMT	C11-C10-C9-C8
29	S1	614	CLA	O1A-CGA-O2A-C1
29	Y1	610	CLA	O1A-CGA-O2A-C1
29	c1	503	CLA	O1A-CGA-O2A-C1
32	b	626	SQD	O10-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
38	B	624	3PH	O32-C31-O31-C3
29	S	613	CLA	C5-C6-C7-C8
29	y1	614	CLA	C15-C16-C17-C18
32	b1	626	SQD	C25-C26-C27-C28
33	C	523	LMG	C16-C17-C18-C19
39	c	524	DGA	CB6-CB7-CB8-CB9
39	C1	524	DGA	CBA-CCA-CDA-CEA
40	N	624	LHG	C11-C12-C13-C14
40	d	410	LHG	C31-C32-C33-C34
40	C1	525	LHG	C9-C10-C11-C12
40	L1	101	LHG	C28-C29-C30-C31
47	I	102	4RF	C46-C47-C48-C49
47	K	101	4RF	C32-C33-C34-C35
47	K	101	4RF	C46-C47-C48-C49
47	k	101	4RF	C30-C31-C32-C33
47	k1	101	4RF	C33-C34-C35-C36
32	b1	626	SQD	O49-C7-O47-C45
33	H1	102	LMG	O9-C10-O7-C8
40	g	624	LHG	O9-C7-O7-C5
40	N1	624	LHG	O9-C7-O7-C5
29	A	405	CLA	C2-C1-O2A-CGA
29	B	607	CLA	C2-C1-O2A-CGA
29	B	608	CLA	C2-C1-O2A-CGA
29	B	611	CLA	C2-C1-O2A-CGA
29	B	617	CLA	C2-C1-O2A-CGA
29	C	503	CLA	C2-C1-O2A-CGA
29	N	611	CLA	C2-C1-O2A-CGA
29	N	613	CLA	C2-C1-O2A-CGA
29	R	603	CLA	C2-C1-O2A-CGA
29	S	603	CLA	C2-C1-O2A-CGA
29	S	614	CLA	C2-C1-O2A-CGA
29	Y	608	CLA	C2-C1-O2A-CGA
29	b	608	CLA	C2-C1-O2A-CGA
29	b	617	CLA	C2-C1-O2A-CGA
29	c	503	CLA	C2-C1-O2A-CGA
29	n	611	CLA	C2-C1-O2A-CGA
29	g	611	CLA	C2-C1-O2A-CGA
29	A1	405	CLA	C2-C1-O2A-CGA
29	B1	611	CLA	C2-C1-O2A-CGA
29	B1	616	CLA	C2-C1-O2A-CGA
29	B1	617	CLA	C2-C1-O2A-CGA
29	C1	502	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
29	C1	504	CLA	C2-C1-O2A-CGA
29	C1	510	CLA	C2-C1-O2A-CGA
29	R1	612	CLA	C2-C1-O2A-CGA
29	S1	603	CLA	C2-C1-O2A-CGA
29	b1	614	CLA	C2-C1-O2A-CGA
29	c1	502	CLA	C2-C1-O2A-CGA
29	c1	509	CLA	C2-C1-O2A-CGA
29	n1	613	CLA	C2-C1-O2A-CGA
29	n1	614	CLA	C2-C1-O2A-CGA
29	g1	611	CLA	C2-C1-O2A-CGA
29	s1	611	CLA	C2-C1-O2A-CGA
29	s1	614	CLA	C2-C1-O2A-CGA
29	y1	604	CLA	C2-C1-O2A-CGA
48	Y1	607	CHL	C2-C1-O2A-CGA
32	B	621	SQD	C12-C13-C14-C15
32	a1	412	SQD	C10-C11-C12-C13
34	y	625	SPH	C11-C10-C9-C8
37	C	519	DGD	C6A-C7A-C8A-C9A
37	C	520	DGD	C9A-CAA-CBA-CCA
38	B	624	3PH	C2A-C2B-C2C-C2D
38	T	101	3PH	C32-C33-C34-C35
38	B1	624	3PH	C2E-C2F-C2G-C2H
38	S1	626	3PH	C29-C2A-C2B-C2C
39	B	625	DGA	CA7-CA8-CA9-CAA
39	J	101	DGA	CA4-CA5-CA6-CA7
39	j	101	DGA	CA2-CA3-CA4-CA5
40	N	624	LHG	C9-C10-C11-C12
40	d	408	LHG	C13-C14-C15-C16
40	N1	624	LHG	C16-C17-C18-C19
40	Y1	624	LHG	C29-C30-C31-C32
40	d1	409	LHG	C27-C28-C29-C30
40	y1	624	LHG	C13-C14-C15-C16
52	r1	625	LMT	C4-C5-C6-C7
29	a	405	CLA	C8-C10-C11-C12
29	b	606	CLA	C10-C11-C12-C13
29	s	611	CLA	C10-C11-C12-C13
29	B1	612	CLA	C5-C6-C7-C8
29	G1	613	CLA	C5-C6-C7-C8
29	Y1	603	CLA	C15-C16-C17-C18
29	b1	612	CLA	C10-C11-C12-C13
29	s1	611	CLA	C10-C11-C12-C13
29	b	612	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	r	610	CLA	O1A-CGA-O2A-C1
40	d1	409	LHG	O10-C23-O8-C6
32	A	412	SQD	C14-C15-C16-C17
32	C1	526	SQD	C25-C26-C27-C28
33	H1	102	LMG	C12-C13-C14-C15
38	S1	626	3PH	C28-C29-C2A-C2B
38	S1	626	3PH	C34-C35-C36-C37
38	s1	626	3PH	C25-C26-C27-C28
39	J	101	DGA	CB7-CB8-CB9-CAB
39	c1	524	DGA	CA9-CAA-CBA-CCA
40	d	408	LHG	C26-C27-C28-C29
40	d	408	LHG	C29-C30-C31-C32
40	D1	408	LHG	C31-C32-C33-C34
40	D1	409	LHG	C13-C14-C15-C16
40	Y1	624	LHG	C33-C34-C35-C36
40	d1	409	LHG	C10-C11-C12-C13
29	C	501	CLA	C16-C17-C18-C19
29	s	604	CLA	C6-C7-C8-C10
29	C1	501	CLA	C16-C17-C18-C20
29	g1	610	CLA	C16-C17-C18-C19
37	C	518	DGD	C1B-C2B-C3B-C4B
37	c1	518	DGD	C1B-C2B-C3B-C4B
39	B1	625	DGA	CB1-CB2-CB3-CB4
31	A	411	BCR	C23-C24-C25-C26
31	A	411	BCR	C23-C24-C25-C30
31	C	514	BCR	C1-C6-C7-C8
31	C	514	BCR	C5-C6-C7-C8
31	C	516	BCR	C1-C6-C7-C8
31	C	516	BCR	C23-C24-C25-C26
31	C	516	BCR	C23-C24-C25-C30
31	C	517	BCR	C23-C24-C25-C26
31	C	517	BCR	C23-C24-C25-C30
31	D	404	BCR	C1-C6-C7-C8
31	D	404	BCR	C5-C6-C7-C8
31	D	404	BCR	C23-C24-C25-C30
31	a	411	BCR	C5-C6-C7-C8
31	a	411	BCR	C23-C24-C25-C26
31	a	411	BCR	C23-C24-C25-C30
31	c	514	BCR	C1-C6-C7-C8
31	c	514	BCR	C5-C6-C7-C8
31	c	514	BCR	C23-C24-C25-C26
31	c	516	BCR	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
31	d	404	BCR	C1-C6-C7-C8
31	d	404	BCR	C5-C6-C7-C8
31	B1	618	BCR	C23-C24-C25-C26
31	B1	618	BCR	C23-C24-C25-C30
31	C1	514	BCR	C1-C6-C7-C8
31	C1	514	BCR	C5-C6-C7-C8
31	C1	515	BCR	C23-C24-C25-C26
31	C1	515	BCR	C23-C24-C25-C30
31	C1	516	BCR	C23-C24-C25-C26
31	C1	516	BCR	C23-C24-C25-C30
31	C1	517	BCR	C23-C24-C25-C26
31	C1	517	BCR	C23-C24-C25-C30
31	D1	404	BCR	C1-C6-C7-C8
31	D1	404	BCR	C5-C6-C7-C8
31	a1	411	BCR	C23-C24-C25-C26
31	a1	411	BCR	C23-C24-C25-C30
31	b1	618	BCR	C23-C24-C25-C26
31	b1	618	BCR	C23-C24-C25-C30
31	c1	514	BCR	C1-C6-C7-C8
31	c1	514	BCR	C5-C6-C7-C8
31	c1	514	BCR	C23-C24-C25-C26
31	c1	514	BCR	C23-C24-C25-C30
31	c1	516	BCR	C1-C6-C7-C8
31	d1	404	BCR	C1-C6-C7-C8
31	d1	404	BCR	C5-C6-C7-C8
36	B	620	C7Z	C1-C6-C7-C8
36	b	620	C7Z	C1-C6-C7-C8
36	b	620	C7Z	C21-C26-C27-C28
36	b	620	C7Z	C25-C26-C27-C28
36	B1	620	C7Z	C1-C6-C7-C8
36	B1	620	C7Z	C21-C26-C27-C28
36	B1	620	C7Z	C25-C26-C27-C28
36	b1	620	C7Z	C1-C6-C7-C8
36	b1	620	C7Z	C5-C6-C7-C8
36	b1	620	C7Z	C25-C26-C27-C28
45	H1	101	RRX	C5-C6-C7-C8
49	G1	620	LUT	C5-C6-C7-C8
49	n1	621	LUT	C5-C6-C7-C8
49	g1	620	LUT	C1-C6-C7-C8
49	g1	620	LUT	C5-C6-C7-C8
49	s1	621	LUT	C5-C6-C7-C8
37	C	519	DGD	O6E-C5E-C6E-O5E

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Mol	Chain	Res	Type	Atoms
33	C	523	LMG	C12-C13-C14-C15
37	C1	519	DGD	CAB-CBB-CCB-CDB
40	S	624	LHG	C9-C10-C11-C12
40	n	624	LHG	C16-C17-C18-C19
40	g	624	LHG	C27-C28-C29-C30
54	S1	625	LPX	C17-C18-C19-C20
29	B	614	CLA	CBA-CGA-O2A-C1
29	B1	613	CLA	CBA-CGA-O2A-C1
37	b1	623	DGD	C2A-C1A-O1G-C1G
39	J1	101	DGA	CA2-CA1-OG1-CG1
29	B	602	CLA	C10-C11-C12-C13
29	B	614	CLA	C8-C10-C11-C12
29	G	602	CLA	C13-C15-C16-C17
29	R	609	CLA	C8-C10-C11-C12
29	S	609	CLA	C5-C6-C7-C8
29	b	613	CLA	C10-C11-C12-C13
29	c	503	CLA	C13-C15-C16-C17
29	A1	405	CLA	C13-C15-C16-C17
29	A1	405	CLA	C15-C16-C17-C18
29	B1	610	CLA	C5-C6-C7-C8
29	Y1	612	CLA	C13-C15-C16-C17
29	b1	602	CLA	C10-C11-C12-C13
29	c1	511	CLA	C10-C11-C12-C13
37	C	518	DGD	O6D-C5D-C6D-O5D
37	c	519	DGD	C4B-C5B-C6B-C7B
38	s1	626	3PH	C3E-C3F-C3G-C3H
39	b	625	DGA	CB3-CB4-CB5-CB6
39	c1	524	DGA	CB7-CB8-CB9-CAB
40	G	624	LHG	C15-C16-C17-C18
40	c	525	LHG	C30-C31-C32-C33
47	I1	102	4RF	C51-C52-C53-C54
47	I1	102	4RF	C52-C53-C54-C55
47	k1	101	4RF	C32-C33-C34-C35
37	c1	518	DGD	C1A-C2A-C3A-C4A
38	B	624	3PH	C21-C22-C23-C24
40	n1	624	LHG	C23-C24-C25-C26
40	C	525	LHG	C25-C26-C27-C28
40	y	624	LHG	C9-C10-C11-C12
29	B	612	CLA	C13-C15-C16-C17
29	C	509	CLA	C15-C16-C17-C18
29	c	501	CLA	C8-C10-C11-C12
29	c	504	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	c	513	CLA	C13-C15-C16-C17
29	N1	604	CLA	C13-C15-C16-C17
29	c1	504	CLA	C8-C10-C11-C12
29	y1	611	CLA	C8-C10-C11-C12
32	A1	412	SQD	C13-C14-C15-C16
37	C1	519	DGD	C6B-C7B-C8B-C9B
40	L	101	LHG	C11-C12-C13-C14
40	n	624	LHG	C13-C14-C15-C16
40	N1	624	LHG	C28-C29-C30-C31
47	K	101	4RF	C03-C04-C05-C06
47	k1	101	4RF	C07-C08-C09-C10
29	G	613	CLA	C4-C3-C5-C6
29	A	410	CLA	C11-C10-C8-C7
29	B	603	CLA	C12-C13-C15-C16
29	B	605	CLA	C11-C12-C13-C15
29	B	607	CLA	C11-C12-C13-C15
29	B	609	CLA	C11-C12-C13-C15
29	B	610	CLA	C11-C12-C13-C15
29	B	612	CLA	C11-C10-C8-C7
29	B	617	CLA	C6-C7-C8-C10
29	C	507	CLA	C6-C7-C8-C10
29	C	513	CLA	C6-C7-C8-C10
29	D	402	CLA	C11-C12-C13-C15
29	D	402	CLA	C12-C13-C15-C16
29	D	403	CLA	C11-C12-C13-C15
29	G	613	CLA	C11-C12-C13-C15
29	R	603	CLA	C11-C10-C8-C7
29	S	603	CLA	C11-C10-C8-C7
29	Y	603	CLA	C6-C7-C8-C10
29	Y	614	CLA	C12-C13-C15-C16
29	a	410	CLA	C6-C7-C8-C10
29	b	602	CLA	C6-C7-C8-C10
29	b	604	CLA	C11-C12-C13-C15
29	b	605	CLA	C6-C7-C8-C10
29	b	612	CLA	C2-C3-C5-C6
29	b	616	CLA	C12-C13-C15-C16
29	c	503	CLA	C12-C13-C15-C16
29	c	509	CLA	C6-C7-C8-C10
29	c	510	CLA	C2-C3-C5-C6
29	c	512	CLA	C12-C13-C15-C16
29	c	513	CLA	C6-C7-C8-C10
29	d	403	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
29	n	603	CLA	C11-C10-C8-C7
29	n	610	CLA	C6-C7-C8-C10
29	g	603	CLA	C6-C7-C8-C10
29	g	611	CLA	C6-C7-C8-C10
29	g	613	CLA	C6-C7-C8-C10
29	r	603	CLA	C11-C10-C8-C7
29	r	610	CLA	C11-C10-C8-C7
29	s	602	CLA	C11-C10-C8-C7
29	y	604	CLA	C2-C3-C5-C6
29	A1	410	CLA	C6-C7-C8-C10
29	B1	606	CLA	C11-C12-C13-C15
29	B1	610	CLA	C11-C12-C13-C15
29	C1	503	CLA	C6-C7-C8-C10
29	C1	505	CLA	C11-C12-C13-C15
29	C1	505	CLA	C12-C13-C15-C16
29	C1	506	CLA	C6-C7-C8-C10
29	G1	611	CLA	C6-C7-C8-C10
29	G1	611	CLA	C11-C10-C8-C7
29	G1	613	CLA	C6-C7-C8-C10
29	R1	603	CLA	C2-C3-C5-C6
29	R1	609	CLA	C11-C10-C8-C7
29	R1	612	CLA	C11-C10-C8-C7
29	b1	602	CLA	C11-C12-C13-C15
29	b1	604	CLA	C6-C7-C8-C10
29	c1	503	CLA	C6-C7-C8-C10
29	c1	505	CLA	C2-C3-C5-C6
29	c1	508	CLA	C11-C12-C13-C15
29	c1	509	CLA	C12-C13-C15-C16
29	c1	510	CLA	C12-C13-C15-C16
29	c1	511	CLA	C11-C12-C13-C15
29	c1	513	CLA	C6-C7-C8-C10
29	n1	613	CLA	C2-C3-C5-C6
29	r1	612	CLA	C6-C7-C8-C10
29	r1	612	CLA	C11-C10-C8-C7
29	y1	602	CLA	C6-C7-C8-C10
29	y1	612	CLA	C12-C13-C15-C16
43	D	405	PL9	C43-C44-C46-C47
43	D1	405	PL9	C28-C29-C31-C32
48	G	601	CHL	C12-C13-C15-C16
48	n	607	CHL	C11-C10-C8-C7
48	g	609	CHL	C12-C13-C15-C16
48	s	608	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
48	y	606	CHL	C11-C10-C8-C7
48	g1	601	CHL	C12-C13-C15-C16
48	y1	609	CHL	C2-C3-C5-C6
29	s	611	CLA	C3-C5-C6-C7
29	b	614	CLA	O1A-CGA-O2A-C1
29	n	602	CLA	O1A-CGA-O2A-C1
29	B1	613	CLA	O1A-CGA-O2A-C1
39	J	101	DGA	OA1-CA1-OG1-CG1
33	C1	523	LMG	C16-C17-C18-C19
34	y1	625	SPH	C6-C7-C8-C9
38	B1	624	3PH	C37-C38-C39-C3A
47	k	101	4RF	C26-C27-C28-C29
29	B	611	CLA	C15-C16-C17-C18
29	C	502	CLA	C8-C10-C11-C12
29	N	603	CLA	C13-C15-C16-C17
29	R1	612	CLA	C5-C6-C7-C8
29	S1	611	CLA	C10-C11-C12-C13
29	r1	608	CLA	C8-C10-C11-C12
31	A	411	BCR	C19-C20-C21-C22
31	D	404	BCR	C9-C10-C11-C12
31	A1	411	BCR	C19-C20-C21-C22
31	c1	514	BCR	C19-C20-C21-C22
36	B	620	C7Z	C29-C30-C31-C32
49	g	621	LUT	C29-C30-C31-C32
49	y	621	LUT	C29-C30-C31-C32
50	y1	622	XAT	C29-C30-C31-C32
51	S1	623	NEX	C9-C10-C11-C12
29	c	510	CLA	C16-C17-C18-C19
29	C1	509	CLA	C16-C17-C18-C20
29	R1	610	CLA	C11-C12-C13-C15
29	A1	406	CLA	O1D-CGD-O2D-CED
29	B1	602	CLA	O1D-CGD-O2D-CED
29	b1	610	CLA	O1D-CGD-O2D-CED
33	C1	521	LMG	O9-C10-O7-C8
40	D1	409	LHG	O9-C7-O7-C5
55	y	626	PTY	O10-C8-O7-C6
38	b	624	3PH	C21-C22-C23-C24
40	d	408	LHG	C7-C8-C9-C10
40	n	624	LHG	C23-C24-C25-C26
40	g1	624	LHG	C7-C8-C9-C10
29	A	410	CLA	CBA-CGA-O2A-C1
29	B	612	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	Y	614	CLA	CBA-CGA-O2A-C1
29	b	605	CLA	CBA-CGA-O2A-C1
29	c	503	CLA	CBA-CGA-O2A-C1
29	G1	603	CLA	CBA-CGA-O2A-C1
29	G1	610	CLA	CBA-CGA-O2A-C1
29	g1	603	CLA	CBA-CGA-O2A-C1
29	y1	602	CLA	CBA-CGA-O2A-C1
29	y1	610	CLA	CBA-CGA-O2A-C1
37	c	519	DGD	C2A-C1A-O1G-C1G
37	c1	518	DGD	C2A-C1A-O1G-C1G
32	A	412	SQD	C31-C32-C33-C34
32	c	526	SQD	C11-C10-C9-C8
33	C1	523	LMG	C13-C14-C15-C16
34	Y	625	SPH	C11-C12-C13-C14
38	B1	624	3PH	C2D-C2E-C2F-C2G
40	g	624	LHG	C31-C32-C33-C34
47	k	101	4RF	C45-C46-C47-C48
47	i1	101	4RF	C52-C53-C54-C55
52	R1	625	LMT	C7-C8-C9-C10
29	N	613	CLA	C2A-CAA-CBA-CGA
29	G	610	CLA	C2A-CAA-CBA-CGA
29	S	603	CLA	C2A-CAA-CBA-CGA
29	b	617	CLA	C2A-CAA-CBA-CGA
29	g	602	CLA	C2A-CAA-CBA-CGA
29	r	602	CLA	C2A-CAA-CBA-CGA
29	y	613	CLA	C2A-CAA-CBA-CGA
29	B1	603	CLA	C2A-CAA-CBA-CGA
29	S1	613	CLA	C2A-CAA-CBA-CGA
29	s1	603	CLA	C2A-CAA-CBA-CGA
29	y1	602	CLA	C2A-CAA-CBA-CGA
29	y1	610	CLA	C2A-CAA-CBA-CGA
48	y1	605	CHL	C2A-CAA-CBA-CGA
29	a	406	CLA	O1D-CGD-O2D-CED
29	B	614	CLA	C5-C6-C7-C8
29	C	510	CLA	C15-C16-C17-C18
29	N	602	CLA	C13-C15-C16-C17
29	Y	612	CLA	C15-C16-C17-C18
29	n	610	CLA	C10-C11-C12-C13
29	n	613	CLA	C10-C11-C12-C13
29	r	610	CLA	C8-C10-C11-C12
29	C1	503	CLA	C15-C16-C17-C18
29	c1	509	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
32	B1	626	SQD	C32-C33-C34-C35
38	b1	624	3PH	C32-C33-C34-C35
39	j	101	DGA	CB6-CB7-CB8-CB9
40	D	408	LHG	C13-C14-C15-C16
40	l	101	LHG	C26-C27-C28-C29
47	K1	101	4RF	C25-C26-C27-C28
47	K1	101	4RF	C32-C33-C34-C35
47	k1	101	4RF	C03-C04-C05-C06
33	d1	411	LMG	C22-C23-C24-C25
37	c1	519	DGD	C4A-C5A-C6A-C7A
38	B1	624	3PH	C39-C3A-C3B-C3C
38	s1	626	3PH	C36-C37-C38-C39
39	j1	101	DGA	CB3-CB4-CB5-CB6
40	d	409	LHG	C34-C35-C36-C37
40	g	624	LHG	C24-C25-C26-C27
40	D1	409	LHG	C28-C29-C30-C31
33	c	523	LMG	C28-C29-C30-C31
37	C	519	DGD	C1A-C2A-C3A-C4A
38	B	624	3PH	C31-C32-C33-C34
40	D	408	LHG	C7-C8-C9-C10
40	N	624	LHG	C23-C24-C25-C26
40	D1	408	LHG	C23-C24-C25-C26
40	N1	624	LHG	C7-C8-C9-C10
54	S1	625	LPX	C3-C4-C5-O6
29	B	613	CLA	C10-C11-C12-C13
29	g	602	CLA	C5-C6-C7-C8
32	b1	626	SQD	C12-C13-C14-C15
33	D1	411	LMG	C19-C20-C21-C22
34	y1	625	SPH	C9-C10-C11-C12
40	D	409	LHG	C11-C12-C13-C14
40	Y	624	LHG	C30-C31-C32-C33
40	L1	101	LHG	C25-C26-C27-C28
41	c1	527	LMK	C12-C13-C14-C15
47	K	101	4RF	C27-C28-C29-C30
47	i1	101	4RF	C27-C28-C29-C30
52	R1	625	LMT	O1'-C1-C2-C3
55	Y	626	PTY	C19-C20-C21-C22
38	B	624	3PH	C27-C28-C29-C2A
39	J	101	DGA	CB6-CB7-CB8-CB9
40	Y1	624	LHG	C13-C14-C15-C16
47	I1	102	4RF	C12-C13-C14-C15
47	K1	101	4RF	C43-C44-C45-C46

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Mol	Chain	Res	Type	Atoms
37	C1	518	DGD	C2A-C1A-O1G-C1G
55	Y	626	PTY	C31-C30-O4-C1
29	C	513	CLA	C16-C17-C18-C19
29	Y	610	CLA	C16-C17-C18-C20
29	s	602	CLA	C11-C12-C13-C15
29	D1	402	CLA	C16-C17-C18-C19
29	D1	403	CLA	C16-C17-C18-C20
29	R1	608	CLA	C11-C12-C13-C15
29	Y1	612	CLA	C16-C17-C18-C20
29	b1	608	CLA	C16-C17-C18-C20
29	b1	614	CLA	C16-C17-C18-C19
33	H	102	LMG	C4-C5-C6-O5
32	M1	101	SQD	O5-C1-O6-C44
37	C	518	DGD	O6E-C1E-O5D-C6D
29	A	405	CLA	C15-C16-C17-C18
29	A	410	CLA	C8-C10-C11-C12
29	g	613	CLA	C13-C15-C16-C17
29	b1	608	CLA	C13-C15-C16-C17
32	c	526	SQD	C12-C13-C14-C15
32	B1	626	SQD	C18-C19-C20-C21
40	c1	525	LHG	C11-C12-C13-C14
47	I1	102	4RF	C09-C10-C11-C12
47	K1	101	4RF	C24-C25-C26-C27
47	i1	101	4RF	C10-C11-C12-C13
55	y1	626	PTY	C38-C39-C40-C41
37	C	519	DGD	C1B-C2B-C3B-C4B
38	T	101	3PH	C31-C32-C33-C34
39	b	625	DGA	CB1-CB2-CB3-CB4
33	A	413	LMG	C11-C10-O7-C8
33	c	521	LMG	C11-C10-O7-C8
33	w	201	LMG	C11-C10-O7-C8
38	B	624	3PH	C22-C21-O21-C2
39	c	524	DGA	CB2-CB1-OG2-CG2
40	C	525	LHG	C8-C7-O7-C5
40	Y	624	LHG	C8-C7-O7-C5
40	s	624	LHG	C8-C7-O7-C5
40	D1	410	LHG	C8-C7-O7-C5
40	c1	525	LHG	C8-C7-O7-C5
47	K	101	4RF	C24-C22-O21-C20
55	y	626	PTY	C11-C8-O7-C6
51	Y	623	NEX	C30-C31-C32-C33
33	A1	413	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
34	a1	414	SPH	C14-C15-C16-C17
40	s	624	LHG	C33-C34-C35-C36
40	D1	409	LHG	C25-C26-C27-C28
29	B	606	CLA	C13-C15-C16-C17
29	N	610	CLA	C13-C15-C16-C17
29	Y	602	CLA	C13-C15-C16-C17
29	c	504	CLA	C5-C6-C7-C8
29	b1	603	CLA	C8-C10-C11-C12
29	g1	603	CLA	C15-C16-C17-C18
29	b1	615	CLA	CBD-CGD-O2D-CED
40	l	101	LHG	C9-C10-C11-C12
40	n	624	LHG	C24-C25-C26-C27
40	S1	624	LHG	C34-C35-C36-C37
33	c	521	LMG	O9-C10-O7-C8
33	h	102	LMG	O9-C10-O7-C8
40	C	525	LHG	O9-C7-O7-C5
40	D1	410	LHG	O9-C7-O7-C5
41	c	527	LMK	C2-C3-C4-O2
41	c1	527	LMK	C2-C3-C4-O2
29	G1	613	CLA	C3-C5-C6-C7
40	L1	101	LHG	C23-C24-C25-C26
32	c1	526	SQD	C18-C19-C20-C21
38	S1	626	3PH	C2D-C2E-C2F-C2G
55	y	626	PTY	C31-C32-C33-C34
53	r1	626	ERG	C21-C20-C22-C23
32	c1	526	SQD	C2-C1-O6-C44
29	C	509	CLA	C8-C10-C11-C12
29	c1	501	CLA	C15-C16-C17-C18
30	a1	408	PHO	C8-C10-C11-C12
33	A	413	LMG	O1-C7-C8-O7
33	a	413	LMG	O1-C7-C8-O7
40	N1	624	LHG	O7-C5-C6-O8
41	c	527	LMK	O1-C7-C8-O7
47	I	102	4RF	O21-C20-C39-O40
47	I1	102	4RF	O18-C19-C20-O21
37	C1	519	DGD	O6E-C5E-C6E-O5E
32	m	101	SQD	C26-C27-C28-C29
38	B	624	3PH	C24-C25-C26-C27
39	C1	524	DGA	CB5-CB6-CB7-CB8
40	D1	409	LHG	C34-C35-C36-C37
40	d1	408	LHG	C25-C26-C27-C28
40	g1	624	LHG	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
52	r	625	LMT	C6-C7-C8-C9
29	C	504	CLA	CBD-CGD-O2D-CED
29	c	509	CLA	C16-C17-C18-C20
29	b1	610	CLA	C16-C17-C18-C19
29	y1	614	CLA	C16-C17-C18-C20
32	b	621	SQD	C24-C25-C26-C27
33	B	622	LMG	C11-C12-C13-C14
34	a	414	SPH	C9-C10-C11-C12
39	C	524	DGA	CA9-CAA-CBA-CCA
47	k1	101	4RF	C11-C12-C13-C14
55	y1	626	PTY	C11-C12-C13-C14
33	D	411	LMG	O6-C5-C6-O5
29	N	613	CLA	C10-C11-C12-C13
29	B1	605	CLA	C15-C16-C17-C18
29	b1	606	CLA	C8-C10-C11-C12
29	r1	602	CLA	C8-C10-C11-C12
29	s1	603	CLA	C5-C6-C7-C8
48	G1	601	CHL	C5-C6-C7-C8
29	B	603	CLA	C4-C3-C5-C6
29	y	604	CLA	C4-C3-C5-C6
29	R1	603	CLA	C4-C3-C5-C6
29	b1	608	CLA	C4-C3-C5-C6
29	n1	613	CLA	C4-C3-C5-C6
40	D	409	LHG	C23-C24-C25-C26
29	G	613	CLA	C2-C3-C5-C6
29	S	602	CLA	C2-C3-C5-C6
29	S	611	CLA	C2-C3-C5-C6
29	b	614	CLA	C2-C3-C5-C6
30	a1	408	PHO	C2-C3-C5-C6
33	A	413	LMG	C36-C37-C38-C39
33	w1	201	LMG	C37-C38-C39-C40
39	C	524	DGA	CCA-CDA-CEA-CFA
47	i	101	4RF	C24-C25-C26-C27
47	k	101	4RF	C28-C29-C30-C31
54	s	625	LPX	C12-C13-C14-C15
29	A	410	CLA	C11-C10-C8-C9
29	B	605	CLA	C11-C12-C13-C14
29	B	609	CLA	C11-C12-C13-C14
29	B	617	CLA	C6-C7-C8-C9
29	C	505	CLA	C14-C13-C15-C16
29	C	509	CLA	C14-C13-C15-C16
29	C	513	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
29	D	402	CLA	C11-C12-C13-C14
29	G	610	CLA	C11-C12-C13-C14
29	G	611	CLA	C6-C7-C8-C9
29	G	611	CLA	C14-C13-C15-C16
29	R	603	CLA	C11-C10-C8-C9
29	Y	612	CLA	C6-C7-C8-C9
29	Y	613	CLA	C6-C7-C8-C9
29	b	615	CLA	C6-C7-C8-C9
29	c	503	CLA	C11-C12-C13-C14
29	c	509	CLA	C14-C13-C15-C16
29	c	513	CLA	C6-C7-C8-C9
29	c	513	CLA	C11-C12-C13-C14
29	n	603	CLA	C11-C10-C8-C9
29	n	604	CLA	C14-C13-C15-C16
29	g	603	CLA	C11-C12-C13-C14
29	g	610	CLA	C11-C10-C8-C9
29	g	613	CLA	C6-C7-C8-C9
29	s	602	CLA	C11-C10-C8-C9
29	y	610	CLA	C11-C12-C13-C14
29	y	613	CLA	C11-C12-C13-C14
29	C1	505	CLA	C11-C12-C13-C14
29	C1	512	CLA	C14-C13-C15-C16
29	G1	602	CLA	C6-C7-C8-C9
29	G1	611	CLA	C6-C7-C8-C9
29	R1	603	CLA	C11-C10-C8-C9
29	R1	609	CLA	C11-C10-C8-C9
29	R1	610	CLA	C11-C10-C8-C9
29	Y1	612	CLA	C14-C13-C15-C16
29	Y1	613	CLA	C14-C13-C15-C16
29	b1	610	CLA	C11-C12-C13-C14
29	c1	503	CLA	C6-C7-C8-C9
29	c1	508	CLA	C11-C12-C13-C14
29	c1	511	CLA	C11-C12-C13-C14
29	c1	513	CLA	C6-C7-C8-C9
29	g1	610	CLA	C11-C10-C8-C9
29	r1	608	CLA	C6-C7-C8-C9
29	r1	609	CLA	C11-C10-C8-C9
29	y1	602	CLA	C6-C7-C8-C9
29	y1	602	CLA	C11-C12-C13-C14
29	y1	612	CLA	C14-C13-C15-C16
29	y1	613	CLA	C11-C10-C8-C9
48	Y	606	CHL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
48	g	601	CHL	C11-C12-C13-C14
48	N1	607	CHL	C11-C10-C8-C9
32	b	626	SQD	C12-C13-C14-C15
38	s	626	3PH	C23-C24-C25-C26
40	l	101	LHG	C28-C29-C30-C31
47	i	101	4RF	C49-C50-C51-C52
47	il	101	4RF	C25-C26-C27-C28
29	n	613	CLA	C3-C5-C6-C7
29	y	614	CLA	C3-C5-C6-C7
29	G1	611	CLA	C3-C5-C6-C7
48	N	607	CHL	C3-C5-C6-C7
29	B	604	CLA	C2A-CAA-CBA-CGA
29	G	614	CLA	C2A-CAA-CBA-CGA
29	R	610	CLA	C2A-CAA-CBA-CGA
29	b	604	CLA	C2A-CAA-CBA-CGA
29	A1	407	CLA	C2A-CAA-CBA-CGA
48	R	607	CHL	C2A-CAA-CBA-CGA
48	r	607	CHL	C2A-CAA-CBA-CGA
29	B1	614	CLA	C4C-C3C-CAC-CBC
32	m1	101	SQD	C10-C11-C12-C13
38	T	101	3PH	C38-C39-C3A-C3B
39	c1	524	DGA	CBB-CCB-CDB-CEB
40	d	408	LHG	C24-C25-C26-C27
40	y1	624	LHG	C11-C10-C9-C8
55	y1	626	PTY	C24-C25-C26-C27
33	h1	102	LMG	O6-C5-C6-O5
37	c	518	DGD	O6E-C5E-C6E-O5E
31	D	404	BCR	C37-C22-C23-C24
29	c1	512	CLA	O1D-CGD-O2D-CED
29	b	614	CLA	C13-C15-C16-C17
29	r	608	CLA	C8-C10-C11-C12
29	g1	611	CLA	C15-C16-C17-C18
29	y1	611	CLA	C10-C11-C12-C13
33	C	521	LMG	C14-C15-C16-C17
33	H1	102	LMG	C14-C15-C16-C17
39	c	524	DGA	CDA-CEA-CFA-CGA
40	d1	409	LHG	C29-C30-C31-C32
40	y1	624	LHG	C33-C34-C35-C36
47	K	101	4RF	C11-C12-C13-C14
47	il	101	4RF	C11-C12-C13-C14
54	s1	625	LPX	C15-C16-C17-C18
31	A	411	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	B	619	BCR	C21-C22-C23-C24
31	D	404	BCR	C21-C22-C23-C24
49	Y	620	LUT	C27-C28-C29-C30
49	N1	620	LUT	C27-C28-C29-C30
29	A	410	CLA	O1A-CGA-O2A-C1
29	B	614	CLA	O1A-CGA-O2A-C1
29	y1	602	CLA	O1A-CGA-O2A-C1
37	c	519	DGD	O1A-C1A-O1G-C1G
37	b1	623	DGD	O1A-C1A-O1G-C1G
37	c1	518	DGD	O1A-C1A-O1G-C1G
39	J1	101	DGA	OA1-CA1-OG1-CG1
40	D	410	LHG	O10-C23-O8-C6
29	A	407	CLA	C1A-C2A-CAA-CBA
29	B	602	CLA	C1A-C2A-CAA-CBA
29	B	604	CLA	C1A-C2A-CAA-CBA
29	B	610	CLA	C1A-C2A-CAA-CBA
29	C	503	CLA	C1A-C2A-CAA-CBA
29	C	511	CLA	C1A-C2A-CAA-CBA
29	D	403	CLA	C1A-C2A-CAA-CBA
29	N	603	CLA	C1A-C2A-CAA-CBA
29	G	603	CLA	C1A-C2A-CAA-CBA
29	G	610	CLA	C1A-C2A-CAA-CBA
29	G	611	CLA	C1A-C2A-CAA-CBA
29	G	614	CLA	C1A-C2A-CAA-CBA
29	R	602	CLA	C1A-C2A-CAA-CBA
29	R	603	CLA	C1A-C2A-CAA-CBA
29	S	602	CLA	C1A-C2A-CAA-CBA
29	S	604	CLA	C1A-C2A-CAA-CBA
29	S	609	CLA	C1A-C2A-CAA-CBA
29	S	610	CLA	C1A-C2A-CAA-CBA
29	S	617	CLA	C1A-C2A-CAA-CBA
29	Y	602	CLA	C1A-C2A-CAA-CBA
29	Y	603	CLA	C1A-C2A-CAA-CBA
29	Y	610	CLA	C1A-C2A-CAA-CBA
29	Y	611	CLA	C1A-C2A-CAA-CBA
29	Y	614	CLA	C1A-C2A-CAA-CBA
29	b	604	CLA	C1A-C2A-CAA-CBA
29	b	606	CLA	C1A-C2A-CAA-CBA
29	b	607	CLA	C1A-C2A-CAA-CBA
29	b	610	CLA	C1A-C2A-CAA-CBA
29	c	501	CLA	C1A-C2A-CAA-CBA
29	c	503	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	c	511	CLA	C1A-C2A-CAA-CBA
29	d	403	CLA	C1A-C2A-CAA-CBA
29	n	602	CLA	C1A-C2A-CAA-CBA
29	n	603	CLA	C1A-C2A-CAA-CBA
29	g	602	CLA	C1A-C2A-CAA-CBA
29	g	603	CLA	C1A-C2A-CAA-CBA
29	g	610	CLA	C1A-C2A-CAA-CBA
29	g	611	CLA	C1A-C2A-CAA-CBA
29	r	610	CLA	C1A-C2A-CAA-CBA
29	y	602	CLA	C1A-C2A-CAA-CBA
29	y	603	CLA	C1A-C2A-CAA-CBA
29	y	610	CLA	C1A-C2A-CAA-CBA
29	y	611	CLA	C1A-C2A-CAA-CBA
29	y	614	CLA	C1A-C2A-CAA-CBA
29	A1	407	CLA	C1A-C2A-CAA-CBA
29	B1	602	CLA	C1A-C2A-CAA-CBA
29	B1	605	CLA	C1A-C2A-CAA-CBA
29	B1	606	CLA	C1A-C2A-CAA-CBA
29	B1	610	CLA	C1A-C2A-CAA-CBA
29	B1	612	CLA	C1A-C2A-CAA-CBA
29	C1	503	CLA	C1A-C2A-CAA-CBA
29	C1	506	CLA	C1A-C2A-CAA-CBA
29	C1	507	CLA	C1A-C2A-CAA-CBA
29	C1	512	CLA	C1A-C2A-CAA-CBA
29	D1	402	CLA	C1A-C2A-CAA-CBA
29	N1	603	CLA	C1A-C2A-CAA-CBA
29	N1	613	CLA	C1A-C2A-CAA-CBA
29	G1	603	CLA	C1A-C2A-CAA-CBA
29	G1	610	CLA	C1A-C2A-CAA-CBA
29	R1	603	CLA	C1A-C2A-CAA-CBA
29	R1	608	CLA	C1A-C2A-CAA-CBA
29	R1	609	CLA	C1A-C2A-CAA-CBA
29	R1	610	CLA	C1A-C2A-CAA-CBA
29	R1	612	CLA	C1A-C2A-CAA-CBA
29	S1	602	CLA	C1A-C2A-CAA-CBA
29	S1	609	CLA	C1A-C2A-CAA-CBA
29	S1	610	CLA	C1A-C2A-CAA-CBA
29	S1	617	CLA	C1A-C2A-CAA-CBA
29	Y1	603	CLA	C1A-C2A-CAA-CBA
29	Y1	608	CLA	C1A-C2A-CAA-CBA
29	Y1	610	CLA	C1A-C2A-CAA-CBA
29	Y1	611	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	Y1	614	CLA	C1A-C2A-CAA-CBA
29	a1	405	CLA	C1A-C2A-CAA-CBA
29	b1	602	CLA	C1A-C2A-CAA-CBA
29	b1	610	CLA	C1A-C2A-CAA-CBA
29	c1	501	CLA	C1A-C2A-CAA-CBA
29	c1	503	CLA	C1A-C2A-CAA-CBA
29	c1	507	CLA	C1A-C2A-CAA-CBA
29	c1	512	CLA	C1A-C2A-CAA-CBA
29	n1	602	CLA	C1A-C2A-CAA-CBA
29	n1	603	CLA	C1A-C2A-CAA-CBA
29	n1	613	CLA	C1A-C2A-CAA-CBA
29	g1	603	CLA	C1A-C2A-CAA-CBA
29	g1	611	CLA	C1A-C2A-CAA-CBA
29	g1	614	CLA	C1A-C2A-CAA-CBA
29	r1	602	CLA	C1A-C2A-CAA-CBA
29	r1	610	CLA	C1A-C2A-CAA-CBA
29	s1	602	CLA	C1A-C2A-CAA-CBA
29	s1	605	CLA	C1A-C2A-CAA-CBA
29	s1	612	CLA	C1A-C2A-CAA-CBA
29	s1	614	CLA	C1A-C2A-CAA-CBA
29	y1	602	CLA	C1A-C2A-CAA-CBA
29	y1	603	CLA	C1A-C2A-CAA-CBA
29	y1	608	CLA	C1A-C2A-CAA-CBA
29	y1	610	CLA	C1A-C2A-CAA-CBA
29	y1	614	CLA	C1A-C2A-CAA-CBA
48	G	606	CHL	C1A-C2A-CAA-CBA
48	n	609	CHL	C1A-C2A-CAA-CBA
48	g	607	CHL	C1A-C2A-CAA-CBA
48	N1	607	CHL	C1A-C2A-CAA-CBA
48	G1	605	CHL	C1A-C2A-CAA-CBA
48	G1	606	CHL	C1A-C2A-CAA-CBA
48	G1	609	CHL	C1A-C2A-CAA-CBA
48	n1	608	CHL	C1A-C2A-CAA-CBA
48	s1	608	CHL	C1A-C2A-CAA-CBA
48	y1	601	CHL	C1A-C2A-CAA-CBA
48	y1	609	CHL	C1A-C2A-CAA-CBA
29	C	509	CLA	C16-C17-C18-C19
29	Y	614	CLA	C16-C17-C18-C20
29	b	602	CLA	C16-C17-C18-C19
29	n	610	CLA	C16-C17-C18-C19
29	r	602	CLA	C11-C12-C13-C15
29	s	610	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
29	B1	605	CLA	C16-C17-C18-C19
29	B1	608	CLA	C16-C17-C18-C19
29	C1	501	CLA	C16-C17-C18-C19
29	C1	509	CLA	C16-C17-C18-C19
29	D1	403	CLA	C16-C17-C18-C19
29	S1	613	CLA	C6-C7-C8-C10
29	Y1	612	CLA	C16-C17-C18-C19
29	Y1	614	CLA	C16-C17-C18-C20
29	b1	614	CLA	C16-C17-C18-C20
29	c1	501	CLA	C16-C17-C18-C20
29	n1	610	CLA	C16-C17-C18-C20
33	A	413	LMG	O9-C10-O7-C8
33	w	201	LMG	O9-C10-O7-C8
40	Y	624	LHG	O9-C7-O7-C5
40	s	624	LHG	O9-C7-O7-C5
40	y	624	LHG	O9-C7-O7-C5
40	c1	525	LHG	O9-C7-O7-C5
32	B	621	SQD	C9-C10-C11-C12
38	t	101	3PH	C22-C23-C24-C25
38	t1	101	3PH	C23-C24-C25-C26
38	t1	101	3PH	C3C-C3D-C3E-C3F
40	Y	624	LHG	C16-C17-C18-C19
31	b	619	BCR	C19-C20-C21-C22
36	b1	620	C7Z	C9-C10-C11-C12
49	G	621	LUT	C9-C10-C11-C12
49	G	621	LUT	C29-C30-C31-C32
49	n	621	LUT	C29-C30-C31-C32
49	N1	621	LUT	C29-C30-C31-C32
49	S1	621	LUT	C29-C30-C31-C32
49	s1	620	LUT	C33-C34-C35-C15
29	B	604	CLA	C10-C11-C12-C13
29	b	612	CLA	C15-C16-C17-C18
29	B1	615	CLA	C10-C11-C12-C13
29	c1	508	CLA	C10-C11-C12-C13
40	l	101	LHG	C3-O3-P-O6
40	g	624	LHG	C4-O6-P-O3
40	L1	101	LHG	C4-O6-P-O3
40	y1	624	LHG	C4-O6-P-O3
54	s	625	LPX	C3-O1-P1-O2
54	s1	625	LPX	C1-O2-P1-O1
55	y	626	PTY	C5-O14-P1-O11
32	C1	526	SQD	C17-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
33	C1	523	LMG	C12-C13-C14-C15
34	a1	414	SPH	C7-C8-C9-C10
38	S	626	3PH	C27-C28-C29-C2A
40	G	624	LHG	C11-C12-C13-C14
40	n	624	LHG	C34-C35-C36-C37
40	d1	410	LHG	C11-C10-C9-C8
37	C1	519	DGD	C1B-C2B-C3B-C4B
40	G	624	LHG	C23-C24-C25-C26
40	g1	624	LHG	C23-C24-C25-C26
37	c	519	DGD	O6E-C5E-C6E-O5E
52	R1	625	LMT	O5B-C5B-C6B-O6B
30	A	408	PHO	C3-C5-C6-C7
32	C	526	SQD	C11-C10-C9-C8
32	A1	412	SQD	C31-C32-C33-C34
40	s	624	LHG	C14-C15-C16-C17
40	D1	409	LHG	C33-C34-C35-C36
41	c1	527	LMK	C11-C12-C13-C14
52	r	625	LMT	C3-C4-C5-C6
54	S1	625	LPX	C13-C14-C15-C16
29	B1	616	CLA	C10-C11-C12-C13
37	c	518	DGD	C2A-C1A-O1G-C1G
40	c	525	LHG	C24-C23-O8-C6
40	s1	624	LHG	C24-C23-O8-C6
47	I	102	4RF	C43-C41-O40-C39
33	B1	622	LMG	O6-C5-C6-O5
38	B	624	3PH	O11-C1-C2-C3
40	C	525	LHG	O6-C4-C5-C6
40	L	101	LHG	O6-C4-C5-C6
40	c	525	LHG	O6-C4-C5-C6
40	l	101	LHG	O6-C4-C5-C6
40	n	624	LHG	O6-C4-C5-C6
40	C1	525	LHG	O6-C4-C5-C6
40	L1	101	LHG	O6-C4-C5-C6
40	c1	525	LHG	O6-C4-C5-C6
40	d1	410	LHG	O6-C4-C5-C6
40	n1	624	LHG	O6-C4-C5-C6
55	y	627	PTY	O14-C5-C6-C1
32	b	626	SQD	C27-C28-C29-C30
33	c1	521	LMG	C18-C19-C20-C21
37	C1	518	DGD	C5A-C6A-C7A-C8A
37	C1	519	DGD	CCB-CDB-CEB-CFB
38	S	626	3PH	C22-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
40	s	624	LHG	C12-C13-C14-C15
40	G1	624	LHG	C31-C32-C33-C34
40	c1	525	LHG	C11-C10-C9-C8
47	i	101	4RF	C46-C47-C48-C49
47	k	101	4RF	C32-C33-C34-C35
32	m	101	SQD	C23-C24-C25-C26
32	a1	412	SQD	C7-C8-C9-C10
33	h1	102	LMG	C10-C11-C12-C13
47	l1	102	4RF	C22-C24-C25-C26
37	C1	520	DGD	CCB-CDB-CEB-CFB
38	T	101	3PH	C2C-C2D-C2E-C2F
38	t1	101	3PH	C3B-C3C-C3D-C3E
39	J	101	DGA	CA2-CA3-CA4-CA5
40	L	101	LHG	C30-C31-C32-C33
40	d1	410	LHG	C30-C31-C32-C33
54	S	625	LPX	C12-C13-C14-C15
29	c	510	CLA	C13-C15-C16-C17
29	b1	604	CLA	C5-C6-C7-C8
29	D	402	CLA	C16-C17-C18-C20
29	N	610	CLA	C16-C17-C18-C19
29	b	605	CLA	C16-C17-C18-C19
29	c	512	CLA	C16-C17-C18-C20
29	c	513	CLA	C16-C17-C18-C20
29	s	602	CLA	C11-C12-C13-C14
29	g1	613	CLA	C16-C17-C18-C20
32	B	621	SQD	C10-C11-C12-C13
33	c1	521	LMG	C13-C14-C15-C16
40	s	624	LHG	C34-C35-C36-C37
32	A	412	SQD	C9-C10-C11-C12
37	C	519	DGD	C4B-C5B-C6B-C7B
38	B1	624	3PH	C2A-C2B-C2C-C2D
40	g1	624	LHG	C25-C26-C27-C28
47	i	101	4RF	C07-C08-C09-C10
55	y	626	PTY	C23-C24-C25-C26
29	C	503	CLA	C10-C11-C12-C13
29	g1	610	CLA	C8-C10-C11-C12
29	y1	612	CLA	C10-C11-C12-C13
32	B1	621	SQD	C11-C12-C13-C14
34	A1	414	SPH	C11-C10-C9-C8
38	T	101	3PH	C2D-C2E-C2F-C2G
40	l	101	LHG	C13-C14-C15-C16
40	n	624	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
40	c1	525	LHG	C14-C15-C16-C17
47	k1	101	4RF	C43-C44-C45-C46
29	Y	614	CLA	C4-C3-C5-C6
29	r1	609	CLA	C4-C3-C5-C6
43	d	405	PL9	C15-C14-C16-C17
48	y1	609	CHL	C4-C3-C5-C6
32	C	526	SQD	C13-C14-C15-C16
33	c	521	LMG	C14-C15-C16-C17
33	w1	201	LMG	C36-C37-C38-C39
34	A	414	SPH	C6-C7-C8-C9
38	t1	101	3PH	C22-C23-C24-C25
39	b	625	DGA	CA9-CAA-CBA-CCA
40	D1	408	LHG	C29-C30-C31-C32
40	D1	408	LHG	C34-C35-C36-C37
40	g1	624	LHG	C13-C14-C15-C16
47	i1	101	4RF	C09-C10-C11-C12
29	b	608	CLA	C15-C16-C17-C18
29	b	614	CLA	C8-C10-C11-C12
29	b	616	CLA	C8-C10-C11-C12
29	N1	604	CLA	C8-C10-C11-C12
29	R1	610	CLA	C10-C11-C12-C13
29	n1	604	CLA	C5-C6-C7-C8
29	r1	603	CLA	C8-C10-C11-C12
38	b1	624	3PH	C39-C3A-C3B-C3C
40	d1	410	LHG	C27-C28-C29-C30
47	K	101	4RF	C01-C02-C03-C04
47	K1	101	4RF	C49-C50-C51-C52
33	w	201	LMG	C28-C29-C30-C31
33	B1	622	LMG	C28-C29-C30-C31
47	K1	101	4RF	C13-C14-C15-C16
40	S	624	LHG	C8-C7-O7-C5
29	B	612	CLA	O1A-CGA-O2A-C1
29	Y	614	CLA	O1A-CGA-O2A-C1
29	c	503	CLA	O1A-CGA-O2A-C1
29	G1	603	CLA	O1A-CGA-O2A-C1
29	g1	603	CLA	O1A-CGA-O2A-C1
29	y1	610	CLA	O1A-CGA-O2A-C1
37	C1	518	DGD	O1A-C1A-O1G-C1G
33	D	411	LMG	C19-C20-C21-C22
38	t1	101	3PH	C37-C38-C39-C3A
38	s1	626	3PH	C2D-C2E-C2F-C2G
40	y	624	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
29	c1	507	CLA	C13-C15-C16-C17
48	S1	608	CHL	C5-C6-C7-C8
29	R	604	CLA	C2A-CAA-CBA-CGA
29	c	501	CLA	C2A-CAA-CBA-CGA
48	G	605	CHL	C2A-CAA-CBA-CGA
48	y	606	CHL	C2A-CAA-CBA-CGA
29	c	507	CLA	C16-C17-C18-C19
29	n	603	CLA	C16-C17-C18-C20
48	s	608	CHL	C11-C12-C13-C14
32	m	101	SQD	C44-C45-C46-O48
32	A1	412	SQD	O6-C44-C45-C46
32	C1	526	SQD	C44-C45-C46-O48
32	a1	412	SQD	C44-C45-C46-O48
32	b1	626	SQD	O6-C44-C45-C46
32	b1	626	SQD	C44-C45-C46-O48
33	a	413	LMG	C7-C8-C9-O8
33	c	523	LMG	C7-C8-C9-O8
33	A1	413	LMG	O1-C7-C8-C9
33	a1	413	LMG	O1-C7-C8-C9
33	c1	523	LMG	C7-C8-C9-O8
33	d1	411	LMG	O1-C7-C8-C9
37	b	623	DGD	O1G-C1G-C2G-C3G
37	c	520	DGD	O1G-C1G-C2G-C3G
37	c1	518	DGD	C2A-C3A-C4A-C5A
37	c1	520	DGD	O1G-C1G-C2G-C3G
38	S1	626	3PH	C35-C36-C37-C38
38	b1	624	3PH	C1-C2-C3-O31
39	c	524	DGA	OG1-CG1-CG2-CG3
39	C1	524	DGA	OG1-CG1-CG2-CG3
39	b1	625	DGA	OG1-CG1-CG2-CG3
40	C	525	LHG	C4-C5-C6-O8
40	L	101	LHG	C4-C5-C6-O8
40	Y	624	LHG	C4-C5-C6-O8
40	c	525	LHG	C4-C5-C6-O8
40	d	410	LHG	C4-C5-C6-O8
40	s	624	LHG	C4-C5-C6-O8
40	S1	624	LHG	C4-C5-C6-O8
40	g1	624	LHG	C4-C5-C6-O8
40	s1	624	LHG	C4-C5-C6-O8
41	c	527	LMK	C7-C8-C9-O8
41	C1	527	LMK	O1-C7-C8-C9
47	I	102	4RF	O18-C19-C20-C39

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Mol	Chain	Res	Type	Atoms
47	I	102	4RF	C19-C20-C39-O40
47	K	101	4RF	C19-C20-C39-O40
47	i	101	4RF	C12-C13-C14-C15
47	i	101	4RF	C19-C20-C39-O40
47	I1	102	4RF	O18-C19-C20-C39
47	i1	101	4RF	C19-C20-C39-O40
54	s1	625	LPX	C18-C19-C20-C21
55	Y	626	PTY	O4-C1-C6-C5
55	Y	627	PTY	O4-C1-C6-C5
55	y	626	PTY	O4-C1-C6-C5
55	y	627	PTY	O4-C1-C6-C5
29	n	603	CLA	C13-C15-C16-C17
29	n	613	CLA	C15-C16-C17-C18
29	B1	611	CLA	C15-C16-C17-C18
29	Y1	602	CLA	C13-C15-C16-C17
29	y1	612	CLA	C15-C16-C17-C18
32	A	412	SQD	C11-C10-C9-C8
38	t1	101	3PH	C38-C39-C3A-C3B
40	D	409	LHG	C28-C29-C30-C31
32	A1	412	SQD	C45-C44-O6-C1
33	W	201	LMG	C8-C7-O1-C1
33	w	201	LMG	C8-C7-O1-C1
33	W1	201	LMG	C8-C7-O1-C1
37	C	519	DGD	C2G-C3G-O3G-C1D
37	c	519	DGD	C5D-C6D-O5D-C1E
29	y1	611	CLA	O1D-CGD-O2D-CED
32	B	626	SQD	C35-C36-C37-C38
33	h1	102	LMG	C11-C12-C13-C14
34	y	625	SPH	C13-C14-C15-C16
37	c1	519	DGD	CDB-CEB-CFB-CGB
39	c1	524	DGA	CA8-CA9-CAA-CBA
40	L	101	LHG	C29-C30-C31-C32
40	L	101	LHG	C33-C34-C35-C36
40	d	408	LHG	C14-C15-C16-C17
40	g1	624	LHG	C35-C36-C37-C38
47	K	101	4RF	C29-C30-C31-C32
29	Y1	603	CLA	C13-C15-C16-C17
32	m	101	SQD	C24-C25-C26-C27
33	C	521	LMG	C19-C20-C21-C22
33	a	413	LMG	C15-C16-C17-C18
34	A1	414	SPH	C14-C15-C16-C17
38	b	624	3PH	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
38	s	626	3PH	C2B-C2C-C2D-C2E
39	B1	625	DGA	CB9-CAB-CBB-CCB
39	J1	101	DGA	CB5-CB6-CB7-CB8
40	L	101	LHG	C14-C15-C16-C17
40	l	101	LHG	C16-C17-C18-C19
40	n1	624	LHG	C28-C29-C30-C31
47	K	101	4RF	C09-C10-C11-C12
47	k1	101	4RF	C01-C02-C03-C04
53	r	626	ERG	C22-C23-C24-C28
33	c1	521	LMG	O7-C10-C11-C12
40	g1	624	LHG	O8-C23-C24-C25
48	N1	605	CHL	CAA-CBA-CGA-O2A
33	b1	622	LMG	C10-C11-C12-C13
40	G	624	LHG	C7-C8-C9-C10
32	c1	526	SQD	C19-C20-C21-C22
33	C	521	LMG	C32-C33-C34-C35
33	A1	413	LMG	C11-C12-C13-C14
38	B	624	3PH	C2F-C2G-C2H-C2I
38	b	624	3PH	C35-C36-C37-C38
38	t1	101	3PH	C2F-C2G-C2H-C2I
39	b	625	DGA	CA3-CA4-CA5-CA6
47	k	101	4RF	C33-C34-C35-C36
32	a	412	SQD	O5-C1-O6-C44
29	G	603	CLA	C8-C10-C11-C12
29	n1	602	CLA	C8-C10-C11-C12
33	a1	413	LMG	C29-C30-C31-C32
39	C1	524	DGA	CB4-CB5-CB6-CB7
40	D1	409	LHG	C19-C20-C21-C22
32	A	412	SQD	C24-C23-O48-C46
40	C	525	LHG	C24-C23-O8-C6
29	S	611	CLA	CBD-CGD-O2D-CED
33	d	411	LMG	O6-C5-C6-O5
37	b1	623	DGD	O6E-C5E-C6E-O5E
40	d	409	LHG	O1-C1-C2-O2
40	n	624	LHG	O1-C1-C2-O2
40	s	624	LHG	O1-C1-C2-O2
38	T	101	3PH	C2B-C2C-C2D-C2E
38	b1	624	3PH	C29-C2A-C2B-C2C
39	c	524	DGA	CA9-CAA-CBA-CCA
39	J1	101	DGA	CB7-CB8-CB9-CAB
40	L1	101	LHG	C35-C36-C37-C38
40	G1	624	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
29	c1	503	CLA	C13-C15-C16-C17
29	R	612	CLA	O1A-CGA-O2A-C1
29	b	605	CLA	O1A-CGA-O2A-C1
37	b	623	DGD	O6E-C5E-C6E-O5E
32	a1	412	SQD	C12-C13-C14-C15
37	C1	518	DGD	C2A-C3A-C4A-C5A
39	c1	524	DGA	CA2-CA3-CA4-CA5
40	D	408	LHG	C26-C27-C28-C29
40	N1	624	LHG	C35-C36-C37-C38
40	n1	624	LHG	O8-C23-C24-C25
33	c	523	LMG	C4-C5-C6-O5
33	a	413	LMG	C11-C10-O7-C8
40	y	624	LHG	C14-C15-C16-C17
40	S1	624	LHG	C15-C16-C17-C18
40	d1	408	LHG	C27-C28-C29-C30
47	K	101	4RF	C51-C52-C53-C54
29	C	505	CLA	C8-C10-C11-C12
29	b	611	CLA	C15-C16-C17-C18
33	C1	521	LMG	O6-C5-C6-O5
50	g1	622	XAT	C40-C33-C34-C35
51	N1	623	NEX	C39-C29-C30-C31
51	Y1	623	NEX	C11-C10-C9-C19
37	b1	623	DGD	O6D-C5D-C6D-O5D
29	y	613	CLA	C4-C3-C5-C6
30	a1	408	PHO	C4-C3-C5-C6
48	Y	609	CHL	C4-C3-C5-C6
48	S	606	CHL	C2A-CAA-CBA-CGA
32	a	412	SQD	C12-C13-C14-C15
33	C	523	LMG	C42-C43-C44-C45
33	w	201	LMG	C29-C30-C31-C32
37	C	520	DGD	CDB-CEB-CFB-CGB
47	K	101	4RF	C45-C46-C47-C48
55	y1	626	PTY	C22-C23-C24-C25
29	y	613	CLA	C2-C3-C5-C6
32	c	526	SQD	C23-C24-C25-C26
33	C	521	LMG	C28-C29-C30-C31
29	C	513	CLA	C16-C17-C18-C20
29	A1	410	CLA	C11-C12-C13-C15
29	N1	602	CLA	C16-C17-C18-C19
29	R	612	CLA	CBA-CGA-O2A-C1
29	c	510	CLA	CBA-CGA-O2A-C1
29	n1	610	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	r1	610	CLA	CBA-CGA-O2A-C1
37	C	518	DGD	C2A-C1A-O1G-C1G
37	c1	519	DGD	C2A-C1A-O1G-C1G
39	C	524	DGA	CA2-CA1-OG1-CG1
32	B1	621	SQD	C14-C15-C16-C17
39	B1	625	DGA	CBA-CCA-CDA-CEA
40	L	101	LHG	C25-C26-C27-C28
40	n	624	LHG	C35-C36-C37-C38
40	D1	410	LHG	C11-C10-C9-C8
47	i	101	4RF	C30-C31-C32-C33
29	B	603	CLA	C13-C15-C16-C17
29	c	505	CLA	C5-C6-C7-C8
29	n	613	CLA	C8-C10-C11-C12
29	b1	604	CLA	C13-C15-C16-C17
29	s1	604	CLA	C5-C6-C7-C8
37	c1	518	DGD	C3A-C4A-C5A-C6A
37	c1	518	DGD	CCB-CDB-CEB-CFB
40	g	624	LHG	C28-C29-C30-C31
47	K	101	4RF	C44-C45-C46-C47
32	b	621	SQD	C46-C45-O47-C7
32	B1	621	SQD	C46-C45-O47-C7
32	M1	101	SQD	C46-C45-O47-C7
33	W1	201	LMG	C7-C8-O7-C10
38	s	626	3PH	C1-C2-O21-C21
38	T1	101	3PH	C3-C2-O21-C21
38	s1	626	3PH	C1-C2-O21-C21
29	N	611	CLA	C2A-CAA-CBA-CGA
29	b	605	CLA	C2A-CAA-CBA-CGA
29	r	609	CLA	C2A-CAA-CBA-CGA
29	c1	502	CLA	C2A-CAA-CBA-CGA
48	r1	607	CHL	C2A-CAA-CBA-CGA
29	B	616	CLA	C13-C15-C16-C17
29	C1	513	CLA	C10-C11-C12-C13
29	D1	402	CLA	C15-C16-C17-C18
29	R1	602	CLA	C8-C10-C11-C12
48	g	601	CHL	C5-C6-C7-C8
29	R	604	CLA	C2-C1-O2A-CGA
29	Y	604	CLA	C2-C1-O2A-CGA
29	b	616	CLA	C2-C1-O2A-CGA
29	r	603	CLA	C2-C1-O2A-CGA
29	s	609	CLA	C2-C1-O2A-CGA
29	B1	602	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
29	B1	603	CLA	C2-C1-O2A-CGA
29	B1	608	CLA	C2-C1-O2A-CGA
29	D1	403	CLA	C2-C1-O2A-CGA
29	R1	610	CLA	C2-C1-O2A-CGA
29	c1	503	CLA	C2-C1-O2A-CGA
29	r1	612	CLA	C2-C1-O2A-CGA
48	G	606	CHL	C2-C1-O2A-CGA
40	l	101	LHG	C19-C20-C21-C22
47	K1	101	4RF	C09-C10-C11-C12
40	l	101	LHG	C7-C8-C9-C10
29	b1	616	CLA	CBD-CGD-O2D-CED
29	a	405	CLA	C3-C5-C6-C7
34	y	625	SPH	C15-C16-C17-C18
38	T	101	3PH	C3A-C3B-C3C-C3D
39	c	524	DGA	CBB-CAB-CB9-CB8
40	d1	410	LHG	C32-C33-C34-C35
47	k1	101	4RF	C26-C27-C28-C29
55	y	626	PTY	C41-C42-C43-C44
29	A	407	CLA	O1D-CGD-O2D-CED
29	y	602	CLA	C15-C16-C17-C18
38	t	101	3PH	C1-O11-P-O12
38	s1	626	3PH	C1-O11-P-O12
40	C	525	LHG	C2-C3-O3-P
32	A	412	SQD	C16-C17-C18-C19
32	c	526	SQD	C14-C15-C16-C17
32	c	526	SQD	C17-C18-C19-C20
33	b	622	LMG	C11-C12-C13-C14
33	c	521	LMG	C29-C30-C31-C32
33	H1	102	LMG	C19-C20-C21-C22
38	T1	101	3PH	C24-C25-C26-C27
38	t1	101	3PH	C2D-C2E-C2F-C2G
40	n	624	LHG	C28-C29-C30-C31
47	i1	101	4RF	C02-C03-C04-C05
55	Y	626	PTY	C21-C22-C23-C24
30	A	409	PHO	CBA-CGA-O2A-C1
47	i	101	4RF	C43-C41-O40-C39
37	c	518	DGD	O1A-C1A-O1G-C1G
38	t	101	3PH	O11-C1-C2-O21
29	b1	608	CLA	C16-C17-C18-C19
29	c1	505	CLA	C16-C17-C18-C20
34	a	414	SPH	C14-C15-C16-C17
34	A1	414	SPH	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
40	L1	101	LHG	C19-C20-C21-C22
40	S1	624	LHG	C13-C14-C15-C16
47	i1	101	4RF	C33-C34-C35-C36
29	R	610	CLA	C8-C10-C11-C12
47	K	101	4RF	C12-C13-C14-C15
47	K	101	4RF	C35-C36-C37-C38
29	r1	610	CLA	O1A-CGA-O2A-C1
55	Y	626	PTY	O30-C30-O4-C1
33	A1	413	LMG	C39-C40-C41-C42
39	c	524	DGA	CFA-CGA-CHA-CIA
34	A	414	SPH	C5-C6-C7-C8
29	B1	616	CLA	C13-C15-C16-C17
29	N1	610	CLA	C15-C16-C17-C18
31	A	411	BCR	C11-C10-C9-C8
32	b	621	SQD	C2-C1-O6-C44
33	A1	413	LMG	C2-C1-O1-C7
37	C	518	DGD	C2E-C1E-O5D-C6D
37	c1	519	DGD	C2E-C1E-O5D-C6D
50	g1	622	XAT	C32-C33-C34-C35
33	d	411	LMG	C33-C34-C35-C36
40	n1	624	LHG	C35-C36-C37-C38
55	y1	626	PTY	C41-C42-C43-C44
38	T1	101	3PH	O21-C2-C3-O31
40	Y	624	LHG	O7-C5-C6-O8
40	g	624	LHG	O7-C5-C6-O8
55	Y	626	PTY	O4-C1-C6-O7
32	B1	626	SQD	C35-C36-C37-C38
33	D	411	LMG	C32-C33-C34-C35
33	d1	411	LMG	C33-C34-C35-C36
38	T1	101	3PH	C25-C26-C27-C28
39	c1	524	DGA	CCA-CDA-CEA-CFA
40	G	624	LHG	C17-C18-C19-C20
47	i1	101	4RF	C32-C33-C34-C35
38	B	624	3PH	O22-C21-O21-C2
39	c	524	DGA	OB1-CB1-OG2-CG2
47	K	101	4RF	O23-C22-O21-C20
29	C	506	CLA	C10-C11-C12-C13
29	b1	602	CLA	C5-C6-C7-C8
29	g1	602	CLA	C8-C10-C11-C12
29	G1	610	CLA	O1A-CGA-O2A-C1
37	C	518	DGD	O1A-C1A-O1G-C1G
29	Y	610	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	D1	402	CLA	C16-C17-C18-C20
30	a	409	PHO	CHA-CBD-CGD-O1D
30	a	409	PHO	CHA-CBD-CGD-O2D
30	A1	408	PHO	CHA-CBD-CGD-O1D
30	A1	408	PHO	CHA-CBD-CGD-O2D
30	A1	409	PHO	CHA-CBD-CGD-O1D
30	A1	409	PHO	CHA-CBD-CGD-O2D
30	a1	409	PHO	CHA-CBD-CGD-O1D
30	a1	409	PHO	CHA-CBD-CGD-O2D
32	b1	626	SQD	C17-C18-C19-C20
33	A	413	LMG	C15-C16-C17-C18
33	w1	201	LMG	C11-C12-C13-C14
37	c1	519	DGD	C4B-C5B-C6B-C7B
38	t	101	3PH	C2B-C2C-C2D-C2E
38	T1	101	3PH	C2B-C2C-C2D-C2E
40	G1	624	LHG	C33-C34-C35-C36
40	c1	525	LHG	C25-C26-C27-C28
47	K1	101	4RF	C05-C06-C07-C08
47	k1	101	4RF	C34-C35-C36-C37
54	s1	625	LPX	C9-C10-C11-C12
29	C	510	CLA	C4-C3-C5-C6
29	N	603	CLA	C4-C3-C5-C6
29	S	610	CLA	C4-C3-C5-C6
29	b	602	CLA	C4-C3-C5-C6
29	y	603	CLA	C4-C3-C5-C6
43	D1	405	PL9	C30-C29-C31-C32
48	N	609	CHL	C4-C3-C5-C6
48	Y1	609	CHL	C4-C3-C5-C6
33	c	521	LMG	C13-C14-C15-C16
40	L1	101	LHG	C13-C14-C15-C16
29	B	603	CLA	C11-C10-C8-C7
29	B	604	CLA	C12-C13-C15-C16
29	B	605	CLA	C6-C7-C8-C10
29	B	605	CLA	C12-C13-C15-C16
29	B	613	CLA	C11-C10-C8-C7
29	B	616	CLA	C11-C12-C13-C15
29	C	504	CLA	C12-C13-C15-C16
29	C	507	CLA	C12-C13-C15-C16
29	C	512	CLA	C11-C10-C8-C7
29	C	513	CLA	C11-C12-C13-C15
29	N	603	CLA	C12-C13-C15-C16
29	N	604	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
29	N	604	CLA	C11-C12-C13-C15
29	G	602	CLA	C6-C7-C8-C10
29	G	610	CLA	C11-C12-C13-C15
29	G	611	CLA	C6-C7-C8-C10
29	G	613	CLA	C6-C7-C8-C10
29	R	610	CLA	C6-C7-C8-C10
29	R	610	CLA	C11-C10-C8-C7
29	S	609	CLA	C6-C7-C8-C10
29	S	610	CLA	C2-C3-C5-C6
29	Y	604	CLA	C11-C10-C8-C7
29	Y	612	CLA	C6-C7-C8-C10
29	Y	613	CLA	C11-C12-C13-C15
29	a	410	CLA	C11-C10-C8-C7
29	b	603	CLA	C6-C7-C8-C10
29	b	603	CLA	C12-C13-C15-C16
29	b	613	CLA	C6-C7-C8-C10
29	b	615	CLA	C6-C7-C8-C10
29	b	616	CLA	C11-C10-C8-C7
29	c	502	CLA	C11-C12-C13-C15
29	c	503	CLA	C11-C12-C13-C15
29	c	505	CLA	C12-C13-C15-C16
29	c	509	CLA	C12-C13-C15-C16
29	c	511	CLA	C11-C12-C13-C15
29	c	512	CLA	C6-C7-C8-C10
29	c	513	CLA	C11-C12-C13-C15
29	n	603	CLA	C6-C7-C8-C10
29	n	610	CLA	C11-C12-C13-C15
29	g	602	CLA	C6-C7-C8-C10
29	g	602	CLA	C12-C13-C15-C16
29	g	603	CLA	C12-C13-C15-C16
29	g	610	CLA	C11-C10-C8-C7
29	g	610	CLA	C12-C13-C15-C16
29	r	608	CLA	C6-C7-C8-C10
29	s	609	CLA	C11-C10-C8-C7
29	y	610	CLA	C11-C12-C13-C15
29	y	611	CLA	C11-C10-C8-C7
29	y	611	CLA	C12-C13-C15-C16
29	y	613	CLA	C11-C12-C13-C15
29	B1	605	CLA	C11-C12-C13-C15
29	B1	607	CLA	C6-C7-C8-C10
29	B1	607	CLA	C11-C10-C8-C7
29	B1	613	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	B1	617	CLA	C12-C13-C15-C16
29	C1	502	CLA	C11-C12-C13-C15
29	C1	504	CLA	C11-C10-C8-C7
29	C1	506	CLA	C11-C10-C8-C7
29	C1	508	CLA	C11-C10-C8-C7
29	C1	509	CLA	C12-C13-C15-C16
29	C1	511	CLA	C6-C7-C8-C10
29	C1	512	CLA	C12-C13-C15-C16
29	D1	402	CLA	C11-C12-C13-C15
29	D1	403	CLA	C11-C12-C13-C15
29	N1	610	CLA	C6-C7-C8-C10
29	G1	602	CLA	C6-C7-C8-C10
29	G1	610	CLA	C11-C10-C8-C7
29	R1	603	CLA	C11-C10-C8-C7
29	R1	610	CLA	C11-C10-C8-C7
29	S1	602	CLA	C11-C10-C8-C7
29	S1	609	CLA	C11-C10-C8-C7
29	S1	610	CLA	C11-C10-C8-C7
29	Y1	602	CLA	C6-C7-C8-C10
29	Y1	602	CLA	C11-C12-C13-C15
29	Y1	612	CLA	C12-C13-C15-C16
29	Y1	614	CLA	C6-C7-C8-C10
29	Y1	614	CLA	C11-C10-C8-C7
29	b1	602	CLA	C11-C10-C8-C7
29	b1	602	CLA	C12-C13-C15-C16
29	b1	613	CLA	C6-C7-C8-C10
29	b1	613	CLA	C12-C13-C15-C16
29	c1	504	CLA	C11-C10-C8-C7
29	c1	513	CLA	C12-C13-C15-C16
29	n1	602	CLA	C11-C10-C8-C7
29	n1	603	CLA	C12-C13-C15-C16
29	n1	610	CLA	C6-C7-C8-C10
29	g1	602	CLA	C6-C7-C8-C10
29	g1	610	CLA	C6-C7-C8-C10
29	g1	610	CLA	C11-C10-C8-C7
29	g1	611	CLA	C6-C7-C8-C10
29	g1	613	CLA	C12-C13-C15-C16
29	r1	603	CLA	C11-C10-C8-C7
29	r1	608	CLA	C6-C7-C8-C10
29	r1	609	CLA	C11-C10-C8-C7
29	s1	609	CLA	C11-C10-C8-C7
29	s1	610	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
29	s1	610	CLA	C11-C12-C13-C15
29	y1	603	CLA	C11-C12-C13-C15
29	y1	611	CLA	C11-C12-C13-C15
29	y1	613	CLA	C11-C10-C8-C7
29	y1	614	CLA	C11-C10-C8-C7
43	d1	405	PL9	C38-C39-C41-C42
48	N	606	CHL	C11-C10-C8-C7
48	N	607	CHL	C11-C12-C13-C15
48	G	601	CHL	C6-C7-C8-C10
48	G	607	CHL	C6-C7-C8-C10
48	Y	607	CHL	C6-C7-C8-C10
48	Y	609	CHL	C2-C3-C5-C6
48	n	606	CHL	C11-C10-C8-C7
48	g	601	CHL	C12-C13-C15-C16
48	y	609	CHL	C11-C12-C13-C15
48	N1	601	CHL	C12-C13-C15-C16
48	N1	607	CHL	C11-C10-C8-C7
48	G1	601	CHL	C11-C12-C13-C15
48	G1	607	CHL	C11-C10-C8-C7
48	Y1	606	CHL	C6-C7-C8-C10
48	Y1	609	CHL	C11-C12-C13-C15
48	n1	606	CHL	C11-C10-C8-C7
48	n1	607	CHL	C11-C12-C13-C15
48	s1	608	CHL	C11-C10-C8-C7
48	y1	607	CHL	C11-C10-C8-C7
33	H	102	LMG	O7-C10-C11-C12
29	C	508	CLA	C3-C5-C6-C7
29	n1	613	CLA	C3-C5-C6-C7
48	Y1	601	CHL	C3-C5-C6-C7
32	M1	101	SQD	C26-C27-C28-C29
32	m1	101	SQD	C11-C10-C9-C8
33	W	201	LMG	C31-C32-C33-C34
37	C	519	DGD	C3B-C4B-C5B-C6B
40	D	410	LHG	C27-C28-C29-C30
29	B	603	CLA	C11-C10-C8-C9
29	C	504	CLA	C14-C13-C15-C16
29	C	507	CLA	C14-C13-C15-C16
29	C	510	CLA	C14-C13-C15-C16
29	C	513	CLA	C11-C12-C13-C14
29	C	513	CLA	C14-C13-C15-C16
29	D	403	CLA	C11-C10-C8-C9
29	N	603	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	N	604	CLA	C11-C10-C8-C9
29	G	602	CLA	C6-C7-C8-C9
29	S	610	CLA	C11-C10-C8-C9
29	Y	602	CLA	C11-C12-C13-C14
29	Y	613	CLA	C11-C12-C13-C14
29	Y	613	CLA	C14-C13-C15-C16
29	a	410	CLA	C11-C10-C8-C9
29	b	603	CLA	C6-C7-C8-C9
29	b	614	CLA	C14-C13-C15-C16
29	b	615	CLA	C11-C10-C8-C9
29	c	502	CLA	C11-C12-C13-C14
29	c	505	CLA	C14-C13-C15-C16
29	c	507	CLA	C6-C7-C8-C9
29	c	512	CLA	C6-C7-C8-C9
29	d	402	CLA	C6-C7-C8-C9
29	d	402	CLA	C11-C12-C13-C14
29	n	610	CLA	C11-C12-C13-C14
29	g	602	CLA	C6-C7-C8-C9
29	g	602	CLA	C14-C13-C15-C16
29	g	603	CLA	C6-C7-C8-C9
29	g	603	CLA	C14-C13-C15-C16
29	y	611	CLA	C14-C13-C15-C16
29	y	612	CLA	C11-C10-C8-C9
29	B1	602	CLA	C11-C10-C8-C9
29	B1	607	CLA	C11-C10-C8-C9
29	B1	609	CLA	C11-C12-C13-C14
29	B1	612	CLA	C11-C12-C13-C14
29	B1	613	CLA	C14-C13-C15-C16
29	B1	615	CLA	C6-C7-C8-C9
29	B1	617	CLA	C6-C7-C8-C9
29	C1	504	CLA	C11-C10-C8-C9
29	C1	508	CLA	C11-C10-C8-C9
29	C1	509	CLA	C14-C13-C15-C16
29	D1	402	CLA	C11-C12-C13-C14
29	D1	403	CLA	C11-C12-C13-C14
29	N1	610	CLA	C11-C12-C13-C14
29	G1	603	CLA	C6-C7-C8-C9
29	G1	603	CLA	C14-C13-C15-C16
29	Y1	602	CLA	C11-C10-C8-C9
29	Y1	602	CLA	C11-C12-C13-C14
29	Y1	611	CLA	C11-C10-C8-C9
29	Y1	613	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	Y1	614	CLA	C11-C10-C8-C9
29	b1	602	CLA	C11-C10-C8-C9
29	b1	613	CLA	C14-C13-C15-C16
29	c1	504	CLA	C11-C10-C8-C9
29	n1	610	CLA	C6-C7-C8-C9
29	g1	610	CLA	C6-C7-C8-C9
29	g1	610	CLA	C14-C13-C15-C16
29	g1	611	CLA	C6-C7-C8-C9
29	g1	613	CLA	C14-C13-C15-C16
29	s1	610	CLA	C6-C7-C8-C9
29	s1	610	CLA	C11-C12-C13-C14
48	N	606	CHL	C11-C10-C8-C9
48	N	606	CHL	C14-C13-C15-C16
48	n	605	CHL	C11-C10-C8-C9
48	n	606	CHL	C11-C10-C8-C9
48	y	606	CHL	C6-C7-C8-C9
48	N1	606	CHL	C11-C10-C8-C9
48	G1	601	CHL	C11-C12-C13-C14
48	n1	606	CHL	C11-C10-C8-C9
48	n1	607	CHL	C11-C12-C13-C14
48	g1	607	CHL	C11-C10-C8-C9
51	G	623	NEX	C9-C10-C11-C12
37	b	623	DGD	C1B-C2B-C3B-C4B
32	c	526	SQD	C19-C20-C21-C22
32	a1	412	SQD	C25-C26-C27-C28
37	c1	519	DGD	C3B-C4B-C5B-C6B
29	G	610	CLA	CBA-CGA-O2A-C1
29	Y	602	CLA	CBA-CGA-O2A-C1
29	b	604	CLA	CBA-CGA-O2A-C1
29	r	612	CLA	CBA-CGA-O2A-C1
29	b1	610	CLA	CBA-CGA-O2A-C1
33	w	201	LMG	C29-C28-O8-C9
39	B1	625	DGA	CA2-CA1-OG1-CG1
40	d1	410	LHG	C24-C23-O8-C6
29	a	406	CLA	C10-C11-C12-C13
29	b	616	CLA	C10-C11-C12-C13
29	g	613	CLA	C10-C11-C12-C13
29	y1	610	CLA	C15-C16-C17-C18
29	b	607	CLA	C2A-CAA-CBA-CGA
29	C	508	CLA	C2C-C3C-CAC-CBC
33	h	102	LMG	C33-C34-C35-C36
37	c1	518	DGD	CDB-CEB-CFB-CGB

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Mol	Chain	Res	Type	Atoms
38	t	101	3PH	C27-C28-C29-C2A
38	S1	626	3PH	C32-C33-C34-C35
54	S1	625	LPX	C18-C19-C20-C21
37	C	518	DGD	C4D-C5D-C6D-O5D
31	C	517	BCR	C7-C8-C9-C34
31	b	618	BCR	C36-C18-C19-C20
31	c	516	BCR	C37-C22-C23-C24
45	H	101	RRX	C36-C18-C19-C20
45	h1	101	RRX	C37-C22-C23-C24
50	g	622	XAT	C11-C12-C13-C20
50	g1	622	XAT	C27-C28-C29-C39
50	g1	622	XAT	C31-C32-C33-C40
29	s	609	CLA	C5-C6-C7-C8
29	D	402	CLA	C16-C17-C18-C19
29	Y	613	CLA	C16-C17-C18-C19
29	A1	410	CLA	C11-C12-C13-C14
29	S1	610	CLA	C16-C17-C18-C19
29	n1	603	CLA	C16-C17-C18-C20
29	r1	612	CLA	C11-C12-C13-C15
32	C	526	SQD	C14-C15-C16-C17
33	C1	523	LMG	C42-C43-C44-C45
38	s	626	3PH	C25-C26-C27-C28
38	s	626	3PH	C27-C28-C29-C2A
40	g	624	LHG	C16-C17-C18-C19
40	d1	409	LHG	C28-C29-C30-C31
47	I1	102	4RF	C26-C27-C28-C29
31	c	514	BCR	C17-C18-C19-C20
31	c	516	BCR	C21-C22-C23-C24
31	c	517	BCR	C21-C22-C23-C24
36	b	620	C7Z	C11-C12-C13-C14
49	n1	620	LUT	C27-C28-C29-C30
50	n	622	XAT	C11-C12-C13-C14
50	r	621	XAT	C27-C28-C29-C30
50	n1	622	XAT	C27-C28-C29-C30
33	W	201	LMG	C32-C33-C34-C35
39	c1	524	DGA	CFA-CGA-CHA-CIA
40	D1	409	LHG	C35-C36-C37-C38
48	N	606	CHL	C3-C5-C6-C7
48	G1	607	CHL	C3-C5-C6-C7
29	b	609	CLA	C15-C16-C17-C18
29	c	510	CLA	C15-C16-C17-C18
29	g	610	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
29	s1	611	CLA	C5-C6-C7-C8
33	c1	523	LMG	C11-C10-O7-C8
33	H	102	LMG	C34-C35-C36-C37
33	d	411	LMG	C15-C16-C17-C18
33	B1	622	LMG	C33-C34-C35-C36
39	j1	101	DGA	CA5-CA6-CA7-CA8
40	c	525	LHG	C17-C18-C19-C20
54	s	625	LPX	C16-C17-C18-C19
32	A	412	SQD	O10-C23-O48-C46
47	I	102	4RF	O42-C41-O40-C39
29	S	614	CLA	CBA-CGA-O2A-C1
29	c	501	CLA	CBA-CGA-O2A-C1
32	C1	526	SQD	C9-C10-C11-C12
33	A	413	LMG	C14-C15-C16-C17
34	Y1	625	SPH	C6-C7-C8-C9
40	D1	408	LHG	C10-C11-C12-C13
47	I	102	4RF	C06-C07-C08-C09
29	N	610	CLA	C8-C10-C11-C12
29	g	602	CLA	C15-C16-C17-C18
29	S1	602	CLA	C10-C11-C12-C13
29	Y1	613	CLA	C13-C15-C16-C17
29	a1	405	CLA	C10-C11-C12-C13
29	d1	403	CLA	C13-C15-C16-C17
29	g1	602	CLA	C15-C16-C17-C18
48	S	608	CHL	C10-C11-C12-C13
32	C	526	SQD	C9-C10-C11-C12
32	a1	412	SQD	C28-C29-C30-C31
33	H1	102	LMG	C13-C14-C15-C16
38	T1	101	3PH	C22-C23-C24-C25
40	g	624	LHG	C9-C10-C11-C12
47	I	102	4RF	C24-C25-C26-C27
52	r	625	LMT	C5-C6-C7-C8
37	B	623	DGD	O6D-C5D-C6D-O5D
29	C1	506	CLA	CBD-CGD-O2D-CED
32	c1	526	SQD	C27-C28-C29-C30
29	S	611	CLA	C16-C17-C18-C20
29	n	604	CLA	C16-C17-C18-C20
29	A1	405	CLA	C16-C17-C18-C19
29	Y	611	CLA	C15-C16-C17-C18
29	c	504	CLA	C15-C16-C17-C18
29	C1	503	CLA	C5-C6-C7-C8
40	D	410	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
40	N	624	LHG	O6-C4-C5-C6
40	N1	624	LHG	O6-C4-C5-C6
40	G1	624	LHG	O6-C4-C5-C6
40	d1	409	LHG	O6-C4-C5-C6
55	y1	627	PTY	O14-C5-C6-C1
29	N	602	CLA	C3-C5-C6-C7
29	R	609	CLA	C3-C5-C6-C7
29	b1	608	CLA	C3-C5-C6-C7
40	d	409	LHG	C13-C14-C15-C16
47	K	101	4RF	C26-C27-C28-C29
32	b1	626	SQD	C7-C8-C9-C10
40	N1	624	LHG	C23-C24-C25-C26
55	y1	627	PTY	N1-C2-C3-O11
39	B1	625	DGA	CA9-CAA-CBA-CCA
54	s1	625	LPX	C13-C14-C15-C16
32	b	621	SQD	C24-C23-O48-C46
37	c1	519	DGD	O1A-C1A-O1G-C1G
29	S	603	CLA	C5-C6-C7-C8
29	y	602	CLA	C5-C6-C7-C8
29	B1	615	CLA	C5-C6-C7-C8
29	N1	603	CLA	C13-C15-C16-C17
29	b1	605	CLA	C13-C15-C16-C17
53	R	626	ERG	C16-C17-C20-C22
29	B	609	CLA	O1D-CGD-O2D-CED
47	i	101	4RF	C11-C12-C13-C14
47	i	101	4RF	C35-C36-C37-C38
29	B	610	CLA	C4-C3-C5-C6
29	B	615	CLA	C4-C3-C5-C6
29	s	602	CLA	C4-C3-C5-C6
43	D	405	PL9	C45-C44-C46-C47
48	y	609	CHL	C4-C3-C5-C6
37	c1	519	DGD	C4E-C5E-C6E-O5E
29	C	510	CLA	C2-C3-C5-C6
29	N	603	CLA	C2-C3-C5-C6
29	b	602	CLA	C2-C3-C5-C6
29	y	603	CLA	C2-C3-C5-C6
43	D	405	PL9	C38-C39-C41-C42
43	d	405	PL9	C38-C39-C41-C42
48	N	609	CHL	C2-C3-C5-C6
48	Y1	609	CHL	C2-C3-C5-C6
32	c	526	SQD	C13-C14-C15-C16
32	c1	526	SQD	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
33	D1	411	LMG	C22-C23-C24-C25
37	c	518	DGD	C4A-C5A-C6A-C7A
40	c1	525	LHG	C30-C31-C32-C33
29	b1	615	CLA	O1D-CGD-O2D-CED
29	g	603	CLA	C13-C15-C16-C17
29	y	603	CLA	C15-C16-C17-C18
33	a	413	LMG	O9-C10-O7-C8
29	n1	610	CLA	O1A-CGA-O2A-C1
47	K1	101	4RF	C44-C45-C46-C47
29	Y1	610	CLA	O1D-CGD-O2D-CED
29	c	507	CLA	C16-C17-C18-C20
29	b1	612	CLA	C16-C17-C18-C19
38	T1	101	3PH	C34-C35-C36-C37
38	b1	624	3PH	C33-C34-C35-C36
47	i	101	4RF	C09-C10-C11-C12
29	C	504	CLA	C8-C10-C11-C12
29	y1	612	CLA	C5-C6-C7-C8
29	g1	610	CLA	CBA-CGA-O2A-C1
47	K	101	4RF	C43-C41-O40-C39
54	S	625	LPX	C7-C6-O6-C5
29	b	602	CLA	CAA-CBA-CGA-O2A
29	b1	602	CLA	CAA-CBA-CGA-O2A
40	G	624	LHG	O8-C23-C24-C25
32	b	626	SQD	C23-C24-C25-C26
38	t	101	3PH	C38-C39-C3A-C3B
38	s1	626	3PH	C2A-C2B-C2C-C2D
40	L	101	LHG	C13-C14-C15-C16
40	N	624	LHG	C35-C36-C37-C38
41	c1	527	LMK	C29-C30-C31-C32
47	i1	101	4RF	C05-C06-C07-C08
40	C1	525	LHG	C2-C3-O3-P
40	L1	101	LHG	C2-C3-O3-P
29	c	510	CLA	O1A-CGA-O2A-C1
40	c	525	LHG	O10-C23-O8-C6
29	N	613	CLA	C3A-C2A-CAA-CBA
29	b	609	CLA	C3A-C2A-CAA-CBA
29	b	610	CLA	C3A-C2A-CAA-CBA
29	r	612	CLA	C3A-C2A-CAA-CBA
29	B1	609	CLA	C3A-C2A-CAA-CBA
29	B1	616	CLA	C3A-C2A-CAA-CBA
29	N1	613	CLA	C3A-C2A-CAA-CBA
29	G1	612	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	S1	603	CLA	C3A-C2A-CAA-CBA
29	a1	405	CLA	C3A-C2A-CAA-CBA
29	b1	615	CLA	C3A-C2A-CAA-CBA
29	r1	612	CLA	C3A-C2A-CAA-CBA
48	Y	601	CHL	C3A-C2A-CAA-CBA
48	n	609	CHL	C3A-C2A-CAA-CBA
48	n1	601	CHL	C3A-C2A-CAA-CBA
48	g1	605	CHL	C3A-C2A-CAA-CBA
33	h1	102	LMG	C39-C40-C41-C42
37	C	520	DGD	CCB-CDB-CEB-CFB
40	y	624	LHG	C31-C32-C33-C34
40	c1	525	LHG	C24-C25-C26-C27
40	y1	624	LHG	C35-C36-C37-C38
31	A1	411	BCR	C9-C10-C11-C12
49	G	620	LUT	C29-C30-C31-C32
49	S1	620	LUT	C29-C30-C31-C32
49	g1	621	LUT	C9-C10-C11-C12
33	b1	622	LMG	C31-C32-C33-C34
37	c1	520	DGD	CCB-CDB-CEB-CFB
38	B	624	3PH	C26-C27-C28-C29
38	s	626	3PH	C22-C23-C24-C25
39	B1	625	DGA	CB6-CB7-CB8-CB9
40	D	409	LHG	C35-C36-C37-C38
40	d1	409	LHG	C19-C20-C21-C22
47	I	102	4RF	C07-C08-C09-C10
29	C	508	CLA	C13-C15-C16-C17
29	C1	509	CLA	C15-C16-C17-C18
29	b1	608	CLA	C8-C10-C11-C12
29	y1	604	CLA	C8-C10-C11-C12
48	G1	607	CHL	C5-C6-C7-C8
38	B	624	3PH	C39-C3A-C3B-C3C
39	B	625	DGA	CA2-CA3-CA4-CA5
39	j	101	DGA	CA5-CA6-CA7-CA8
39	B1	625	DGA	CA7-CA8-CA9-CAA
39	c1	524	DGA	CAB-CBB-CCB-CDB
40	Y	624	LHG	C35-C36-C37-C38
29	B1	610	CLA	C16-C17-C18-C19
29	C	510	CLA	CBA-CGA-O2A-C1
32	b1	626	SQD	C24-C23-O48-C46
39	b1	625	DGA	CA4-CA5-CA6-CA7
40	S	624	LHG	C29-C30-C31-C32
47	k1	101	4RF	C02-C03-C04-C05

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Mol	Chain	Res	Type	Atoms
29	B	606	CLA	C5-C6-C7-C8
29	a	406	CLA	C15-C16-C17-C18
29	b	615	CLA	C8-C10-C11-C12
29	y	603	CLA	C8-C10-C11-C12
32	B	626	SQD	O6-C44-C45-C46
32	M	101	SQD	C44-C45-C46-O48
32	a	412	SQD	O6-C44-C45-C46
32	a	412	SQD	C44-C45-C46-O48
33	A	413	LMG	O1-C7-C8-C9
33	B	622	LMG	C7-C8-C9-O8
33	a	413	LMG	O1-C7-C8-C9
33	b	622	LMG	C7-C8-C9-O8
33	w	201	LMG	O1-C7-C8-C9
33	B1	622	LMG	C7-C8-C9-O8
33	a1	413	LMG	C7-C8-C9-O8
37	B1	623	DGD	O1G-C1G-C2G-C3G
38	T1	101	3PH	C1-C2-C3-O31
38	S1	626	3PH	C1-C2-C3-O31
40	D	410	LHG	C4-C5-C6-O8
40	N	624	LHG	C4-C5-C6-O8
40	l	101	LHG	C4-C5-C6-O8
40	N1	624	LHG	C4-C5-C6-O8
40	c1	525	LHG	C4-C5-C6-O8
40	n1	624	LHG	C4-C5-C6-O8
41	c	527	LMK	O1-C7-C8-C9
47	i	101	4RF	O18-C19-C20-C39
47	K1	101	4RF	C19-C20-C39-O40
55	Y1	627	PTY	O4-C1-C6-C5
55	y1	627	PTY	O4-C1-C6-C5
38	t1	101	3PH	C32-C33-C34-C35
39	B	625	DGA	CAA-CBA-CCA-CDA
39	C	524	DGA	CB5-CB6-CB7-CB8
33	w	201	LMG	C10-C11-C12-C13
32	b1	626	SQD	C15-C16-C17-C18
38	t1	101	3PH	C27-C28-C29-C2A
40	Y	624	LHG	C11-C12-C13-C14
40	d	410	LHG	C34-C35-C36-C37
40	s1	624	LHG	C10-C11-C12-C13
40	s1	624	LHG	C33-C34-C35-C36
52	r	625	LMT	C9-C10-C11-C12
32	C1	526	SQD	C24-C25-C26-C27
32	c1	526	SQD	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
40	G	624	LHG	C30-C31-C32-C33
40	L1	101	LHG	C31-C32-C33-C34
29	Y	611	CLA	C3-C5-C6-C7
32	b1	626	SQD	C30-C31-C32-C33
39	J1	101	DGA	CA4-CA5-CA6-CA7
40	d	409	LHG	C33-C34-C35-C36
40	g1	624	LHG	C26-C27-C28-C29
55	Y	626	PTY	C37-C38-C39-C40
29	n	604	CLA	C4-C3-C5-C6
29	C1	505	CLA	C4-C3-C5-C6
48	S	608	CHL	C11-C12-C13-C15
38	T1	101	3PH	C29-C2A-C2B-C2C
38	b1	624	3PH	C25-C26-C27-C28
40	D	409	LHG	C19-C20-C21-C22
40	N1	624	LHG	C32-C33-C34-C35
33	h1	102	LMG	C19-C20-C21-C22
40	y	624	LHG	C10-C11-C12-C13
47	K	101	4RF	C25-C26-C27-C28
29	B1	611	CLA	C13-C15-C16-C17
40	y	624	LHG	C3-O3-P-O6
40	Y1	624	LHG	C3-O3-P-O6
41	C	527	LMK	C9-C8-O7-C10
41	C1	527	LMK	C9-C8-O7-C10
32	m	101	SQD	O47-C7-C8-C9
39	C	524	DGA	OA1-CA1-OG1-CG1
39	B1	625	DGA	OA1-CA1-OG1-CG1
40	C	525	LHG	O10-C23-O8-C6
38	S	626	3PH	C32-C33-C34-C35
29	C	504	CLA	O1D-CGD-O2D-CED
29	C1	504	CLA	C3-C5-C6-C7
29	B	602	CLA	C2A-CAA-CBA-CGA
29	r	603	CLA	C2A-CAA-CBA-CGA
29	N1	611	CLA	C2A-CAA-CBA-CGA
40	N	624	LHG	O1-C1-C2-O2
40	g	624	LHG	O1-C1-C2-O2
40	N1	624	LHG	O1-C1-C2-O2
32	B	621	SQD	C13-C14-C15-C16
38	b	624	3PH	C22-C23-C24-C25
38	B1	624	3PH	C34-C35-C36-C37
38	T1	101	3PH	C23-C24-C25-C26
40	l	101	LHG	C32-C33-C34-C35
40	n	624	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
40	L1	101	LHG	C33-C34-C35-C36
40	G1	624	LHG	C35-C36-C37-C38
40	c1	525	LHG	C34-C35-C36-C37
47	I1	102	4RF	C01-C02-C03-C04
47	K1	101	4RF	C31-C32-C33-C34
40	C	525	LHG	O6-C4-C5-O7
40	D	410	LHG	O6-C4-C5-O7
40	G	624	LHG	O6-C4-C5-O7
40	c	525	LHG	O6-C4-C5-O7
40	C1	525	LHG	O6-C4-C5-O7
40	N1	624	LHG	O6-C4-C5-O7
40	c1	525	LHG	O6-C4-C5-O7
40	g1	624	LHG	O6-C4-C5-O7
55	Y	627	PTY	O14-C5-C6-O7
53	R1	626	ERG	C23-C24-C25-C27
33	A1	413	LMG	C29-C28-O8-C9
32	M	101	SQD	C11-C12-C13-C14
29	b	604	CLA	O1A-CGA-O2A-C1
29	b1	610	CLA	O1A-CGA-O2A-C1
40	s1	624	LHG	O10-C23-O8-C6
33	A1	413	LMG	C10-C11-C12-C13
47	k1	101	4RF	C13-C14-C15-C16
29	c1	504	CLA	C16-C17-C18-C20
29	y1	611	CLA	C15-C16-C17-C18
32	C1	526	SQD	C33-C34-C35-C36
38	t	101	3PH	C24-C25-C26-C27
39	j	101	DGA	CBB-CAB-CB9-CB8
32	A1	412	SQD	C16-C17-C18-C19
40	D	409	LHG	C30-C31-C32-C33
47	k	101	4RF	C01-C02-C03-C04
47	k	101	4RF	C03-C04-C05-C06
52	R	625	LMT	C3-C4-C5-C6
29	b	613	CLA	C8-C10-C11-C12
29	G	610	CLA	O1A-CGA-O2A-C1
30	A	409	PHO	O1A-CGA-O2A-C1
47	i	101	4RF	O42-C41-O40-C39
37	C	519	DGD	CAB-CBB-CCB-CDB
38	S	626	3PH	C37-C38-C39-C3A
38	S	626	3PH	C3F-C3G-C3H-C3I
40	l	101	LHG	C29-C30-C31-C32
40	S1	624	LHG	C33-C34-C35-C36
48	R	607	CHL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
29	S1	614	CLA	C3-C5-C6-C7
32	m	101	SQD	C28-C29-C30-C31
38	B	624	3PH	C3E-C3F-C3G-C3H
40	C	525	LHG	C35-C36-C37-C38
40	C1	525	LHG	C26-C27-C28-C29
32	C1	526	SQD	O47-C45-C46-O48
32	b1	626	SQD	O47-C45-C46-O48
33	C	523	LMG	O1-C7-C8-O7
33	c	523	LMG	O1-C7-C8-O7
33	w	201	LMG	O1-C7-C8-O7
33	w1	201	LMG	O7-C8-C9-O8
37	c1	519	DGD	O1G-C1G-C2G-O2G
38	s	626	3PH	O21-C2-C3-O31
38	S1	626	3PH	O21-C2-C3-O31
39	c	524	DGA	OG1-CG1-CG2-OG2
40	L	101	LHG	O7-C5-C6-O8
40	l	101	LHG	O7-C5-C6-O8
40	n	624	LHG	O7-C5-C6-O8
40	s	624	LHG	O7-C5-C6-O8
40	D1	408	LHG	O7-C5-C6-O8
41	C	527	LMK	O1-C7-C8-O7
41	c1	527	LMK	O1-C7-C8-O7
55	Y	627	PTY	O4-C1-C6-O7
29	B	613	CLA	C13-C15-C16-C17
33	c	523	LMG	C14-C15-C16-C17
33	d	411	LMG	C22-C23-C24-C25
38	b	624	3PH	C39-C3A-C3B-C3C
40	g	624	LHG	C34-C35-C36-C37
55	Y	626	PTY	C36-C37-C38-C39
29	S	602	CLA	C11-C12-C13-C14
29	n1	610	CLA	C16-C17-C18-C19
33	b	622	LMG	C12-C13-C14-C15
33	h1	102	LMG	C29-C30-C31-C32
37	c	520	DGD	CCB-CDB-CEB-CFB
40	Y	624	LHG	C9-C10-C11-C12
32	M	101	SQD	O5-C1-O6-C44
39	B1	625	DGA	CG1-CG2-CG3-OXT
39	b1	625	DGA	CG1-CG2-CG3-OXT
40	S1	624	LHG	C1-C2-C3-O3
43	D	405	PL9	C39-C41-C42-C43
43	d1	405	PL9	C19-C21-C22-C23
43	d1	405	PL9	C34-C36-C37-C38

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Mol	Chain	Res	Type	Atoms
54	s1	625	LPX	O1-C3-C4-C5
32	m1	101	SQD	C28-C29-C30-C31
38	T	101	3PH	C34-C35-C36-C37
39	c	524	DGA	CCB-CDB-CEB-CFB
39	B1	625	DGA	CEA-CFA-CGA-CHA
40	C	525	LHG	C24-C25-C26-C27
47	k	101	4RF	C44-C45-C46-C47
33	c1	523	LMG	O9-C10-O7-C8
29	B1	615	CLA	C4-C3-C5-C6
48	G	607	CHL	C4-C3-C5-C6
29	C	501	CLA	C2-C1-O2A-CGA
29	R	609	CLA	C2-C1-O2A-CGA
29	n	603	CLA	C2-C1-O2A-CGA
29	g	603	CLA	C2-C1-O2A-CGA
29	B1	604	CLA	C2-C1-O2A-CGA
29	B1	615	CLA	C2-C1-O2A-CGA
29	N1	604	CLA	C2-C1-O2A-CGA
29	b1	612	CLA	C2-C1-O2A-CGA
29	c1	505	CLA	C2-C1-O2A-CGA
48	R	607	CHL	C2-C1-O2A-CGA
43	d	405	PL9	C47-C48-C49-C51
48	y	609	CHL	C2-C3-C5-C6
32	M1	101	SQD	C28-C29-C30-C31
40	L	101	LHG	C10-C11-C12-C13
40	G1	624	LHG	C24-C25-C26-C27
52	r1	625	LMT	C9-C10-C11-C12
29	r	612	CLA	O1A-CGA-O2A-C1
29	c	512	CLA	C8-C10-C11-C12
29	B	607	CLA	C6-C7-C8-C9
29	B	614	CLA	C14-C13-C15-C16
29	B	616	CLA	C11-C12-C13-C14
29	C	511	CLA	C11-C12-C13-C14
29	N	602	CLA	C6-C7-C8-C9
29	S	609	CLA	C6-C7-C8-C9
29	S	610	CLA	C6-C7-C8-C9
29	Y	611	CLA	C6-C7-C8-C9
29	b	602	CLA	C14-C13-C15-C16
29	b	612	CLA	C11-C12-C13-C14
29	b	617	CLA	C14-C13-C15-C16
29	c	510	CLA	C14-C13-C15-C16
29	n	603	CLA	C14-C13-C15-C16
29	g	610	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	g	613	CLA	C11-C12-C13-C14
29	r	608	CLA	C6-C7-C8-C9
29	y	603	CLA	C14-C13-C15-C16
29	y	613	CLA	C11-C10-C8-C9
29	B1	616	CLA	C11-C10-C8-C9
29	B1	616	CLA	C14-C13-C15-C16
29	C1	501	CLA	C14-C13-C15-C16
29	C1	510	CLA	C14-C13-C15-C16
29	C1	513	CLA	C11-C12-C13-C14
29	D1	403	CLA	C6-C7-C8-C9
29	N1	610	CLA	C6-C7-C8-C9
29	Y1	612	CLA	C11-C10-C8-C9
29	b1	609	CLA	C6-C7-C8-C9
29	b1	610	CLA	C6-C7-C8-C9
29	b1	617	CLA	C14-C13-C15-C16
29	c1	507	CLA	C11-C12-C13-C14
29	c1	507	CLA	C14-C13-C15-C16
29	c1	511	CLA	C14-C13-C15-C16
29	n1	602	CLA	C11-C10-C8-C9
29	n1	603	CLA	C14-C13-C15-C16
29	g1	602	CLA	C14-C13-C15-C16
29	g1	603	CLA	C11-C12-C13-C14
29	r1	603	CLA	C11-C10-C8-C9
29	y1	603	CLA	C11-C12-C13-C14
29	y1	611	CLA	C14-C13-C15-C16
48	N	605	CHL	C11-C10-C8-C9
48	G	601	CHL	C14-C13-C15-C16
48	g	607	CHL	C11-C10-C8-C9
48	N1	607	CHL	C11-C12-C13-C14
48	G1	601	CHL	C6-C7-C8-C9
32	M	101	SQD	C24-C25-C26-C27
38	b	624	3PH	C26-C27-C28-C29
37	c1	519	DGD	C3A-C4A-C5A-C6A
38	B	624	3PH	C35-C36-C37-C38
29	C	510	CLA	C10-C11-C12-C13
29	g	603	CLA	C15-C16-C17-C18
29	y	613	CLA	C8-C10-C11-C12
29	Y1	604	CLA	C10-C11-C12-C13
29	y1	603	CLA	C5-C6-C7-C8
30	a1	408	PHO	C10-C11-C12-C13
48	S	608	CHL	C5-C6-C7-C8
48	Y1	607	CHL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
30	A	409	PHO	C1A-C2A-CAA-CBA
30	a	409	PHO	C1A-C2A-CAA-CBA
40	D	410	LHG	C2-C3-O3-P
40	L	101	LHG	C2-C3-O3-P
40	S	624	LHG	C5-C4-O6-P
40	D1	409	LHG	C5-C4-O6-P
40	S1	624	LHG	C2-C3-O3-P
40	c1	525	LHG	C2-C3-O3-P
40	d1	408	LHG	C2-C3-O3-P
40	d1	409	LHG	C2-C3-O3-P
29	Y	602	CLA	O1A-CGA-O2A-C1
29	c	501	CLA	O1A-CGA-O2A-C1
33	w	201	LMG	O10-C28-O8-C9
38	b	624	3PH	C38-C39-C3A-C3B
40	D1	408	LHG	C24-C25-C26-C27
29	S1	617	CLA	C2A-CAA-CBA-CGA
29	r1	604	CLA	C2A-CAA-CBA-CGA
29	C	507	CLA	C16-C17-C18-C19
29	G	611	CLA	C16-C17-C18-C20
29	n	610	CLA	C16-C17-C18-C20
29	N1	602	CLA	C16-C17-C18-C20
29	Y1	611	CLA	C16-C17-C18-C19
38	t	101	3PH	C31-C32-C33-C34
29	c	508	CLA	C3-C5-C6-C7
31	C	514	BCR	C23-C24-C25-C26
31	C	515	BCR	C23-C24-C25-C26
31	C	517	BCR	C5-C6-C7-C8
31	b	619	BCR	C23-C24-C25-C26
31	c	515	BCR	C23-C24-C25-C26
31	B1	618	BCR	C5-C6-C7-C8
31	C1	514	BCR	C23-C24-C25-C26
31	b1	618	BCR	C5-C6-C7-C8
31	b1	619	BCR	C23-C24-C25-C26
31	b1	619	BCR	C23-C24-C25-C30
31	c1	515	BCR	C23-C24-C25-C26
31	c1	515	BCR	C23-C24-C25-C30
36	B	620	C7Z	C5-C6-C7-C8
49	N	620	LUT	C1-C6-C7-C8
49	N	620	LUT	C5-C6-C7-C8
49	S	620	LUT	C1-C6-C7-C8
49	S	620	LUT	C5-C6-C7-C8
49	Y	620	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
49	Y	620	LUT	C5-C6-C7-C8
49	g	621	LUT	C1-C6-C7-C8
49	G1	621	LUT	C1-C6-C7-C8
49	Y1	621	LUT	C1-C6-C7-C8
49	Y1	621	LUT	C5-C6-C7-C8
49	g1	621	LUT	C1-C6-C7-C8
49	g1	621	LUT	C5-C6-C7-C8
29	C	511	CLA	C8-C10-C11-C12
29	R	610	CLA	C5-C6-C7-C8
29	b	617	CLA	C8-C10-C11-C12
29	d	402	CLA	C15-C16-C17-C18
29	a1	405	CLA	C13-C15-C16-C17
29	c1	503	CLA	C8-C10-C11-C12
29	s1	610	CLA	C8-C10-C11-C12
48	n1	607	CHL	C5-C6-C7-C8
32	b1	626	SQD	C13-C14-C15-C16
33	W1	201	LMG	C33-C34-C35-C36
39	b1	625	DGA	CAA-CBA-CCA-CDA
40	l	101	LHG	C12-C13-C14-C15
47	I1	102	4RF	C27-C28-C29-C30
29	s	610	CLA	O1D-CGD-O2D-CED
33	C	521	LMG	O7-C10-C11-C12
31	c	517	BCR	C37-C22-C23-C24
31	c1	515	BCR	C11-C12-C13-C35
49	G1	620	LUT	C27-C28-C29-C39
48	R	606	CHL	C2A-CAA-CBA-CGA
33	w1	201	LMG	C39-C40-C41-C42
39	B	625	DGA	CFB-CGB-CHB-CIB
39	c1	524	DGA	CB2-CB3-CB4-CB5
31	B	618	BCR	C21-C22-C23-C24
31	C	514	BCR	C17-C18-C19-C20
31	C	517	BCR	C7-C8-C9-C10
31	D	404	BCR	C17-C18-C19-C20
31	C1	514	BCR	C11-C12-C13-C14
48	S1	607	CHL	C1A-C2A-CAA-CBA
49	S1	621	LUT	C11-C12-C13-C14
49	S1	621	LUT	C27-C28-C29-C30
49	s1	620	LUT	C31-C32-C33-C34
49	y1	620	LUT	C27-C28-C29-C30
51	y	623	NEX	C11-C12-C13-C14
29	c	512	CLA	C15-C16-C17-C18
29	n	602	CLA	C13-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
29	b1	615	CLA	C8-C10-C11-C12
29	d1	403	CLA	C15-C16-C17-C18
40	S	624	LHG	O9-C7-O7-C5
40	C1	525	LHG	O9-C7-O7-C5
51	r1	622	NEX	C14-C15-C35-C34
40	C1	525	LHG	C8-C7-O7-C5
33	d	411	LMG	C32-C33-C34-C35
37	c	519	DGD	CAB-CBB-CCB-CDB
38	S	626	3PH	C3B-C3C-C3D-C3E
40	G	624	LHG	C31-C32-C33-C34
40	n1	624	LHG	C34-C35-C36-C37
29	A1	410	CLA	C10-C11-C12-C13
48	Y1	606	CHL	C5-C6-C7-C8
32	A1	412	SQD	C11-C10-C9-C8
40	L1	101	LHG	C9-C10-C11-C12
29	S	611	CLA	C16-C17-C18-C19
29	B1	612	CLA	C16-C17-C18-C19
29	S1	610	CLA	C16-C17-C18-C20
29	r1	612	CLA	C11-C12-C13-C14
29	y1	613	CLA	C16-C17-C18-C19
34	A	414	SPH	C12-C13-C14-C15
40	C1	525	LHG	C35-C36-C37-C38
37	C1	520	DGD	C4D-C5D-C6D-O5D
29	b	604	CLA	C5-C6-C7-C8
29	b	608	CLA	C13-C15-C16-C17
29	y	612	CLA	C8-C10-C11-C12
29	c1	509	CLA	C5-C6-C7-C8
30	a1	408	PHO	C5-C6-C7-C8
53	r1	626	ERG	C22-C23-C24-C28
34	Y1	625	SPH	C12-C13-C14-C15
40	D1	409	LHG	C30-C31-C32-C33
29	c	506	CLA	C10-C11-C12-C13
29	b1	615	CLA	C13-C15-C16-C17
38	t	101	3PH	O11-C1-C2-C3
40	G	624	LHG	O6-C4-C5-C6
40	d	410	LHG	O6-C4-C5-C6
40	d1	408	LHG	O6-C4-C5-C6
40	g1	624	LHG	O6-C4-C5-C6
55	Y1	626	PTY	O14-C5-C6-C1
32	m1	101	SQD	O47-C7-C8-C9
40	l	101	LHG	O2-C2-C3-O3
29	C1	506	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
33	D1	411	LMG	C18-C19-C20-C21
37	C1	519	DGD	C2A-C3A-C4A-C5A
29	B	602	CLA	C11-C12-C13-C15
29	B	604	CLA	C11-C12-C13-C15
29	B	607	CLA	C11-C10-C8-C7
29	B	608	CLA	C11-C10-C8-C7
29	B	615	CLA	C6-C7-C8-C10
29	B	617	CLA	C11-C12-C13-C15
29	C	502	CLA	C12-C13-C15-C16
29	C	509	CLA	C6-C7-C8-C10
29	C	509	CLA	C11-C10-C8-C7
29	C	510	CLA	C12-C13-C15-C16
29	C	511	CLA	C11-C12-C13-C15
29	D	402	CLA	C11-C10-C8-C7
29	D	403	CLA	C11-C10-C8-C7
29	N	602	CLA	C6-C7-C8-C10
29	G	603	CLA	C12-C13-C15-C16
29	R	602	CLA	C6-C7-C8-C10
29	S	602	CLA	C6-C7-C8-C10
29	S	610	CLA	C11-C10-C8-C7
29	Y	602	CLA	C11-C12-C13-C15
29	Y	611	CLA	C6-C7-C8-C10
29	Y	613	CLA	C6-C7-C8-C10
29	Y	613	CLA	C12-C13-C15-C16
29	b	602	CLA	C11-C10-C8-C7
29	b	602	CLA	C12-C13-C15-C16
29	b	607	CLA	C11-C12-C13-C15
29	b	608	CLA	C11-C10-C8-C7
29	b	613	CLA	C11-C10-C8-C7
29	b	616	CLA	C11-C12-C13-C15
29	b	617	CLA	C6-C7-C8-C10
29	c	501	CLA	C11-C12-C13-C15
29	c	507	CLA	C6-C7-C8-C10
29	c	510	CLA	C12-C13-C15-C16
29	c	513	CLA	C11-C10-C8-C7
29	d	402	CLA	C11-C12-C13-C15
29	n	613	CLA	C11-C10-C8-C7
29	n	613	CLA	C12-C13-C15-C16
29	g	611	CLA	C12-C13-C15-C16
29	g	613	CLA	C12-C13-C15-C16
29	r	602	CLA	C6-C7-C8-C10
29	r	609	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
29	r	612	CLA	C6-C7-C8-C10
29	y	603	CLA	C12-C13-C15-C16
29	y	604	CLA	C6-C7-C8-C10
29	y	612	CLA	C11-C10-C8-C7
29	y	613	CLA	C12-C13-C15-C16
29	A1	406	CLA	C12-C13-C15-C16
29	B1	603	CLA	C11-C10-C8-C7
29	B1	609	CLA	C11-C10-C8-C7
29	B1	609	CLA	C11-C12-C13-C15
29	B1	611	CLA	C11-C12-C13-C15
29	B1	615	CLA	C6-C7-C8-C10
29	B1	616	CLA	C11-C12-C13-C15
29	B1	617	CLA	C6-C7-C8-C10
29	C1	501	CLA	C12-C13-C15-C16
29	C1	510	CLA	C12-C13-C15-C16
29	C1	513	CLA	C11-C12-C13-C15
29	D1	403	CLA	C6-C7-C8-C10
29	D1	403	CLA	C11-C10-C8-C7
29	N1	602	CLA	C12-C13-C15-C16
29	N1	604	CLA	C6-C7-C8-C10
29	N1	604	CLA	C12-C13-C15-C16
29	N1	610	CLA	C11-C12-C13-C15
29	N1	610	CLA	C12-C13-C15-C16
29	G1	603	CLA	C6-C7-C8-C10
29	G1	610	CLA	C6-C7-C8-C10
29	S1	610	CLA	C11-C12-C13-C15
29	Y1	604	CLA	C11-C10-C8-C7
29	Y1	611	CLA	C6-C7-C8-C10
29	Y1	612	CLA	C11-C10-C8-C7
29	Y1	613	CLA	C11-C12-C13-C15
29	a1	405	CLA	C11-C10-C8-C7
29	a1	410	CLA	C11-C10-C8-C7
29	b1	603	CLA	C6-C7-C8-C10
29	b1	603	CLA	C11-C10-C8-C7
29	b1	609	CLA	C6-C7-C8-C10
29	b1	613	CLA	C11-C10-C8-C7
29	b1	616	CLA	C11-C10-C8-C7
29	c1	504	CLA	C6-C7-C8-C10
29	c1	507	CLA	C11-C12-C13-C15
29	c1	507	CLA	C12-C13-C15-C16
29	c1	513	CLA	C11-C10-C8-C7
29	n1	604	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	n1	610	CLA	C12-C13-C15-C16
29	n1	613	CLA	C11-C12-C13-C15
29	g1	602	CLA	C12-C13-C15-C16
29	g1	603	CLA	C11-C12-C13-C15
29	s1	603	CLA	C11-C10-C8-C7
29	s1	609	CLA	C6-C7-C8-C10
29	y1	604	CLA	C11-C10-C8-C7
29	y1	611	CLA	C12-C13-C15-C16
30	a1	408	PHO	C11-C10-C8-C7
30	a1	409	PHO	C11-C10-C8-C7
48	N	601	CHL	C12-C13-C15-C16
48	N	605	CHL	C11-C10-C8-C7
48	G	607	CHL	C2-C3-C5-C6
48	G	609	CHL	C11-C12-C13-C15
48	Y	606	CHL	C11-C10-C8-C7
48	Y	609	CHL	C12-C13-C15-C16
48	n	605	CHL	C11-C10-C8-C7
48	n	606	CHL	C11-C12-C13-C15
48	y	606	CHL	C6-C7-C8-C10
48	y	607	CHL	C11-C10-C8-C7
48	y	609	CHL	C12-C13-C15-C16
48	N1	605	CHL	C11-C10-C8-C7
48	N1	606	CHL	C11-C10-C8-C7
48	N1	606	CHL	C11-C12-C13-C15
48	N1	607	CHL	C11-C12-C13-C15
48	G1	601	CHL	C6-C7-C8-C10
48	G1	609	CHL	C11-C12-C13-C15
48	Y1	601	CHL	C6-C7-C8-C10
48	n1	601	CHL	C12-C13-C15-C16
48	n1	605	CHL	C12-C13-C15-C16
48	g1	601	CHL	C6-C7-C8-C10
48	g1	607	CHL	C11-C10-C8-C7
48	y1	606	CHL	C12-C13-C15-C16
29	S	614	CLA	O1A-CGA-O2A-C1
32	M	101	SQD	C28-C29-C30-C31
47	I	102	4RF	C44-C45-C46-C47
31	a	411	BCR	C19-C20-C21-C22
31	b	618	BCR	C13-C14-C15-C16
31	c	514	BCR	C13-C14-C15-C16
31	c	516	BCR	C9-C10-C11-C12
31	C1	514	BCR	C15-C16-C17-C18
31	C1	516	BCR	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
31	c1	516	BCR	C9-C10-C11-C12
31	c1	517	BCR	C15-C16-C17-C18
45	H	101	RRX	C19-C20-C21-C22
45	h	101	RRX	C19-C20-C21-C22
49	Y	621	LUT	C29-C30-C31-C32
49	n	620	LUT	C29-C30-C31-C32
49	s	621	LUT	C29-C30-C31-C32
49	g1	620	LUT	C29-C30-C31-C32
49	y1	621	LUT	C9-C10-C11-C12
51	G1	623	NEX	C13-C14-C15-C35
29	B	603	CLA	C16-C17-C18-C20
29	B	612	CLA	C16-C17-C18-C19
29	B	615	CLA	C16-C17-C18-C19
29	R	603	CLA	C11-C12-C13-C15
29	g	610	CLA	C16-C17-C18-C20
29	A1	405	CLA	C16-C17-C18-C20
29	n1	603	CLA	C16-C17-C18-C19
33	W1	201	LMG	O6-C5-C6-O5
33	H	102	LMG	C37-C38-C39-C40
38	t1	101	3PH	C26-C27-C28-C29
39	j1	101	DGA	CBB-CAB-CB9-CB8
32	m1	101	SQD	C23-C24-C25-C26
38	t	101	3PH	C21-C22-C23-C24
32	C	526	SQD	C15-C16-C17-C18
33	A	413	LMG	C31-C32-C33-C34
33	d	411	LMG	C34-C35-C36-C37
33	a1	413	LMG	C36-C37-C38-C39
47	I	102	4RF	C02-C03-C04-C05
29	B	615	CLA	C8-C10-C11-C12
29	N	602	CLA	C15-C16-C17-C18
29	n	604	CLA	C2A-CAA-CBA-CGA
29	n	611	CLA	C2A-CAA-CBA-CGA
29	r1	602	CLA	C2A-CAA-CBA-CGA
33	c1	523	LMG	C31-C32-C33-C34
34	a1	414	SPH	C12-C13-C14-C15
40	D	409	LHG	C29-C30-C31-C32
40	d	408	LHG	C34-C35-C36-C37
29	g	613	CLA	C8-C10-C11-C12
29	y	602	CLA	C10-C11-C12-C13
29	B1	603	CLA	C15-C16-C17-C18
38	B	624	3PH	C3F-C3G-C3H-C3I
38	b	624	3PH	C1-O11-P-O13

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Mol	Chain	Res	Type	Atoms
39	C	524	DGA	CB7-CB8-CB9-CAB
40	S	624	LHG	C30-C31-C32-C33
40	c	525	LHG	C25-C26-C27-C28
47	k	101	4RF	C49-C50-C51-C52
51	S	623	NEX	C11-C10-C9-C19
51	y	623	NEX	C11-C10-C9-C19
51	G1	623	NEX	C11-C10-C9-C19
51	G1	623	NEX	C40-C33-C34-C35
29	b1	611	CLA	C3-C5-C6-C7
48	G	609	CHL	C3-C5-C6-C7
29	S	602	CLA	C11-C12-C13-C15
29	Y	613	CLA	C16-C17-C18-C20
29	b	603	CLA	C16-C17-C18-C19
29	C1	510	CLA	C16-C17-C18-C19
30	A	408	PHO	C16-C17-C18-C20
29	Y	603	CLA	C8-C10-C11-C12
29	B	604	CLA	CBA-CGA-O2A-C1
29	B1	616	CLA	CBA-CGA-O2A-C1
39	c1	524	DGA	CA2-CA1-OG1-CG1
39	J	101	DGA	CB3-CB4-CB5-CB6
39	C1	524	DGA	CA2-CA3-CA4-CA5
40	n1	624	LHG	C14-C15-C16-C17
47	I	102	4RF	C47-C48-C49-C50
37	C	520	DGD	C1B-C2B-C3B-C4B
32	b	626	SQD	C19-C20-C21-C22
34	y1	625	SPH	C12-C13-C14-C15
38	t	101	3PH	C3A-C3B-C3C-C3D
39	B1	625	DGA	CA5-CA6-CA7-CA8
29	C	509	CLA	C10-C11-C12-C13
29	g1	602	CLA	C10-C11-C12-C13
39	c	524	DGA	CA7-CA8-CA9-CAA
40	d1	409	LHG	C35-C36-C37-C38
47	i1	101	4RF	C49-C50-C51-C52
29	B	606	CLA	CAD-CBD-CGD-O2D
29	C	503	CLA	CAD-CBD-CGD-O2D
29	N	602	CLA	CAD-CBD-CGD-O2D
29	N	614	CLA	CAD-CBD-CGD-O2D
29	G	602	CLA	CAD-CBD-CGD-O2D
29	G	603	CLA	CAD-CBD-CGD-O2D
29	G	612	CLA	CAD-CBD-CGD-O2D
29	b	615	CLA	CAD-CBD-CGD-O2D
29	c	507	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
29	n	602	CLA	CAD-CBD-CGD-O2D
29	n	612	CLA	CAD-CBD-CGD-O2D
29	g	603	CLA	CAD-CBD-CGD-O2D
29	g	604	CLA	CAD-CBD-CGD-O2D
29	g	614	CLA	CAD-CBD-CGD-O2D
29	r	602	CLA	CAD-CBD-CGD-O2D
29	r	612	CLA	CAD-CBD-CGD-O2D
29	y	602	CLA	CAD-CBD-CGD-O2D
29	y	614	CLA	CAD-CBD-CGD-O2D
29	B1	608	CLA	CAD-CBD-CGD-O2D
29	B1	617	CLA	CAD-CBD-CGD-O2D
29	C1	509	CLA	CAD-CBD-CGD-O2D
29	G1	604	CLA	CAD-CBD-CGD-O2D
29	R1	612	CLA	CAD-CBD-CGD-O2D
29	b1	611	CLA	CAD-CBD-CGD-O2D
29	b1	615	CLA	CAD-CBD-CGD-O2D
29	c1	504	CLA	CAD-CBD-CGD-O2D
29	c1	509	CLA	CAD-CBD-CGD-O2D
29	n1	602	CLA	CAD-CBD-CGD-O2D
29	r1	612	CLA	CAD-CBD-CGD-O2D
33	B	622	LMG	C9-C8-O7-C10
38	T	101	3PH	C3-C2-O21-C21
38	t	101	3PH	C3-C2-O21-C21
39	b	625	DGA	CG1-CG2-OG2-CB1
39	b1	625	DGA	CG1-CG2-OG2-CB1
48	N	605	CHL	CAD-CBD-CGD-O2D
48	N	608	CHL	CAD-CBD-CGD-O2D
48	Y	605	CHL	CAD-CBD-CGD-O2D
48	N1	606	CHL	CAD-CBD-CGD-O2D
48	G1	606	CHL	CAD-CBD-CGD-O2D
51	G1	623	NEX	C7-C8-C9-C19
32	C1	526	SQD	C12-C13-C14-C15
33	C1	523	LMG	C39-C40-C41-C42
38	b1	624	3PH	C2D-C2E-C2F-C2G
29	B1	609	CLA	C15-C16-C17-C18
29	R1	609	CLA	C10-C11-C12-C13
32	A	412	SQD	C24-C25-C26-C27
33	a	413	LMG	C39-C40-C41-C42
37	C	519	DGD	CDB-CEB-CFB-CGB
38	T1	101	3PH	C27-C28-C29-C2A
39	c1	524	DGA	CFB-CGB-CHB-CIB
29	C	510	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	B	617	CLA	CBA-CGA-O2A-C1
48	N	606	CHL	C4-C3-C5-C6
48	g	601	CHL	C4-C3-C5-C6
33	H	102	LMG	C29-C30-C31-C32
39	J	101	DGA	CB2-CB3-CB4-CB5
39	c	524	DGA	CFB-CGB-CHB-CIB
40	d1	409	LHG	C11-C12-C13-C14
33	H	102	LMG	O6-C1-O1-C7
37	c1	519	DGD	O6E-C1E-O5D-C6D
29	b1	608	CLA	C2-C3-C5-C6
32	C	526	SQD	O6-C44-C45-C46
32	C	526	SQD	C44-C45-C46-O48
32	m1	101	SQD	C44-C45-C46-O48
33	C	523	LMG	O1-C7-C8-C9
33	c	523	LMG	O1-C7-C8-C9
33	H1	102	LMG	C7-C8-C9-O8
33	d1	411	LMG	C7-C8-C9-O8
39	j	101	DGA	OG1-CG1-CG2-CG3
40	D	409	LHG	C4-C5-C6-O8
40	G	624	LHG	C4-C5-C6-O8
40	n	624	LHG	C4-C5-C6-O8
40	s	624	LHG	C2-C3-O3-P
40	C1	525	LHG	C4-C5-C6-O8
40	D1	408	LHG	C4-C5-C6-O8
40	G1	624	LHG	C4-C5-C6-O8
40	d1	408	LHG	C4-C5-C6-O8
40	d1	410	LHG	C4-C5-C6-O8
41	C	527	LMK	O1-C7-C8-C9
41	C1	527	LMK	C4-C3-N4-C6
41	c1	527	LMK	C7-C8-C9-O8
47	k	101	4RF	C19-C20-C39-O40
55	Y1	626	PTY	O4-C1-C6-C5
55	y1	626	PTY	O4-C1-C6-C5
33	A1	413	LMG	O10-C28-O8-C9
40	L	101	LHG	O6-C4-C5-O7
40	N	624	LHG	O6-C4-C5-O7
40	l	101	LHG	O6-C4-C5-O7
40	n	624	LHG	O6-C4-C5-O7
40	G1	624	LHG	O6-C4-C5-O7
40	d1	408	LHG	O6-C4-C5-O7
40	d1	409	LHG	O6-C4-C5-O7
40	n1	624	LHG	O6-C4-C5-O7

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Mol	Chain	Res	Type	Atoms
55	Y	626	PTY	O14-C5-C6-O7
55	y1	627	PTY	O14-C5-C6-O7
29	A	405	CLA	C5-C6-C7-C8
29	B1	612	CLA	C10-C11-C12-C13
48	N1	601	CHL	C3-C5-C6-C7
33	A1	413	LMG	O7-C10-C11-C12
29	g	614	CLA	O2A-C1-C2-C3
37	c	519	DGD	C2B-C3B-C4B-C5B
29	C1	508	CLA	CBA-CGA-O2A-C1
29	S	610	CLA	C2A-CAA-CBA-CGA
29	B1	602	CLA	C2A-CAA-CBA-CGA
48	Y	605	CHL	C2A-CAA-CBA-CGA
29	b1	605	CLA	C5-C6-C7-C8
32	M	101	SQD	C11-C10-C9-C8
32	C1	526	SQD	C19-C20-C21-C22
40	L1	101	LHG	C10-C11-C12-C13
29	B	605	CLA	C16-C17-C18-C19
29	a	406	CLA	C16-C17-C18-C20
29	n	604	CLA	C16-C17-C18-C19
30	A	408	PHO	C16-C17-C18-C19
33	c	523	LMG	C12-C13-C14-C15
37	C	519	DGD	C2A-C3A-C4A-C5A
40	d	409	LHG	C15-C16-C17-C18
40	n	624	LHG	C14-C15-C16-C17
55	y1	626	PTY	C37-C38-C39-C40
29	b1	616	CLA	O1D-CGD-O2D-CED
40	c	525	LHG	O9-C7-O7-C5
29	A	406	CLA	CHA-CBD-CGD-O1D
29	A	406	CLA	CHA-CBD-CGD-O2D
29	B	605	CLA	CHA-CBD-CGD-O1D
29	B	605	CLA	CHA-CBD-CGD-O2D
29	B	608	CLA	CHA-CBD-CGD-O1D
29	B	608	CLA	CHA-CBD-CGD-O2D
29	B	611	CLA	CHA-CBD-CGD-O1D
29	B	611	CLA	CHA-CBD-CGD-O2D
29	B	613	CLA	CHA-CBD-CGD-O1D
29	C	505	CLA	CHA-CBD-CGD-O2D
29	C	506	CLA	CHA-CBD-CGD-O1D
29	C	506	CLA	CHA-CBD-CGD-O2D
29	C	507	CLA	CHA-CBD-CGD-O1D
29	C	507	CLA	CHA-CBD-CGD-O2D
29	C	509	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
29	C	509	CLA	CHA-CBD-CGD-O2D
29	C	511	CLA	CHA-CBD-CGD-O1D
29	C	511	CLA	CHA-CBD-CGD-O2D
29	C	512	CLA	CHA-CBD-CGD-O1D
29	C	512	CLA	CHA-CBD-CGD-O2D
29	N	604	CLA	CHA-CBD-CGD-O1D
29	N	604	CLA	CHA-CBD-CGD-O2D
29	N	612	CLA	CHA-CBD-CGD-O1D
29	R	603	CLA	CHA-CBD-CGD-O1D
29	R	603	CLA	CHA-CBD-CGD-O2D
29	R	608	CLA	CHA-CBD-CGD-O2D
29	R	609	CLA	CHA-CBD-CGD-O1D
29	R	609	CLA	CHA-CBD-CGD-O2D
29	S	602	CLA	CHA-CBD-CGD-O1D
29	S	605	CLA	CHA-CBD-CGD-O1D
29	S	605	CLA	CHA-CBD-CGD-O2D
29	S	612	CLA	CHA-CBD-CGD-O1D
29	S	612	CLA	CHA-CBD-CGD-O2D
29	Y	602	CLA	CHA-CBD-CGD-O1D
29	Y	602	CLA	CHA-CBD-CGD-O2D
29	Y	612	CLA	CHA-CBD-CGD-O1D
29	Y	612	CLA	CHA-CBD-CGD-O2D
29	a	406	CLA	CHA-CBD-CGD-O1D
29	a	406	CLA	CHA-CBD-CGD-O2D
29	b	607	CLA	CHA-CBD-CGD-O1D
29	b	607	CLA	CHA-CBD-CGD-O2D
29	b	609	CLA	CHA-CBD-CGD-O1D
29	b	609	CLA	CHA-CBD-CGD-O2D
29	b	610	CLA	CHA-CBD-CGD-O1D
29	b	610	CLA	CHA-CBD-CGD-O2D
29	c	503	CLA	CHA-CBD-CGD-O1D
29	c	506	CLA	CHA-CBD-CGD-O1D
29	c	506	CLA	CHA-CBD-CGD-O2D
29	n	613	CLA	CHA-CBD-CGD-O1D
29	n	613	CLA	CHA-CBD-CGD-O2D
29	g	602	CLA	CHA-CBD-CGD-O1D
29	g	602	CLA	CHA-CBD-CGD-O2D
29	g	611	CLA	CHA-CBD-CGD-O1D
29	g	611	CLA	CHA-CBD-CGD-O2D
29	r	603	CLA	CHA-CBD-CGD-O1D
29	s	602	CLA	CHA-CBD-CGD-O1D
29	s	602	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
29	s	605	CLA	CHA-CBD-CGD-O1D
29	y	603	CLA	CHA-CBD-CGD-O1D
29	y	603	CLA	CHA-CBD-CGD-O2D
29	y	612	CLA	CHA-CBD-CGD-O1D
29	y	612	CLA	CHA-CBD-CGD-O2D
29	B1	602	CLA	CHA-CBD-CGD-O1D
29	B1	602	CLA	CHA-CBD-CGD-O2D
29	B1	604	CLA	CHA-CBD-CGD-O1D
29	B1	604	CLA	CHA-CBD-CGD-O2D
29	B1	605	CLA	CHA-CBD-CGD-O1D
29	B1	605	CLA	CHA-CBD-CGD-O2D
29	B1	609	CLA	CHA-CBD-CGD-O1D
29	B1	616	CLA	CHA-CBD-CGD-O2D
29	C1	502	CLA	CHA-CBD-CGD-O1D
29	C1	502	CLA	CHA-CBD-CGD-O2D
29	C1	505	CLA	CHA-CBD-CGD-O1D
29	C1	512	CLA	CHA-CBD-CGD-O1D
29	C1	512	CLA	CHA-CBD-CGD-O2D
29	G1	612	CLA	CHA-CBD-CGD-O1D
29	G1	612	CLA	CHA-CBD-CGD-O2D
29	G1	613	CLA	CHA-CBD-CGD-O1D
29	G1	613	CLA	CHA-CBD-CGD-O2D
29	S1	602	CLA	CHA-CBD-CGD-O1D
29	S1	602	CLA	CHA-CBD-CGD-O2D
29	S1	604	CLA	CHA-CBD-CGD-O1D
29	S1	611	CLA	CHA-CBD-CGD-O1D
29	S1	611	CLA	CHA-CBD-CGD-O2D
29	Y1	604	CLA	CHA-CBD-CGD-O1D
29	Y1	612	CLA	CHA-CBD-CGD-O1D
29	Y1	612	CLA	CHA-CBD-CGD-O2D
29	b1	605	CLA	CHA-CBD-CGD-O1D
29	b1	608	CLA	CHA-CBD-CGD-O2D
29	b1	610	CLA	CHA-CBD-CGD-O1D
29	b1	610	CLA	CHA-CBD-CGD-O2D
29	b1	612	CLA	CHA-CBD-CGD-O1D
29	b1	613	CLA	CHA-CBD-CGD-O1D
29	b1	613	CLA	CHA-CBD-CGD-O2D
29	c1	501	CLA	CHA-CBD-CGD-O1D
29	c1	501	CLA	CHA-CBD-CGD-O2D
29	c1	505	CLA	CHA-CBD-CGD-O1D
29	c1	505	CLA	CHA-CBD-CGD-O2D
29	g1	612	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
29	r1	603	CLA	CHA-CBD-CGD-O1D
29	r1	603	CLA	CHA-CBD-CGD-O2D
29	r1	608	CLA	CHA-CBD-CGD-O2D
29	s1	604	CLA	CHA-CBD-CGD-O1D
29	s1	604	CLA	CHA-CBD-CGD-O2D
29	s1	605	CLA	CHA-CBD-CGD-O1D
29	s1	605	CLA	CHA-CBD-CGD-O2D
29	y1	612	CLA	CHA-CBD-CGD-O1D
29	y1	612	CLA	CHA-CBD-CGD-O2D
48	G	605	CHL	CHA-CBD-CGD-O1D
48	G	605	CHL	CHA-CBD-CGD-O2D
48	r	606	CHL	CHA-CBD-CGD-O2D
48	N1	601	CHL	CHA-CBD-CGD-O1D
48	n1	601	CHL	CHA-CBD-CGD-O2D
48	n1	608	CHL	CHA-CBD-CGD-O1D
48	n1	608	CHL	CHA-CBD-CGD-O2D
48	r1	606	CHL	CHA-CBD-CGD-O2D
48	y1	609	CHL	CHA-CBD-CGD-O1D
48	y1	609	CHL	CHA-CBD-CGD-O2D
29	Y1	611	CLA	C15-C16-C17-C18
47	K1	101	4RF	C01-C02-C03-C04
29	C	501	CLA	O1A-CGA-O2A-C1
29	B1	616	CLA	O1A-CGA-O2A-C1
32	b	621	SQD	O10-C23-O48-C46
32	b1	626	SQD	O10-C23-O48-C46
40	d1	410	LHG	O10-C23-O8-C6
54	S	625	LPX	O7-C6-O6-C5
40	g1	624	LHG	C24-C25-C26-C27
32	M1	101	SQD	C2-C1-O6-C44
33	a	413	LMG	C2-C1-O1-C7
51	S	623	NEX	C11-C10-C9-C8
29	C1	503	CLA	C10-C11-C12-C13
32	B1	621	SQD	C25-C26-C27-C28
32	A	412	SQD	O6-C44-C45-O47
32	B	626	SQD	O6-C44-C45-O47
32	C	526	SQD	O6-C44-C45-O47
32	C	526	SQD	O47-C45-C46-O48
32	a	412	SQD	O6-C44-C45-O47
32	m	101	SQD	O47-C45-C46-O48
32	b1	626	SQD	O6-C44-C45-O47
33	b	622	LMG	O1-C7-C8-O7
33	c	523	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
33	A1	413	LMG	O1-C7-C8-O7
33	B1	622	LMG	O7-C8-C9-O8
37	B	623	DGD	O1G-C1G-C2G-O2G
37	b	623	DGD	O1G-C1G-C2G-O2G
37	c	520	DGD	O1G-C1G-C2G-O2G
37	B1	623	DGD	O1G-C1G-C2G-O2G
37	C1	520	DGD	O2G-C2G-C3G-O3G
39	j	101	DGA	OG1-CG1-CG2-OG2
40	C1	525	LHG	O7-C5-C6-O8
40	S1	624	LHG	O7-C5-C6-O8
40	c1	525	LHG	O7-C5-C6-O8
41	c	527	LMK	O7-C8-C9-O8
47	i1	101	4RF	O18-C19-C20-O21
47	k1	101	4RF	O18-C19-C20-O21
55	Y1	627	PTY	O4-C1-C6-O7
55	y1	626	PTY	O4-C1-C6-O7
55	y1	627	PTY	O4-C1-C6-O7
38	s1	626	3PH	C22-C23-C24-C25
29	C	505	CLA	C13-C15-C16-C17
29	g1	610	CLA	O1A-CGA-O2A-C1
39	B1	625	DGA	CB7-CB8-CB9-CAB
40	d1	408	LHG	C26-C27-C28-C29
40	d1	408	LHG	C33-C34-C35-C36
40	n1	624	LHG	C30-C31-C32-C33
29	s	614	CLA	C6-C7-C8-C10
29	y	603	CLA	C16-C17-C18-C19
29	Y1	611	CLA	C16-C17-C18-C20
34	y1	625	SPH	N2-C2-C3-O3
40	S1	624	LHG	O1-C1-C2-O2
32	B	626	SQD	C14-C15-C16-C17
37	c	519	DGD	C6B-C7B-C8B-C9B
39	J1	101	DGA	CB2-CB3-CB4-CB5
39	c1	524	DGA	CA3-CA4-CA5-CA6
29	d1	402	CLA	C3-C5-C6-C7
29	B	615	CLA	C5-C6-C7-C8
29	y	611	CLA	C4-C3-C5-C6
48	n1	609	CHL	C4-C3-C5-C6
37	C	519	DGD	C9A-CAA-CBA-CCA
47	k	101	4RF	C54-C55-C56-C57
29	C1	501	CLA	C2-C3-C5-C6
43	D1	405	PL9	C13-C14-C16-C17
48	g	601	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
32	C1	526	SQD	C32-C33-C34-C35
33	d1	411	LMG	O9-C10-O7-C8
29	B	604	CLA	C11-C12-C13-C14
29	B	606	CLA	C6-C7-C8-C9
29	B	607	CLA	C11-C10-C8-C9
29	B	608	CLA	C11-C10-C8-C9
29	B	608	CLA	C11-C12-C13-C14
29	B	615	CLA	C6-C7-C8-C9
29	B	617	CLA	C11-C12-C13-C14
29	C	511	CLA	C14-C13-C15-C16
29	B1	605	CLA	C14-C13-C15-C16
29	N1	603	CLA	C14-C13-C15-C16
29	N1	604	CLA	C14-C13-C15-C16
29	G1	610	CLA	C11-C12-C13-C14
29	Y1	611	CLA	C6-C7-C8-C9
29	a1	410	CLA	C11-C10-C8-C9
29	c1	512	CLA	C11-C10-C8-C9
29	g1	603	CLA	C14-C13-C15-C16
29	g1	611	CLA	C11-C10-C8-C9
29	y1	604	CLA	C11-C10-C8-C9
30	a1	408	PHO	C11-C10-C8-C9
48	N	607	CHL	C11-C12-C13-C14
48	n	607	CHL	C11-C12-C13-C14
48	N1	605	CHL	C11-C10-C8-C9
29	S	611	CLA	O1D-CGD-O2D-CED
33	w	201	LMG	C11-C12-C13-C14
40	C1	525	LHG	C34-C35-C36-C37
40	d1	409	LHG	C33-C34-C35-C36
37	c	520	DGD	O6D-C5D-C6D-O5D
29	B	604	CLA	O1A-CGA-O2A-C1
29	B	617	CLA	O1A-CGA-O2A-C1
39	c1	524	DGA	OA1-CA1-OG1-CG1
47	K	101	4RF	O42-C41-O40-C39
40	c1	525	LHG	C23-C24-C25-C26
40	d	409	LHG	C29-C30-C31-C32
32	B	621	SQD	C4-C5-C6-S
32	C	526	SQD	C4-C5-C6-S
32	b	621	SQD	C4-C5-C6-S
32	C1	526	SQD	C4-C5-C6-S
32	b1	626	SQD	C5-C6-S-O8
32	c1	526	SQD	C4-C5-C6-S
32	a	412	SQD	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
40	C	525	LHG	C28-C29-C30-C31
29	B1	608	CLA	C2A-CAA-CBA-CGA
48	g	605	CHL	C2A-CAA-CBA-CGA
48	S1	608	CHL	CAA-CBA-CGA-O2A
38	B	624	3PH	C2E-C2F-C2G-C2H
38	s1	626	3PH	C3A-C3B-C3C-C3D
39	B	625	DGA	CA8-CA9-CAA-CBA
31	b	618	BCR	C37-C22-C23-C24
49	G	620	LUT	C27-C28-C29-C39
50	Y	622	XAT	C31-C32-C33-C40
47	i	101	4RF	C47-C48-C49-C50
40	S1	624	LHG	O1-C1-C2-C3
46	I1	101	GOL	C1-C2-C3-O3
29	Y	613	CLA	C13-C15-C16-C17
29	c1	508	CLA	C8-C10-C11-C12
30	a1	408	PHO	C13-C15-C16-C17
34	Y1	625	SPH	C13-C14-C15-C16
39	B	625	DGA	CBB-CAB-CB9-CB8
47	k1	101	4RF	C35-C36-C37-C38
31	c1	515	BCR	C11-C12-C13-C14
49	G1	620	LUT	C27-C28-C29-C30
50	R	621	XAT	C27-C28-C29-C30
33	A	413	LMG	C37-C38-C39-C40
37	C1	519	DGD	C9B-CAB-CBB-CCB
38	T1	101	3PH	C26-C27-C28-C29
41	C	527	LMK	C34-C16-C17-C18
29	A	410	CLA	C1A-C2A-CAA-CBA
29	B	605	CLA	C1A-C2A-CAA-CBA
29	N	602	CLA	C1A-C2A-CAA-CBA
29	R	609	CLA	C1A-C2A-CAA-CBA
29	b	612	CLA	C1A-C2A-CAA-CBA
29	r	612	CLA	C1A-C2A-CAA-CBA
29	y	604	CLA	C1A-C2A-CAA-CBA
29	B1	616	CLA	C1A-C2A-CAA-CBA
29	C1	511	CLA	C1A-C2A-CAA-CBA
29	D1	403	CLA	C1A-C2A-CAA-CBA
29	G1	612	CLA	C1A-C2A-CAA-CBA
29	S1	604	CLA	C1A-C2A-CAA-CBA
29	r1	612	CLA	C1A-C2A-CAA-CBA
48	N	609	CHL	C1A-C2A-CAA-CBA
48	G	609	CHL	C1A-C2A-CAA-CBA
48	s	608	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
48	N1	606	CHL	C1A-C2A-CAA-CBA
29	B	613	CLA	C16-C17-C18-C19
29	B1	607	CLA	C16-C17-C18-C19
29	g	602	CLA	C13-C15-C16-C17
29	r	602	CLA	C10-C11-C12-C13
29	r	608	CLA	C5-C6-C7-C8
40	y	624	LHG	C34-C35-C36-C37
29	R	608	CLA	C2-C1-O2A-CGA
29	n	613	CLA	C2-C1-O2A-CGA
29	s	610	CLA	C2-C1-O2A-CGA
29	R1	604	CLA	C2-C1-O2A-CGA
29	a1	405	CLA	C2-C1-O2A-CGA
29	a1	406	CLA	C2-C1-O2A-CGA
29	c1	501	CLA	C2-C1-O2A-CGA
29	r1	609	CLA	C2-C1-O2A-CGA
29	r1	610	CLA	C2-C1-O2A-CGA
29	C	501	CLA	CBA-CGA-O2A-C1
29	b	615	CLA	CBA-CGA-O2A-C1
38	S	626	3PH	C34-C35-C36-C37
38	t1	101	3PH	C3A-C3B-C3C-C3D
40	s	624	LHG	C28-C29-C30-C31
40	d1	410	LHG	C9-C10-C11-C12
40	d1	410	LHG	C34-C35-C36-C37
31	d	404	BCR	C19-C20-C21-C22
45	H1	101	RRX	C9-C10-C11-C12
49	Y1	620	LUT	C9-C10-C11-C12
49	Y1	621	LUT	C33-C34-C35-C15
49	n1	621	LUT	C29-C30-C31-C32
41	c	527	LMK	C10-C11-C12-C13
29	b1	611	CLA	C13-C15-C16-C17
40	D	409	LHG	C4-O6-P-O3
40	D	410	LHG	C4-O6-P-O3
40	L	101	LHG	C4-O6-P-O3
40	N	624	LHG	C3-O3-P-O6
40	S	624	LHG	C3-O3-P-O6
40	s	624	LHG	C3-O3-P-O6
40	C1	525	LHG	C3-O3-P-O6
40	N1	624	LHG	C3-O3-P-O6
40	S1	624	LHG	C3-O3-P-O6
40	s1	624	LHG	C3-O3-P-O6
32	b1	626	SQD	C14-C15-C16-C17
37	C	519	DGD	CDA-CEA-CFA-CGA

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Mol	Chain	Res	Type	Atoms
38	b1	624	3PH	C3D-C3E-C3F-C3G
40	L	101	LHG	C27-C28-C29-C30
40	n	624	LHG	C31-C32-C33-C34
54	s	625	LPX	C18-C19-C20-C21
29	r	609	CLA	C4-C3-C5-C6
29	y1	603	CLA	C4-C3-C5-C6
33	w1	201	LMG	O7-C10-C11-C12
29	Y1	611	CLA	C3-C5-C6-C7
29	b1	604	CLA	C3-C5-C6-C7
40	l	101	LHG	C2-C3-O3-P
40	D1	408	LHG	C2-C3-O3-P
40	s1	624	LHG	C2-C3-O3-P
29	B	603	CLA	C2-C3-C5-C6
29	B	610	CLA	C2-C3-C5-C6
29	r1	609	CLA	C2-C3-C5-C6
32	m1	101	SQD	C26-C27-C28-C29
39	c	524	DGA	CA2-CA3-CA4-CA5
39	j1	101	DGA	CA4-CA5-CA6-CA7
40	D	408	LHG	C4-O6-P-O4
40	D	409	LHG	C3-O3-P-O4
40	D	410	LHG	C3-O3-P-O4
40	Y	624	LHG	C4-O6-P-O4
40	d	408	LHG	C3-O3-P-O5
40	d	408	LHG	C4-O6-P-O4
40	d	409	LHG	C3-O3-P-O5
40	l	101	LHG	C3-O3-P-O5
40	n	624	LHG	C3-O3-P-O4
40	g	624	LHG	C4-O6-P-O4
40	s	624	LHG	C4-O6-P-O5
40	C1	525	LHG	C4-O6-P-O4
40	D1	409	LHG	C4-O6-P-O4
40	D1	410	LHG	C4-O6-P-O4
40	L1	101	LHG	C3-O3-P-O5
40	L1	101	LHG	C4-O6-P-O5
40	N1	624	LHG	C4-O6-P-O4
40	G1	624	LHG	C4-O6-P-O4
40	d1	408	LHG	C4-O6-P-O4
40	d1	409	LHG	C3-O3-P-O5
40	d1	409	LHG	C4-O6-P-O4
40	d1	410	LHG	C4-O6-P-O4
40	y1	624	LHG	C4-O6-P-O4
54	S1	625	LPX	C3-O1-P1-O3

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Mol	Chain	Res	Type	Atoms
54	s1	625	LPX	C3-O1-P1-O3
55	Y	626	PTY	C3-O11-P1-O13
55	Y	627	PTY	C5-O14-P1-O12
55	y	627	PTY	C3-O11-P1-O12
55	Y1	626	PTY	C3-O11-P1-O13
55	y1	626	PTY	C3-O11-P1-O12
55	y1	626	PTY	C5-O14-P1-O13
55	y1	627	PTY	C3-O11-P1-O13
29	c	505	CLA	C16-C17-C18-C20
29	y	613	CLA	C16-C17-C18-C19
29	C1	503	CLA	C16-C17-C18-C20
29	R1	602	CLA	C11-C12-C13-C14
29	R1	612	CLA	C11-C12-C13-C15
29	a1	405	CLA	C16-C17-C18-C20
29	b1	605	CLA	C16-C17-C18-C20
29	s1	614	CLA	C6-C7-C8-C9
33	B1	622	LMG	C19-C20-C21-C22
33	w1	201	LMG	C34-C35-C36-C37
38	s	626	3PH	C35-C36-C37-C38
29	N1	611	CLA	O2A-C1-C2-C3
29	G1	604	CLA	O2A-C1-C2-C3
29	n1	611	CLA	O2A-C1-C2-C3
29	A	410	CLA	C10-C11-C12-C13
29	B	612	CLA	C5-C6-C7-C8
29	B	617	CLA	C15-C16-C17-C18
29	r1	609	CLA	C5-C6-C7-C8
29	B	602	CLA	CBA-CGA-O2A-C1
38	s1	626	3PH	O11-C1-C2-C3
40	D1	410	LHG	O6-C4-C5-C6
55	Y	627	PTY	O14-C5-C6-C1
55	y1	626	PTY	O14-C5-C6-C1
33	h1	102	LMG	C16-C17-C18-C19
38	T	101	3PH	C3B-C3C-C3D-C3E
39	c	524	DGA	CA4-CA5-CA6-CA7
39	j1	101	DGA	CB4-CB5-CB6-CB7
47	i1	101	4RF	C48-C49-C50-C51
34	A1	414	SPH	C15-C16-C17-C18
55	y1	626	PTY	C36-C37-C38-C39
29	R	609	CLA	C5-C6-C7-C8
48	g	609	CHL	C13-C15-C16-C17
53	R	626	ERG	C21-C20-C22-C23
43	D	405	PL9	C47-C48-C49-C51

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Mol	Chain	Res	Type	Atoms
29	G1	603	CLA	C2A-CAA-CBA-CGA
29	Y1	604	CLA	C3-C5-C6-C7
29	b	602	CLA	C5-C6-C7-C8
32	C	526	SQD	C32-C33-C34-C35
37	c	519	DGD	C5A-C6A-C7A-C8A
40	d	408	LHG	C32-C33-C34-C35
55	y	626	PTY	C32-C33-C34-C35
32	B	621	SQD	C28-C29-C30-C31
33	a1	413	LMG	C33-C34-C35-C36
38	B	624	3PH	C23-C24-C25-C26
29	B	605	CLA	CAD-CBD-CGD-O1D
29	B	608	CLA	CAD-CBD-CGD-O1D
29	B	613	CLA	CAD-CBD-CGD-O1D
29	B	617	CLA	CAD-CBD-CGD-O1D
29	C	505	CLA	CAD-CBD-CGD-O1D
29	C	506	CLA	CAD-CBD-CGD-O1D
29	C	512	CLA	CAD-CBD-CGD-O1D
29	G	604	CLA	CAD-CBD-CGD-O1D
29	b	610	CLA	CAD-CBD-CGD-O1D
29	c	501	CLA	CAD-CBD-CGD-O1D
29	c	503	CLA	CAD-CBD-CGD-O1D
29	c	505	CLA	CAD-CBD-CGD-O1D
29	c	506	CLA	CAD-CBD-CGD-O1D
29	B1	602	CLA	CAD-CBD-CGD-O1D
29	B1	605	CLA	CAD-CBD-CGD-O1D
29	C1	502	CLA	CAD-CBD-CGD-O1D
29	C1	503	CLA	CAD-CBD-CGD-O1D
29	C1	505	CLA	CAD-CBD-CGD-O1D
29	b1	605	CLA	CAD-CBD-CGD-O1D
29	b1	610	CLA	CAD-CBD-CGD-O1D
29	b1	613	CLA	CAD-CBD-CGD-O1D
29	c1	501	CLA	CAD-CBD-CGD-O1D
29	c1	505	CLA	CAD-CBD-CGD-O1D
29	c1	506	CLA	CAD-CBD-CGD-O1D
29	g1	604	CLA	CAD-CBD-CGD-O1D
32	b	626	SQD	C5-C6-S-O7
32	b1	626	SQD	C5-C6-S-O7
32	m1	101	SQD	C5-C6-S-O7
32	m1	101	SQD	C5-C6-S-O9
41	C1	527	LMK	C29-C28-O8-C9
48	N	609	CHL	CAD-CBD-CGD-O1D
48	n	601	CHL	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
48	r	606	CHL	CAD-CBD-CGD-O1D
48	N1	601	CHL	CAD-CBD-CGD-O1D
48	R1	606	CHL	CAD-CBD-CGD-O1D
48	n1	601	CHL	CAD-CBD-CGD-O1D
48	r1	606	CHL	CAD-CBD-CGD-O1D
51	s	623	NEX	C7-C8-C9-C10
51	R1	622	NEX	C7-C8-C9-C10
51	s1	623	NEX	C7-C8-C9-C10
55	Y	626	PTY	C2-C3-O11-P1
55	y	626	PTY	C2-C3-O11-P1
55	y1	626	PTY	C2-C3-O11-P1
33	B1	622	LMG	C10-C11-C12-C13
41	C	527	LMK	C28-C29-C30-C31
33	h1	102	LMG	O7-C10-C11-C12
29	B	606	CLA	C8-C10-C11-C12
29	G1	611	CLA	C13-C15-C16-C17
38	B1	624	3PH	C3B-C3C-C3D-C3E
40	L	101	LHG	C19-C20-C21-C22
33	H1	102	LMG	C4-C5-C6-O5
29	B	602	CLA	O1A-CGA-O2A-C1
29	s1	611	CLA	O1A-CGA-O2A-C1
37	C1	520	DGD	C4B-C5B-C6B-C7B
37	c1	519	DGD	C7A-C8A-C9A-CAA
29	C	505	CLA	C5-C6-C7-C8
29	S	603	CLA	C8-C10-C11-C12
37	C1	518	DGD	C9B-CAB-CBB-CCB
40	G	624	LHG	C24-C25-C26-C27
32	c1	526	SQD	C7-C8-C9-C10
33	C1	523	LMG	C10-C11-C12-C13
37	C1	518	DGD	C6B-C7B-C8B-C9B
29	s1	611	CLA	CBA-CGA-O2A-C1
47	K1	101	4RF	C15-C16-O18-C19
29	C1	508	CLA	O1A-CGA-O2A-C1
33	B	622	LMG	C15-C16-C17-C18
33	b1	622	LMG	C13-C14-C15-C16
39	b1	625	DGA	CDA-CEA-CFA-CGA
48	N	606	CHL	C16-C17-C18-C19
48	N1	605	CHL	C4-C3-C5-C6
29	B	602	CLA	C12-C13-C15-C16
29	B	606	CLA	C12-C13-C15-C16
29	B	608	CLA	C11-C12-C13-C15
29	B	608	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	B	614	CLA	C11-C10-C8-C7
29	C	501	CLA	C11-C12-C13-C15
29	C	511	CLA	C12-C13-C15-C16
29	G	610	CLA	C6-C7-C8-C10
29	Y	603	CLA	C11-C12-C13-C15
29	Y	610	CLA	C12-C13-C15-C16
29	b	605	CLA	C12-C13-C15-C16
29	c	501	CLA	C12-C13-C15-C16
29	c	504	CLA	C6-C7-C8-C10
29	c	504	CLA	C12-C13-C15-C16
29	c	507	CLA	C12-C13-C15-C16
29	n	603	CLA	C12-C13-C15-C16
29	s	609	CLA	C6-C7-C8-C10
29	s	610	CLA	C11-C10-C8-C7
29	s	610	CLA	C11-C12-C13-C15
29	y	613	CLA	C11-C10-C8-C7
29	B1	602	CLA	C6-C7-C8-C10
29	B1	605	CLA	C12-C13-C15-C16
29	B1	606	CLA	C11-C10-C8-C7
29	B1	608	CLA	C12-C13-C15-C16
29	B1	610	CLA	C12-C13-C15-C16
29	B1	617	CLA	C11-C12-C13-C15
29	C1	505	CLA	C6-C7-C8-C10
29	N1	603	CLA	C12-C13-C15-C16
29	N1	604	CLA	C11-C12-C13-C15
29	G1	602	CLA	C12-C13-C15-C16
29	G1	610	CLA	C11-C12-C13-C15
29	G1	611	CLA	C11-C12-C13-C15
29	S1	603	CLA	C11-C12-C13-C15
29	S1	611	CLA	C11-C10-C8-C7
29	Y1	602	CLA	C12-C13-C15-C16
29	Y1	603	CLA	C12-C13-C15-C16
29	a1	406	CLA	C11-C12-C13-C15
29	b1	608	CLA	C11-C10-C8-C7
29	b1	616	CLA	C11-C12-C13-C15
29	c1	501	CLA	C11-C12-C13-C15
29	c1	501	CLA	C12-C13-C15-C16
29	c1	503	CLA	C12-C13-C15-C16
29	c1	504	CLA	C12-C13-C15-C16
29	c1	509	CLA	C6-C7-C8-C10
29	c1	509	CLA	C11-C10-C8-C7
29	c1	512	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
29	d1	403	CLA	C11-C10-C8-C7
29	d1	403	CLA	C11-C12-C13-C15
29	n1	602	CLA	C11-C12-C13-C15
29	g1	603	CLA	C12-C13-C15-C16
29	y1	610	CLA	C12-C13-C15-C16
30	A	409	PHO	C6-C7-C8-C10
30	a1	409	PHO	C6-C7-C8-C10
38	B	624	3PH	O11-C1-C2-O21
38	s1	626	3PH	O11-C1-C2-O21
40	d	410	LHG	O6-C4-C5-O7
40	d1	410	LHG	O6-C4-C5-O7
48	N	605	CHL	C11-C12-C13-C15
48	Y	607	CHL	C11-C10-C8-C7
48	n	607	CHL	C11-C12-C13-C15
48	g	601	CHL	C6-C7-C8-C10
48	g	607	CHL	C11-C10-C8-C7
48	g	609	CHL	C11-C12-C13-C15
48	y	601	CHL	C3A-C2A-CAA-CBA
48	y	606	CHL	C11-C12-C13-C15
48	y	607	CHL	C12-C13-C15-C16
48	N1	609	CHL	C12-C13-C15-C16
48	G1	607	CHL	C6-C7-C8-C10
48	Y1	607	CHL	C11-C10-C8-C7
48	n1	601	CHL	C11-C12-C13-C15
48	g1	609	CHL	C12-C13-C15-C16
48	y1	609	CHL	C11-C12-C13-C15
49	R	620	LUT	C25-C26-C27-C28
49	S	620	LUT	C25-C26-C27-C28
49	Y	620	LUT	C25-C26-C27-C28
49	y	620	LUT	C25-C26-C27-C28
49	R1	620	LUT	C25-C26-C27-C28
49	g1	620	LUT	C25-C26-C27-C28
49	r1	620	LUT	C25-C26-C27-C28
49	s1	621	LUT	C25-C26-C27-C28
49	y1	620	LUT	C25-C26-C27-C28
55	y	626	PTY	O14-C5-C6-O7
55	y	627	PTY	O14-C5-C6-O7
55	Y1	626	PTY	O14-C5-C6-O7
55	y1	626	PTY	O14-C5-C6-O7
38	B1	624	3PH	C28-C29-C2A-C2B
29	B	613	CLA	C3-C5-C6-C7
29	b	615	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
36	b	620	C7Z	C13-C14-C15-C35
32	b1	621	SQD	O47-C7-C8-C9
33	C1	521	LMG	O7-C10-C11-C12
32	c	526	SQD	C18-C19-C20-C21
37	c1	520	DGD	CAB-CBB-CCB-CDB
29	G	613	CLA	C13-C15-C16-C17
40	S	624	LHG	C23-C24-C25-C26
40	D	410	LHG	C8-C7-O7-C5
40	d1	410	LHG	O2-C2-C3-O3
32	B	621	SQD	C26-C27-C28-C29
38	s1	626	3PH	C35-C36-C37-C38
39	j	101	DGA	CB4-CB5-CB6-CB7
39	J1	101	DGA	CA2-CA3-CA4-CA5
29	N1	602	CLA	C8-C10-C11-C12
29	A	405	CLA	C2A-CAA-CBA-CGA
29	B	610	CLA	C2A-CAA-CBA-CGA
29	n	602	CLA	C2A-CAA-CBA-CGA
29	r	610	CLA	C2A-CAA-CBA-CGA
48	G	607	CHL	C2A-CAA-CBA-CGA
34	A	414	SPH	C11-C12-C13-C14
38	T1	101	3PH	C2F-C2G-C2H-C2I
40	D	409	LHG	C32-C33-C34-C35
40	g1	624	LHG	C16-C17-C18-C19
29	Y	614	CLA	C3-C5-C6-C7
29	A1	405	CLA	CAA-CBA-CGA-O2A
48	g	606	CHL	CAA-CBA-CGA-O2A
29	R1	608	CLA	C8-C10-C11-C12
32	C1	526	SQD	O6-C44-C45-C46
33	B	622	LMG	O1-C7-C8-C9
33	H	102	LMG	C7-C8-C9-O8
33	h1	102	LMG	C40-C41-C42-C43
33	w1	201	LMG	C7-C8-C9-O8
34	a1	414	SPH	C1-C2-C3-C4
37	c1	519	DGD	O1G-C1G-C2G-C3G
40	D	409	LHG	C34-C35-C36-C37
40	d	410	LHG	C11-C10-C9-C8
40	d1	408	LHG	C34-C35-C36-C37
32	A1	412	SQD	O6-C44-C45-O47
32	C1	526	SQD	O6-C44-C45-O47
33	B	622	LMG	O7-C8-C9-O8
33	H	102	LMG	O7-C8-C9-O8
33	b	622	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
33	b1	622	LMG	O7-C8-C9-O8
33	c1	523	LMG	O7-C8-C9-O8
37	c1	520	DGD	O1G-C1G-C2G-O2G
38	t1	101	3PH	O21-C2-C3-O31
39	C1	524	DGA	OG1-CG1-CG2-OG2
39	b1	625	DGA	OG1-CG1-CG2-OG2
40	s1	624	LHG	O7-C5-C6-O8
41	C1	527	LMK	O1-C7-C8-O7
47	k	101	4RF	O21-C20-C39-O40
55	y	626	PTY	O4-C1-C6-O7
55	y	627	PTY	O4-C1-C6-O7
32	A	412	SQD	C28-C29-C30-C31
32	m1	101	SQD	C11-C12-C13-C14
33	C1	521	LMG	C29-C30-C31-C32
33	A	413	LMG	C29-C30-C31-C32
40	y1	624	LHG	C26-C27-C28-C29
40	N1	624	LHG	C12-C13-C14-C15
33	w1	201	LMG	C8-C7-O1-C1
37	C	519	DGD	C5D-C6D-O5D-C1E
37	c	519	DGD	C2G-C3G-O3G-C1D
37	C1	519	DGD	C5D-C6D-O5D-C1E
37	c1	519	DGD	C5D-C6D-O5D-C1E
29	s1	617	CLA	CAA-CBA-CGA-O2A
29	C	507	CLA	C16-C17-C18-C20
29	b	603	CLA	C16-C17-C18-C20
29	c1	505	CLA	C16-C17-C18-C19
29	G	602	CLA	C5-C6-C7-C8
29	b	614	CLA	C15-C16-C17-C18
29	c	512	CLA	C5-C6-C7-C8
47	i	101	4RF	C53-C54-C55-C56
38	T	101	3PH	C2-C1-O11-P
40	c	525	LHG	C2-C3-O3-P
29	B1	617	CLA	C15-C16-C17-C18
29	G1	613	CLA	C4-C3-C5-C6
29	s1	611	CLA	C4-C3-C5-C6
48	n1	605	CHL	C4-C3-C5-C6
39	j	101	DGA	CA2-CA1-OG1-CG1
40	g1	624	LHG	C24-C23-O8-C6
37	C	520	DGD	C4A-C5A-C6A-C7A
37	C	520	DGD	C5A-C6A-C7A-C8A
40	L1	101	LHG	C26-C27-C28-C29
29	Y	614	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
48	Y1	607	CHL	C2-C3-C5-C6
40	L	101	LHG	C35-C36-C37-C38
47	i	101	4RF	C03-C04-C05-C06
29	c	505	CLA	C13-C15-C16-C17
29	B1	605	CLA	C10-C11-C12-C13
29	C	502	CLA	C6-C7-C8-C9
29	C	502	CLA	C14-C13-C15-C16
29	C	504	CLA	C11-C10-C8-C9
29	C	509	CLA	C11-C10-C8-C9
29	D	402	CLA	C11-C10-C8-C9
29	G	603	CLA	C14-C13-C15-C16
29	b	602	CLA	C11-C10-C8-C9
29	b	607	CLA	C11-C12-C13-C14
29	b	609	CLA	C11-C10-C8-C9
29	b	612	CLA	C14-C13-C15-C16
29	b	613	CLA	C11-C10-C8-C9
29	b	616	CLA	C11-C12-C13-C14
29	b	617	CLA	C6-C7-C8-C9
29	c	511	CLA	C11-C12-C13-C14
29	c	513	CLA	C14-C13-C15-C16
29	n	613	CLA	C11-C10-C8-C9
29	r	609	CLA	C11-C10-C8-C9
29	r	612	CLA	C6-C7-C8-C9
29	s	610	CLA	C11-C10-C8-C9
29	y	613	CLA	C14-C13-C15-C16
29	A1	406	CLA	C14-C13-C15-C16
29	B1	603	CLA	C11-C10-C8-C9
29	B1	609	CLA	C11-C10-C8-C9
29	B1	611	CLA	C11-C12-C13-C14
29	B1	616	CLA	C11-C12-C13-C14
29	C1	502	CLA	C11-C12-C13-C14
29	C1	511	CLA	C6-C7-C8-C9
29	D1	403	CLA	C11-C10-C8-C9
29	N1	602	CLA	C14-C13-C15-C16
29	N1	610	CLA	C14-C13-C15-C16
29	G1	602	CLA	C14-C13-C15-C16
29	G1	610	CLA	C6-C7-C8-C9
29	S1	610	CLA	C11-C12-C13-C14
29	a1	405	CLA	C11-C10-C8-C9
29	b1	603	CLA	C6-C7-C8-C9
29	b1	603	CLA	C11-C10-C8-C9
29	b1	613	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
29	n1	610	CLA	C14-C13-C15-C16
48	G	607	CHL	C6-C7-C8-C9
48	G	609	CHL	C11-C12-C13-C14
48	G	609	CHL	C14-C13-C15-C16
48	Y	609	CHL	C11-C10-C8-C9
48	Y	609	CHL	C14-C13-C15-C16
48	n	606	CHL	C11-C12-C13-C14
48	y	607	CHL	C11-C10-C8-C9
48	N1	606	CHL	C11-C12-C13-C14
48	Y1	601	CHL	C6-C7-C8-C9
48	n1	601	CHL	C14-C13-C15-C16
48	n1	605	CHL	C14-C13-C15-C16
48	n1	606	CHL	C14-C13-C15-C16
48	g1	601	CHL	C6-C7-C8-C9
48	y1	606	CHL	C11-C10-C8-C9
47	K1	101	4RF	O17-C16-O18-C19
39	C	524	DGA	CAB-CBB-CCB-CDB
39	c	524	DGA	CEA-CFA-CGA-CHA
29	B1	606	CLA	C3-C5-C6-C7
29	c1	501	CLA	C3-C5-C6-C7
30	a1	408	PHO	C3-C5-C6-C7
32	a1	412	SQD	O5-C1-O6-C44
33	d	411	LMG	O6-C1-O1-C7
32	b1	621	SQD	C23-C24-C25-C26
29	s1	614	CLA	C2A-CAA-CBA-CGA
46	I1	101	GOL	O2-C2-C3-O3
47	i	101	4RF	C25-C26-C27-C28
49	r	620	LUT	C33-C34-C35-C15
51	R1	622	NEX	C13-C14-C15-C35
32	B	626	SQD	C32-C33-C34-C35
34	a	414	SPH	C6-C7-C8-C9
40	n	624	LHG	C33-C34-C35-C36
49	N1	620	LUT	C31-C32-C33-C40
40	Y	624	LHG	C32-C33-C34-C35
39	B	625	DGA	CA1-CA2-CA3-CA4
29	s1	609	CLA	C11-C12-C13-C14
39	b	625	DGA	CA2-CA3-CA4-CA5
40	N1	624	LHG	C30-C31-C32-C33
31	c1	514	BCR	C17-C18-C19-C20
29	n1	613	CLA	C8-C10-C11-C12
32	B	626	SQD	C15-C16-C17-C18
38	B	624	3PH	C3A-C3B-C3C-C3D

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Mol	Chain	Res	Type	Atoms
39	B	625	DGA	CBA-CCA-CDA-CEA
40	D	409	LHG	C33-C34-C35-C36
40	S1	624	LHG	C24-C25-C26-C27
55	y	626	PTY	C40-C41-C42-C43
39	j1	101	DGA	OA1-CA1-OG1-CG1
29	C1	505	CLA	C10-C11-C12-C13
51	y	623	NEX	C39-C29-C30-C31
34	A	414	SPH	C11-C10-C9-C8
47	K1	101	4RF	C35-C36-C37-C38
29	B	616	CLA	C4-C3-C5-C6
29	C	506	CLA	C4-C3-C5-C6
48	n	605	CHL	C4-C3-C5-C6
40	N	624	LHG	C16-C17-C18-C19
40	S	624	LHG	C31-C32-C33-C34
40	d1	408	LHG	C32-C33-C34-C35
29	y	611	CLA	C2-C3-C5-C6
29	g1	603	CLA	C5-C6-C7-C8
47	k	101	4RF	C13-C14-C15-C16
29	G	611	CLA	C16-C17-C18-C19
29	R1	602	CLA	C11-C12-C13-C15
33	c	523	LMG	C30-C31-C32-C33
33	A1	413	LMG	C16-C17-C18-C19
40	l	101	LHG	C17-C18-C19-C20
41	C1	527	LMK	C31-C32-C33-C34
40	d	410	LHG	C29-C30-C31-C32
29	c1	506	CLA	C8-C10-C11-C12
29	N	611	CLA	C1-C2-C3-C4
29	G	604	CLA	C1-C2-C3-C4
29	G	614	CLA	C1-C2-C3-C4
29	n	611	CLA	C1-C2-C3-C4
29	g	604	CLA	C1-C2-C3-C4
29	g	614	CLA	C1-C2-C3-C4
29	N1	611	CLA	C1-C2-C3-C4
29	G1	604	CLA	C1-C2-C3-C4
29	G1	614	CLA	C1-C2-C3-C4
29	n1	611	CLA	C1-C2-C3-C4
29	g1	604	CLA	C1-C2-C3-C4
29	g1	614	CLA	C1-C2-C3-C4
34	A1	414	SPH	C2-C3-C4-C5
48	N	608	CHL	C1-C2-C3-C4
48	G	606	CHL	C1-C2-C3-C4
48	R	607	CHL	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
48	n	608	CHL	C1-C2-C3-C4
48	g	606	CHL	C1-C2-C3-C4
48	r	607	CHL	C1-C2-C3-C4
48	N1	608	CHL	C1-C2-C3-C4
48	G1	606	CHL	C1-C2-C3-C4
48	R1	607	CHL	C1-C2-C3-C4
48	n1	608	CHL	C1-C2-C3-C4
48	g1	606	CHL	C1-C2-C3-C4
48	r1	607	CHL	C1-C2-C3-C4
34	y1	625	SPH	C14-C15-C16-C17
39	c	524	DGA	CB4-CB5-CB6-CB7
39	b1	625	DGA	CFB-CGB-CHB-CIB
29	D	402	CLA	CAA-CBA-CGA-O2A
33	h	102	LMG	C15-C16-C17-C18
29	C	505	CLA	C15-C16-C17-C18
29	B1	607	CLA	C15-C16-C17-C18
32	B	621	SQD	C46-C45-O47-C7
32	M	101	SQD	C46-C45-O47-C7
32	m	101	SQD	C46-C45-O47-C7
32	b1	621	SQD	C46-C45-O47-C7
32	m1	101	SQD	C46-C45-O47-C7
33	b	622	LMG	C9-C8-O7-C10
33	C1	523	LMG	C7-C8-O7-C10
39	B1	625	DGA	CG1-CG2-OG2-CB1
40	L	101	LHG	C6-C5-O7-C7
55	y	626	PTY	O14-C5-C6-C1
29	B	615	CLA	C2A-CAA-CBA-CGA
29	s	611	CLA	C2A-CAA-CBA-CGA
29	B1	607	CLA	C2A-CAA-CBA-CGA
29	G1	610	CLA	C2A-CAA-CBA-CGA
29	c1	510	CLA	C2A-CAA-CBA-CGA
48	N1	607	CHL	C2A-CAA-CBA-CGA
48	n1	608	CHL	C2A-CAA-CBA-CGA
32	c1	526	SQD	C16-C17-C18-C19
41	C	527	LMK	C13-C14-C15-C27
40	D	410	LHG	O9-C7-O7-C5
39	j1	101	DGA	CA2-CA1-OG1-CG1
29	a	405	CLA	C10-C11-C12-C13
29	B	610	CLA	C2-C1-O2A-CGA
29	C	513	CLA	C2-C1-O2A-CGA
29	N	602	CLA	C2-C1-O2A-CGA
29	N	604	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
29	S	611	CLA	C2-C1-O2A-CGA
29	y	602	CLA	C2-C1-O2A-CGA
29	N1	614	CLA	C2-C1-O2A-CGA
29	S1	617	CLA	C2-C1-O2A-CGA
29	r1	603	CLA	C2-C1-O2A-CGA
30	a	409	PHO	C2-C1-O2A-CGA
48	N	609	CHL	C2-C1-O2A-CGA
48	Y	601	CHL	C2-C1-O2A-CGA
48	y	601	CHL	C2-C1-O2A-CGA
48	Y1	609	CHL	C2-C1-O2A-CGA
48	n1	608	CHL	C2-C1-O2A-CGA
38	b1	624	3PH	C35-C36-C37-C38
40	d1	410	LHG	C31-C32-C33-C34
29	g	613	CLA	C16-C17-C18-C19
40	S1	624	LHG	C7-C8-C9-C10
32	C1	526	SQD	C34-C35-C36-C37
38	t	101	3PH	C35-C36-C37-C38
40	C	525	LHG	C12-C13-C14-C15
32	M	101	SQD	O47-C7-C8-C9
48	G	607	CHL	CAA-CBA-CGA-O2A
29	b1	614	CLA	C5-C6-C7-C8
29	A	406	CLA	C3-C5-C6-C7
32	b	626	SQD	C16-C17-C18-C19
40	S	624	LHG	C14-C15-C16-C17
29	B	610	CLA	C5-C6-C7-C8
41	C	527	LMK	C30-C31-C32-C33
31	B	619	BCR	C19-C20-C21-C22
53	R	626	ERG	C22-C23-C24-C28
29	n1	613	CLA	O1A-CGA-O2A-C1
39	j	101	DGA	OA1-CA1-OG1-CG1
32	b1	621	SQD	C14-C15-C16-C17
34	y	625	SPH	C10-C11-C12-C13
48	g1	601	CHL	C16-C17-C18-C19
40	s1	624	LHG	C23-C24-C25-C26
48	g1	606	CHL	O2A-C1-C2-C3
29	B	605	CLA	C4-C3-C5-C6
29	C1	506	CLA	C4-C3-C5-C6
29	c1	513	CLA	C4-C3-C5-C6
29	n1	610	CLA	C4-C3-C5-C6
38	t	101	3PH	C23-C24-C25-C26
39	C1	524	DGA	CB9-CAB-CBB-CCB
31	C	514	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
31	C	517	BCR	C1-C6-C7-C8
31	b	619	BCR	C23-C24-C25-C30
31	B1	618	BCR	C1-C6-C7-C8
31	C1	514	BCR	C23-C24-C25-C30
31	b1	618	BCR	C1-C6-C7-C8
49	N	621	LUT	C1-C6-C7-C8
49	N	621	LUT	C5-C6-C7-C8
49	S	621	LUT	C5-C6-C7-C8
49	g	621	LUT	C5-C6-C7-C8
49	N1	620	LUT	C5-C6-C7-C8
49	G1	621	LUT	C5-C6-C7-C8
49	n1	620	LUT	C1-C6-C7-C8
49	n1	620	LUT	C5-C6-C7-C8
29	s	602	CLA	C2-C3-C5-C6
29	B1	615	CLA	C2-C3-C5-C6
29	C1	505	CLA	C2-C3-C5-C6
29	y1	603	CLA	C2-C3-C5-C6
48	N	606	CHL	C2-C3-C5-C6
48	n1	609	CHL	C2-C3-C5-C6
40	g	624	LHG	C35-C36-C37-C38
40	N1	624	LHG	C33-C34-C35-C36
40	g1	624	LHG	O10-C23-O8-C6
55	Y	626	PTY	C35-C36-C37-C38
29	b1	615	CLA	CBA-CGA-O2A-C1
40	N	624	LHG	O8-C23-C24-C25
39	C	524	DGA	CEA-CFA-CGA-CHA
39	B1	625	DGA	CFB-CGB-CHB-CIB
29	B	613	CLA	C16-C17-C18-C20
29	g	610	CLA	C16-C17-C18-C19
29	a1	405	CLA	C16-C17-C18-C19
29	n1	604	CLA	C16-C17-C18-C20
29	C1	513	CLA	C3-C5-C6-C7
33	d1	411	LMG	C11-C10-O7-C8
47	I1	102	4RF	C46-C47-C48-C49
29	B	606	CLA	C2A-CAA-CBA-CGA
29	B	613	CLA	C2A-CAA-CBA-CGA
29	B1	613	CLA	C2A-CAA-CBA-CGA
29	R1	608	CLA	C2A-CAA-CBA-CGA
30	a1	408	PHO	C2A-CAA-CBA-CGA
48	G1	601	CHL	C2A-CAA-CBA-CGA
51	y	623	NEX	C28-C29-C30-C31
51	G1	623	NEX	C11-C10-C9-C8

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Mol	Chain	Res	Type	Atoms
51	s1	623	NEX	C28-C29-C30-C31
33	a	413	LMG	C31-C32-C33-C34
55	y	626	PTY	C13-C14-C15-C16
32	A	412	SQD	O47-C45-C46-O48
33	B	622	LMG	O1-C7-C8-O7
33	a	413	LMG	O7-C8-C9-O8
33	a1	413	LMG	O7-C8-C9-O8
37	c	519	DGD	O1G-C1G-C2G-O2G
39	j1	101	DGA	OG1-CG1-CG2-OG2
40	C	525	LHG	O7-C5-C6-O8
40	c	525	LHG	O7-C5-C6-O8
29	n1	604	CLA	C8-C10-C11-C12
33	B	622	LMG	C14-C15-C16-C17
33	C	521	LMG	C31-C32-C33-C34
39	J1	101	DGA	CA5-CA6-CA7-CA8
40	D1	409	LHG	C31-C32-C33-C34
40	G	624	LHG	C3-O3-P-O6
40	Y	624	LHG	C3-O3-P-O6
40	c	525	LHG	C3-O3-P-O6
40	l	101	LHG	C4-O6-P-O3
40	g	624	LHG	C3-O3-P-O6
40	G1	624	LHG	C3-O3-P-O6
40	c1	525	LHG	C3-O3-P-O6
40	n1	624	LHG	C3-O3-P-O6
40	g1	624	LHG	C3-O3-P-O6
40	y1	624	LHG	C3-O3-P-O6
54	S	625	LPX	C1-O2-P1-O1
55	Y	626	PTY	C5-O14-P1-O11
55	Y	627	PTY	C3-O11-P1-O14
55	Y1	626	PTY	C5-O14-P1-O11
55	Y1	627	PTY	C3-O11-P1-O14
32	C1	526	SQD	C30-C31-C32-C33
38	T	101	3PH	C3F-C3G-C3H-C3I
40	C	525	LHG	C17-C18-C19-C20
37	C	520	DGD	O6D-C5D-C6D-O5D
33	A	413	LMG	C34-C35-C36-C37
55	Y	626	PTY	C23-C24-C25-C26
37	C1	520	DGD	C1A-C2A-C3A-C4A
47	I	102	4RF	C22-C24-C25-C26
53	R1	626	ERG	C23-C24-C25-C26
40	Y	624	LHG	C19-C20-C21-C22
40	c	525	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
54	S1	625	LPX	C7-C6-O6-C5
32	A	412	SQD	O6-C44-C45-C46
33	b	622	LMG	O1-C7-C8-C9
29	Y	603	CLA	C4-C3-C5-C6
29	Y1	603	CLA	C4-C3-C5-C6
34	A1	414	SPH	C7-C8-C9-C10
47	I	102	4RF	C29-C30-C31-C32
47	k	101	4RF	C34-C35-C36-C37
29	A	405	CLA	C12-C13-C15-C16
29	A	406	CLA	C11-C10-C8-C7
29	B	615	CLA	C2-C3-C5-C6
29	D	402	CLA	C6-C7-C8-C10
29	b	612	CLA	C12-C13-C15-C16
29	n	610	CLA	C12-C13-C15-C16
29	s	611	CLA	C11-C12-C13-C15
29	B1	602	CLA	C11-C12-C13-C15
29	B1	616	CLA	C11-C10-C8-C7
29	B1	616	CLA	C12-C13-C15-C16
29	Y1	610	CLA	C11-C12-C13-C15
29	Y1	611	CLA	C11-C10-C8-C7
29	b1	614	CLA	C11-C10-C8-C7
29	g1	603	CLA	C6-C7-C8-C10
29	g1	610	CLA	C12-C13-C15-C16
30	a	408	PHO	C11-C12-C13-C15
43	D	405	PL9	C13-C14-C16-C17
43	D	405	PL9	C18-C19-C21-C22
48	Y	601	CHL	C6-C7-C8-C10
48	g	607	CHL	C12-C13-C15-C16
40	g1	624	LHG	C33-C34-C35-C36
47	I1	102	4RF	C53-C54-C55-C56
29	B	605	CLA	C14-C13-C15-C16
29	B	613	CLA	C11-C10-C8-C9
29	C	501	CLA	C11-C10-C8-C9
29	C	512	CLA	C11-C10-C8-C9
29	G	610	CLA	C6-C7-C8-C9
29	R	610	CLA	C11-C10-C8-C9
29	S	602	CLA	C6-C7-C8-C9
29	Y	603	CLA	C11-C12-C13-C14
29	a	410	CLA	C6-C7-C8-C9
29	c	502	CLA	C6-C7-C8-C9
29	c	507	CLA	C14-C13-C15-C16
29	g	613	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	B1	602	CLA	C6-C7-C8-C9
29	C1	506	CLA	C11-C10-C8-C9
29	G1	611	CLA	C11-C10-C8-C9
29	S1	610	CLA	C11-C10-C8-C9
29	Y1	602	CLA	C6-C7-C8-C9
29	Y1	602	CLA	C14-C13-C15-C16
29	a1	410	CLA	C6-C7-C8-C9
29	b1	602	CLA	C14-C13-C15-C16
29	b1	616	CLA	C11-C12-C13-C14
29	c1	503	CLA	C14-C13-C15-C16
29	n1	602	CLA	C11-C12-C13-C14
29	r1	609	CLA	C6-C7-C8-C9
29	s1	603	CLA	C11-C10-C8-C9
29	y1	610	CLA	C14-C13-C15-C16
29	y1	611	CLA	C11-C12-C13-C14
29	y1	614	CLA	C11-C10-C8-C9
48	N	601	CHL	C14-C13-C15-C16
48	G	601	CHL	C6-C7-C8-C9
48	y	609	CHL	C14-C13-C15-C16
48	G1	607	CHL	C6-C7-C8-C9
48	G1	609	CHL	C11-C12-C13-C14
48	Y1	606	CHL	C6-C7-C8-C9
48	y1	606	CHL	C14-C13-C15-C16
29	b1	603	CLA	C13-C15-C16-C17
31	c	514	BCR	C15-C16-C17-C18
31	C1	517	BCR	C9-C10-C11-C12
49	S	621	LUT	C29-C30-C31-C32
49	r	620	LUT	C9-C10-C11-C12
49	y1	621	LUT	C33-C34-C35-C15
50	Y1	622	XAT	C13-C14-C15-C35
51	S	623	NEX	C33-C34-C35-C15
29	B1	613	CLA	C16-C17-C18-C19
29	y1	613	CLA	C16-C17-C18-C20
32	B	626	SQD	C27-C28-C29-C30
32	b1	621	SQD	C10-C11-C12-C13
54	S	625	LPX	C10-C11-C12-C13
32	C	526	SQD	C28-C29-C30-C31
40	y	624	LHG	C24-C25-C26-C27
40	y1	624	LHG	C11-C12-C13-C14
32	C	526	SQD	C24-C23-O48-C46
32	m	101	SQD	O49-C7-C8-C9
33	a	413	LMG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
38	B1	624	3PH	C36-C37-C38-C39
55	Y1	626	PTY	C24-C25-C26-C27
33	D	411	LMG	C33-C34-C35-C36
33	w	201	LMG	C33-C34-C35-C36
34	A	414	SPH	C15-C16-C17-C18
37	c	518	DGD	CCB-CDB-CEB-CFB
40	D	410	LHG	C10-C11-C12-C13
40	l	101	LHG	C11-C12-C13-C14
40	D1	409	LHG	C14-C15-C16-C17
40	n1	624	LHG	C17-C18-C19-C20
29	n	602	CLA	C8-C10-C11-C12
29	c	505	CLA	C16-C17-C18-C19
29	y	613	CLA	C16-C17-C18-C20
29	b1	609	CLA	C16-C17-C18-C19
29	s1	614	CLA	C6-C7-C8-C10
32	C1	526	SQD	C35-C36-C37-C38
40	d	409	LHG	C30-C31-C32-C33
47	k1	101	4RF	C43-C41-O40-C39
40	d	409	LHG	C2-C3-O3-P
40	D1	408	LHG	C5-C4-O6-P
40	G1	624	LHG	C2-C3-O3-P
47	k1	101	4RF	C45-C46-C47-C48
29	Y1	610	CLA	C10-C11-C12-C13
29	c1	504	CLA	C13-C15-C16-C17
49	G	620	LUT	C27-C28-C29-C30
50	g	622	XAT	C11-C12-C13-C14
50	g1	622	XAT	C27-C28-C29-C30
32	B1	621	SQD	C26-C27-C28-C29
33	b1	622	LMG	C33-C34-C35-C36
37	c1	518	DGD	CAB-CBB-CCB-CDB
38	S1	626	3PH	C3C-C3D-C3E-C3F
38	s1	626	3PH	C2C-C2D-C2E-C2F
40	d1	410	LHG	C1-C2-C3-O3
33	H1	102	LMG	C15-C16-C17-C18
29	n	603	CLA	C4-C3-C5-C6
29	y	612	CLA	C4-C3-C5-C6
38	B1	624	3PH	C21-C22-C23-C24
29	n	604	CLA	C2-C3-C5-C6
29	n	613	CLA	C2-C3-C5-C6
48	n	605	CHL	C2-C3-C5-C6
38	T	101	3PH	C25-C26-C27-C28
29	s1	609	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
29	c	508	CLA	CBA-CGA-O2A-C1
30	a	408	PHO	C10-C11-C12-C13
29	b1	615	CLA	O1A-CGA-O2A-C1
47	k1	101	4RF	O42-C41-O40-C39
52	r	625	LMT	C4'-C5'-C6'-O6'
33	h	102	LMG	C11-C12-C13-C14
33	b1	622	LMG	C19-C20-C21-C22
41	C1	527	LMK	C2-C1-O1-C7
33	D1	411	LMG	C16-C17-C18-C19
38	s	626	3PH	C28-C29-C2A-C2B
39	C1	524	DGA	CBB-CCB-CDB-CEB
29	s	610	CLA	CBD-CGD-O2D-CED
33	h1	102	LMG	C29-C28-O8-C9
55	Y	626	PTY	C30-C31-C32-C33
32	b1	621	SQD	C27-C28-C29-C30
40	D	408	LHG	C11-C10-C9-C8
29	r	608	CLA	C2A-CAA-CBA-CGA
29	s	605	CLA	C2A-CAA-CBA-CGA
48	n	607	CHL	C2A-CAA-CBA-CGA
48	N1	605	CHL	CAA-CBA-CGA-O1A
32	m1	101	SQD	O5-C1-O6-C44
37	C1	519	DGD	O6D-C1D-O3G-C3G
31	D	404	BCR	C19-C20-C21-C22
31	d	404	BCR	C9-C10-C11-C12
31	C1	515	BCR	C19-C20-C21-C22
31	C1	516	BCR	C19-C20-C21-C22
31	b1	618	BCR	C19-C20-C21-C22
36	b	620	C7Z	C9-C10-C11-C12
49	R1	620	LUT	C29-C30-C31-C32
49	Y1	621	LUT	C13-C14-C15-C35
49	y1	621	LUT	C29-C30-C31-C32
50	Y	622	XAT	C13-C14-C15-C35
51	r	622	NEX	C33-C34-C35-C15
51	N1	623	NEX	C13-C14-C15-C35
51	R1	622	NEX	C9-C10-C11-C12
51	R1	622	NEX	C29-C30-C31-C32
51	n1	623	NEX	C9-C10-C11-C12
32	C	526	SQD	O10-C23-O48-C46
29	C	509	CLA	C5-C6-C7-C8
29	G	602	CLA	C10-C11-C12-C13
29	b	615	CLA	C15-C16-C17-C18
47	i1	101	4RF	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
38	S1	626	3PH	C3D-C3E-C3F-C3G
40	D	410	LHG	C26-C27-C28-C29
40	L	101	LHG	C12-C13-C14-C15
31	C1	514	BCR	C18-C19-C20-C21
50	y1	622	XAT	C10-C11-C12-C13
51	G	623	NEX	C10-C11-C12-C13
51	r	622	NEX	C30-C31-C32-C33
51	y1	623	NEX	C30-C31-C32-C33
54	S1	625	LPX	O7-C6-O6-C5
29	c1	505	CLA	C15-C16-C17-C18
53	R	626	ERG	C13-C17-C20-C22
29	C	508	CLA	C16-C17-C18-C20
32	B1	621	SQD	O47-C7-C8-C9
38	S1	626	3PH	O31-C31-C32-C33
29	B1	602	CLA	C3-C5-C6-C7
32	B	626	SQD	C31-C32-C33-C34
40	D1	409	LHG	C29-C30-C31-C32
29	R	608	CLA	C4-C3-C5-C6
29	n	613	CLA	C4-C3-C5-C6
29	B1	610	CLA	C4-C3-C5-C6
29	g1	613	CLA	C4-C3-C5-C6
48	y1	601	CHL	C4-C3-C5-C6
48	G	601	CHL	C5-C6-C7-C8
32	m1	101	SQD	C9-C10-C11-C12
33	C1	523	LMG	C36-C37-C38-C39
40	D	409	LHG	C24-C25-C26-C27
47	k	101	4RF	C53-C54-C55-C56
33	h1	102	LMG	O10-C28-O8-C9
33	d	411	LMG	C11-C12-C13-C14
29	B	617	CLA	C13-C15-C16-C17
29	S	614	CLA	C5-C6-C7-C8
40	D1	408	LHG	O9-C7-O7-C5
33	c	521	LMG	C36-C37-C38-C39
39	c1	524	DGA	CA6-CA7-CA8-CA9
40	S1	624	LHG	C35-C36-C37-C38
47	k1	101	4RF	C46-C47-C48-C49
55	Y1	626	PTY	C37-C38-C39-C40
29	b	610	CLA	C2-C1-O2A-CGA
29	y	610	CLA	C2-C1-O2A-CGA
29	G1	610	CLA	C2-C1-O2A-CGA
29	c1	513	CLA	C2-C1-O2A-CGA
29	y1	610	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
48	n	608	CHL	C2-C1-O2A-CGA
48	g	606	CHL	C2-C1-O2A-CGA
48	y	606	CHL	C2-C1-O2A-CGA
48	Y1	606	CHL	C2-C1-O2A-CGA
48	n1	607	CHL	C2-C1-O2A-CGA
38	S	626	3PH	C26-C27-C28-C29
39	b	625	DGA	CFB-CGB-CHB-CIB
29	B1	612	CLA	C16-C17-C18-C20
33	D	411	LMG	C12-C13-C14-C15
33	d1	411	LMG	C11-C12-C13-C14
43	D1	405	PL9	C22-C23-C24-C25
53	R1	626	ERG	C22-C23-C24-C28
32	M	101	SQD	C2-C1-O6-C44
29	c	505	CLA	C2A-CAA-CBA-CGA
29	s	604	CLA	C2A-CAA-CBA-CGA
29	G1	602	CLA	C2A-CAA-CBA-CGA
29	S1	611	CLA	C2A-CAA-CBA-CGA
29	c1	506	CLA	C2A-CAA-CBA-CGA
38	b	624	3PH	O21-C2-C3-O31
40	D1	410	LHG	O7-C5-C6-O8
48	Y	606	CHL	C2A-CAA-CBA-CGA
48	G1	607	CHL	C2A-CAA-CBA-CGA
48	R1	607	CHL	C2A-CAA-CBA-CGA
48	n1	607	CHL	C2A-CAA-CBA-CGA
32	c	526	SQD	C30-C31-C32-C33
38	S1	626	3PH	C39-C3A-C3B-C3C
29	n1	613	CLA	CBA-CGA-O2A-C1
55	Y1	626	PTY	C30-C31-C32-C33
32	C	526	SQD	C18-C19-C20-C21
33	B	622	LMG	C33-C34-C35-C36
38	S1	626	3PH	C3E-C3F-C3G-C3H
39	c	524	DGA	CA8-CA9-CAA-CBA
40	s1	624	LHG	C25-C26-C27-C28
40	n1	624	LHG	O10-C23-C24-C25
29	g	612	CLA	C3A-C2A-CAA-CBA
29	b1	607	CLA	C3A-C2A-CAA-CBA
29	c1	511	CLA	C3A-C2A-CAA-CBA
29	s1	609	CLA	C3A-C2A-CAA-CBA
48	g	601	CHL	C3A-C2A-CAA-CBA
48	n1	609	CHL	C3A-C2A-CAA-CBA
29	b1	616	CLA	C16-C17-C18-C20
29	r1	610	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
29	s1	611	CLA	C16-C17-C18-C19
37	c	519	DGD	C3A-C4A-C5A-C6A
48	n	608	CHL	O2A-C1-C2-C3
29	R1	609	CLA	CAA-CBA-CGA-O2A
39	c1	524	DGA	CEB-CFB-CGB-CHB
40	s	624	LHG	C32-C33-C34-C35
40	C1	525	LHG	C25-C26-C27-C28
29	d	402	CLA	CBA-CGA-O2A-C1
29	c	503	CLA	C8-C10-C11-C12
32	B	626	SQD	C18-C19-C20-C21
40	y	624	LHG	C19-C20-C21-C22
41	c	527	LMK	C32-C33-C34-C16
47	k	101	4RF	C51-C52-C53-C54
48	y	605	CHL	CAA-CBA-CGA-O1A
40	D1	408	LHG	C26-C27-C28-C29
40	g1	624	LHG	C29-C30-C31-C32
41	C1	527	LMK	C28-C29-C30-C31
29	B	610	CLA	C14-C13-C15-C16
29	B	616	CLA	C6-C7-C8-C9
29	G	602	CLA	C11-C12-C13-C14
29	a	406	CLA	C14-C13-C15-C16
29	b	604	CLA	C11-C10-C8-C9
29	b	614	CLA	C11-C12-C13-C14
29	r	603	CLA	C6-C7-C8-C9
29	A1	406	CLA	C6-C7-C8-C9
29	B1	603	CLA	C11-C12-C13-C14
29	B1	603	CLA	C14-C13-C15-C16
29	B1	614	CLA	C11-C12-C13-C14
29	D1	402	CLA	C6-C7-C8-C9
29	G1	611	CLA	C14-C13-C15-C16
29	S1	603	CLA	C11-C12-C13-C14
29	S1	611	CLA	C11-C10-C8-C9
29	S1	611	CLA	C14-C13-C15-C16
29	Y1	613	CLA	C6-C7-C8-C9
29	b1	604	CLA	C14-C13-C15-C16
29	b1	615	CLA	C11-C10-C8-C9
29	n1	613	CLA	C14-C13-C15-C16
29	g1	603	CLA	C11-C10-C8-C9
29	r1	603	CLA	C6-C7-C8-C9
29	y1	603	CLA	C6-C7-C8-C9
29	y1	611	CLA	C6-C7-C8-C9
30	A	409	PHO	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
30	a	409	PHO	C6-C7-C8-C9
48	N	607	CHL	C14-C13-C15-C16
48	Y	601	CHL	C6-C7-C8-C9
48	Y	606	CHL	C11-C12-C13-C14
48	g	601	CHL	C6-C7-C8-C9
48	g	601	CHL	C11-C10-C8-C9
48	g	609	CHL	C6-C7-C8-C9
48	n1	601	CHL	C11-C10-C8-C9
32	B1	626	SQD	C9-C10-C11-C12
33	c1	523	LMG	C16-C17-C18-C19
39	C	524	DGA	CB6-CB7-CB8-CB9
48	y	605	CHL	CAA-CBA-CGA-O2A
33	B1	622	LMG	C14-C15-C16-C17
40	N	624	LHG	C31-C32-C33-C34
47	I	102	4RF	C32-C33-C34-C35
29	S	613	CLA	C2C-C3C-CAC-CBC
37	B1	623	DGD	C2A-C3A-C4A-C5A
39	c1	524	DGA	CDB-CEB-CFB-CGB
40	n	624	LHG	C30-C31-C32-C33
48	y1	609	CHL	C2C-C3C-CAC-CBC
29	c	506	CLA	C8-C10-C11-C12
29	c	509	CLA	C13-C15-C16-C17
33	w1	201	LMG	O1-C7-C8-C9
49	n	621	LUT	C21-C26-C27-C28
49	g	621	LUT	C21-C26-C27-C28
49	s1	620	LUT	C21-C26-C27-C28
50	y1	622	XAT	C40-C33-C34-C35
51	N	623	NEX	C39-C29-C30-C31
51	G	623	NEX	C39-C29-C30-C31
51	R	622	NEX	C40-C33-C34-C35
51	S	623	NEX	C39-C29-C30-C31
51	Y	623	NEX	C20-C13-C14-C15
51	n	623	NEX	C39-C29-C30-C31
51	r	622	NEX	C39-C29-C30-C31
51	r	622	NEX	C40-C33-C34-C35
51	g1	623	NEX	C39-C29-C30-C31
51	s1	623	NEX	C39-C29-C30-C31
29	N	613	CLA	C3-C5-C6-C7
29	G	613	CLA	C3-C5-C6-C7
32	c1	526	SQD	O49-C7-O47-C45
33	W1	201	LMG	C32-C33-C34-C35
40	S	624	LHG	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
32	M1	101	SQD	O47-C7-C8-C9
29	n	612	CLA	CAA-CBA-CGA-O1A
29	y1	604	CLA	C2A-CAA-CBA-CGA
29	g1	613	CLA	C5-C6-C7-C8
40	g1	624	LHG	O10-C23-C24-C25
33	B	622	LMG	C29-C30-C31-C32
47	K	101	4RF	C04-C05-C06-C07
29	C1	503	CLA	C16-C17-C18-C19
29	R1	612	CLA	C11-C12-C13-C14
29	b1	605	CLA	C16-C17-C18-C19
29	n1	604	CLA	C16-C17-C18-C19
53	r	626	ERG	C22-C23-C24-C25
40	S1	624	LHG	C24-C23-O8-C6
33	c	523	LMG	O6-C1-O1-C7
33	C1	523	LMG	O6-C1-O1-C7
32	A	412	SQD	C33-C34-C35-C36
33	C1	523	LMG	C18-C19-C20-C21
33	a1	413	LMG	C13-C14-C15-C16
38	t1	101	3PH	C28-C29-C2A-C2B
40	d	410	LHG	C26-C27-C28-C29
55	Y	626	PTY	C25-C26-C27-C28
29	C	509	CLA	C13-C15-C16-C17
40	D	410	LHG	C30-C31-C32-C33
49	N1	620	LUT	C31-C32-C33-C34
32	a	412	SQD	C29-C30-C31-C32
32	B1	626	SQD	C11-C12-C13-C14
33	a	413	LMG	C30-C31-C32-C33
33	c1	521	LMG	C34-C35-C36-C37
55	Y1	626	PTY	C38-C39-C40-C41
29	n	612	CLA	CAA-CBA-CGA-O2A
37	b	623	DGD	C1G-C2G-O2G-C1B
37	b1	623	DGD	C1G-C2G-O2G-C1B
40	l	101	LHG	C6-C5-O7-C7
29	N1	603	CLA	C4-C3-C5-C6
29	B	612	CLA	C1A-C2A-CAA-CBA
29	N	613	CLA	C1A-C2A-CAA-CBA
29	a	410	CLA	C1A-C2A-CAA-CBA
29	b	609	CLA	C1A-C2A-CAA-CBA
29	c	506	CLA	C1A-C2A-CAA-CBA
29	d	402	CLA	C1A-C2A-CAA-CBA
29	g	612	CLA	C1A-C2A-CAA-CBA
29	r	602	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
29	s	602	CLA	C1A-C2A-CAA-CBA
29	C1	504	CLA	C1A-C2A-CAA-CBA
29	G1	611	CLA	C1A-C2A-CAA-CBA
29	a1	410	CLA	C1A-C2A-CAA-CBA
29	b1	612	CLA	C1A-C2A-CAA-CBA
29	c1	506	CLA	C1A-C2A-CAA-CBA
48	N	606	CHL	C1A-C2A-CAA-CBA
48	N	607	CHL	C1A-C2A-CAA-CBA
48	Y	601	CHL	C1A-C2A-CAA-CBA
48	g	608	CHL	C1A-C2A-CAA-CBA
48	r	607	CHL	C1A-C2A-CAA-CBA
48	y	601	CHL	C1A-C2A-CAA-CBA
48	n1	601	CHL	C1A-C2A-CAA-CBA
48	n1	609	CHL	C1A-C2A-CAA-CBA
40	n	624	LHG	C29-C30-C31-C32
55	Y	626	PTY	C15-C16-C17-C18
48	Y1	606	CHL	C16-C17-C18-C20
29	B	602	CLA	C11-C10-C8-C7
29	B	613	CLA	C6-C7-C8-C10
29	B	617	CLA	C12-C13-C15-C16
29	C	506	CLA	C2-C3-C5-C6
29	N	603	CLA	C11-C12-C13-C15
29	N	604	CLA	C6-C7-C8-C10
29	G	603	CLA	C11-C10-C8-C7
29	R	602	CLA	C11-C10-C8-C7
29	Y	602	CLA	C12-C13-C15-C16
29	a	405	CLA	C11-C10-C8-C7
29	b	606	CLA	C11-C10-C8-C7
29	c	502	CLA	C11-C10-C8-C7
29	c	507	CLA	C11-C12-C13-C15
29	c	508	CLA	C11-C10-C8-C7
29	y	613	CLA	C6-C7-C8-C10
29	C1	513	CLA	C12-C13-C15-C16
29	S1	610	CLA	C6-C7-C8-C10
29	b1	604	CLA	C11-C10-C8-C7
29	b1	605	CLA	C11-C10-C8-C7
29	b1	617	CLA	C6-C7-C8-C10
29	c1	513	CLA	C11-C12-C13-C15
29	s1	611	CLA	C6-C7-C8-C10
29	y1	611	CLA	C11-C10-C8-C7
43	d1	405	PL9	C12-C11-C9-C8
48	N	607	CHL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
48	G	601	CHL	C11-C12-C13-C15
48	y	601	CHL	C12-C13-C15-C16
48	N1	605	CHL	C11-C12-C13-C15
48	N1	606	CHL	C12-C13-C15-C16
48	S1	608	CHL	C11-C10-C8-C7
29	C1	510	CLA	C3-C5-C6-C7
33	C	523	LMG	C30-C31-C32-C33
55	Y1	626	PTY	C33-C34-C35-C36
31	c	517	BCR	C9-C10-C11-C12
51	Y	623	NEX	C9-C10-C11-C12
51	Y1	623	NEX	C9-C10-C11-C12
41	c1	527	LMK	C9-C8-O7-C10
47	K1	101	4RF	C34-C35-C36-C37
47	i1	101	4RF	C24-C25-C26-C27
29	N	613	CLA	CAA-CBA-CGA-O2A
48	S	601	CHL	CAA-CBA-CGA-O2A
40	D	409	LHG	C15-C16-C17-C18
40	G	624	LHG	C10-C11-C12-C13
29	B	607	CLA	C16-C17-C18-C19
29	b	608	CLA	C16-C17-C18-C20
29	s1	603	CLA	C16-C17-C18-C20
33	b	622	LMG	C31-C32-C33-C34
33	h1	102	LMG	C33-C34-C35-C36
29	b1	615	CLA	C3-C5-C6-C7
40	d	408	LHG	C2-C3-O3-P
29	S	611	CLA	C2A-CAA-CBA-CGA
29	B1	606	CLA	C2A-CAA-CBA-CGA
48	g	607	CHL	C2A-CAA-CBA-CGA
37	C	519	DGD	O6D-C5D-C6D-O5D
41	c	527	LMK	O10-C28-C29-C30
29	R	612	CLA	C10-C11-C12-C13
29	C1	504	CLA	C5-C6-C7-C8
29	a1	410	CLA	C5-C6-C7-C8
32	B	626	SQD	C19-C20-C21-C22
40	n	624	LHG	C32-C33-C34-C35
47	K	101	4RF	C50-C51-C52-C53
53	R1	626	ERG	C28-C24-C25-C26
29	S	612	CLA	CAA-CBA-CGA-O1A
38	S1	626	3PH	C2A-C2B-C2C-C2D
55	Y	626	PTY	C12-C13-C14-C15
32	C	526	SQD	O49-C7-O47-C45
29	b	605	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
30	a	408	PHO	CBA-CGA-O2A-C1
40	D	410	LHG	C34-C35-C36-C37
55	Y	626	PTY	O14-C5-C6-C1
38	t	101	3PH	C29-C2A-C2B-C2C
40	D	408	LHG	C30-C31-C32-C33
47	k1	101	4RF	C27-C28-C29-C30
29	g	613	CLA	C16-C17-C18-C20
29	C1	510	CLA	C16-C17-C18-C20
29	c1	507	CLA	C8-C10-C11-C12
38	T1	101	3PH	C2E-C2F-C2G-C2H
29	B	612	CLA	C4-C3-C5-C6
29	S1	604	CLA	C4-C3-C5-C6
29	c1	506	CLA	C4-C3-C5-C6
29	y1	614	CLA	C4-C3-C5-C6
48	Y1	601	CHL	C4-C3-C5-C6
33	C	521	LMG	C37-C38-C39-C40
33	b1	622	LMG	C11-C12-C13-C14
39	C1	524	DGA	CFA-CGA-CHA-CIA
47	I1	102	4RF	C10-C11-C12-C13
55	Y1	626	PTY	C11-C12-C13-C14
29	C	502	CLA	C10-C11-C12-C13
29	B	616	CLA	C2-C3-C5-C6
29	Y	603	CLA	C2-C3-C5-C6
29	Y1	603	CLA	C2-C3-C5-C6
43	d	405	PL9	C28-C29-C31-C32
40	L1	101	LHG	C12-C13-C14-C15
40	Y1	624	LHG	C17-C18-C19-C20
29	R1	609	CLA	C5-C6-C7-C8
32	B1	626	SQD	C7-C8-C9-C10
40	Y	624	LHG	C7-C8-C9-C10
40	Y1	624	LHG	O9-C7-O7-C5
38	b	624	3PH	C2A-C2B-C2C-C2D
33	c1	521	LMG	O9-C10-C11-C12
33	B1	622	LMG	C2-C1-O1-C7
34	a1	414	SPH	N2-C2-C3-C4
51	N	623	NEX	C28-C29-C30-C31
51	G	623	NEX	C28-C29-C30-C31
51	S	623	NEX	C28-C29-C30-C31
51	n	623	NEX	C28-C29-C30-C31
51	r	622	NEX	C28-C29-C30-C31
51	Y1	623	NEX	C11-C10-C9-C8
51	g1	623	NEX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
29	y	602	CLA	C8-C10-C11-C12
30	a	409	PHO	C8-C10-C11-C12
48	S	601	CHL	CAA-CBA-CGA-O1A
48	s	601	CHL	CAA-CBA-CGA-O2A
32	M	101	SQD	O47-C45-C46-O48
32	m1	101	SQD	O47-C45-C46-O48
33	C1	521	LMG	O7-C8-C9-O8
33	d1	411	LMG	O7-C8-C9-O8
55	Y1	626	PTY	O4-C1-C6-O7
40	y1	624	LHG	C30-C31-C32-C33
47	k	101	4RF	C22-C24-C25-C26
31	c	516	BCR	C15-C16-C17-C18
49	N1	621	LUT	C33-C34-C35-C15
49	R1	620	LUT	C33-C34-C35-C15
49	Y1	621	LUT	C29-C30-C31-C32
49	n1	620	LUT	C29-C30-C31-C32
50	g	622	XAT	C9-C10-C11-C12
51	N	623	NEX	C29-C30-C31-C32
29	S	612	CLA	CAA-CBA-CGA-O2A
29	B1	604	CLA	C10-C11-C12-C13
29	c1	502	CLA	C13-C15-C16-C17
48	N1	601	CHL	C10-C11-C12-C13
39	J1	101	DGA	CA6-CA7-CA8-CA9
32	C	526	SQD	C31-C32-C33-C34
32	c1	526	SQD	C34-C35-C36-C37
34	a	414	SPH	C11-C10-C9-C8
39	c	524	DGA	CA3-CA4-CA5-CA6
40	g1	624	LHG	C34-C35-C36-C37
47	k1	101	4RF	C29-C30-C31-C32
33	w	201	LMG	O6-C1-O1-C7
29	B	605	CLA	C10-C11-C12-C13
37	c	519	DGD	C6A-C7A-C8A-C9A
39	c	524	DGA	CA5-CA6-CA7-CA8
40	D	408	LHG	C14-C15-C16-C17
40	C1	525	LHG	C17-C18-C19-C20
40	s1	624	LHG	C27-C28-C29-C30
30	a	408	PHO	O1A-CGA-O2A-C1
39	C1	524	DGA	CG1-CG2-CG3-OXT
39	c1	524	DGA	CG1-CG2-CG3-OXT
43	d1	405	PL9	C14-C16-C17-C18
33	c1	523	LMG	C30-C31-C32-C33
37	C	520	DGD	C4B-C5B-C6B-C7B

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Mol	Chain	Res	Type	Atoms
29	R1	609	CLA	C4-C3-C5-C6
29	b1	612	CLA	C4-C3-C5-C6
43	d1	405	PL9	C32-C33-C34-C35
48	N1	607	CHL	C4-C3-C5-C6
32	c	526	SQD	C27-C28-C29-C30
38	t1	101	3PH	C3F-C3G-C3H-C3I
29	A	410	CLA	C2-C1-O2A-CGA
29	B	605	CLA	C2-C1-O2A-CGA
29	a	410	CLA	C2-C1-O2A-CGA
29	b	606	CLA	C2-C1-O2A-CGA
29	c	513	CLA	C2-C1-O2A-CGA
29	b1	609	CLA	C2-C1-O2A-CGA
29	b1	610	CLA	C2-C1-O2A-CGA
48	n	601	CHL	C2-C1-O2A-CGA
48	g	601	CHL	C2-C1-O2A-CGA
48	g	609	CHL	C2-C1-O2A-CGA
29	G1	613	CLA	C2-C3-C5-C6
43	d1	405	PL9	C13-C14-C16-C17
48	N1	605	CHL	C2-C3-C5-C6
48	Y1	601	CHL	C2-C3-C5-C6
38	t1	101	3PH	C2E-C2F-C2G-C2H
29	d	402	CLA	O1A-CGA-O2A-C1
29	g1	611	CLA	C5-C6-C7-C8
41	c1	527	LMK	C14-C15-C27-C35
55	y1	626	PTY	C20-C21-C22-C23
29	S	614	CLA	CAA-CBA-CGA-O2A
40	g	624	LHG	O8-C23-C24-C25
29	A	405	CLA	C14-C13-C15-C16
29	C	512	CLA	C11-C12-C13-C14
29	b	608	CLA	C11-C12-C13-C14
29	b	611	CLA	C11-C12-C13-C14
29	d	403	CLA	C14-C13-C15-C16
29	n	604	CLA	C6-C7-C8-C9
29	y	602	CLA	C11-C12-C13-C14
29	B1	610	CLA	C11-C12-C13-C14
29	b1	611	CLA	C11-C12-C13-C14
29	s1	602	CLA	C11-C10-C8-C9
48	S1	608	CHL	C11-C10-C8-C9
48	y1	606	CHL	C11-C12-C13-C14
34	Y	625	SPH	C13-C14-C15-C16
34	a	414	SPH	C12-C13-C14-C15
37	C	519	DGD	C2B-C3B-C4B-C5B

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Mol	Chain	Res	Type	Atoms
37	c1	520	DGD	C4B-C5B-C6B-C7B
29	D	402	CLA	C3-C5-C6-C7
29	C	503	CLA	C5-C6-C7-C8
38	S	626	3PH	C22-C21-O21-C2
40	D1	408	LHG	C8-C7-O7-C5
29	N1	613	CLA	CAA-CBA-CGA-O2A
32	B	621	SQD	O47-C7-C8-C9
33	c	521	LMG	O7-C10-C11-C12
33	b	622	LMG	C22-C23-C24-C25
37	C	519	DGD	CCA-CDA-CEA-CFA
47	K	101	4RF	C33-C34-C35-C36
33	C	523	LMG	O6-C5-C6-O5
29	C1	510	CLA	C10-C11-C12-C13
29	R1	608	CLA	C10-C11-C12-C13
48	N1	609	CHL	C13-C15-C16-C17
29	C	502	CLA	C2A-CAA-CBA-CGA
29	y1	613	CLA	C2A-CAA-CBA-CGA
30	a	408	PHO	C2A-CAA-CBA-CGA
48	S	601	CHL	C2A-CAA-CBA-CGA
48	N1	605	CHL	C2A-CAA-CBA-CGA
48	s	601	CHL	CAA-CBA-CGA-O1A
40	Y	624	LHG	C34-C35-C36-C37
29	c	508	CLA	O1A-CGA-O2A-C1
31	A	411	BCR	C1-C6-C7-C8
31	A	411	BCR	C5-C6-C7-C8
31	B	619	BCR	C23-C24-C25-C30
31	c	517	BCR	C23-C24-C25-C30
31	A1	411	BCR	C23-C24-C25-C30
45	H	101	RRX	C23-C24-C25-C30
49	G	621	LUT	C1-C6-C7-C8
49	R	620	LUT	C1-C6-C7-C8
49	S	621	LUT	C1-C6-C7-C8
49	Y	621	LUT	C1-C6-C7-C8
49	s	620	LUT	C1-C6-C7-C8
49	y	620	LUT	C1-C6-C7-C8
49	N1	620	LUT	C1-C6-C7-C8
49	S1	620	LUT	C1-C6-C7-C8
49	Y1	620	LUT	C1-C6-C7-C8
29	y1	613	CLA	C13-C15-C16-C17
29	A1	410	CLA	C2C-C3C-CAC-CBC
47	I	102	4RF	C26-C27-C28-C29
49	y	620	LUT	C27-C28-C29-C39

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Mol	Chain	Res	Type	Atoms
29	A	406	CLA	C15-C16-C17-C18
40	N	624	LHG	O1-C1-C2-C3
33	b1	622	LMG	C14-C15-C16-C17
37	C	519	DGD	CCB-CDB-CEB-CFB
52	r	625	LMT	C7-C8-C9-C10
40	S1	624	LHG	O10-C23-O8-C6
31	B	618	BCR	C15-C16-C17-C18
31	B1	618	BCR	C13-C14-C15-C16
31	b1	619	BCR	C9-C10-C11-C12
49	N1	620	LUT	C33-C34-C35-C15
32	M	101	SQD	C10-C11-C12-C13
33	b1	622	LMG	C15-C16-C17-C18
29	r1	603	CLA	C4-C3-C5-C6
29	s1	613	CLA	C4-C3-C5-C6
43	d1	405	PL9	C12-C11-C9-C10
43	d1	405	PL9	C15-C14-C16-C17
48	n	609	CHL	C4-C3-C5-C6
48	g	607	CHL	C4-C3-C5-C6
48	N1	609	CHL	C4-C3-C5-C6
49	y	620	LUT	C27-C28-C29-C30
50	g1	622	XAT	C31-C32-C33-C34
29	C	508	CLA	C16-C17-C18-C19
29	B1	613	CLA	C16-C17-C18-C20
29	C	510	CLA	C5-C6-C7-C8
29	N1	613	CLA	C15-C16-C17-C18
29	c1	502	CLA	C2C-C3C-CAC-CBC
29	n	603	CLA	C2-C3-C5-C6
29	C1	506	CLA	C2-C3-C5-C6
29	s1	611	CLA	C2-C3-C5-C6
48	n1	605	CHL	C2-C3-C5-C6
29	D1	402	CLA	CAA-CBA-CGA-O2A
38	T	101	3PH	C23-C24-C25-C26
39	j1	101	DGA	CA7-CA8-CA9-CAA
33	a1	413	LMG	C8-C7-O1-C1
37	C	518	DGD	C5D-C6D-O5D-C1E
40	c	525	LHG	C8-C7-O7-C5
40	d	409	LHG	C8-C7-O7-C5
37	C1	520	DGD	C3A-C4A-C5A-C6A
33	d1	411	LMG	C4-C5-C6-O5
37	c1	519	DGD	C9A-CAA-CBA-CCA
33	d1	411	LMG	O10-C28-O8-C9
29	s1	602	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
33	a1	413	LMG	C14-C15-C16-C17
33	d1	411	LMG	C14-C15-C16-C17
29	A	410	CLA	C11-C12-C13-C14
29	B	602	CLA	C16-C17-C18-C20
29	B	603	CLA	C16-C17-C18-C19
29	y	612	CLA	C16-C17-C18-C19
29	r1	603	CLA	C11-C12-C13-C15
29	B	610	CLA	C3-C5-C6-C7
29	c	501	CLA	C3-C5-C6-C7
34	A1	414	SPH	C4-C5-C6-C7
29	B1	613	CLA	C8-C10-C11-C12
29	G1	602	CLA	C15-C16-C17-C18
38	T	101	3PH	O11-C1-C2-O21
40	D1	410	LHG	O6-C4-C5-O7
33	d	411	LMG	C10-C11-C12-C13
39	B	625	DGA	CDA-CEA-CFA-CGA
29	s	612	CLA	CAA-CBA-CGA-O2A
48	s1	601	CHL	CAA-CBA-CGA-O2A
29	N	603	CLA	C2A-CAA-CBA-CGA
29	N	604	CLA	C2A-CAA-CBA-CGA
29	B1	610	CLA	C2A-CAA-CBA-CGA
29	R1	603	CLA	C2A-CAA-CBA-CGA
37	C	518	DGD	C4A-C5A-C6A-C7A
40	c1	525	LHG	C17-C18-C19-C20
40	g1	624	LHG	C30-C31-C32-C33
29	s1	614	CLA	CAA-CBA-CGA-O2A
54	s	625	LPX	C6-C7-C8-C9
40	d	409	LHG	O9-C7-O7-C5
29	s	605	CLA	C4C-C3C-CAC-CBC
41	C1	527	LMK	O7-C10-C11-C12
29	C1	501	CLA	C3-C5-C6-C7
29	B	612	CLA	C16-C17-C18-C20
32	A	412	SQD	C32-C33-C34-C35
34	a1	414	SPH	C11-C10-C9-C8
40	s1	624	LHG	C35-C36-C37-C38
47	K	101	4RF	C54-C55-C56-C57
47	i	101	4RF	C26-C27-C28-C29
38	B	624	3PH	C2D-C2E-C2F-C2G
38	T	101	3PH	C3C-C3D-C3E-C3F
38	s	626	3PH	C31-C32-C33-C34
29	C	512	CLA	C4-C3-C5-C6
29	R	609	CLA	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	C1	510	CLA	C4-C3-C5-C6
48	y1	606	CHL	C4-C3-C5-C6
40	Y1	624	LHG	C8-C7-O7-C5
29	b1	602	CLA	CAA-CBA-CGA-O1A
29	g	613	CLA	C11-C12-C13-C15
29	y	602	CLA	C11-C12-C13-C15
29	y	614	CLA	C6-C7-C8-C10
29	N1	603	CLA	C2-C3-C5-C6
29	a1	410	CLA	C6-C7-C8-C10
29	b1	608	CLA	C11-C12-C13-C15
29	b1	612	CLA	C2-C3-C5-C6
29	n1	613	CLA	C12-C13-C15-C16
29	y1	614	CLA	C2-C3-C5-C6
48	n	609	CHL	C2-C3-C5-C6
48	G1	607	CHL	C11-C12-C13-C15
29	b1	613	CLA	C15-C16-C17-C18
40	l	101	LHG	C33-C34-C35-C36
39	B1	625	DGA	OG2-CG2-CG3-OXT
39	C1	524	DGA	OG2-CG2-CG3-OXT
39	b1	625	DGA	OG2-CG2-CG3-OXT
33	H	102	LMG	O9-C10-C11-C12
36	b	620	C7Z	C33-C34-C35-C15
50	y	622	XAT	C9-C10-C11-C12
38	B	624	3PH	O31-C31-C32-C33
48	n1	607	CHL	CAA-CBA-CGA-O2A
33	W	201	LMG	C2-C1-O1-C7
29	B	606	CLA	C16-C17-C18-C19
38	S1	626	3PH	C2-C1-O11-P
40	L1	101	LHG	C1-C2-C3-O3
32	a	412	SQD	C26-C27-C28-C29
33	H1	102	LMG	O7-C8-C9-O8
37	C1	519	DGD	O1G-C1G-C2G-O2G
29	Y	610	CLA	CBA-CGA-O2A-C1
39	c1	524	DGA	CCB-CDB-CEB-CFB
40	G	624	LHG	C35-C36-C37-C38
29	b	602	CLA	CAA-CBA-CGA-O1A
33	c	521	LMG	C33-C34-C35-C36
29	y	604	CLA	C13-C15-C16-C17
29	b1	602	CLA	C8-C10-C11-C12
48	s1	601	CHL	CAA-CBA-CGA-O1A
48	r	607	CHL	O2A-C1-C2-C3
48	n1	608	CHL	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
29	R	612	CLA	CAA-CBA-CGA-O2A
29	g	613	CLA	CAA-CBA-CGA-O2A
29	g	614	CLA	CAA-CBA-CGA-O2A
29	Y1	613	CLA	CAA-CBA-CGA-O2A
37	C1	518	DGD	O1G-C1A-C2A-C3A
38	s	626	3PH	O21-C21-C22-C23
39	c	524	DGA	OG2-CB1-CB2-CB3
40	D1	409	LHG	O7-C7-C8-C9
33	C1	521	LMG	C33-C34-C35-C36
29	B	607	CLA	O1A-CGA-O2A-C1
29	b1	609	CLA	C10-C11-C12-C13
48	n	607	CHL	C8-C10-C11-C12
29	b1	606	CLA	C16-C17-C18-C19
29	b1	609	CLA	C16-C17-C18-C20
29	c1	513	CLA	C16-C17-C18-C19
43	D1	405	PL9	C2-C3-C7-C8
33	C	523	LMG	C36-C37-C38-C39
29	N1	610	CLA	C8-C10-C11-C12
32	c1	526	SQD	C9-C10-C11-C12
38	T	101	3PH	C1-O11-P-O13
39	J1	101	DGA	CA7-CA8-CA9-CAA
47	i	101	4RF	C08-C09-C10-C11
50	y	622	XAT	C40-C33-C34-C35
50	y1	622	XAT	C20-C13-C14-C15
51	g	623	NEX	C20-C13-C14-C15
51	y1	623	NEX	C39-C29-C30-C31
29	b1	608	CLA	CAA-CBA-CGA-O2A
29	b1	615	CLA	CAA-CBA-CGA-O2A
29	c1	505	CLA	CAA-CBA-CGA-O2A
30	A	409	PHO	CAA-CBA-CGA-O2A
37	b	623	DGD	O1G-C1A-C2A-C3A
38	S1	626	3PH	O21-C21-C22-C23
38	t1	101	3PH	O31-C31-C32-C33
40	D	408	LHG	O7-C7-C8-C9
29	s	605	CLA	C2C-C3C-CAC-CBC
47	I1	102	4RF	C03-C04-C05-C06
29	c	506	CLA	C4-C3-C5-C6
29	c	513	CLA	C4-C3-C5-C6
30	A1	408	PHO	C4-C3-C5-C6
48	y	601	CHL	C4-C3-C5-C6
48	S1	608	CHL	C4-C3-C5-C6
48	g1	607	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
29	N	603	CLA	C10-C11-C12-C13
29	B	612	CLA	C2-C3-C5-C6
29	r	609	CLA	C2-C3-C5-C6
29	c1	506	CLA	C2-C3-C5-C6
29	n1	610	CLA	C2-C3-C5-C6
29	r1	603	CLA	C2-C3-C5-C6
43	d1	405	PL9	C28-C29-C31-C32
48	N1	607	CHL	C2-C3-C5-C6
33	h1	102	LMG	C34-C35-C36-C37
38	B1	624	3PH	C33-C34-C35-C36
29	B	615	CLA	C16-C17-C18-C20
29	Y1	610	CLA	C16-C17-C18-C19
30	a1	409	PHO	C16-C17-C18-C19
38	b1	624	3PH	O21-C21-C22-C23
29	S	613	CLA	C4C-C3C-CAC-CBC
29	A	406	CLA	C11-C10-C8-C9
29	B	602	CLA	C14-C13-C15-C16
29	B	606	CLA	C14-C13-C15-C16
29	B	608	CLA	C14-C13-C15-C16
29	B	610	CLA	C11-C12-C13-C14
29	N	604	CLA	C6-C7-C8-C9
29	G	611	CLA	C11-C10-C8-C9
29	Y	602	CLA	C14-C13-C15-C16
29	Y	604	CLA	C6-C7-C8-C9
29	Y	610	CLA	C14-C13-C15-C16
29	b	605	CLA	C14-C13-C15-C16
29	c	501	CLA	C14-C13-C15-C16
29	c	504	CLA	C14-C13-C15-C16
29	c	507	CLA	C11-C12-C13-C14
29	c	508	CLA	C11-C10-C8-C9
29	y	611	CLA	C11-C10-C8-C9
29	y	613	CLA	C6-C7-C8-C9
29	B1	605	CLA	C6-C7-C8-C9
29	B1	608	CLA	C14-C13-C15-C16
29	B1	617	CLA	C11-C12-C13-C14
29	C1	505	CLA	C6-C7-C8-C9
29	C1	506	CLA	C6-C7-C8-C9
29	N1	604	CLA	C6-C7-C8-C9
29	G1	611	CLA	C11-C12-C13-C14
29	R1	612	CLA	C6-C7-C8-C9
29	S1	610	CLA	C6-C7-C8-C9
29	Y1	603	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
29	a1	406	CLA	C14-C13-C15-C16
29	b1	617	CLA	C6-C7-C8-C9
29	b1	617	CLA	C11-C12-C13-C14
29	c1	501	CLA	C14-C13-C15-C16
29	c1	504	CLA	C14-C13-C15-C16
29	c1	509	CLA	C11-C10-C8-C9
29	c1	511	CLA	C6-C7-C8-C9
29	c1	513	CLA	C14-C13-C15-C16
29	d1	403	CLA	C11-C10-C8-C9
29	d1	403	CLA	C11-C12-C13-C14
29	s1	602	CLA	C6-C7-C8-C9
48	N	605	CHL	C11-C12-C13-C14
48	Y	606	CHL	C11-C10-C8-C9
48	Y	607	CHL	C11-C10-C8-C9
48	y	606	CHL	C11-C12-C13-C14
48	N1	601	CHL	C14-C13-C15-C16
29	b	613	CLA	C3-C5-C6-C7
40	g1	624	LHG	C18-C19-C20-C21
29	G	612	CLA	C3A-C2A-CAA-CBA
29	b	617	CLA	C3A-C2A-CAA-CBA
29	s	605	CLA	C3A-C2A-CAA-CBA
29	y	608	CLA	C3A-C2A-CAA-CBA
29	S1	605	CLA	C3A-C2A-CAA-CBA
29	b1	603	CLA	C3A-C2A-CAA-CBA
29	s1	617	CLA	C3A-C2A-CAA-CBA
29	y1	613	CLA	C3A-C2A-CAA-CBA
30	A	408	PHO	C3A-C2A-CAA-CBA
30	A1	409	PHO	C3A-C2A-CAA-CBA
48	N	607	CHL	C3A-C2A-CAA-CBA
48	g	608	CHL	C3A-C2A-CAA-CBA
48	G1	609	CHL	C3A-C2A-CAA-CBA
48	n1	608	CHL	C3A-C2A-CAA-CBA
48	g1	601	CHL	C3A-C2A-CAA-CBA
39	b	625	DGA	CBB-CAB-CB9-CB8
40	y1	624	LHG	C17-C18-C19-C20
48	g1	605	CHL	C2-C1-O2A-CGA
29	Y	613	CLA	CAA-CBA-CGA-O2A
29	B1	603	CLA	CAA-CBA-CGA-O2A
29	n1	604	CLA	CAA-CBA-CGA-O2A
33	C	523	LMG	O7-C10-C11-C12
33	d	411	LMG	O7-C10-C11-C12
48	y	606	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
32	a1	412	SQD	C32-C33-C34-C35
33	A1	413	LMG	C34-C35-C36-C37
40	y	624	LHG	C27-C28-C29-C30
40	s1	624	LHG	C11-C10-C9-C8
29	s	612	CLA	CAA-CBA-CGA-O1A
29	C	502	CLA	CAD-CBD-CGD-O2D
29	C	504	CLA	CAD-CBD-CGD-O2D
29	C	510	CLA	CAD-CBD-CGD-O2D
29	R	602	CLA	CAD-CBD-CGD-O2D
29	Y	603	CLA	CAD-CBD-CGD-O2D
29	Y	614	CLA	CAD-CBD-CGD-O2D
29	b	605	CLA	CAD-CBD-CGD-O2D
29	b	606	CLA	CAD-CBD-CGD-O2D
29	c	510	CLA	CAD-CBD-CGD-O2D
29	c	512	CLA	CAD-CBD-CGD-O2D
29	n	611	CLA	CAD-CBD-CGD-O2D
29	r	603	CLA	CAD-CBD-CGD-O2D
29	C1	506	CLA	CAD-CBD-CGD-O2D
29	N1	602	CLA	CAD-CBD-CGD-O2D
29	N1	604	CLA	CAD-CBD-CGD-O2D
29	G1	603	CLA	CAD-CBD-CGD-O2D
29	G1	614	CLA	CAD-CBD-CGD-O2D
29	n1	603	CLA	CAD-CBD-CGD-O2D
29	n1	612	CLA	CAD-CBD-CGD-O2D
29	g1	602	CLA	CAD-CBD-CGD-O2D
29	g1	614	CLA	CAD-CBD-CGD-O2D
29	y1	614	CLA	CAD-CBD-CGD-O2D
30	a	408	PHO	CAD-CBD-CGD-O2D
34	y1	625	SPH	O3-C3-C4-C5
37	b1	623	DGD	C3G-C2G-O2G-C1B
38	t1	101	3PH	C1-C2-O21-C21
38	t1	101	3PH	C3-C2-O21-C21
40	l	101	LHG	C4-C5-O7-C7
48	G	606	CHL	CAD-CBD-CGD-O2D
48	S	606	CHL	CAD-CBD-CGD-O2D
48	g	607	CHL	CAD-CBD-CGD-O2D
48	g	609	CHL	CAD-CBD-CGD-O2D
48	S1	606	CHL	CAD-CBD-CGD-O2D
29	B	602	CLA	C16-C17-C18-C19
29	r1	610	CLA	C11-C12-C13-C14
29	s1	603	CLA	C16-C17-C18-C19
47	k	101	4RF	C31-C32-C33-C34

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Mol	Chain	Res	Type	Atoms
49	S1	620	LUT	C9-C10-C11-C12
29	b	608	CLA	C2A-CAA-CBA-CGA
29	Y1	612	CLA	C3-C5-C6-C7
29	g1	613	CLA	C3-C5-C6-C7
32	A1	412	SQD	C33-C34-C35-C36
32	B1	626	SQD	C12-C13-C14-C15
29	c	505	CLA	C2-C1-O2A-CGA
29	C1	501	CLA	C2-C1-O2A-CGA
29	d1	403	CLA	C2-C1-O2A-CGA
29	n1	612	CLA	CAA-CBA-CGA-O2A
39	c	524	DGA	CB2-CB3-CB4-CB5
29	C	503	CLA	CAA-CBA-CGA-O2A
29	c	503	CLA	CAA-CBA-CGA-O2A
29	c1	512	CLA	CAA-CBA-CGA-O2A
33	c	523	LMG	O7-C10-C11-C12
33	W1	201	LMG	O7-C10-C11-C12
39	b1	625	DGA	OG1-CA1-CA2-CA3
48	n1	605	CHL	CAA-CBA-CGA-O2A
29	b1	614	CLA	O1D-CGD-O2D-CED
29	c	511	CLA	C4-C3-C5-C6
43	d1	405	PL9	C35-C34-C36-C37
30	a1	408	PHO	C16-C17-C18-C19
29	c1	502	CLA	C4C-C3C-CAC-CBC
40	s	624	LHG	C9-C10-C11-C12
29	c	508	CLA	C8-C10-C11-C12
29	S1	604	CLA	C2-C3-C5-C6
43	D1	405	PL9	C33-C34-C36-C37
48	g	607	CHL	C2-C3-C5-C6
48	N1	609	CHL	C2-C3-C5-C6
29	y	613	CLA	CAA-CBA-CGA-O2A
29	B1	609	CLA	CAA-CBA-CGA-O2A
29	B1	615	CLA	CAA-CBA-CGA-O2A
30	A1	409	PHO	CAA-CBA-CGA-O2A
32	b	621	SQD	O47-C7-C8-C9
39	b1	625	DGA	OG2-CB1-CB2-CB3
40	N	624	LHG	O7-C7-C8-C9
40	c	525	LHG	O7-C7-C8-C9
33	C	523	LMG	C13-C14-C15-C16
33	c	523	LMG	C31-C32-C33-C34
38	t1	101	3PH	C33-C34-C35-C36
40	Y	624	LHG	C10-C11-C12-C13
31	C	514	BCR	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
31	b	618	BCR	C17-C18-C19-C20
31	b	618	BCR	C21-C22-C23-C24
31	C1	516	BCR	C17-C18-C19-C20
31	D1	404	BCR	C7-C8-C9-C10
45	H	101	RRX	C17-C18-C19-C20
45	h1	101	RRX	C21-C22-C23-C24
49	R1	620	LUT	C27-C28-C29-C30
50	Y	622	XAT	C31-C32-C33-C34
34	a1	414	SPH	C4-C5-C6-C7
34	A1	414	SPH	C5-C6-C7-C8
38	b	624	3PH	C3D-C3E-C3F-C3G
30	a	408	PHO	C2C-C3C-CAC-CBC
37	B	623	DGD	O1G-C1G-C2G-C3G
37	C1	520	DGD	C1G-C2G-C3G-O3G
38	t1	101	3PH	C1-C2-C3-O31
41	C	527	LMK	C4-C3-N4-C5
41	C	527	LMK	C4-C3-N4-C6
41	c	527	LMK	C11-C10-O7-C8
41	c1	527	LMK	O1-C7-C8-C9
41	c1	527	LMK	C11-C10-O7-C8
50	Y	622	XAT	O24-C26-C27-C28
50	G1	622	XAT	O24-C26-C27-C28
51	S	623	NEX	O24-C26-C27-C28
51	g1	623	NEX	O24-C26-C27-C28
51	y1	623	NEX	O24-C26-C27-C28
48	Y1	605	CHL	CAA-CBA-CGA-O1A
47	i	101	4RF	C48-C49-C50-C51
29	B	607	CLA	CBA-CGA-O2A-C1
52	r1	625	LMT	C4'-C5'-C6'-O6'
29	a	410	CLA	C10-C11-C12-C13
29	G	611	CLA	C3-C5-C6-C7
29	b	610	CLA	C3-C5-C6-C7
29	B	608	CLA	CAA-CBA-CGA-O2A
29	G	613	CLA	CAA-CBA-CGA-O2A
29	G	614	CLA	CAA-CBA-CGA-O2A
29	c	505	CLA	CAA-CBA-CGA-O2A
29	C1	502	CLA	CAA-CBA-CGA-O2A
29	R1	604	CLA	CAA-CBA-CGA-O2A
29	b1	603	CLA	CAA-CBA-CGA-O2A
29	r1	604	CLA	CAA-CBA-CGA-O2A
29	y1	613	CLA	CAA-CBA-CGA-O2A
32	A	412	SQD	O47-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
37	C	518	DGD	O2G-C1B-C2B-C3B
40	S	624	LHG	O8-C23-C24-C25
40	y	624	LHG	O8-C23-C24-C25
48	g1	605	CHL	CAA-CBA-CGA-O2A
38	T1	101	3PH	C3C-C3D-C3E-C3F
40	d	408	LHG	C11-C10-C9-C8
40	L1	101	LHG	C14-C15-C16-C17
38	s	626	3PH	C21-C22-C23-C24
48	R	607	CHL	O2A-C1-C2-C3
40	G	624	LHG	O10-C23-C24-C25
33	b1	622	LMG	C16-C17-C18-C19
29	b	616	CLA	C13-C15-C16-C17
30	A	408	PHO	O2A-C1-C2-C3
48	y	607	CHL	O2A-C1-C2-C3
48	G1	609	CHL	O2A-C1-C2-C3
48	Y1	607	CHL	O2A-C1-C2-C3
32	A	412	SQD	C15-C16-C17-C18
32	B1	626	SQD	C31-C32-C33-C34
38	T1	101	3PH	C2A-C2B-C2C-C2D
33	d1	411	LMG	C29-C28-O8-C9
29	Y	610	CLA	C2A-CAA-CBA-CGA
29	r	612	CLA	C2A-CAA-CBA-CGA
29	S	610	CLA	C8-C10-C11-C12
29	c	507	CLA	C15-C16-C17-C18
29	d	403	CLA	C13-C15-C16-C17
48	G	607	CHL	C5-C6-C7-C8
32	a1	412	SQD	C9-C10-C11-C12
37	C	519	DGD	C5A-C6A-C7A-C8A
29	N	604	CLA	CAA-CBA-CGA-O2A
29	b	607	CLA	O1A-CGA-O2A-C1
29	n1	612	CLA	CAA-CBA-CGA-O1A
32	c	526	SQD	C35-C36-C37-C38
39	B	625	DGA	CDB-CEB-CFB-CGB
40	Y	624	LHG	C15-C16-C17-C18
34	Y	625	SPH	C4-C5-C6-C7
29	b	612	CLA	C16-C17-C18-C19
29	r1	603	CLA	C11-C12-C13-C14
29	A	405	CLA	CHA-CBD-CGD-O2D
29	B	609	CLA	CHA-CBD-CGD-O1D
29	B	609	CLA	CHA-CBD-CGD-O2D
29	B	614	CLA	CHA-CBD-CGD-O1D
29	B	614	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
29	B	617	CLA	CHA-CBD-CGD-O1D
29	D	402	CLA	CHA-CBD-CGD-O1D
29	D	402	CLA	CHA-CBD-CGD-O2D
29	N	610	CLA	CHA-CBD-CGD-O1D
29	N	610	CLA	CHA-CBD-CGD-O2D
29	G	604	CLA	CHA-CBD-CGD-O1D
29	G	610	CLA	CHA-CBD-CGD-O1D
29	G	610	CLA	CHA-CBD-CGD-O2D
29	R	604	CLA	CHA-CBD-CGD-O1D
29	R	604	CLA	CHA-CBD-CGD-O2D
29	R	612	CLA	CHA-CBD-CGD-O1D
29	S	604	CLA	CHA-CBD-CGD-O2D
29	S	613	CLA	CHA-CBD-CGD-O1D
29	S	613	CLA	CHA-CBD-CGD-O2D
29	b	604	CLA	CHA-CBD-CGD-O1D
29	b	604	CLA	CHA-CBD-CGD-O2D
29	b	611	CLA	CHA-CBD-CGD-O1D
29	b	611	CLA	CHA-CBD-CGD-O2D
29	c	503	CLA	CHA-CBD-CGD-O2D
29	d	402	CLA	CHA-CBD-CGD-O1D
29	d	402	CLA	CHA-CBD-CGD-O2D
29	n	610	CLA	CHA-CBD-CGD-O1D
29	n	610	CLA	CHA-CBD-CGD-O2D
29	g	612	CLA	CHA-CBD-CGD-O1D
29	g	612	CLA	CHA-CBD-CGD-O2D
29	r	603	CLA	CHA-CBD-CGD-O2D
29	s	603	CLA	CHA-CBD-CGD-O1D
29	y	604	CLA	CHA-CBD-CGD-O1D
29	y	611	CLA	CHA-CBD-CGD-O1D
29	y	611	CLA	CHA-CBD-CGD-O2D
29	A1	406	CLA	CHA-CBD-CGD-O1D
29	A1	406	CLA	CHA-CBD-CGD-O2D
29	B1	610	CLA	CHA-CBD-CGD-O1D
29	B1	610	CLA	CHA-CBD-CGD-O2D
29	B1	611	CLA	CHA-CBD-CGD-O1D
29	C1	503	CLA	CHA-CBD-CGD-O1D
29	C1	505	CLA	CHA-CBD-CGD-O2D
29	N1	610	CLA	CHA-CBD-CGD-O1D
29	N1	610	CLA	CHA-CBD-CGD-O2D
29	N1	611	CLA	CHA-CBD-CGD-O1D
29	N1	611	CLA	CHA-CBD-CGD-O2D
29	N1	612	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
29	G1	602	CLA	CHA-CBD-CGD-O1D
29	G1	611	CLA	CHA-CBD-CGD-O1D
29	G1	611	CLA	CHA-CBD-CGD-O2D
29	R1	602	CLA	CHA-CBD-CGD-O1D
29	R1	609	CLA	CHA-CBD-CGD-O1D
29	R1	609	CLA	CHA-CBD-CGD-O2D
29	S1	604	CLA	CHA-CBD-CGD-O2D
29	S1	612	CLA	CHA-CBD-CGD-O1D
29	S1	612	CLA	CHA-CBD-CGD-O2D
29	Y1	602	CLA	CHA-CBD-CGD-O1D
29	Y1	602	CLA	CHA-CBD-CGD-O2D
29	a1	407	CLA	CHA-CBD-CGD-O1D
29	a1	407	CLA	CHA-CBD-CGD-O2D
29	b1	605	CLA	CHA-CBD-CGD-O2D
29	b1	606	CLA	CHA-CBD-CGD-O2D
29	b1	617	CLA	CHA-CBD-CGD-O1D
29	b1	617	CLA	CHA-CBD-CGD-O2D
29	c1	502	CLA	CHA-CBD-CGD-O1D
29	c1	502	CLA	CHA-CBD-CGD-O2D
29	c1	506	CLA	CHA-CBD-CGD-O1D
29	c1	507	CLA	CHA-CBD-CGD-O1D
29	c1	508	CLA	CHA-CBD-CGD-O1D
29	c1	508	CLA	CHA-CBD-CGD-O2D
29	n1	604	CLA	CHA-CBD-CGD-O1D
29	n1	610	CLA	CHA-CBD-CGD-O1D
29	n1	610	CLA	CHA-CBD-CGD-O2D
29	n1	614	CLA	CHA-CBD-CGD-O1D
29	n1	614	CLA	CHA-CBD-CGD-O2D
29	g1	604	CLA	CHA-CBD-CGD-O1D
29	g1	604	CLA	CHA-CBD-CGD-O2D
29	g1	613	CLA	CHA-CBD-CGD-O2D
29	r1	609	CLA	CHA-CBD-CGD-O2D
29	s1	603	CLA	CHA-CBD-CGD-O1D
29	s1	609	CLA	CHA-CBD-CGD-O1D
29	s1	609	CLA	CHA-CBD-CGD-O2D
29	s1	612	CLA	CHA-CBD-CGD-O2D
29	s1	613	CLA	CHA-CBD-CGD-O1D
29	s1	613	CLA	CHA-CBD-CGD-O2D
29	y1	602	CLA	CHA-CBD-CGD-O1D
29	y1	602	CLA	CHA-CBD-CGD-O2D
29	y1	610	CLA	CHA-CBD-CGD-O1D
29	y1	610	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
29	y1	613	CLA	CHA-CBD-CGD-O1D
29	y1	613	CLA	CHA-CBD-CGD-O2D
31	C	516	BCR	C13-C14-C15-C16
31	c1	517	BCR	C9-C10-C11-C12
41	C	527	LMK	C2-C3-C4-O3
41	C1	527	LMK	C2-C3-C4-O3
48	y	601	CHL	CHA-CBD-CGD-O1D
48	y	601	CHL	CHA-CBD-CGD-O2D
48	N1	601	CHL	CHA-CBD-CGD-O2D
48	R1	607	CHL	CHA-CBD-CGD-O1D
48	R1	607	CHL	CHA-CBD-CGD-O2D
48	Y1	607	CHL	CHA-CBD-CGD-O1D
48	Y1	607	CHL	CHA-CBD-CGD-O2D
48	y1	605	CHL	CHA-CBD-CGD-O1D
48	y1	605	CHL	CHA-CBD-CGD-O2D
49	n1	621	LUT	C33-C34-C35-C15
29	c1	502	CLA	CAA-CBA-CGA-O2A
38	s1	626	3PH	O21-C21-C22-C23
39	C1	524	DGA	OG2-CB1-CB2-CB3
29	s1	605	CLA	C2C-C3C-CAC-CBC
38	B1	624	3PH	C27-C28-C29-C2A
40	S1	624	LHG	C29-C30-C31-C32
29	c	506	CLA	C2-C3-C5-C6
29	C1	510	CLA	C2-C3-C5-C6
30	A1	408	PHO	C2-C3-C5-C6
48	g1	607	CHL	C2-C3-C5-C6
29	A1	405	CLA	C3-C5-C6-C7
33	c	523	LMG	C2-C1-O1-C7
51	y1	623	NEX	C28-C29-C30-C31
48	G	608	CHL	C2A-CAA-CBA-CGA
39	B	625	DGA	CCB-CDB-CEB-CFB
40	d1	410	LHG	C24-C25-C26-C27
29	b	608	CLA	C16-C17-C18-C19
29	G1	613	CLA	C16-C17-C18-C20
29	d	402	CLA	C13-C15-C16-C17
29	C1	501	CLA	C15-C16-C17-C18
29	A	406	CLA	CAA-CBA-CGA-O2A
29	b	603	CLA	CAA-CBA-CGA-O2A
29	b	609	CLA	CAA-CBA-CGA-O2A
29	r	612	CLA	CAA-CBA-CGA-O2A
38	t	101	3PH	O31-C31-C32-C33
39	c1	524	DGA	OG1-CA1-CA2-CA3

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Mol	Chain	Res	Type	Atoms
40	Y	624	LHG	O8-C23-C24-C25
40	d1	408	LHG	O7-C7-C8-C9
40	y1	624	LHG	O8-C23-C24-C25
55	y	626	PTY	O4-C30-C31-C32
33	C	523	LMG	C11-C12-C13-C14
39	B1	625	DGA	CFA-CGA-CHA-CIA
47	k1	101	4RF	C08-C09-C10-C11
40	D	409	LHG	C7-C8-C9-C10
40	N	624	LHG	C34-C35-C36-C37
40	S	624	LHG	C32-C33-C34-C35
29	b	603	CLA	C8-C10-C11-C12
29	B1	603	CLA	C8-C10-C11-C12
29	C1	504	CLA	C10-C11-C12-C13
29	s1	605	CLA	C4C-C3C-CAC-CBC
33	D1	411	LMG	C21-C22-C23-C24
40	Y	624	LHG	C33-C34-C35-C36
29	b	612	CLA	C8-C10-C11-C12
29	B	603	CLA	CAA-CBA-CGA-O2A
29	B	609	CLA	CAA-CBA-CGA-O2A
29	R	604	CLA	CAA-CBA-CGA-O2A
29	a	405	CLA	CAA-CBA-CGA-O2A
29	b	608	CLA	CAA-CBA-CGA-O2A
29	B1	608	CLA	CAA-CBA-CGA-O2A
29	n1	614	CLA	CAA-CBA-CGA-O2A
29	g1	603	CLA	CAA-CBA-CGA-O2A
33	D	411	LMG	O7-C10-C11-C12
33	h1	102	LMG	O8-C28-C29-C30
37	c	519	DGD	O2G-C1B-C2B-C3B
40	d	408	LHG	O8-C23-C24-C25
47	K	101	4RF	C14-C15-C16-O18
47	K1	101	4RF	O21-C22-C24-C25
55	Y	626	PTY	O4-C30-C31-C32
38	S	626	3PH	C33-C34-C35-C36
38	S1	626	3PH	C38-C39-C3A-C3B
38	s1	626	3PH	C26-C27-C28-C29
40	c	525	LHG	C12-C13-C14-C15
29	B	607	CLA	C2A-CAA-CBA-CGA
29	c	502	CLA	C2A-CAA-CBA-CGA
48	Y1	605	CHL	CAA-CBA-CGA-O2A
30	A	409	PHO	CHA-CBD-CGD-O1D
30	A	409	PHO	CHA-CBD-CGD-O2D
34	a1	414	SPH	N2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
41	C	527	LMK	O9-C10-C11-C12
44	f1	101	HEM	C4D-C3D-CAD-CBD
29	G1	613	CLA	C15-C16-C17-C18
29	s1	610	CLA	C5-C6-C7-C8
37	C	520	DGD	CAA-CBA-CCA-CDA
40	g	624	LHG	C26-C27-C28-C29
33	h1	102	LMG	C30-C31-C32-C33
32	C	526	SQD	C8-C7-O47-C45
32	c1	526	SQD	C8-C7-O47-C45
29	B	610	CLA	CAA-CBA-CGA-O2A
29	c	513	CLA	CAA-CBA-CGA-O2A
29	d	402	CLA	CAA-CBA-CGA-O2A
29	g	603	CLA	CAA-CBA-CGA-O2A
29	g1	613	CLA	CAA-CBA-CGA-O2A
39	j1	101	DGA	OG1-CA1-CA2-CA3
47	K1	101	4RF	O40-C41-C43-C44
32	c1	526	SQD	C11-C10-C9-C8
47	i1	101	4RF	C46-C47-C48-C49
29	A1	406	CLA	C4-C3-C5-C6
29	c1	511	CLA	C4-C3-C5-C6
37	c1	519	DGD	C2B-C3B-C4B-C5B
40	D	410	LHG	C31-C32-C33-C34
39	b1	625	DGA	CEB-CFB-CGB-CHB
29	C	504	CLA	C11-C10-C8-C7
29	N	613	CLA	C12-C13-C15-C16
29	R	608	CLA	C11-C10-C8-C7
29	y	614	CLA	C11-C10-C8-C7
29	A1	406	CLA	C11-C10-C8-C7
29	B1	610	CLA	C2-C3-C5-C6
29	B1	615	CLA	C11-C10-C8-C7
29	c1	502	CLA	C6-C7-C8-C10
29	r1	602	CLA	C6-C7-C8-C10
30	a1	408	PHO	C6-C7-C8-C10
48	N1	605	CHL	C6-C7-C8-C10
48	N1	609	CHL	C11-C12-C13-C15
48	Y1	609	CHL	C12-C13-C15-C16
43	d1	405	PL9	C4-C3-C7-C8
32	b1	626	SQD	C19-C20-C21-C22
38	B1	624	3PH	C22-C23-C24-C25
39	j	101	DGA	OB1-CB1-OG2-CG2
33	c	521	LMG	O6-C1-O1-C7
29	B	615	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
32	c1	526	SQD	O47-C7-C8-C9
33	a	413	LMG	O7-C10-C11-C12
33	B1	622	LMG	O8-C28-C29-C30
47	I	102	4RF	C14-C15-C16-O18
54	s1	625	LPX	O6-C6-C7-C8
29	c1	509	CLA	C4C-C3C-CAC-CBC
40	N1	624	LHG	C15-C16-C17-C18
29	N	613	CLA	C14-C13-C15-C16
29	c	502	CLA	C11-C10-C8-C9
29	n	603	CLA	C6-C7-C8-C9
29	s	609	CLA	C6-C7-C8-C9
29	s	610	CLA	C11-C12-C13-C14
29	s	611	CLA	C11-C12-C13-C14
29	y	614	CLA	C11-C10-C8-C9
29	B1	612	CLA	C14-C13-C15-C16
29	a1	406	CLA	C11-C12-C13-C14
29	s1	609	CLA	C6-C7-C8-C9
48	N1	609	CHL	C14-C13-C15-C16
48	g1	601	CHL	C11-C12-C13-C14
29	b1	603	CLA	CAA-CBA-CGA-O1A
29	b1	615	CLA	CAA-CBA-CGA-O1A
36	B	620	C7Z	C9-C10-C11-C12
48	N1	608	CHL	O2A-C1-C2-C3
29	B	605	CLA	O1A-CGA-O2A-C1
29	Y	610	CLA	O1A-CGA-O2A-C1
29	S1	612	CLA	CAA-CBA-CGA-O2A
33	w1	201	LMG	C28-C29-C30-C31
33	B	622	LMG	C18-C19-C20-C21
40	y1	624	LHG	C34-C35-C36-C37
37	C1	519	DGD	C2A-C1A-O1G-C1G
29	S	610	CLA	CAA-CBA-CGA-O2A
29	b	615	CLA	CAA-CBA-CGA-O2A
29	b1	607	CLA	CAA-CBA-CGA-O2A
39	C	524	DGA	OG1-CA1-CA2-CA3
39	j1	101	DGA	OG2-CB1-CB2-CB3
40	L1	101	LHG	O7-C7-C8-C9
29	Y	613	CLA	CAA-CBA-CGA-O1A
32	M	101	SQD	C4-C5-C6-S
32	b	626	SQD	C5-C6-S-O8
32	m	101	SQD	C4-C5-C6-S
32	b1	626	SQD	C4-C5-C6-S
29	G1	603	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
32	b	621	SQD	C11-C10-C9-C8
33	a1	413	LMG	C32-C33-C34-C35
37	C	518	DGD	C6B-C7B-C8B-C9B
29	a1	405	CLA	C3-C5-C6-C7
29	B	610	CLA	O1A-CGA-O2A-C1
29	y	613	CLA	O1A-CGA-O2A-C1
37	C1	519	DGD	O1A-C1A-O1G-C1G
34	y1	625	SPH	C13-C14-C15-C16
38	b1	624	3PH	C2A-C2B-C2C-C2D
29	n1	602	CLA	C15-C16-C17-C18
29	A	406	CLA	C2A-CAA-CBA-CGA
29	C	512	CLA	C2A-CAA-CBA-CGA
29	a	406	CLA	C2A-CAA-CBA-CGA
29	b	606	CLA	C2A-CAA-CBA-CGA
29	C1	506	CLA	C2A-CAA-CBA-CGA
29	R1	610	CLA	C2A-CAA-CBA-CGA
29	g	613	CLA	CAA-CBA-CGA-O1A
29	c1	505	CLA	CAA-CBA-CGA-O1A
33	C	523	LMG	O9-C10-C11-C12
33	C1	523	LMG	C30-C31-C32-C33
40	Y1	624	LHG	C27-C28-C29-C30
29	g1	614	CLA	CAA-CBA-CGA-O2A
32	a1	412	SQD	O47-C7-C8-C9
38	S	626	3PH	O21-C21-C22-C23
40	N1	624	LHG	O7-C7-C8-C9
33	C	521	LMG	C13-C14-C15-C16
47	K	101	4RF	C24-C25-C26-C27
47	I1	102	4RF	C32-C33-C34-C35
40	d	409	LHG	C24-C23-O8-C6
33	H1	102	LMG	C37-C38-C39-C40
31	C1	516	BCR	C36-C18-C19-C20
32	M	101	SQD	C23-C24-C25-C26
49	R1	620	LUT	C27-C28-C29-C39
50	Y	622	XAT	C27-C28-C29-C39
29	g	614	CLA	CAA-CBA-CGA-O1A
29	b1	608	CLA	CAA-CBA-CGA-O1A
37	C1	518	DGD	O1A-C1A-C2A-C3A
38	S1	626	3PH	O22-C21-C22-C23
38	t1	101	3PH	O32-C31-C32-C33
30	a1	409	PHO	C16-C17-C18-C20
40	d1	410	LHG	C33-C34-C35-C36
48	Y1	607	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
44	f1	101	HEM	C2D-C3D-CAD-CBD
40	c1	525	LHG	O7-C7-C8-C9
41	C	527	LMK	C11-C12-C13-C14
32	b1	621	SQD	O49-C7-C8-C9
33	C	521	LMG	O9-C10-C11-C12
33	A1	413	LMG	O9-C10-C11-C12
40	N	624	LHG	O9-C7-C8-C9
31	b1	618	BCR	C21-C22-C23-C24
29	C	508	CLA	CBA-CGA-O2A-C1
38	S1	626	3PH	C32-C31-O31-C3
32	M1	101	SQD	C25-C26-C27-C28
29	G	612	CLA	C1A-C2A-CAA-CBA
29	b	617	CLA	C1A-C2A-CAA-CBA
29	B1	615	CLA	C1A-C2A-CAA-CBA
29	N1	612	CLA	C1A-C2A-CAA-CBA
29	b1	603	CLA	C1A-C2A-CAA-CBA
29	d1	402	CLA	C1A-C2A-CAA-CBA
29	g1	613	CLA	C1A-C2A-CAA-CBA
29	s1	609	CLA	C1A-C2A-CAA-CBA
48	G	607	CHL	C1A-C2A-CAA-CBA
48	Y	605	CHL	C1A-C2A-CAA-CBA
48	n	607	CHL	C1A-C2A-CAA-CBA
48	g	601	CHL	C1A-C2A-CAA-CBA
48	y	607	CHL	C1A-C2A-CAA-CBA
48	n1	607	CHL	C1A-C2A-CAA-CBA
48	g1	601	CHL	C1A-C2A-CAA-CBA
48	g1	606	CHL	C1A-C2A-CAA-CBA
48	g1	608	CHL	C1A-C2A-CAA-CBA
32	a	412	SQD	C7-C8-C9-C10
38	B1	624	3PH	C38-C39-C3A-C3B
40	Y1	624	LHG	C9-C10-C11-C12
29	B	608	CLA	CAA-CBA-CGA-O1A
29	R	612	CLA	CAA-CBA-CGA-O1A
29	R1	604	CLA	CAA-CBA-CGA-O1A
29	r1	604	CLA	CAA-CBA-CGA-O1A
38	B	624	3PH	O32-C31-C32-C33
38	S	626	3PH	O22-C21-C22-C23
38	s	626	3PH	O22-C21-C22-C23
39	j1	101	DGA	OB1-CB1-CB2-CB3
40	c	525	LHG	O9-C7-C8-C9
48	n1	605	CHL	CAA-CBA-CGA-O1A
48	g1	605	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
29	N1	614	CLA	CAA-CBA-CGA-O2A
29	c1	502	CLA	C8-C10-C11-C12
48	G	607	CHL	C15-C16-C17-C18
47	K1	101	4RF	C03-C04-C05-C06
29	b	604	CLA	C2-C1-O2A-CGA
40	d1	409	LHG	C15-C16-C17-C18
33	W1	201	LMG	C4-C5-C6-O5
29	y1	604	CLA	C10-C11-C12-C13
29	G	613	CLA	CAA-CBA-CGA-O1A
29	c	503	CLA	CAA-CBA-CGA-O1A
29	B1	609	CLA	CAA-CBA-CGA-O1A
29	C1	502	CLA	CAA-CBA-CGA-O1A
29	Y1	613	CLA	CAA-CBA-CGA-O1A
29	c1	512	CLA	CAA-CBA-CGA-O1A
29	y1	613	CLA	CAA-CBA-CGA-O1A
30	A	409	PHO	CAA-CBA-CGA-O1A
37	C	518	DGD	O1B-C1B-C2B-C3B
37	b	623	DGD	O1A-C1A-C2A-C3A
39	c	524	DGA	OB1-CB1-CB2-CB3
39	b1	625	DGA	OB1-CB1-CB2-CB3
40	D1	409	LHG	O9-C7-C8-C9
39	J1	101	DGA	CBB-CAB-CB9-CB8
39	j1	101	DGA	OG1-CG1-CG2-CG3
40	d1	409	LHG	C4-C5-C6-O8
47	i1	101	4RF	O18-C19-C20-C39
37	c1	518	DGD	O1G-C1A-C2A-C3A
29	B1	610	CLA	C10-C11-C12-C13
30	a1	409	PHO	C8-C10-C11-C12
29	B	608	CLA	C2A-CAA-CBA-CGA
29	N1	603	CLA	C2A-CAA-CBA-CGA
32	B	626	SQD	C30-C31-C32-C33
32	b	626	SQD	C10-C11-C12-C13
33	h	102	LMG	C18-C19-C20-C21
38	S	626	3PH	C2F-C2G-C2H-C2I
54	s1	625	LPX	C7-C8-C9-C10
29	b1	617	CLA	C16-C17-C18-C19
29	y1	602	CLA	C16-C17-C18-C19
29	c	505	CLA	CAA-CBA-CGA-O1A
29	y	613	CLA	CAA-CBA-CGA-O1A
39	C1	524	DGA	OB1-CB1-CB2-CB3
39	c1	524	DGA	OA1-CA1-CA2-CA3
40	D	408	LHG	O9-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
54	s1	625	LPX	O7-C6-C7-C8
29	n	610	CLA	C13-C15-C16-C17
29	G1	603	CLA	C5-C6-C7-C8
33	B	622	LMG	C21-C22-C23-C24
29	A	405	CLA	C4-C3-C5-C6
29	A	405	CLA	CAA-CBA-CGA-O2A
29	b	607	CLA	CAA-CBA-CGA-O2A
29	C1	503	CLA	CAA-CBA-CGA-O2A
29	r1	612	CLA	CAA-CBA-CGA-O2A
33	c1	523	LMG	O7-C10-C11-C12
39	J	101	DGA	OG2-CB1-CB2-CB3
48	n	605	CHL	CAA-CBA-CGA-O2A
32	A1	412	SQD	O49-C7-O47-C45
55	Y	627	PTY	C6-C5-O14-P1
38	b	624	3PH	C2C-C2D-C2E-C2F
29	B	603	CLA	CAA-CBA-CGA-O1A
29	c1	502	CLA	CAA-CBA-CGA-O1A
40	N1	624	LHG	O9-C7-C8-C9
29	B	605	CLA	C2-C3-C5-C6
29	R	608	CLA	C2-C3-C5-C6
29	c1	513	CLA	C2-C3-C5-C6
29	g1	613	CLA	C2-C3-C5-C6
48	y1	605	CHL	CAA-CBA-CGA-O2A
29	B	609	CLA	C13-C15-C16-C17
29	N	610	CLA	C5-C6-C7-C8
29	B1	602	CLA	C8-C10-C11-C12
48	g1	601	CHL	C13-C15-C16-C17
29	c1	509	CLA	C2C-C3C-CAC-CBC
33	C	523	LMG	C14-C15-C16-C17
47	k1	101	4RF	C06-C07-C08-C09
40	D	410	LHG	C4-O6-P-O4
40	g	624	LHG	C3-O3-P-O5
40	C1	525	LHG	C3-O3-P-O4
40	n1	624	LHG	C3-O3-P-O5
54	s	625	LPX	C3-O1-P1-O3
54	s1	625	LPX	C1-O2-P1-O4
55	Y	627	PTY	C3-O11-P1-O13
55	Y1	626	PTY	C5-O14-P1-O13
41	c1	527	LMK	O7-C8-C9-O8
37	B	623	DGD	C2B-C3B-C4B-C5B
37	C1	520	DGD	CDB-CEB-CFB-CGB
39	j	101	DGA	CB5-CB6-CB7-CB8

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Mol	Chain	Res	Type	Atoms
29	N	604	CLA	CAA-CBA-CGA-O1A
29	c	513	CLA	CAA-CBA-CGA-O1A
29	r	612	CLA	CAA-CBA-CGA-O1A
29	B1	608	CLA	CAA-CBA-CGA-O1A
30	A1	409	PHO	CAA-CBA-CGA-O1A
32	c1	526	SQD	O49-C7-C8-C9
33	d	411	LMG	O9-C10-C11-C12
39	C	524	DGA	OA1-CA1-CA2-CA3
39	j1	101	DGA	OA1-CA1-CA2-CA3
40	d	408	LHG	O10-C23-C24-C25
40	y	624	LHG	O10-C23-C24-C25
48	y	606	CHL	CAA-CBA-CGA-O1A
55	y	626	PTY	O30-C30-C31-C32
29	B1	602	CLA	CAA-CBA-CGA-O2A
29	B1	602	CLA	C15-C16-C17-C18
29	g1	610	CLA	C13-C15-C16-C17
48	G	607	CHL	C13-C15-C16-C17
33	C	523	LMG	C37-C38-C39-C40
33	h	102	LMG	C39-C40-C41-C42
37	C	520	DGD	C9B-CAB-CBB-CCB
31	c	517	BCR	C23-C24-C25-C26
31	A1	411	BCR	C23-C24-C25-C26
31	C1	517	BCR	C1-C6-C7-C8
49	Y	621	LUT	C5-C6-C7-C8
49	Y1	620	LUT	C5-C6-C7-C8
43	d	405	PL9	C24-C26-C27-C28
41	C	527	LMK	C10-C11-C12-C13
29	r	608	CLA	C10-C11-C12-C13
55	y1	626	PTY	N1-C2-C3-O11
29	B	615	CLA	CAA-CBA-CGA-O1A
29	C	503	CLA	CAA-CBA-CGA-O1A
29	G	614	CLA	CAA-CBA-CGA-O1A
29	S	610	CLA	CAA-CBA-CGA-O1A
29	b	603	CLA	CAA-CBA-CGA-O1A
29	b	609	CLA	CAA-CBA-CGA-O1A
29	B1	603	CLA	CAA-CBA-CGA-O1A
29	n1	604	CLA	CAA-CBA-CGA-O1A
29	n1	614	CLA	CAA-CBA-CGA-O1A
33	W1	201	LMG	O9-C10-C11-C12
33	h1	102	LMG	O10-C28-C29-C30
40	d1	408	LHG	O9-C7-C8-C9
47	K	101	4RF	C14-C15-C16-O17

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Mol	Chain	Res	Type	Atoms
38	S1	626	3PH	O32-C31-O31-C3
29	C1	501	CLA	CAA-CBA-CGA-O2A
29	G1	603	CLA	CAA-CBA-CGA-O2A
33	a1	413	LMG	O7-C10-C11-C12
40	n	624	LHG	O7-C7-C8-C9
32	A	412	SQD	C30-C31-C32-C33
40	N1	624	LHG	C17-C18-C19-C20
29	N	613	CLA	CBA-CGA-O2A-C1
53	r	626	ERG	C21-C20-C22-C23
51	n	623	NEX	C30-C31-C32-C33
33	c	523	LMG	O9-C10-C11-C12
39	b1	625	DGA	OA1-CA1-CA2-CA3
40	Y	624	LHG	O10-C23-C24-C25
40	D1	410	LHG	C34-C35-C36-C37
38	b1	624	3PH	C38-C39-C3A-C3B
29	S1	612	CLA	CAA-CBA-CGA-O1A
29	G	603	CLA	CAA-CBA-CGA-O2A
37	C	519	DGD	O2G-C1B-C2B-C3B
37	c1	519	DGD	O2G-C1B-C2B-C3B
40	S1	624	LHG	O8-C23-C24-C25
29	S	610	CLA	C5-C6-C7-C8
29	Y1	612	CLA	C15-C16-C17-C18
38	s	626	3PH	C2E-C2F-C2G-C2H
39	B1	625	DGA	CBB-CAB-CB9-CB8
40	L	101	LHG	C17-C18-C19-C20
55	Y	626	PTY	C41-C42-C43-C44
32	A	412	SQD	O49-C7-C8-C9
38	b1	624	3PH	O22-C21-C22-C23
29	c	509	CLA	C4-C3-C5-C6
29	A1	410	CLA	C4-C3-C5-C6
48	S	608	CHL	C4-C3-C5-C6
32	b	626	SQD	C9-C10-C11-C12
43	D1	405	PL9	C26-C27-C28-C29
29	y	612	CLA	C2-C3-C5-C6
29	b1	607	CLA	C15-C16-C17-C18
47	k1	101	4RF	C50-C51-C52-C53
29	A	410	CLA	CAD-CBD-CGD-O1D
29	B	614	CLA	CAD-CBD-CGD-O1D
29	B	615	CLA	CAD-CBD-CGD-O1D
29	N	603	CLA	CAD-CBD-CGD-O1D
29	n	603	CLA	CAD-CBD-CGD-O1D
29	s	604	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
29	s	610	CLA	CAD-CBD-CGD-O1D
29	A1	406	CLA	CAD-CBD-CGD-O1D
29	N1	603	CLA	CAD-CBD-CGD-O1D
29	G1	611	CLA	CAD-CBD-CGD-O1D
29	Y1	603	CLA	CAD-CBD-CGD-O1D
29	c1	510	CLA	CAD-CBD-CGD-O1D
29	n1	611	CLA	CAD-CBD-CGD-O1D
29	g1	613	CLA	CAD-CBD-CGD-O1D
29	s1	609	CLA	CAD-CBD-CGD-O1D
32	B	626	SQD	O5-C5-C6-S
32	M	101	SQD	O5-C5-C6-S
32	c	526	SQD	O5-C5-C6-S
32	m	101	SQD	O5-C5-C6-S
32	b1	626	SQD	O5-C5-C6-S
32	b1	626	SQD	C5-C6-S-O9
48	S	607	CHL	CAD-CBD-CGD-O1D
48	n1	606	CHL	CAD-CBD-CGD-O1D
55	Y	627	PTY	C2-C3-O11-P1
55	y	627	PTY	C2-C3-O11-P1
55	Y1	627	PTY	C2-C3-O11-P1
33	b	622	LMG	C10-C11-C12-C13
29	N	613	CLA	O1A-CGA-O2A-C1
29	B	609	CLA	CAA-CBA-CGA-O1A
29	b	608	CLA	CAA-CBA-CGA-O1A
29	B1	615	CLA	CAA-CBA-CGA-O1A
29	g1	603	CLA	CAA-CBA-CGA-O1A
38	t	101	3PH	O32-C31-C32-C33
40	S	624	LHG	O10-C23-C24-C25
37	c1	519	DGD	C5B-C6B-C7B-C8B
55	Y	626	PTY	C13-C14-C15-C16
33	w	201	LMG	O7-C10-C11-C12
48	N	605	CHL	CAA-CBA-CGA-O2A
54	S1	625	LPX	O6-C6-C7-C8
29	A1	410	CLA	C5-C6-C7-C8
29	n1	610	CLA	C13-C15-C16-C17
29	B	606	CLA	C11-C12-C13-C14
29	B	614	CLA	C11-C10-C8-C9
29	C	508	CLA	C11-C10-C8-C9
29	D	403	CLA	C14-C13-C15-C16
29	G	610	CLA	C11-C10-C8-C9
29	g	610	CLA	C6-C7-C8-C9
29	g	610	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
29	y	604	CLA	C14-C13-C15-C16
29	A1	406	CLA	C11-C10-C8-C9
29	B1	613	CLA	C11-C12-C13-C14
29	C1	507	CLA	C14-C13-C15-C16
29	C1	512	CLA	C11-C10-C8-C9
29	G1	603	CLA	C11-C12-C13-C14
29	b1	605	CLA	C11-C10-C8-C9
29	b1	612	CLA	C6-C7-C8-C9
29	c1	513	CLA	C11-C12-C13-C14
29	d1	402	CLA	C11-C12-C13-C14
29	n1	613	CLA	C11-C10-C8-C9
37	C	518	DGD	CCB-CDB-CEB-CFB
29	S	605	CLA	C4C-C3C-CAC-CBC
37	C	520	DGD	C6A-C7A-C8A-C9A
40	c1	525	LHG	C35-C36-C37-C38
29	A	406	CLA	CAA-CBA-CGA-O1A
33	D	411	LMG	O9-C10-C11-C12
40	L1	101	LHG	O9-C7-C8-C9
40	c1	525	LHG	O9-C7-C8-C9
29	r1	602	CLA	C11-C12-C13-C14
29	C	505	CLA	CAA-CBA-CGA-O2A
29	a	406	CLA	CAA-CBA-CGA-O2A
29	C1	513	CLA	CAA-CBA-CGA-O2A
29	r1	609	CLA	CAA-CBA-CGA-O2A
32	c1	526	SQD	O48-C23-C24-C25
37	C1	519	DGD	O2G-C1B-C2B-C3B
39	j	101	DGA	OG1-CA1-CA2-CA3
39	B1	625	DGA	OG2-CB1-CB2-CB3
29	b	606	CLA	C5-C6-C7-C8
55	Y1	626	PTY	C35-C36-C37-C38
29	s1	610	CLA	C2A-CAA-CBA-CGA
40	Y	624	LHG	C17-C18-C19-C20
29	c	508	CLA	CAA-CBA-CGA-O2A
29	B1	613	CLA	CAA-CBA-CGA-O2A
29	C1	508	CLA	CAA-CBA-CGA-O2A
29	R1	612	CLA	CAA-CBA-CGA-O2A
29	c1	508	CLA	CAA-CBA-CGA-O2A
32	M1	101	SQD	O48-C23-C24-C25
32	b1	621	SQD	O48-C23-C24-C25
33	W	201	LMG	O7-C10-C11-C12
37	C1	520	DGD	O1G-C1A-C2A-C3A
39	b	625	DGA	OG1-CA1-CA2-CA3

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Mol	Chain	Res	Type	Atoms
48	G1	601	CHL	CAA-CBA-CGA-O2A
48	y1	606	CHL	CAA-CBA-CGA-O2A
32	b	621	SQD	C14-C15-C16-C17
29	B	610	CLA	CAA-CBA-CGA-O1A
29	R	604	CLA	CAA-CBA-CGA-O1A
32	a1	412	SQD	O49-C7-C8-C9
33	a	413	LMG	O9-C10-C11-C12
40	y1	624	LHG	O10-C23-C24-C25
47	K1	101	4RF	O42-C41-C43-C44
33	c	521	LMG	C4-C5-C6-O5
40	d1	410	LHG	C10-C11-C12-C13
29	b	615	CLA	C16-C17-C18-C20
40	n	624	LHG	C2-C3-O3-P
29	s	604	CLA	C4-C3-C5-C6
29	Y1	604	CLA	C4-C3-C5-C6
48	G1	601	CHL	C4-C3-C5-C6
29	g	611	CLA	C8-C10-C11-C12
31	C	514	BCR	C11-C12-C13-C35
33	d1	411	LMG	C31-C32-C33-C34
38	B1	624	3PH	C3F-C3G-C3H-C3I
29	B	606	CLA	C11-C12-C13-C15
29	B	611	CLA	C12-C13-C15-C16
29	C	503	CLA	C12-C13-C15-C16
29	C	508	CLA	C11-C10-C8-C7
29	C	513	CLA	C11-C10-C8-C7
29	N	610	CLA	C11-C10-C8-C7
29	G	610	CLA	C11-C10-C8-C7
29	S	605	CLA	C3A-C2A-CAA-CBA
29	c	505	CLA	C11-C10-C8-C7
29	c	513	CLA	C12-C13-C15-C16
29	n	614	CLA	C3A-C2A-CAA-CBA
29	g	610	CLA	C6-C7-C8-C10
29	g	610	CLA	C11-C12-C13-C15
29	r	610	CLA	C6-C7-C8-C10
29	y	612	CLA	C11-C12-C13-C15
29	B1	603	CLA	C11-C12-C13-C15
29	C1	506	CLA	C12-C13-C15-C16
29	C1	507	CLA	C11-C10-C8-C7
29	C1	507	CLA	C12-C13-C15-C16
29	C1	512	CLA	C11-C10-C8-C7
29	N1	613	CLA	C12-C13-C15-C16
29	G1	603	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
29	b1	612	CLA	C6-C7-C8-C10
29	c1	507	CLA	C11-C10-C8-C7
29	c1	511	CLA	C11-C10-C8-C7
29	d1	402	CLA	C12-C13-C15-C16
29	n1	613	CLA	C11-C10-C8-C7
29	s1	611	CLA	C11-C12-C13-C15
29	y1	611	CLA	C3A-C2A-CAA-CBA
29	y1	612	CLA	C11-C12-C13-C15
29	y1	614	CLA	C11-C12-C13-C15
37	B	623	DGD	C1B-C2B-C3B-C4B
38	B1	624	3PH	O11-C1-C2-O21
48	N	601	CHL	C11-C12-C13-C15
48	n	605	CHL	C6-C7-C8-C10
48	G1	601	CHL	C12-C13-C15-C16
48	Y1	606	CHL	C11-C12-C13-C15
48	g1	609	CHL	C11-C12-C13-C15
29	a	405	CLA	CAA-CBA-CGA-O1A
29	b	613	CLA	CAA-CBA-CGA-O1A
29	b1	607	CLA	CAA-CBA-CGA-O1A
37	c	519	DGD	O1B-C1B-C2B-C3B
47	K1	101	4RF	O23-C22-C24-C25
55	Y	626	PTY	C20-C21-C22-C23
29	b	613	CLA	CAA-CBA-CGA-O2A
29	s	603	CLA	CAA-CBA-CGA-O2A
29	A1	406	CLA	CAA-CBA-CGA-O2A
29	B1	606	CLA	CAA-CBA-CGA-O2A
29	C1	505	CLA	CAA-CBA-CGA-O2A
29	G1	614	CLA	CAA-CBA-CGA-O2A
29	c1	503	CLA	CAA-CBA-CGA-O2A
29	c1	513	CLA	CAA-CBA-CGA-O2A
33	B1	622	LMG	O7-C10-C11-C12
39	j	101	DGA	OG2-CB1-CB2-CB3
55	y1	626	PTY	C12-C11-C8-O7
33	C1	521	LMG	C19-C20-C21-C22
33	C1	523	LMG	C21-C22-C23-C24
38	S1	626	3PH	C27-C28-C29-C2A
29	G	604	CLA	O2A-C1-C2-C3
29	r	609	CLA	C3-C5-C6-C7
48	g	609	CHL	C3-C5-C6-C7
47	i	101	4RF	C01-C02-C03-C04
41	c1	527	LMK	N4-C3-C4-O2
31	A	411	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
45	H1	101	RRX	C17-C18-C19-C20
50	Y	622	XAT	C27-C28-C29-C30
50	r1	621	XAT	C27-C28-C29-C30
50	y1	622	XAT	C27-C28-C29-C30
51	g	623	NEX	C11-C12-C13-C14
29	g	603	CLA	CAA-CBA-CGA-O1A
29	G1	603	CLA	CAA-CBA-CGA-O1A
29	g1	613	CLA	CAA-CBA-CGA-O1A
33	B1	622	LMG	O9-C10-C11-C12
37	C	519	DGD	O1B-C1B-C2B-C3B
39	J	101	DGA	OB1-CB1-CB2-CB3
39	j	101	DGA	OA1-CA1-CA2-CA3
55	Y	626	PTY	O30-C30-C31-C32
45	h	101	RRX	C15-C16-C17-C18
49	g	620	LUT	C9-C10-C11-C12
49	G1	620	LUT	C33-C34-C35-C15
51	y1	623	NEX	C29-C30-C31-C32
40	C	525	LHG	C15-C16-C17-C18
52	r	625	LMT	O1'-C1-C2-C3
41	c1	527	LMK	C2-C1-O1-C7
32	A	412	SQD	O48-C23-C24-C25
32	c	526	SQD	O47-C7-C8-C9
33	d1	411	LMG	O7-C10-C11-C12
37	b1	623	DGD	O1G-C1A-C2A-C3A
40	G1	624	LHG	O8-C23-C24-C25
47	i1	101	4RF	C14-C15-C16-O18
48	n1	606	CHL	CAA-CBA-CGA-O2A
29	y	611	CLA	C13-C15-C16-C17
29	C1	507	CLA	C8-C10-C11-C12
29	Y1	610	CLA	C13-C15-C16-C17
29	r1	603	CLA	C5-C6-C7-C8
29	r1	612	CLA	C10-C11-C12-C13
29	C	508	CLA	O1A-CGA-O2A-C1
29	b	616	CLA	O1A-CGA-O2A-C1
29	b1	614	CLA	O1A-CGA-O2A-C1
29	a	406	CLA	CAA-CBA-CGA-O1A
29	C1	503	CLA	CAA-CBA-CGA-O1A
29	N1	614	CLA	CAA-CBA-CGA-O1A
29	R1	612	CLA	CAA-CBA-CGA-O1A
29	c1	503	CLA	CAA-CBA-CGA-O1A
37	C1	519	DGD	O1B-C1B-C2B-C3B
39	b	625	DGA	OA1-CA1-CA2-CA3

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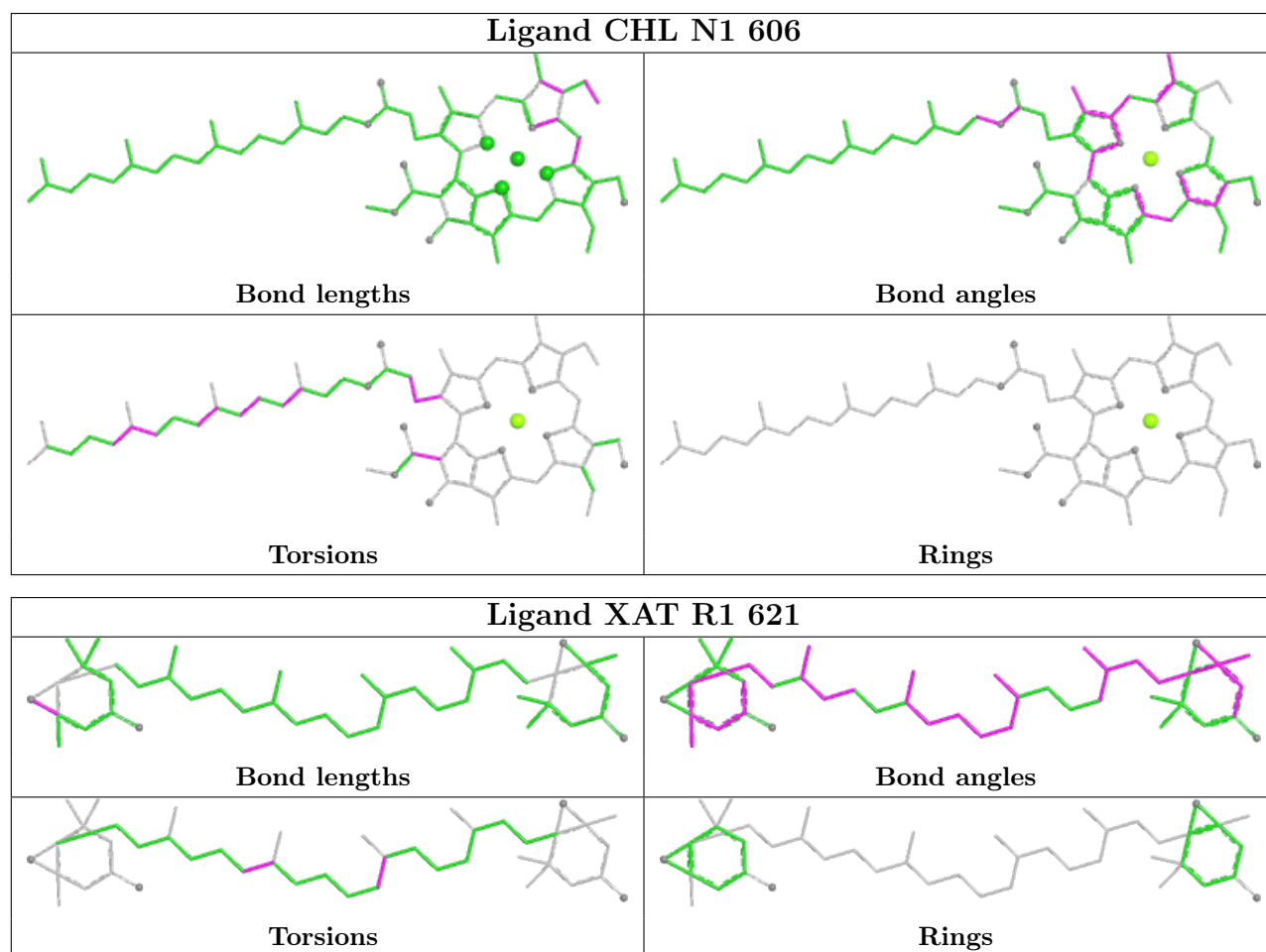
Mol	Chain	Res	Type	Atoms
48	n	605	CHL	CAA-CBA-CGA-O1A
48	G1	601	CHL	CAA-CBA-CGA-O1A
41	C1	527	LMK	C8-C7-O1-C1
29	B	605	CLA	CBA-CGA-O2A-C1
29	G1	611	CLA	C5-C6-C7-C8
48	G	609	CHL	C15-C16-C17-C18
29	N1	604	CLA	CAA-CBA-CGA-O2A
29	b1	606	CLA	CAA-CBA-CGA-O2A
37	c1	518	DGD	O2G-C1B-C2B-C3B
38	S	626	3PH	O31-C31-C32-C33
48	n	607	CHL	CAA-CBA-CGA-O2A
29	s	603	CLA	C10-C11-C12-C13
29	b	607	CLA	CAA-CBA-CGA-O1A
29	b	615	CLA	CAA-CBA-CGA-O1A
29	c	508	CLA	CAA-CBA-CGA-O1A
29	B1	613	CLA	CAA-CBA-CGA-O1A
29	c1	513	CLA	CAA-CBA-CGA-O1A
29	g1	614	CLA	CAA-CBA-CGA-O1A
33	c1	523	LMG	O9-C10-C11-C12
40	n	624	LHG	O9-C7-C8-C9
43	D1	405	PL9	C42-C43-C44-C45
29	S	613	CLA	C6-C7-C8-C10
33	B1	622	LMG	C11-C12-C13-C14
29	a	406	CLA	C8-C10-C11-C12
48	G1	609	CHL	C15-C16-C17-C18
40	G	624	LHG	C16-C17-C18-C19
40	G	624	LHG	C18-C19-C20-C21
29	C	505	CLA	CAA-CBA-CGA-O1A
29	B1	606	CLA	CAA-CBA-CGA-O1A
48	S1	608	CHL	CAA-CBA-CGA-O1A
29	C	513	CLA	C4-C3-C5-C6
32	c1	526	SQD	C31-C32-C33-C34
33	C	523	LMG	C34-C35-C36-C37
38	S	626	3PH	C2E-C2F-C2G-C2H
29	s	617	CLA	CAA-CBA-CGA-O2A
37	C	518	DGD	O1G-C1A-C2A-C3A
39	b	625	DGA	OG2-CB1-CB2-CB3
48	G	601	CHL	CAA-CBA-CGA-O2A
48	G	605	CHL	CAA-CBA-CGA-O2A
55	y1	626	PTY	O4-C30-C31-C32

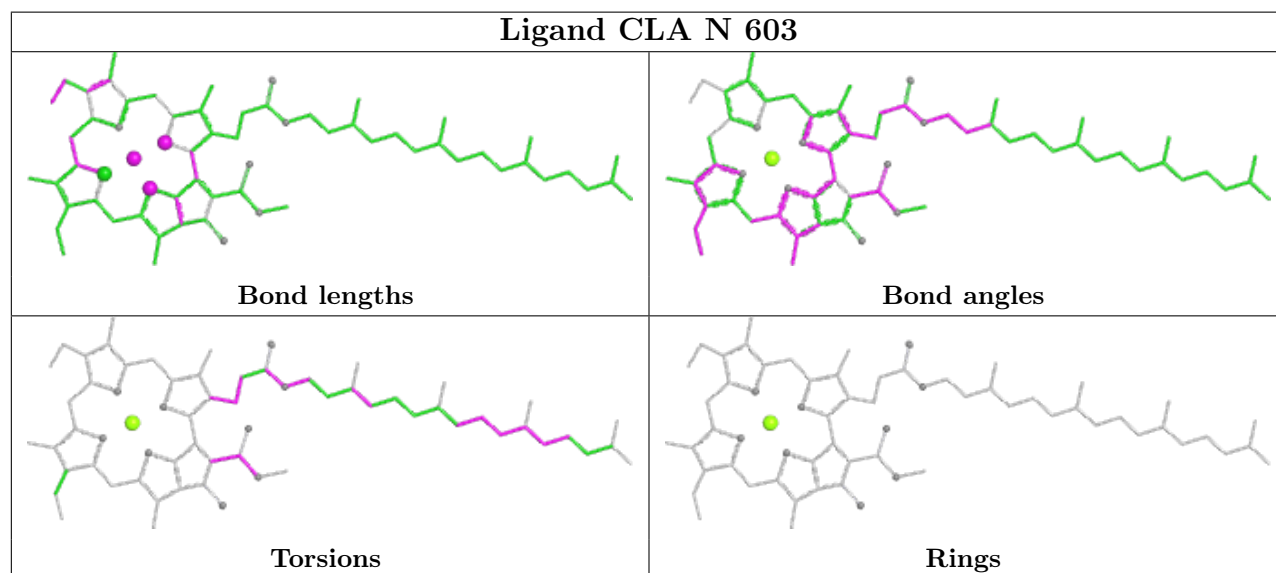
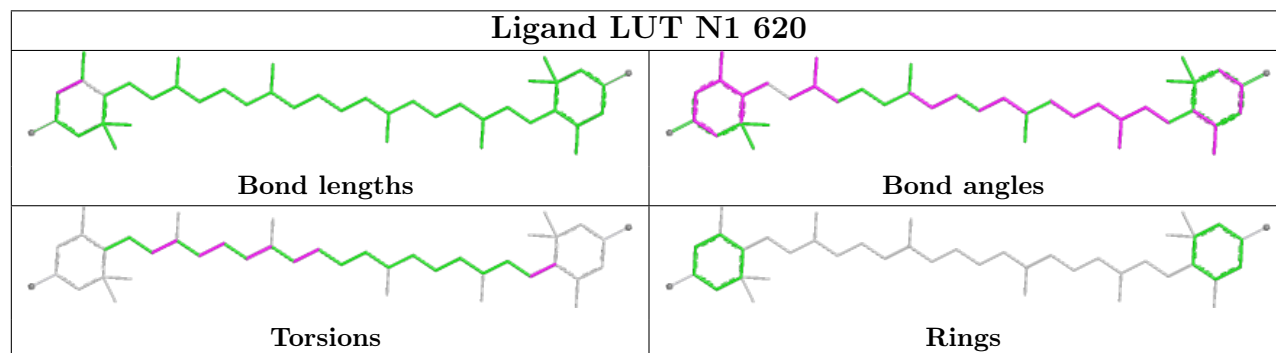
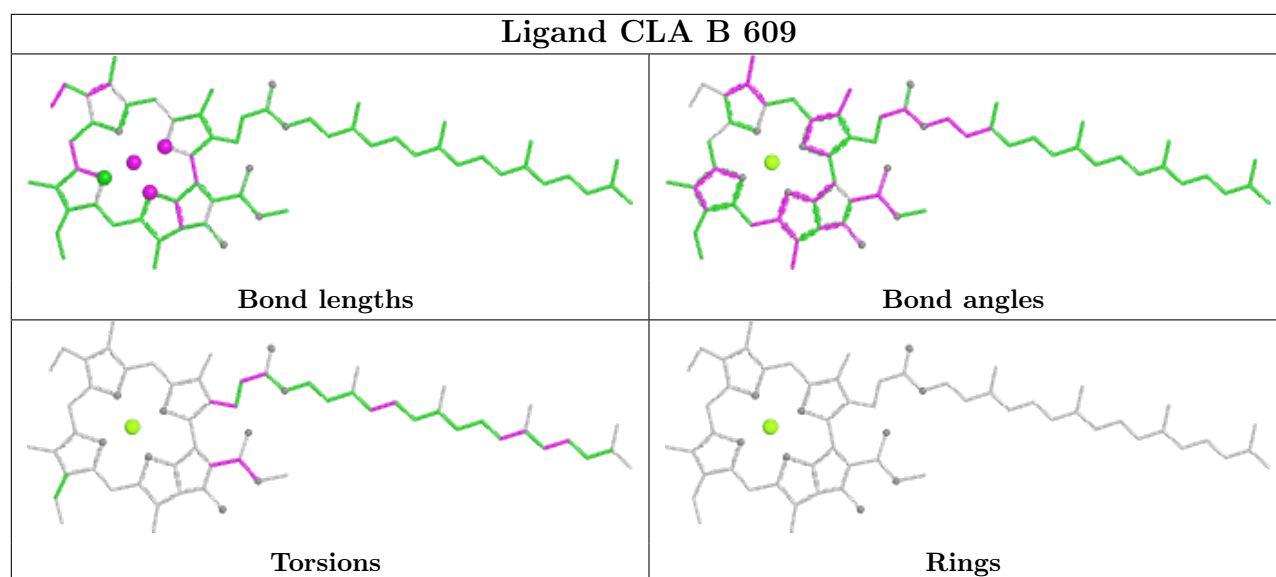
All (2) ring outliers are listed below:

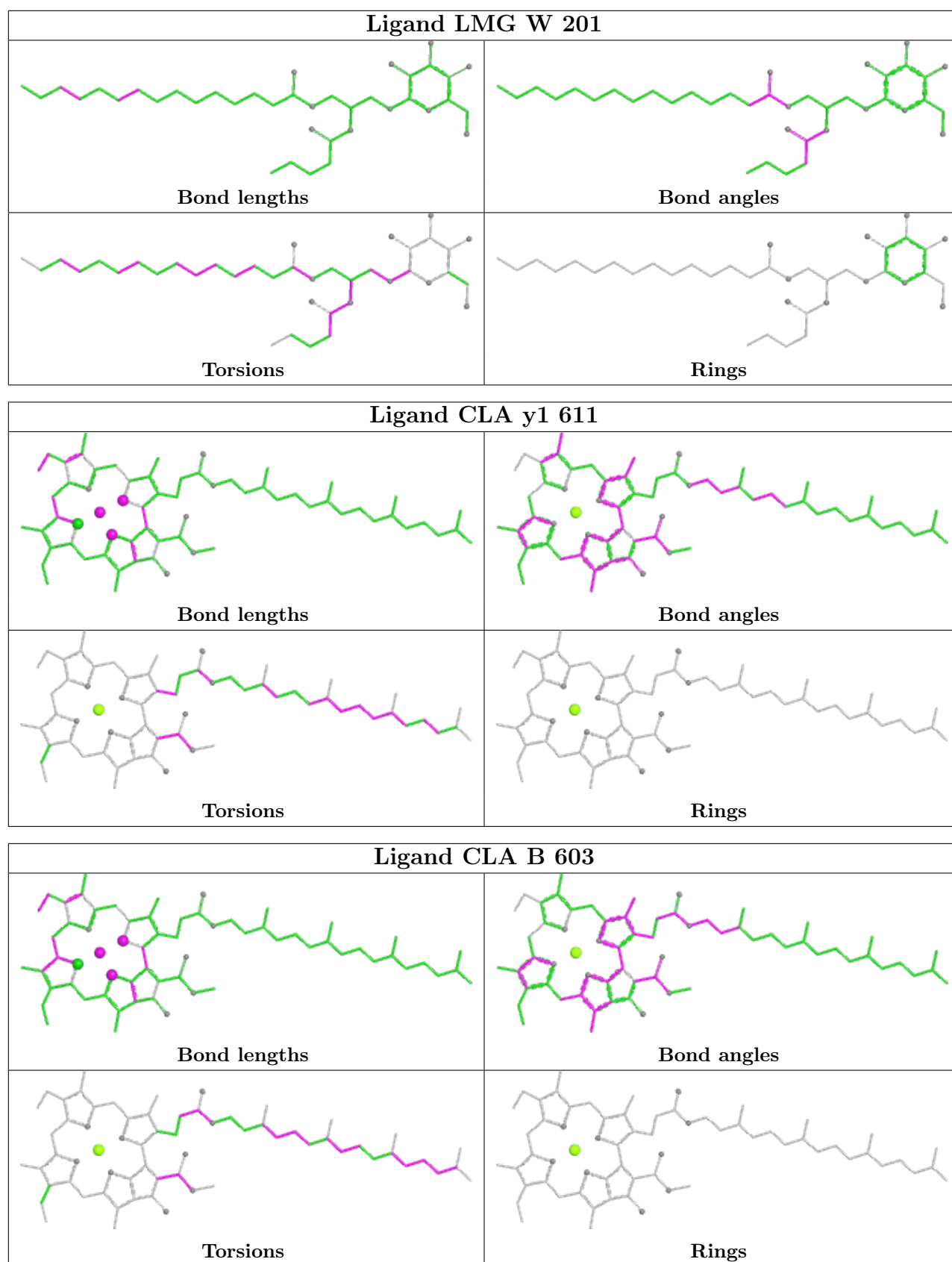
Mol	Chain	Res	Type	Atoms
51	N	623	NEX	C1-C2-C3-C4-C5-C6
51	n	623	NEX	C1-C2-C3-C4-C5-C6

No monomer is involved in short contacts.

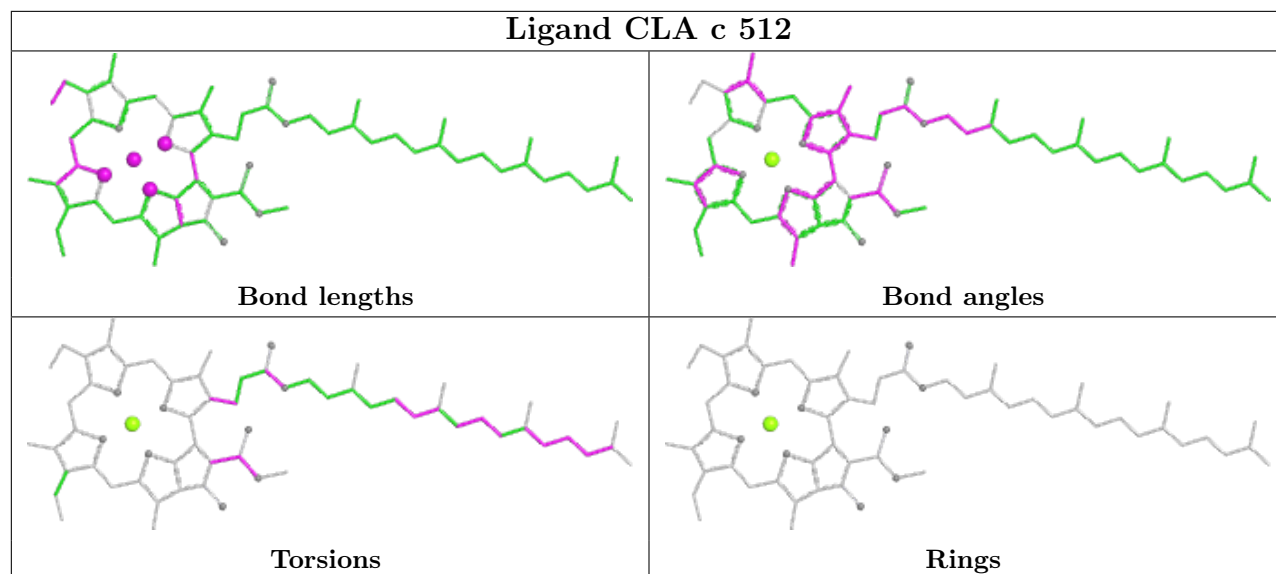
The following is a two-dimensional graphical depiction of Mogul quality analysis of bond lengths, bond angles, torsion angles, and ring geometry for all instances of the Ligand of Interest. In addition, ligands with molecular weight > 250 and outliers as shown on the validation Tables will also be included.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



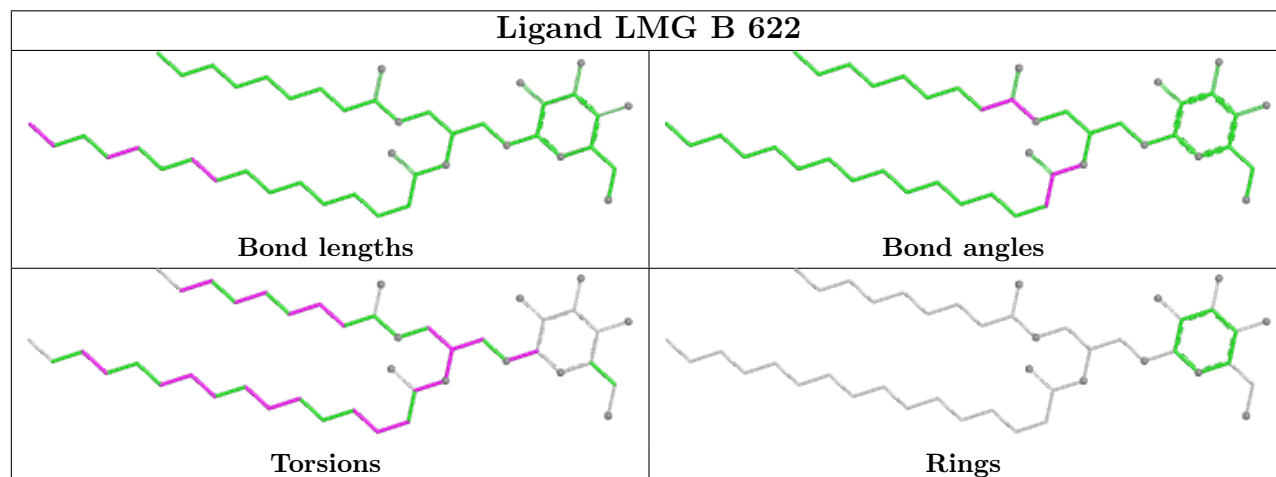




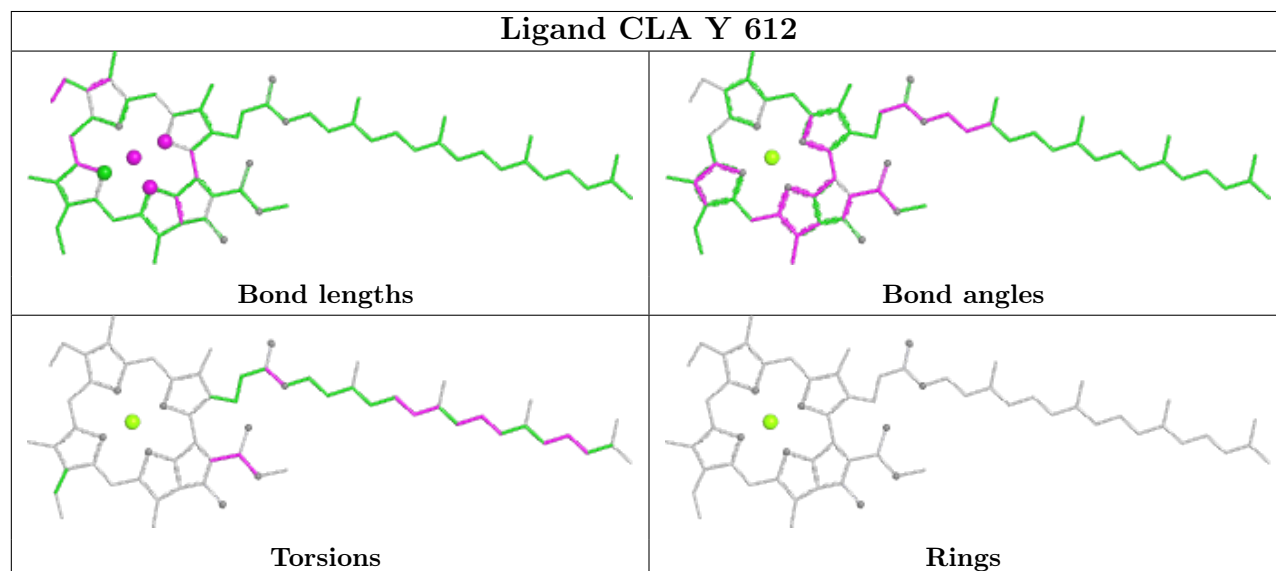
## Ligand CLA c 512

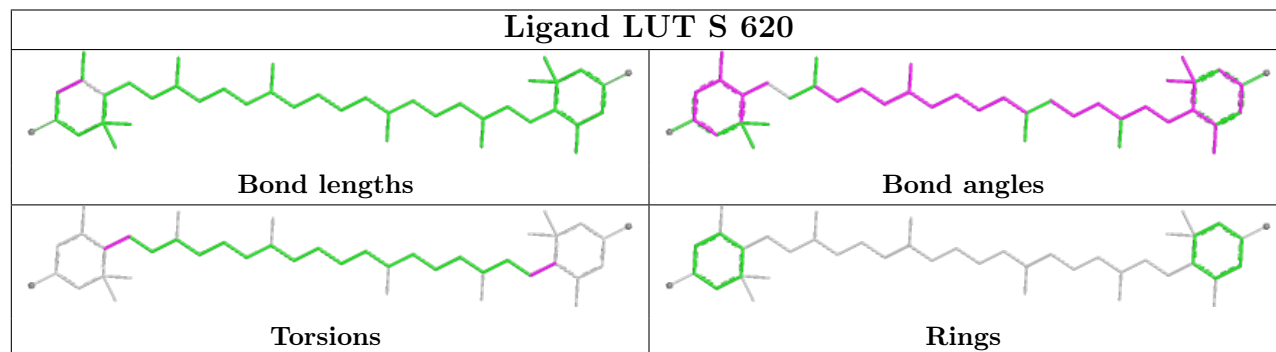
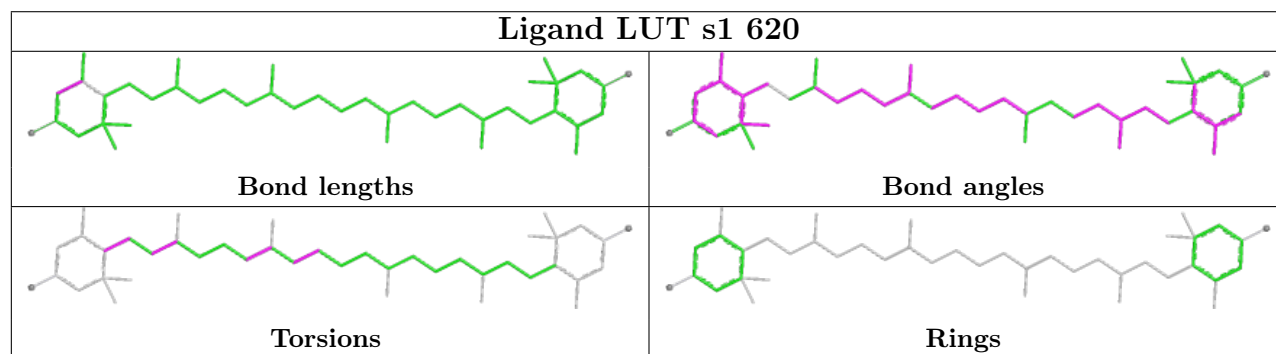
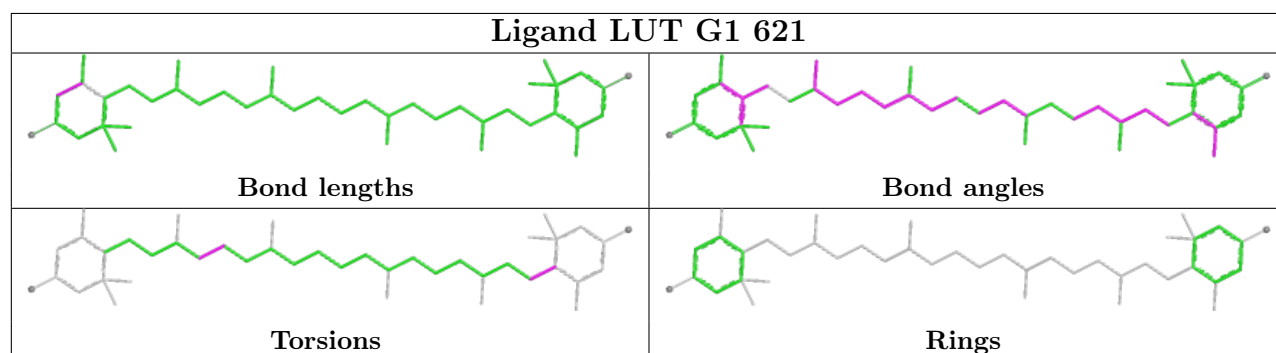
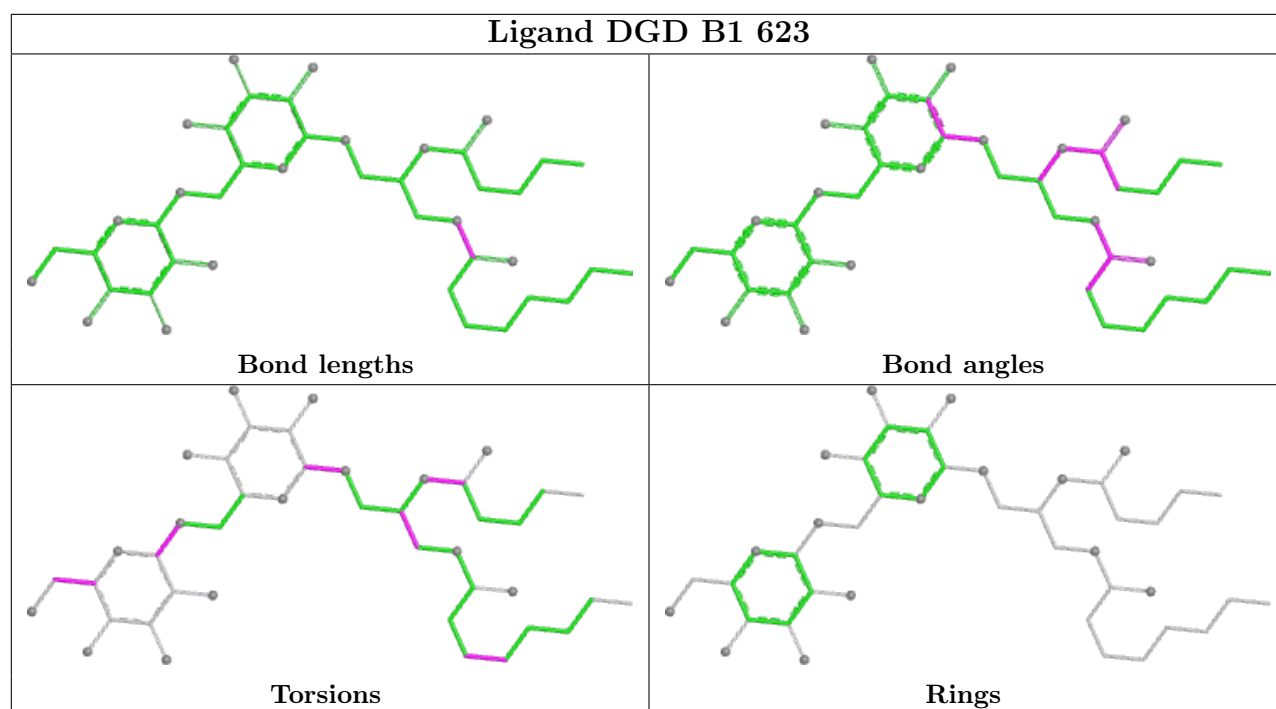


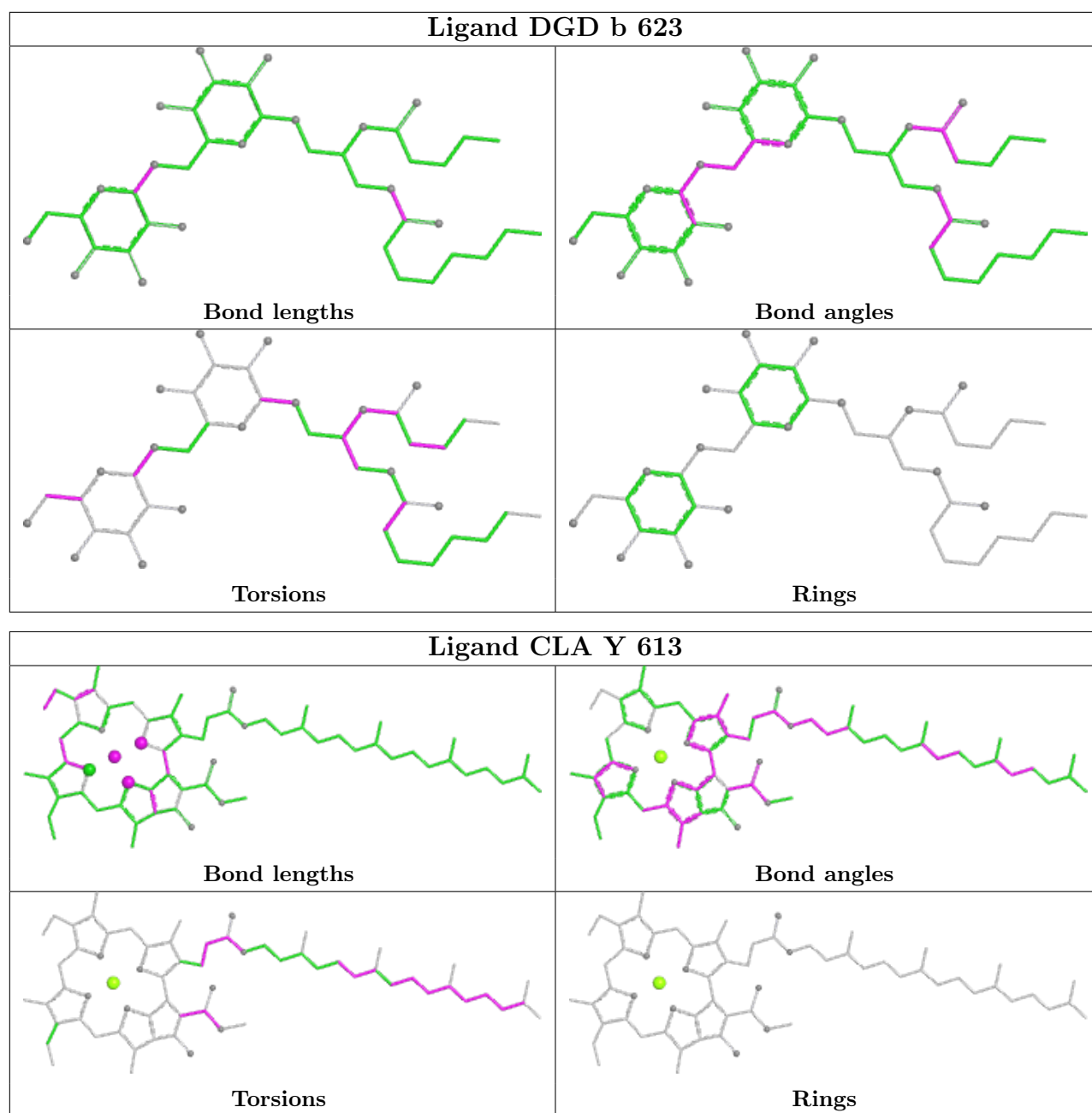
## Ligand LMG B 622



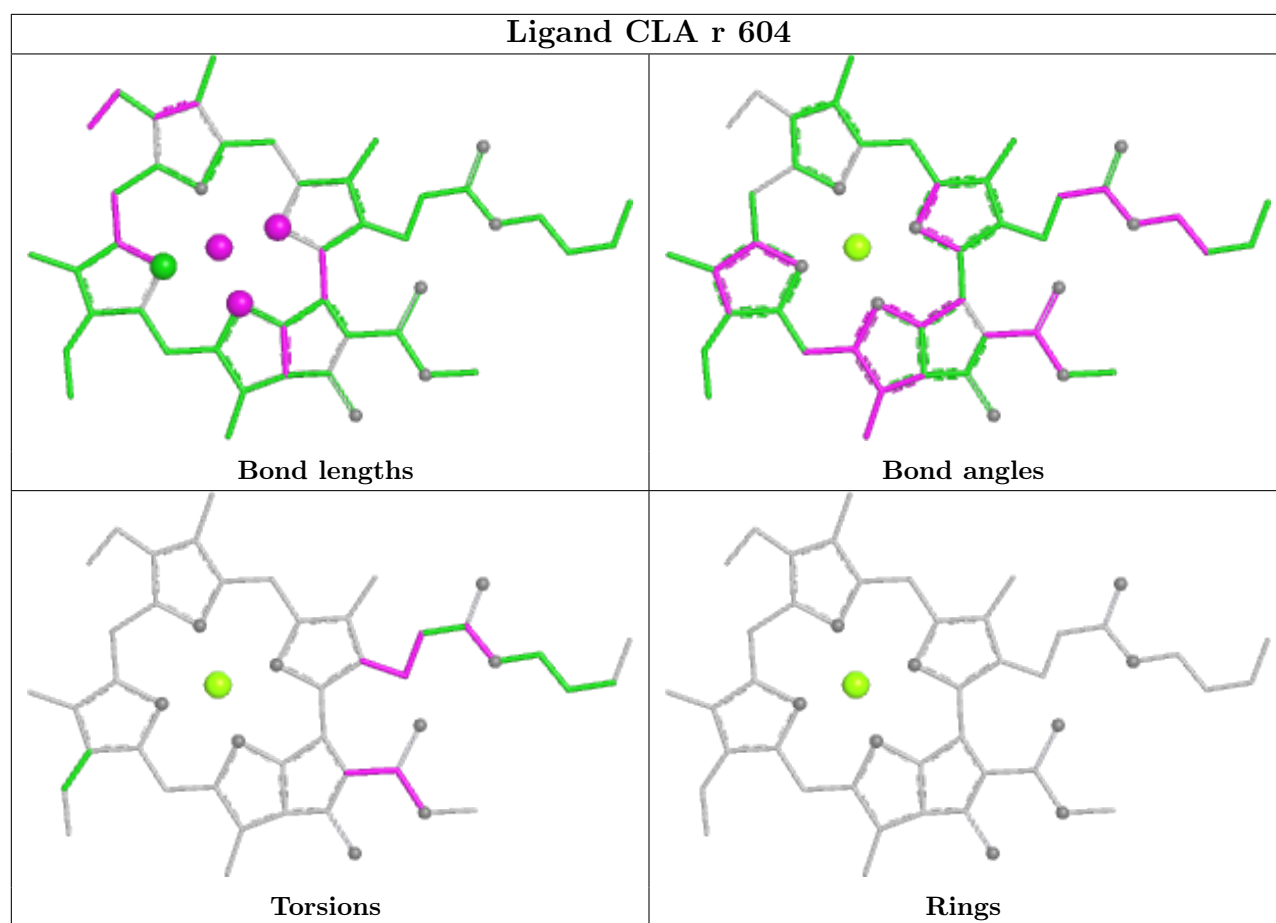
## Ligand CLA Y 612

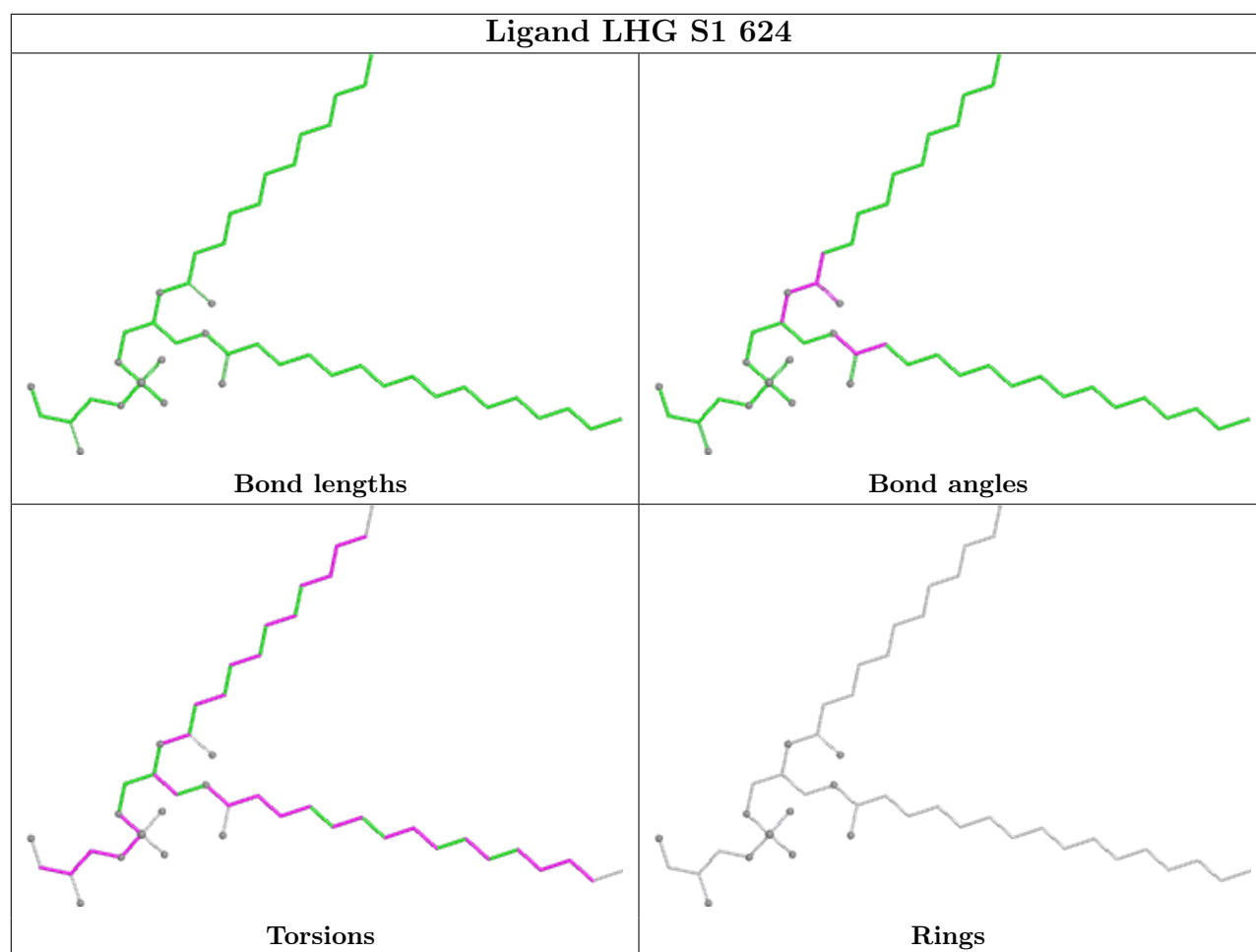


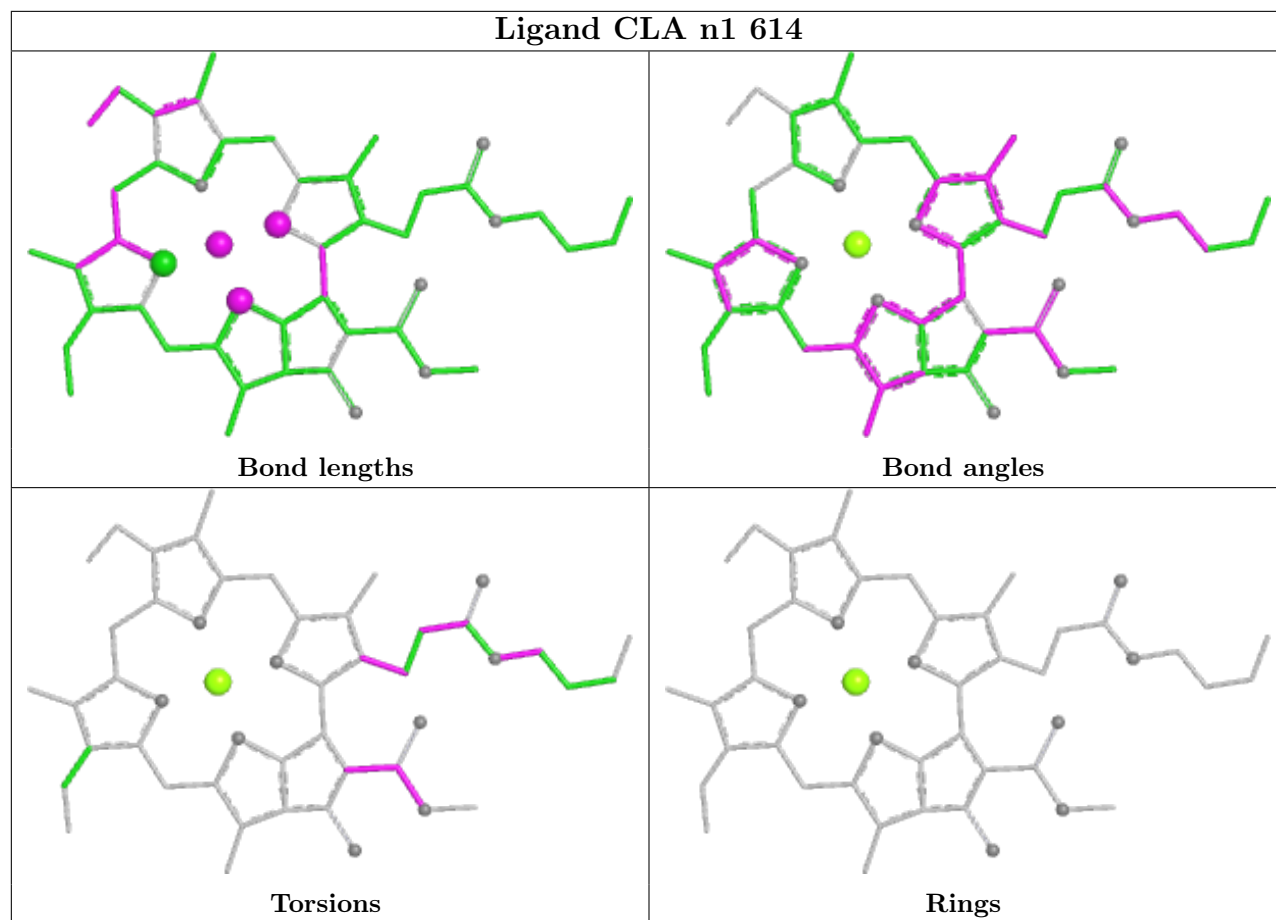


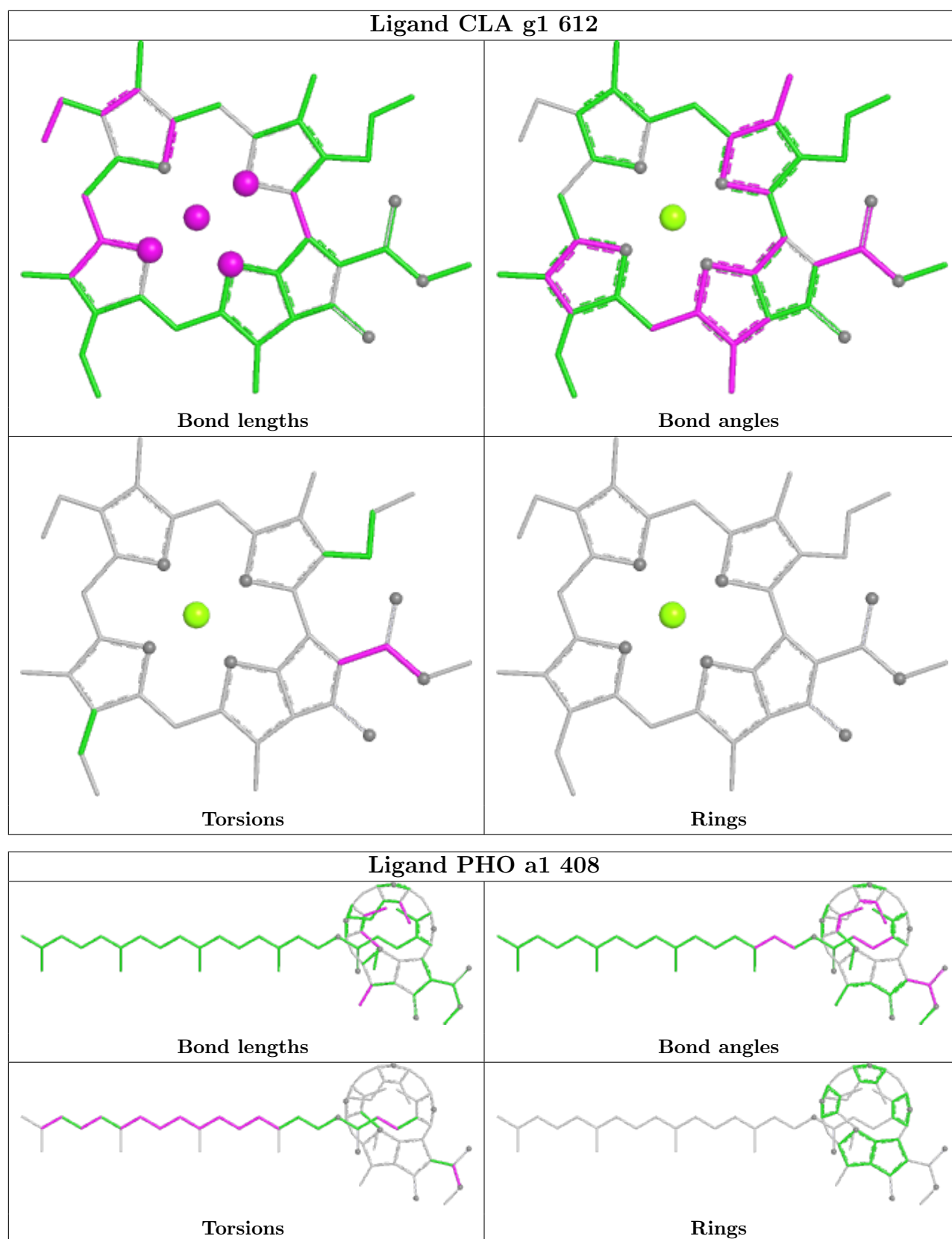


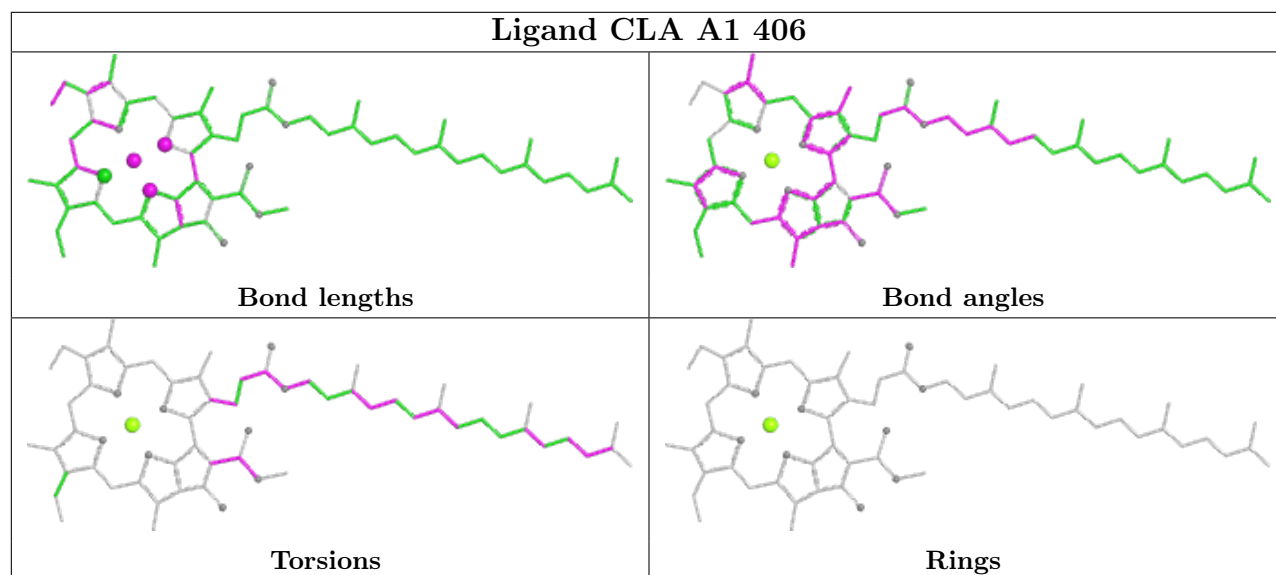
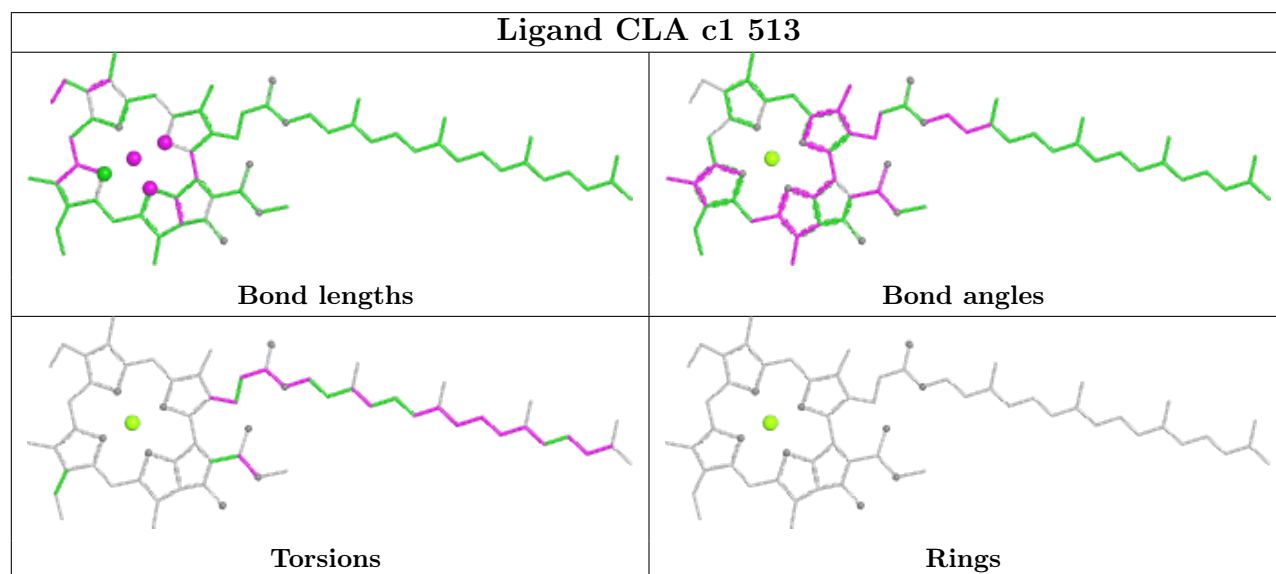
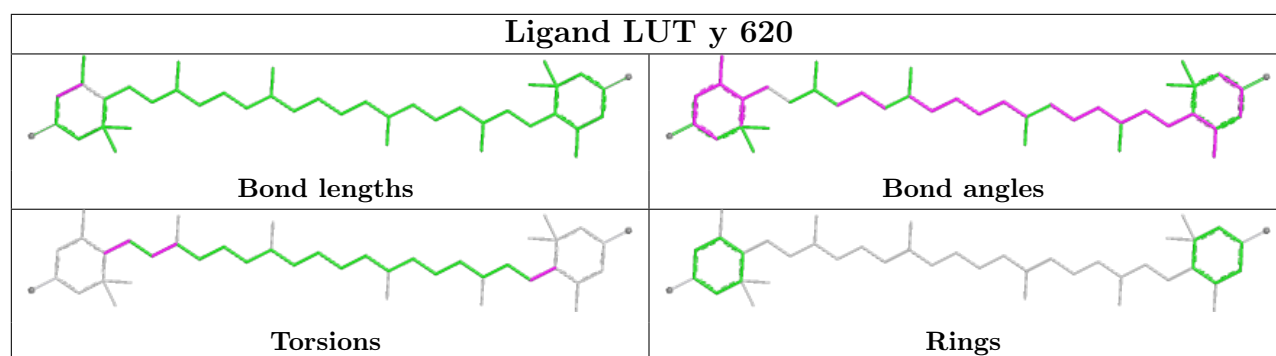


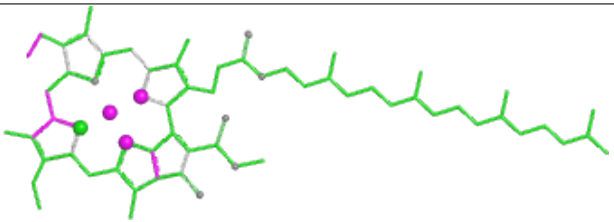
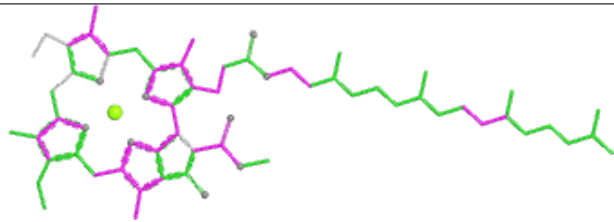
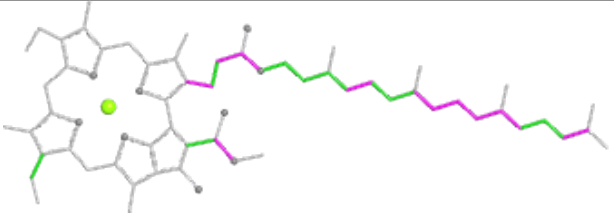
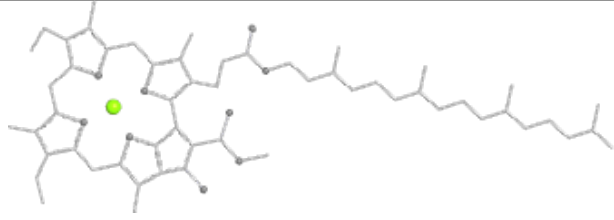


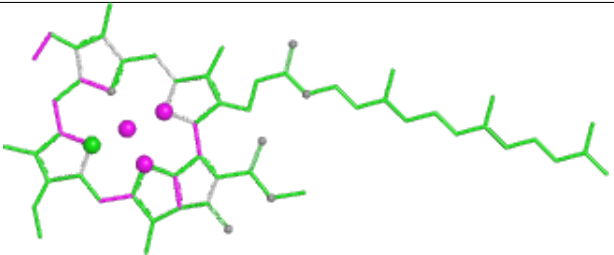
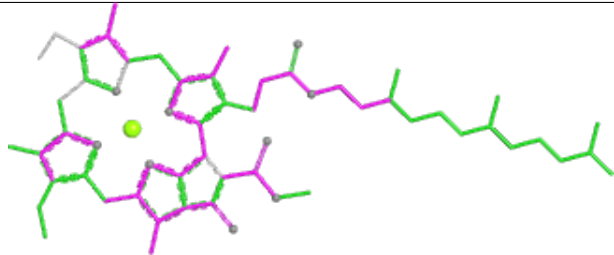
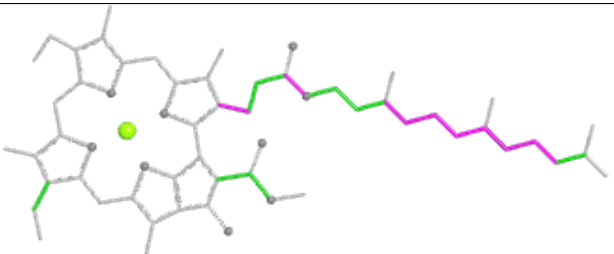
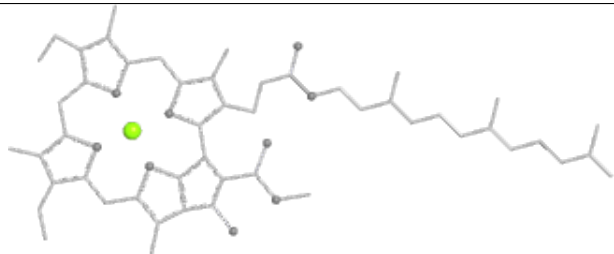


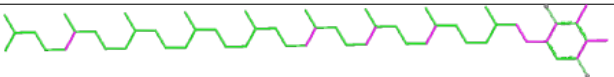
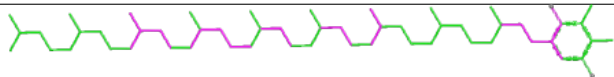
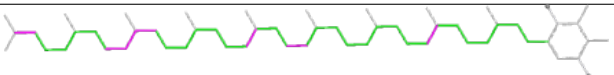
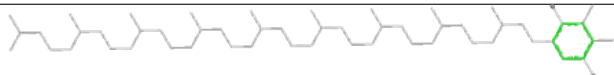


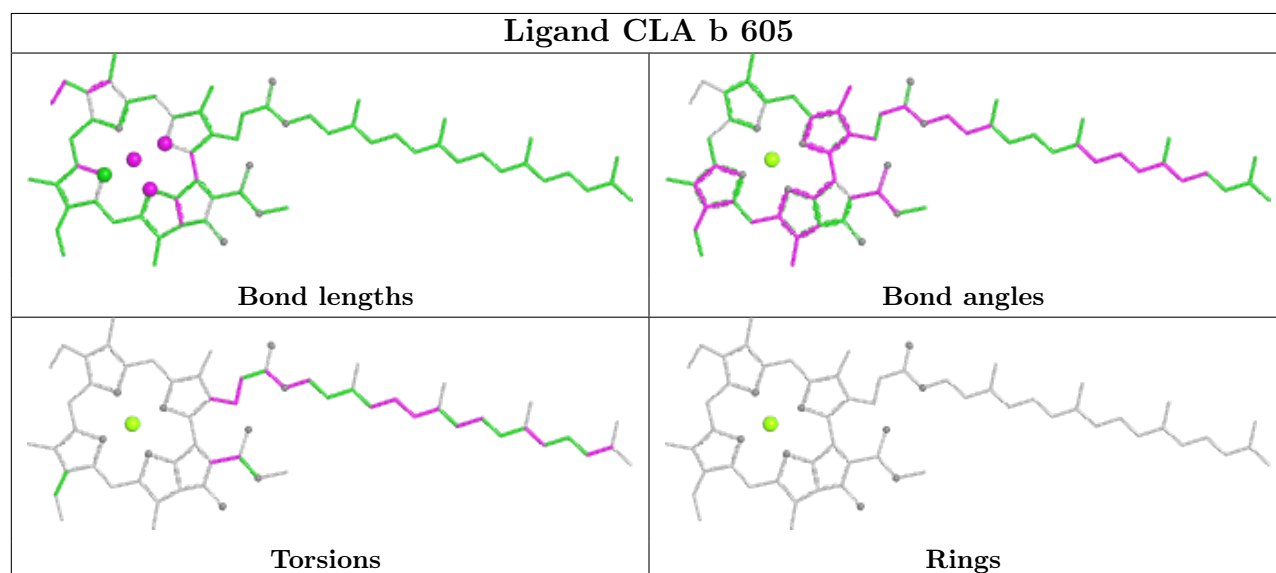
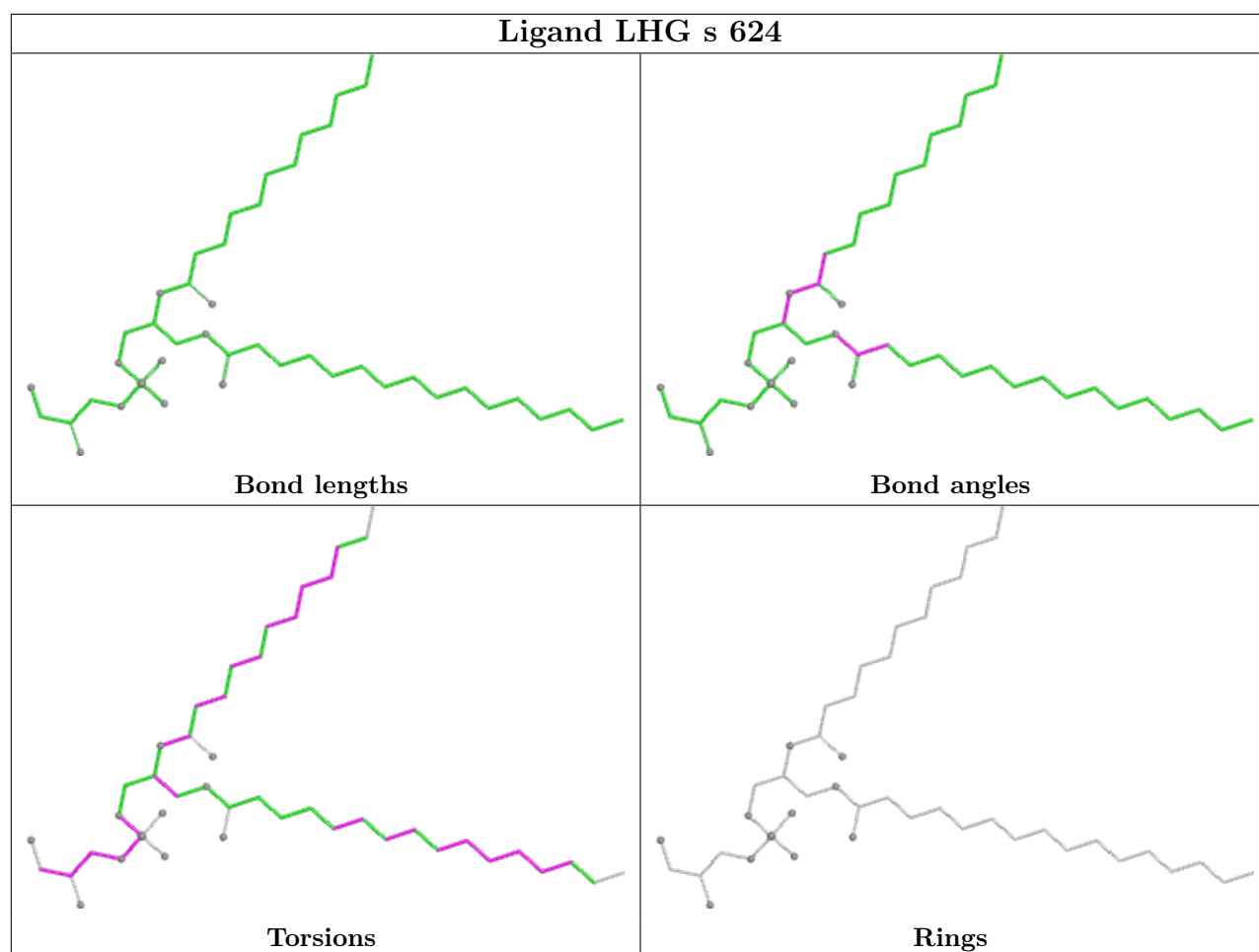


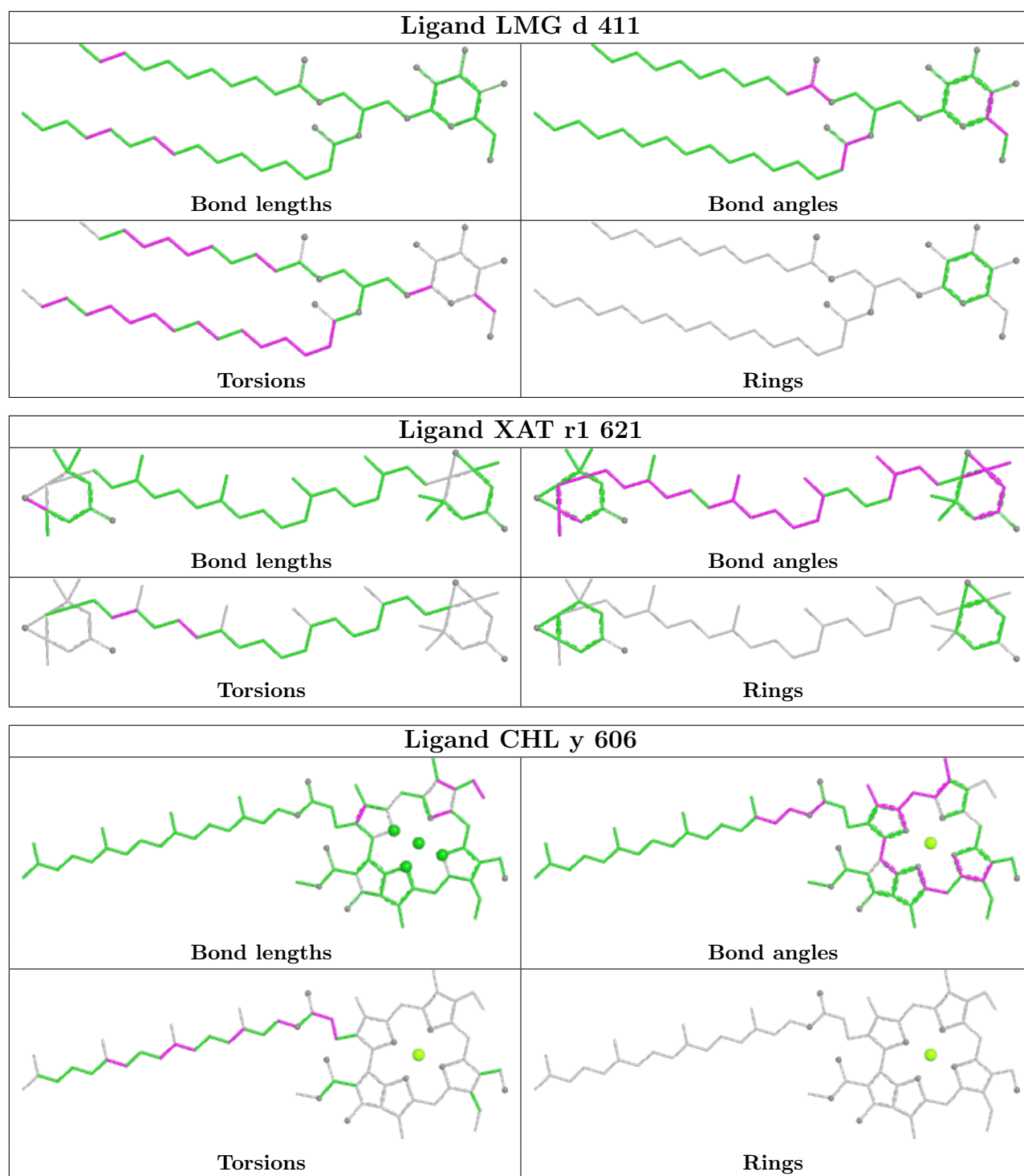


Ligand CLA C1 513	
	
Bond lengths	Bond angles
	
Torsions	Rings

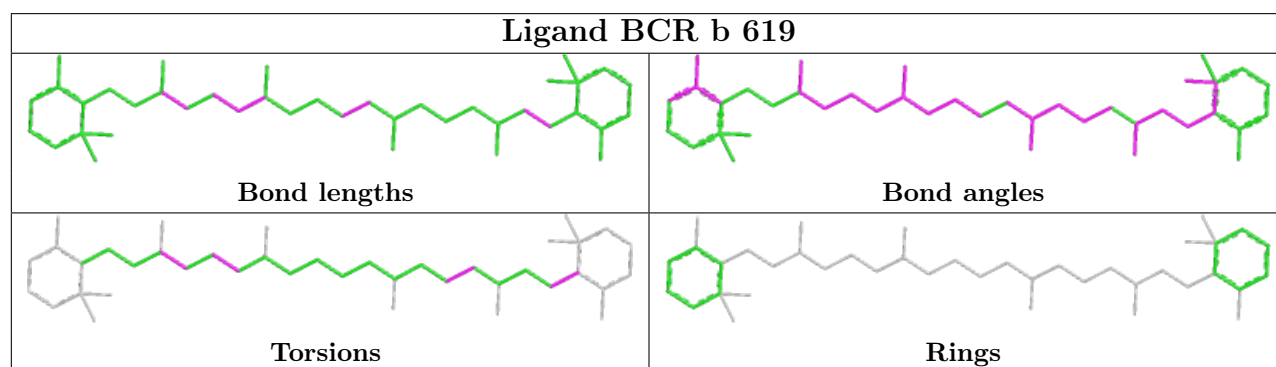
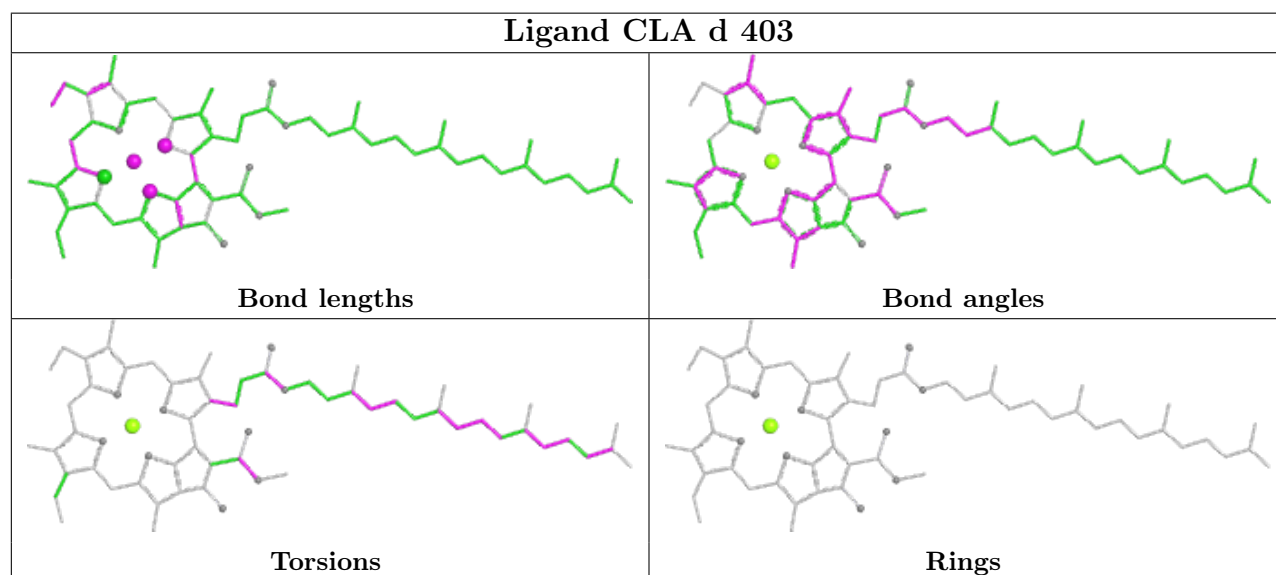
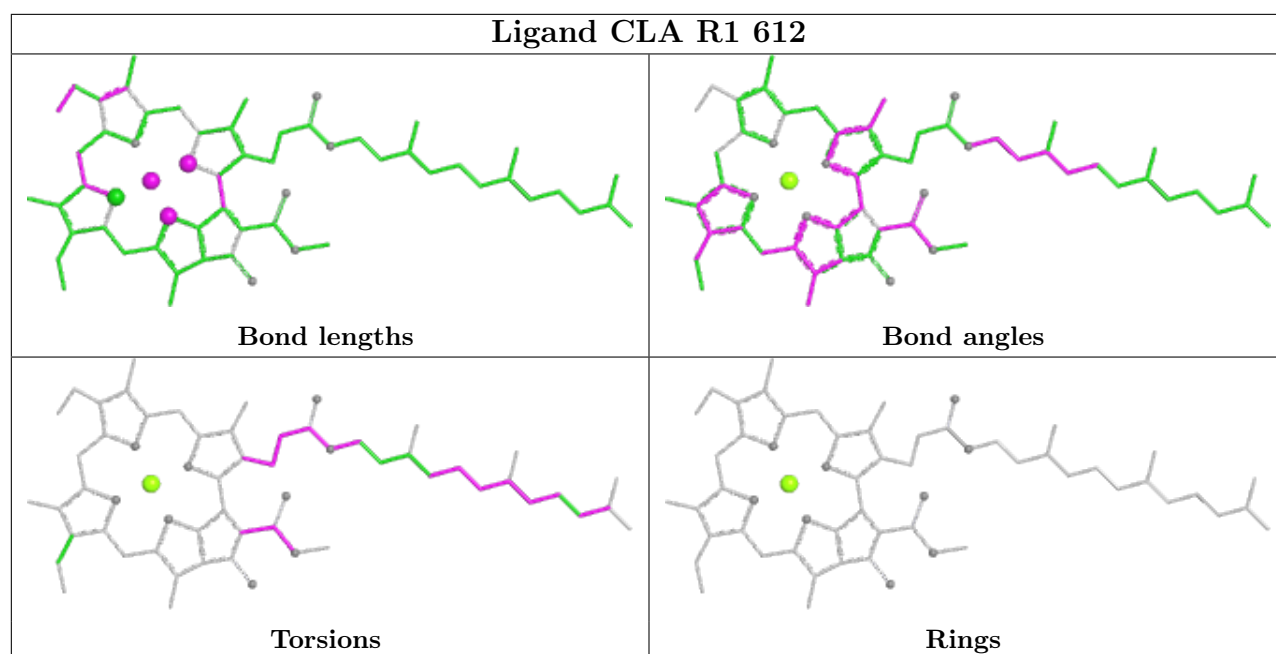
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Bond lengths	Bond angles
	
Torsions	Rings

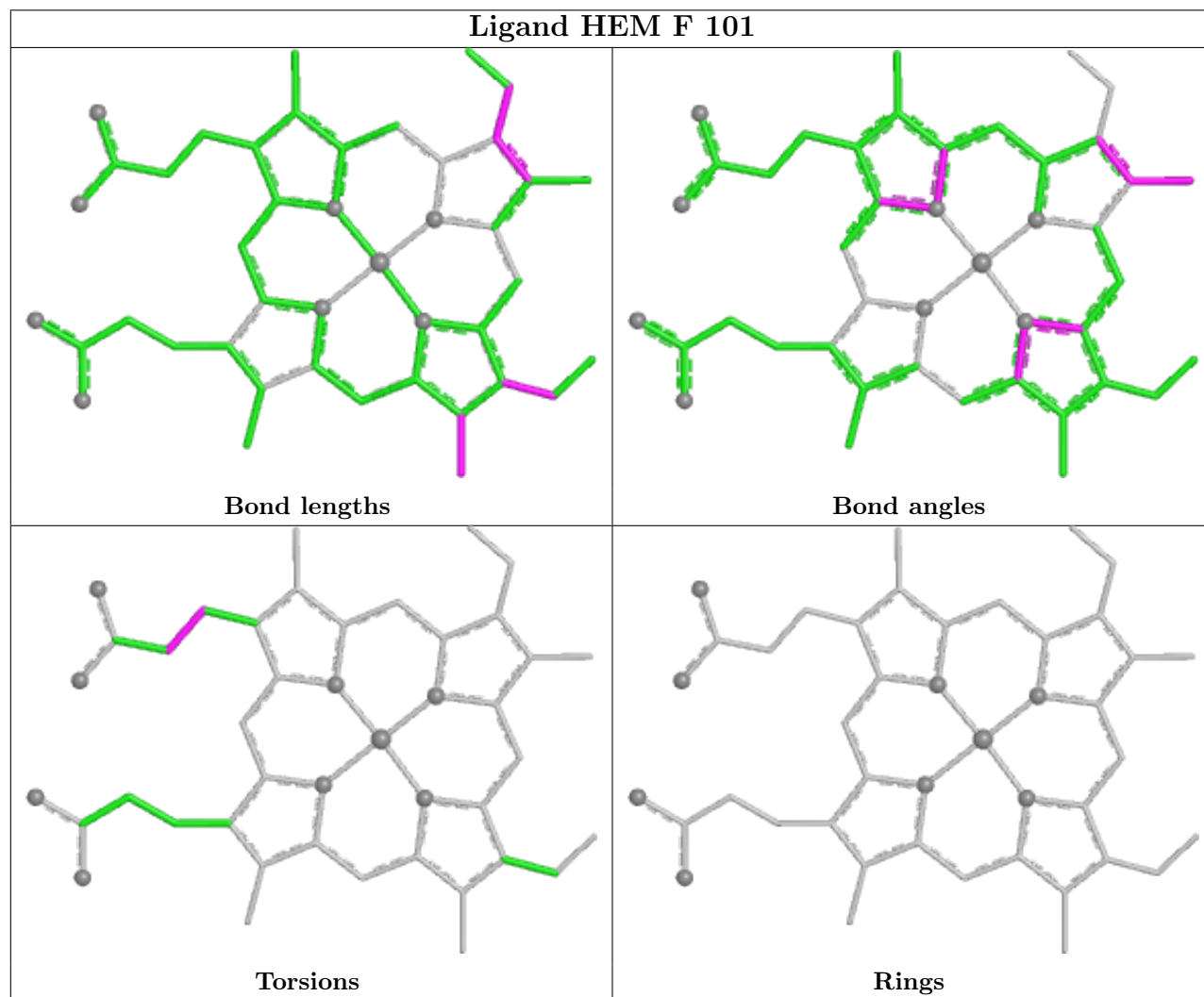
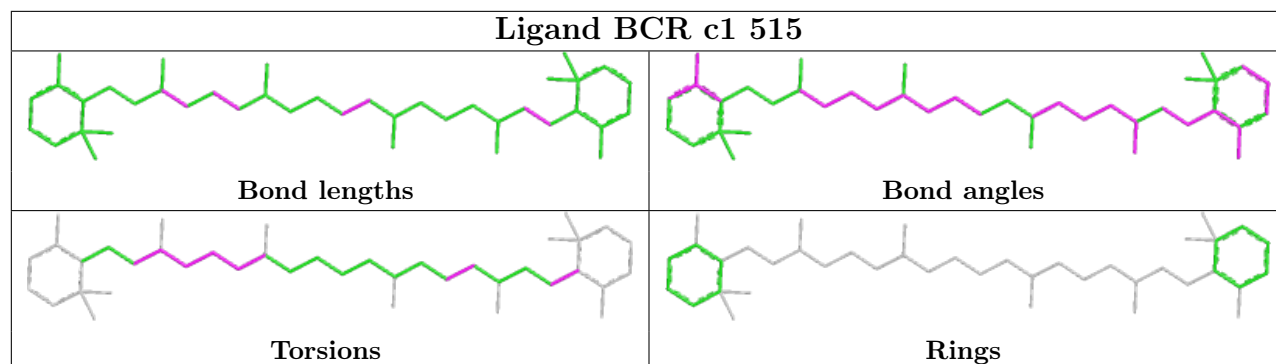
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Bond lengths	Bond angles
	
Torsions	Rings

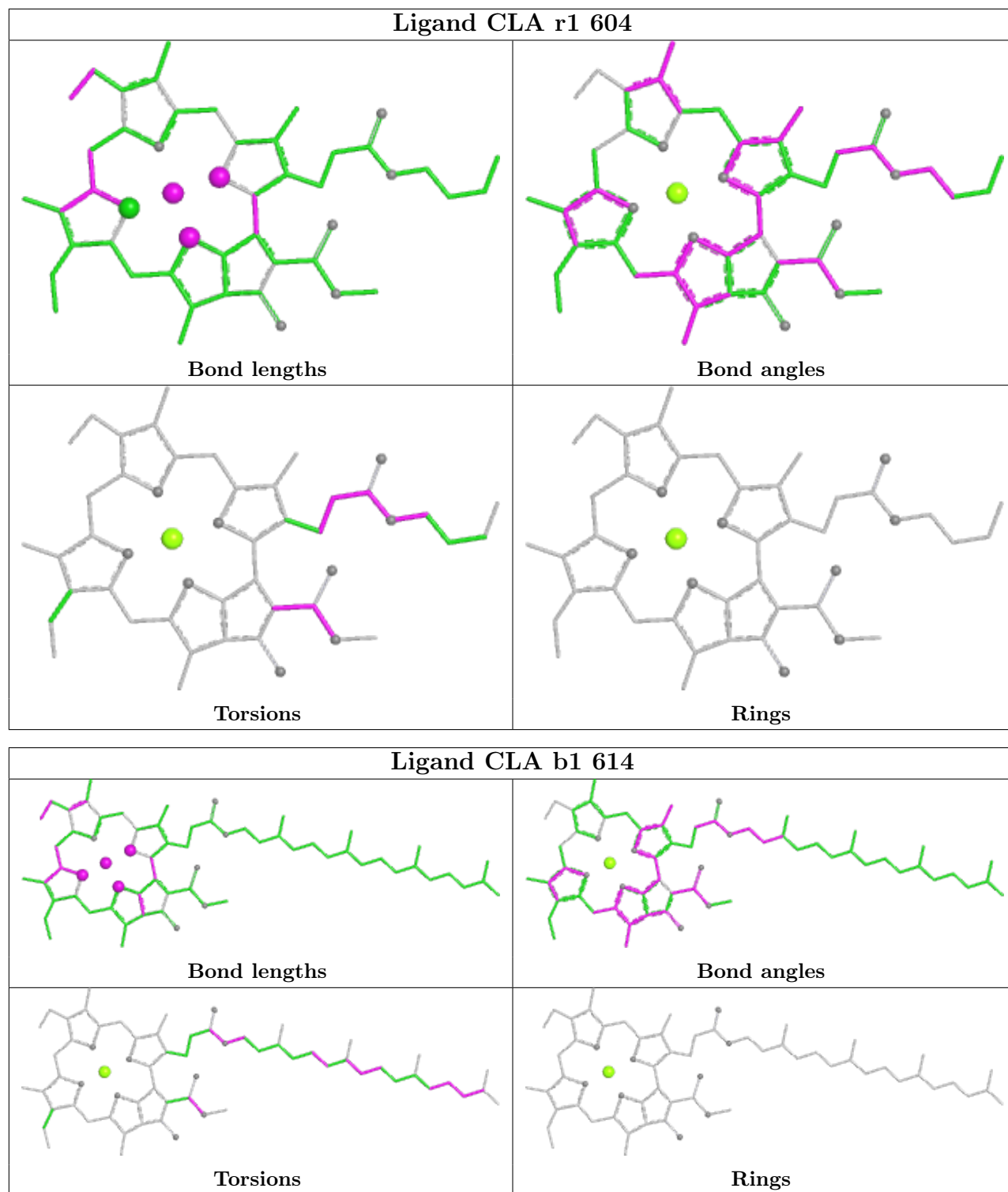


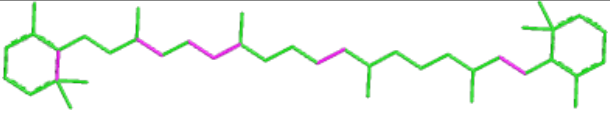
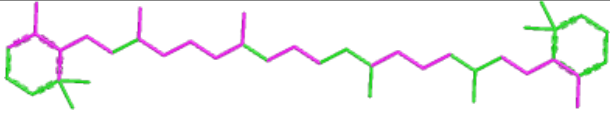
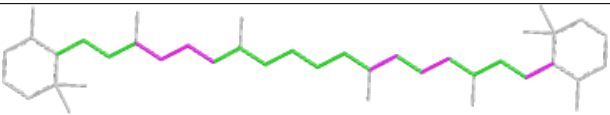
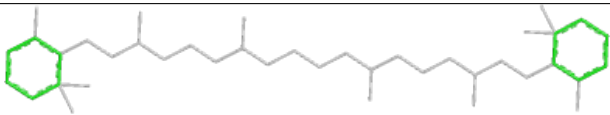
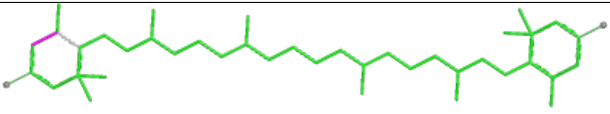
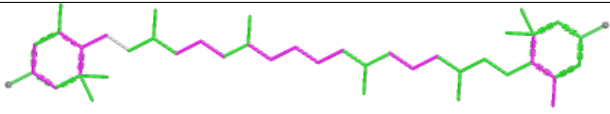
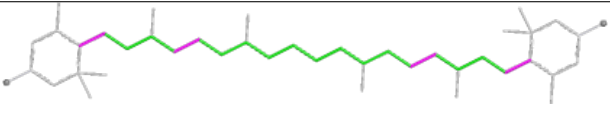
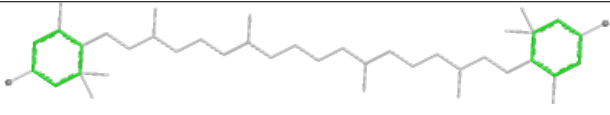
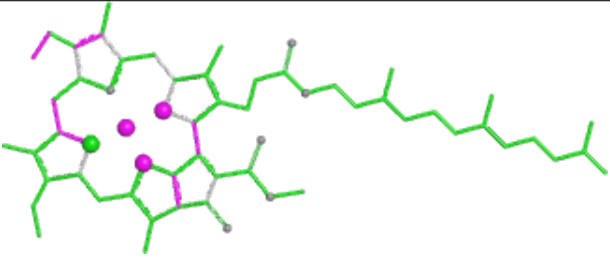
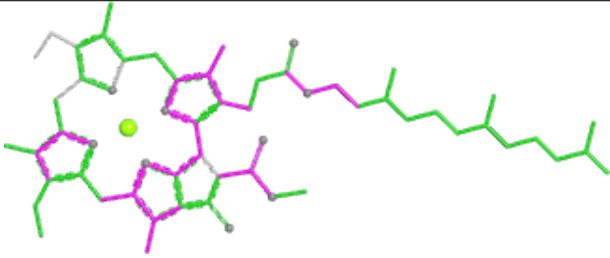
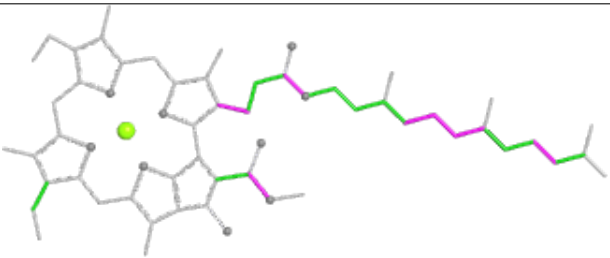
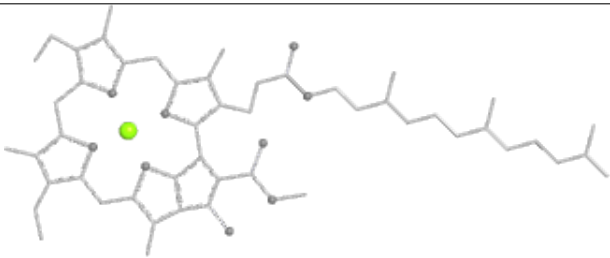


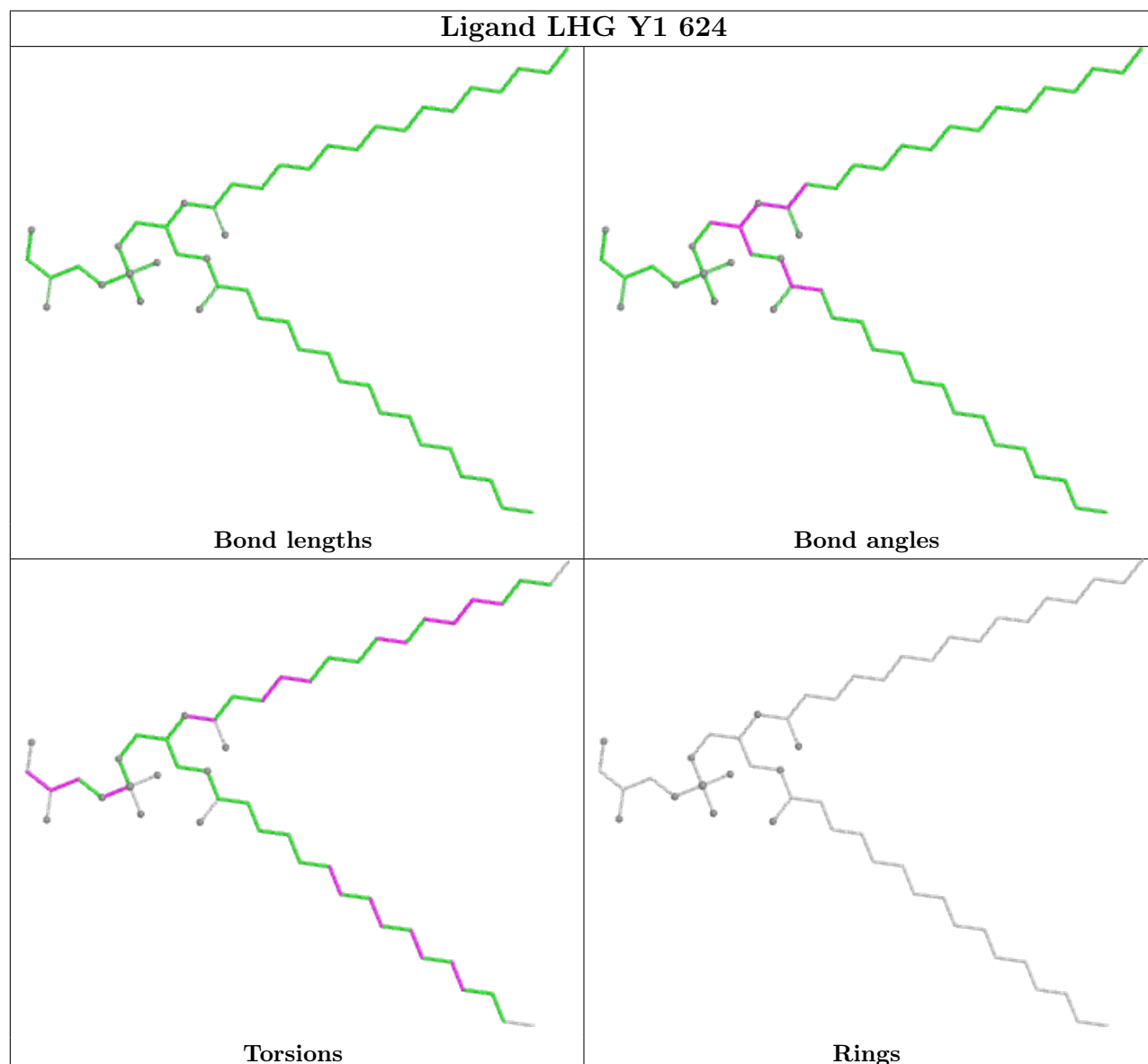
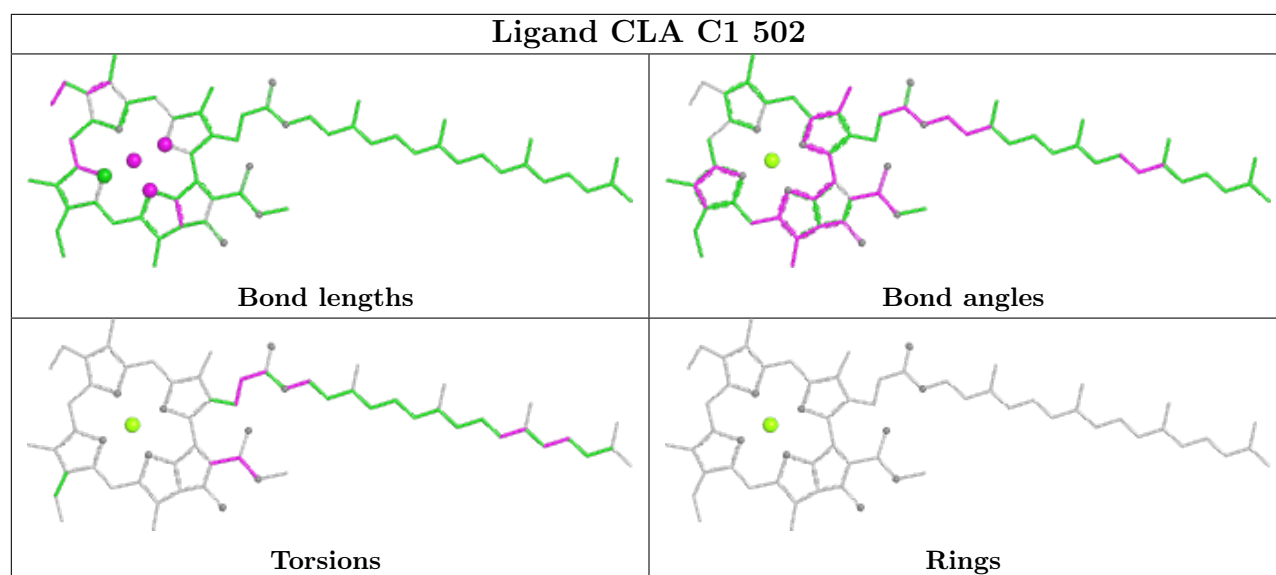


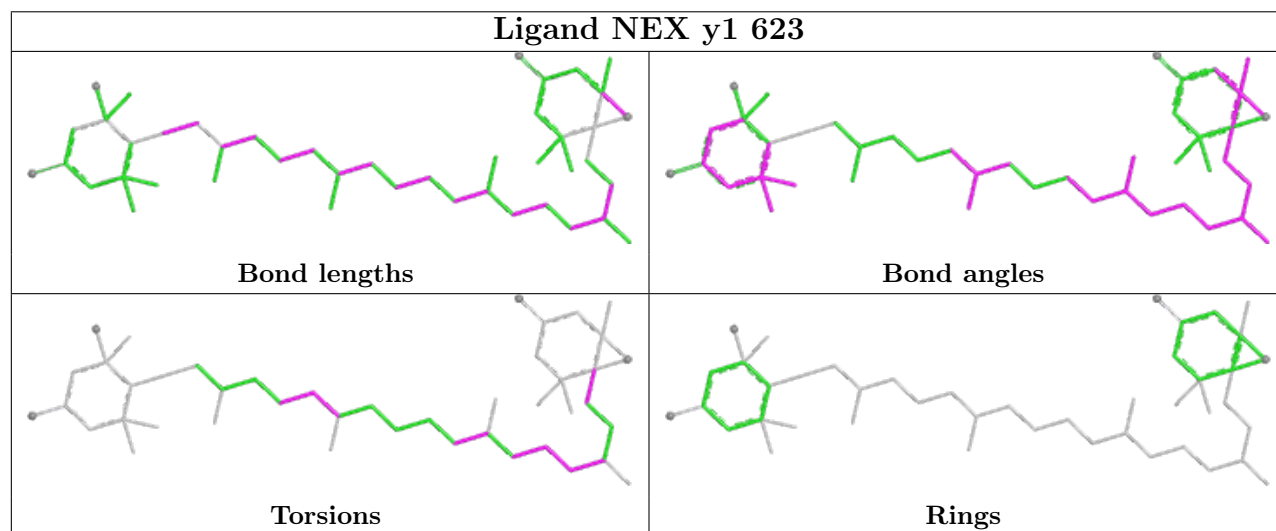
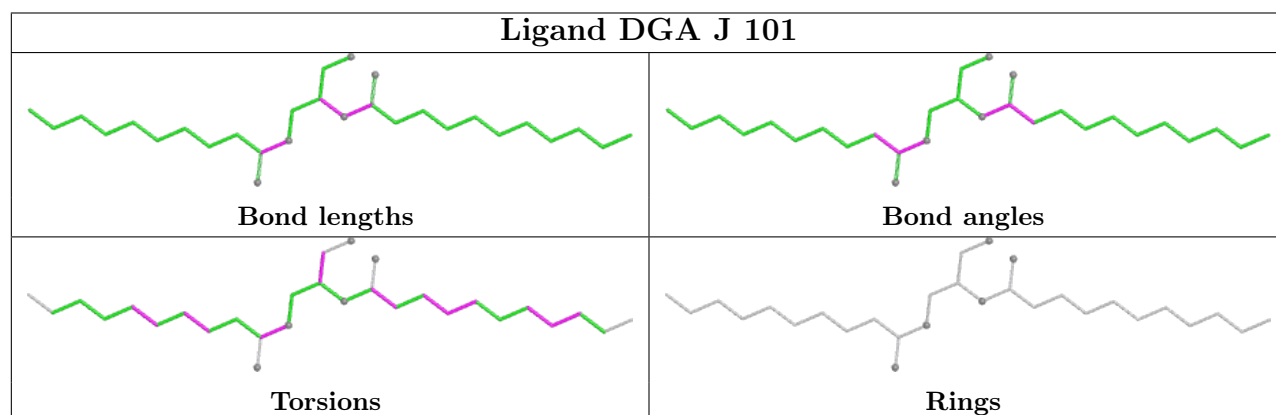
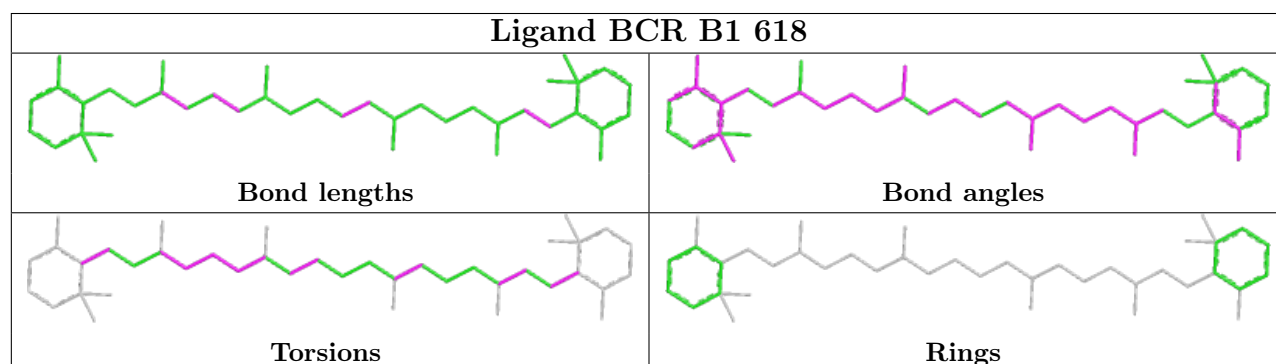
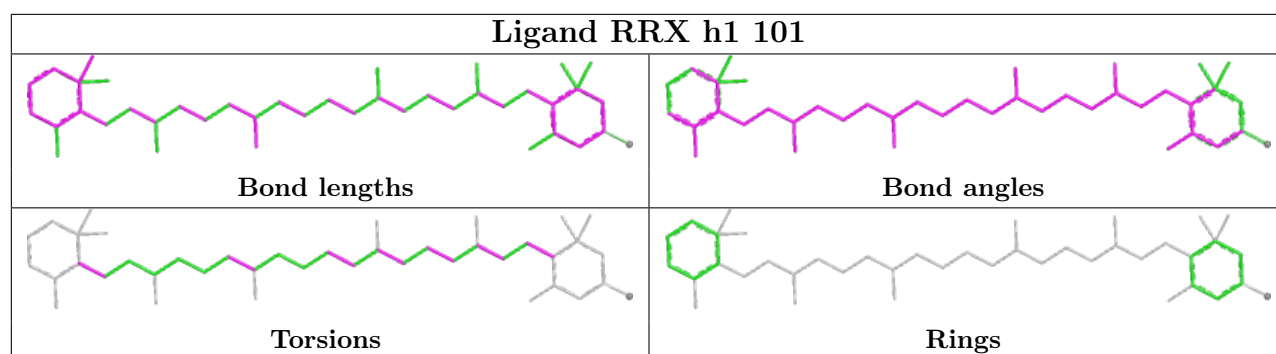




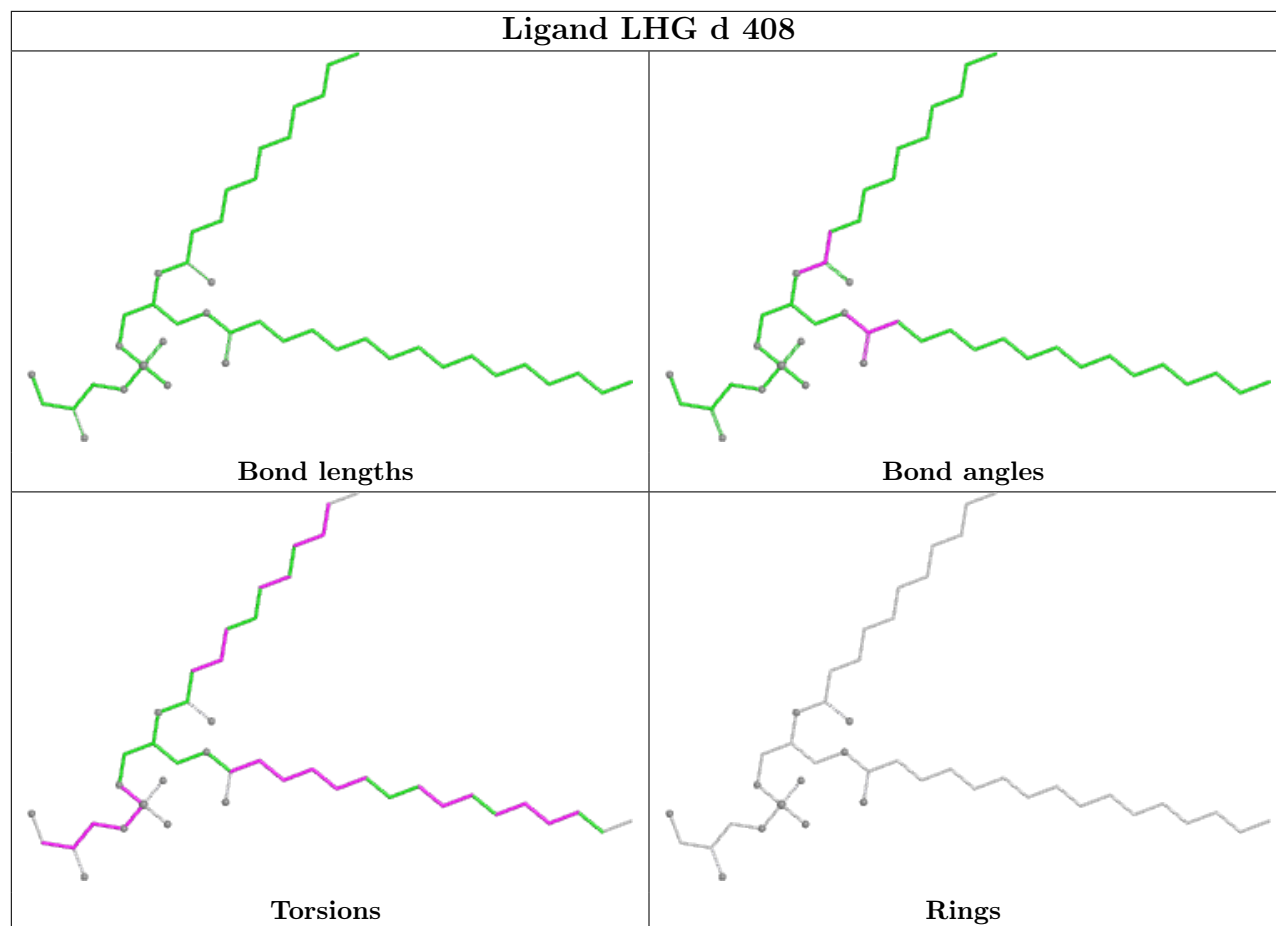


Ligand BCR C 515	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LUT S1 620	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA S 609	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

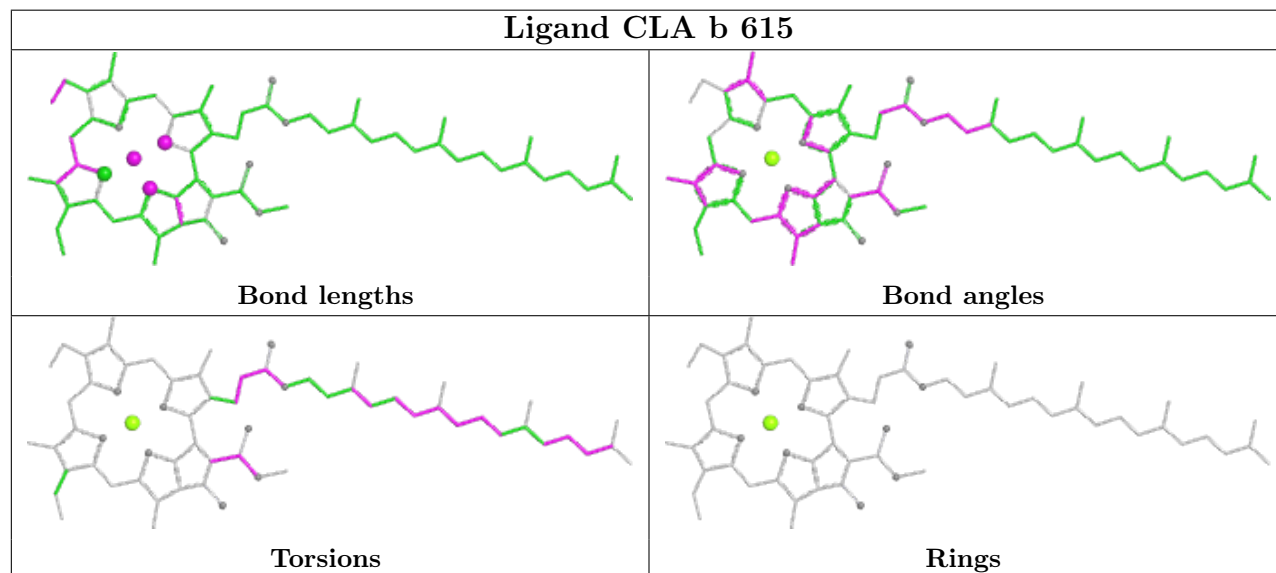


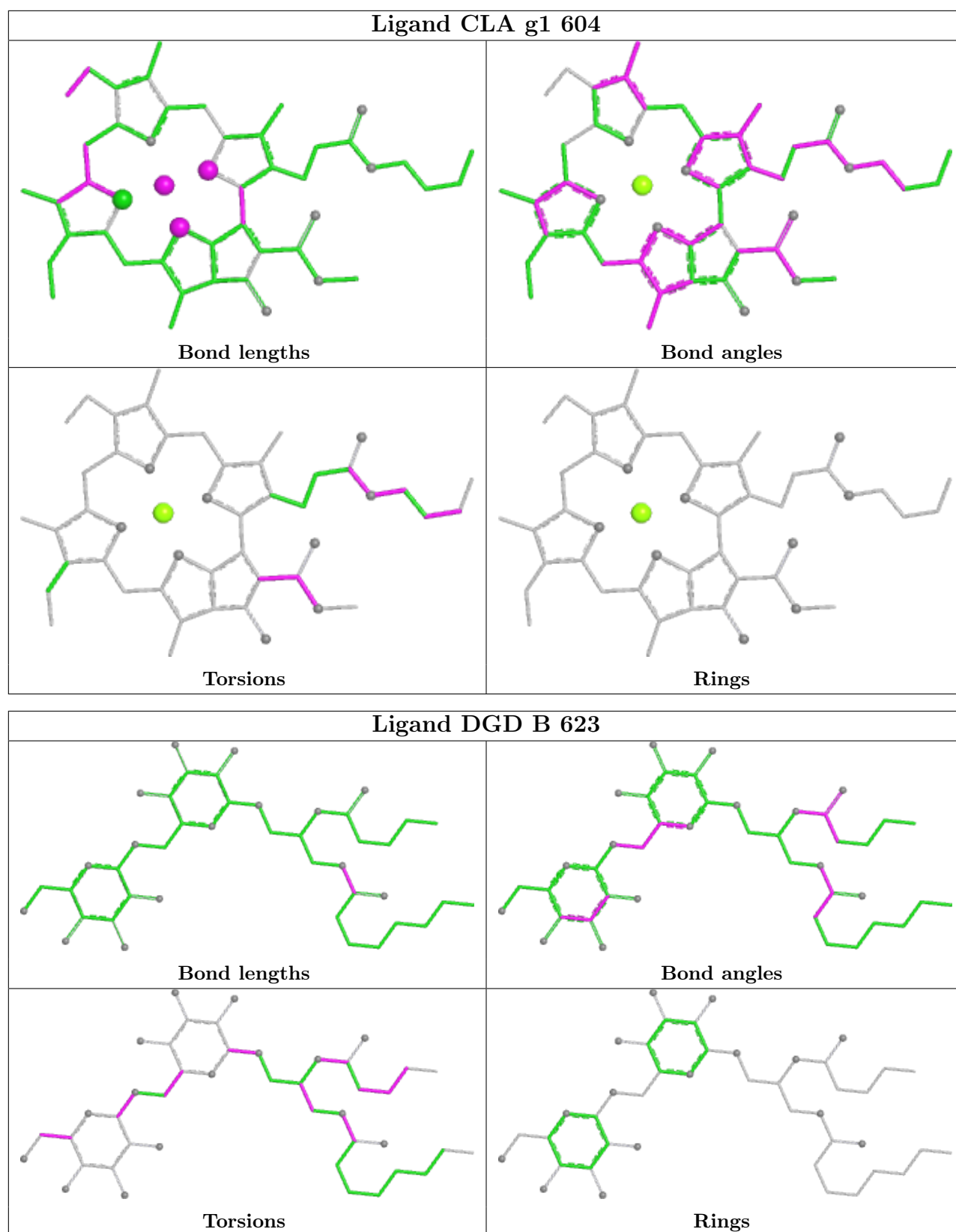


## Ligand LHG d 408

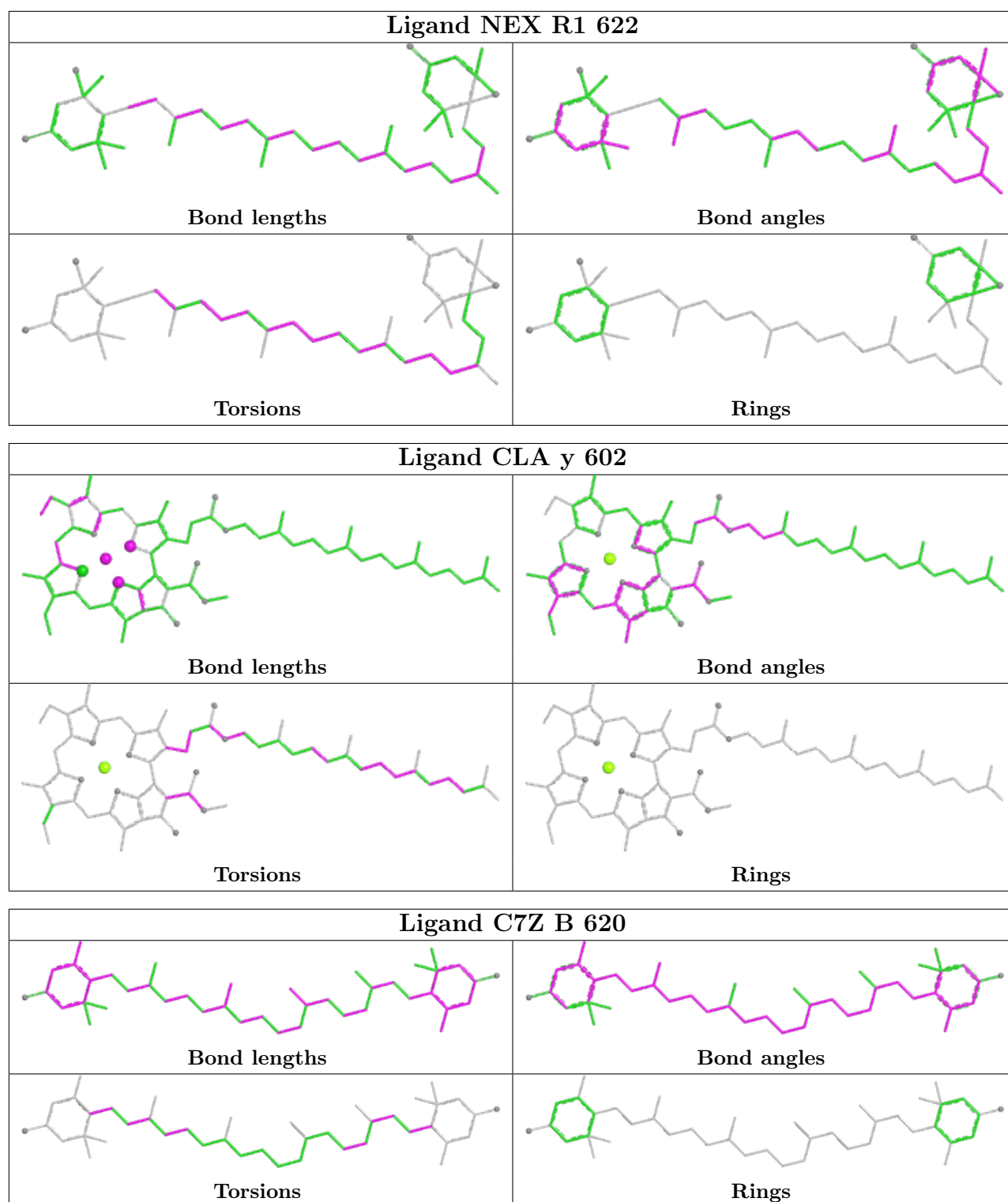


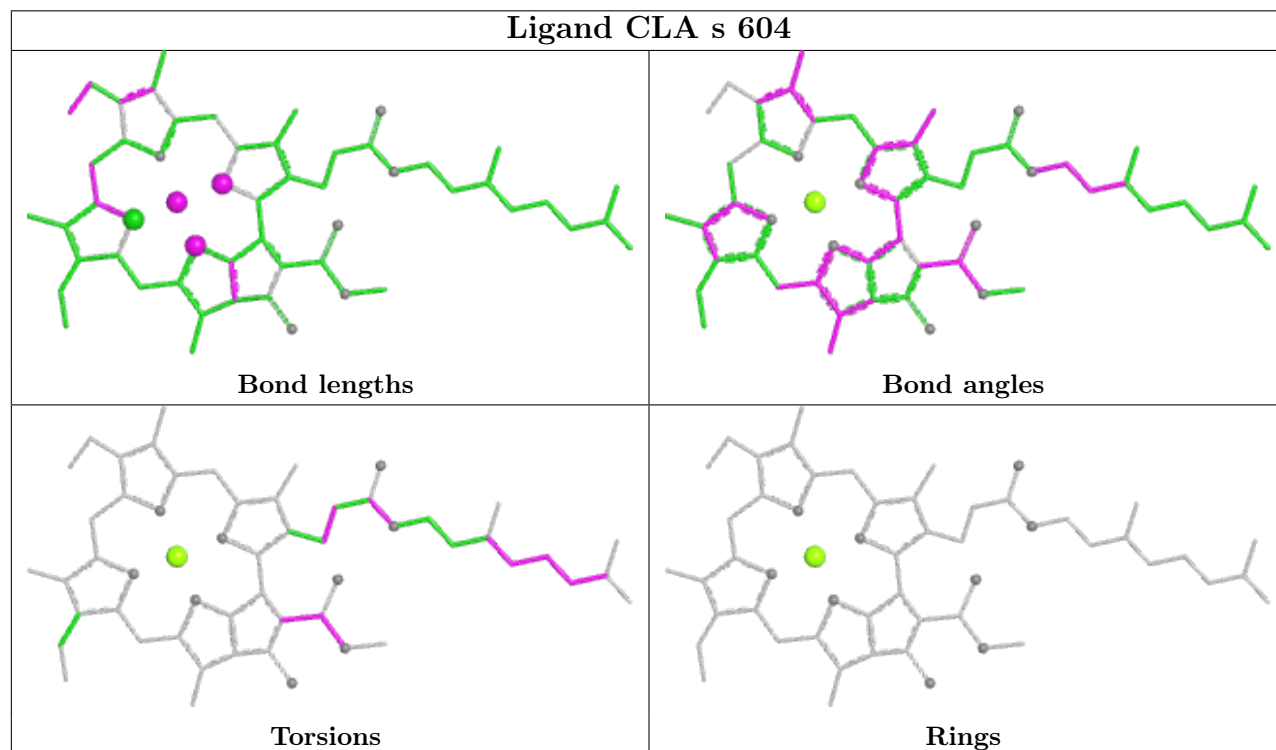
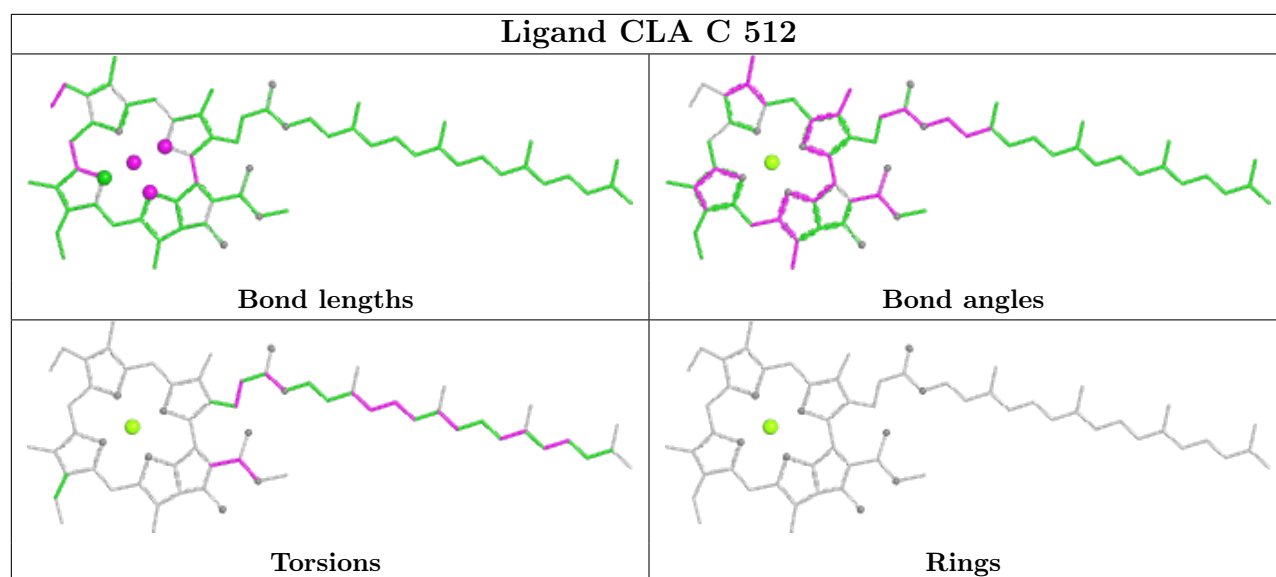
## Ligand CLA b 615

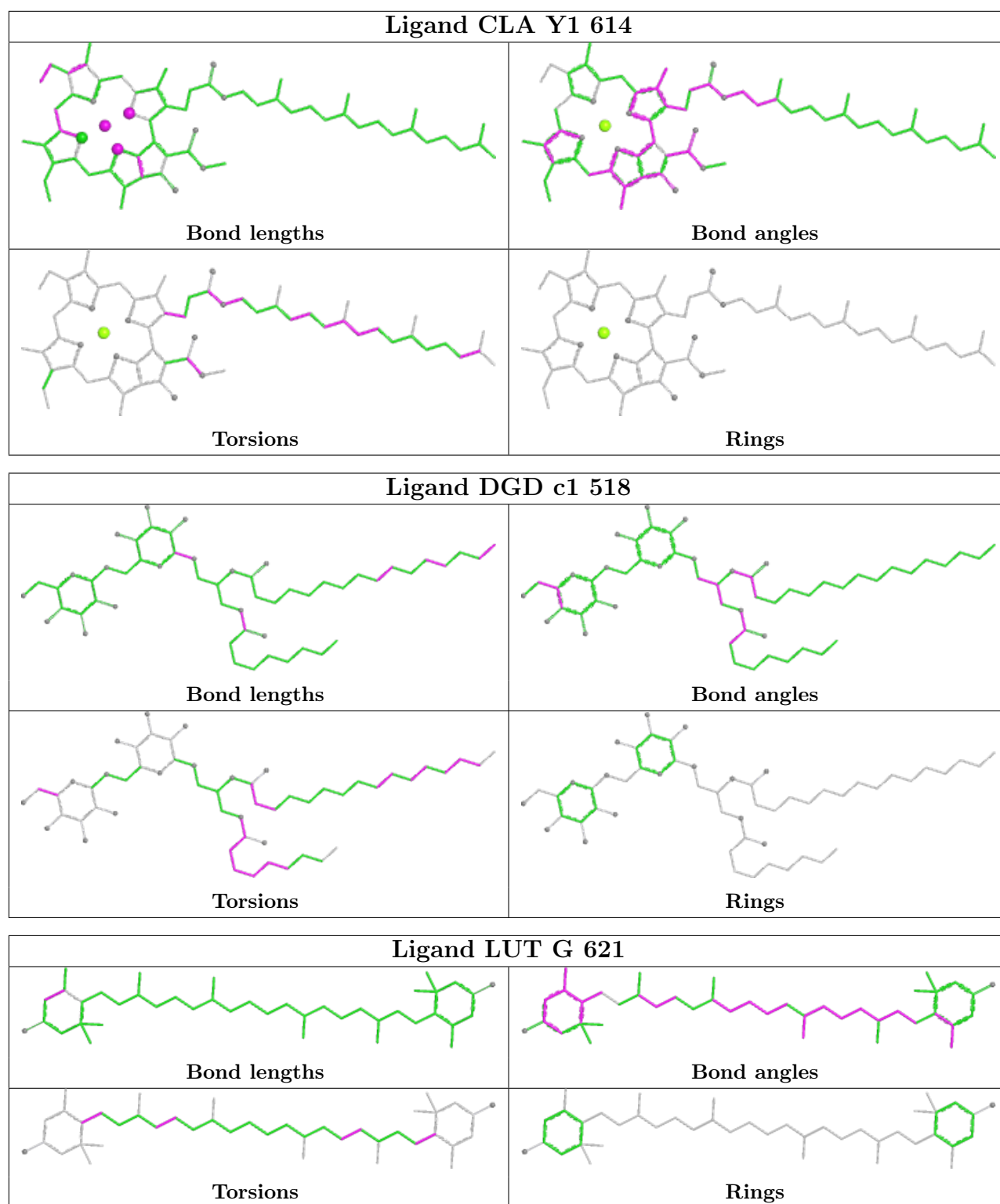




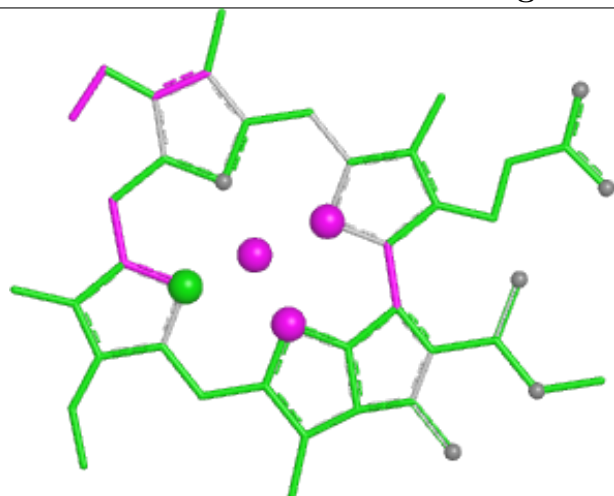




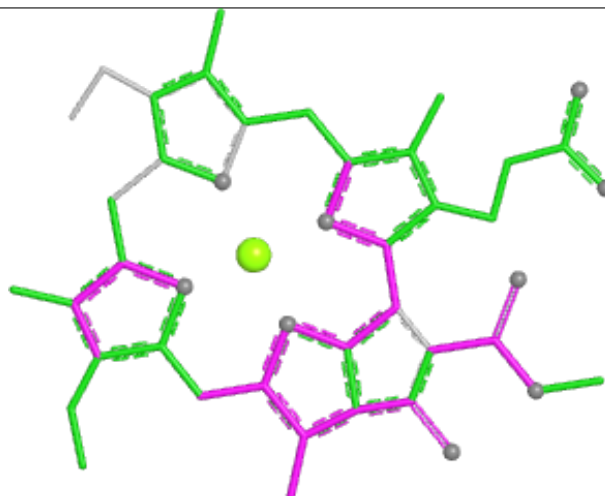




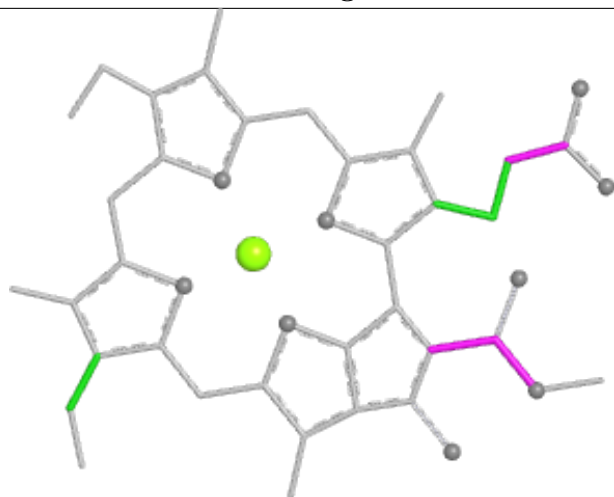
## Ligand CLA n 612



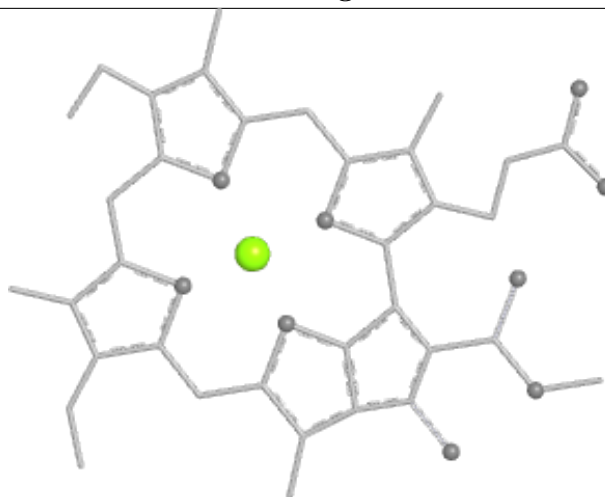
Bond lengths



Bond angles

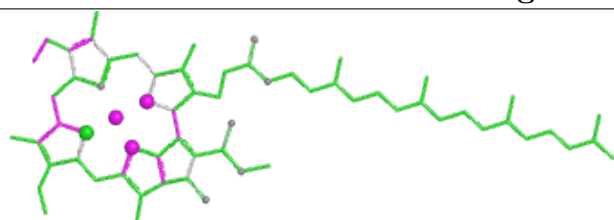


Torsions

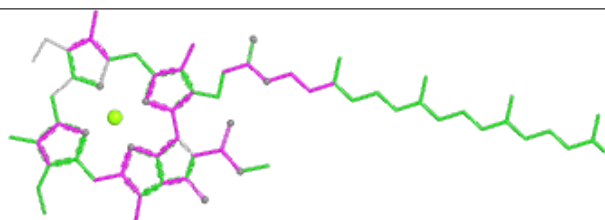


Rings

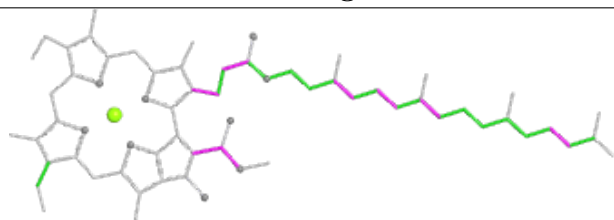
## Ligand CLA b 609



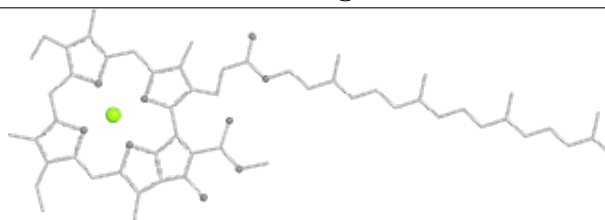
Bond lengths



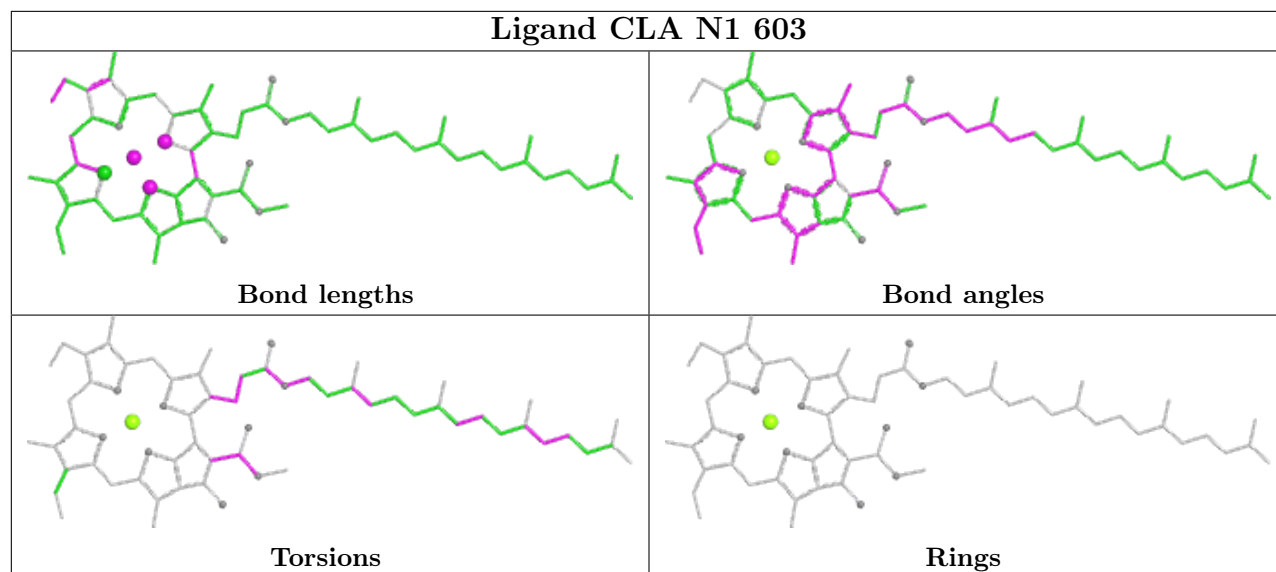
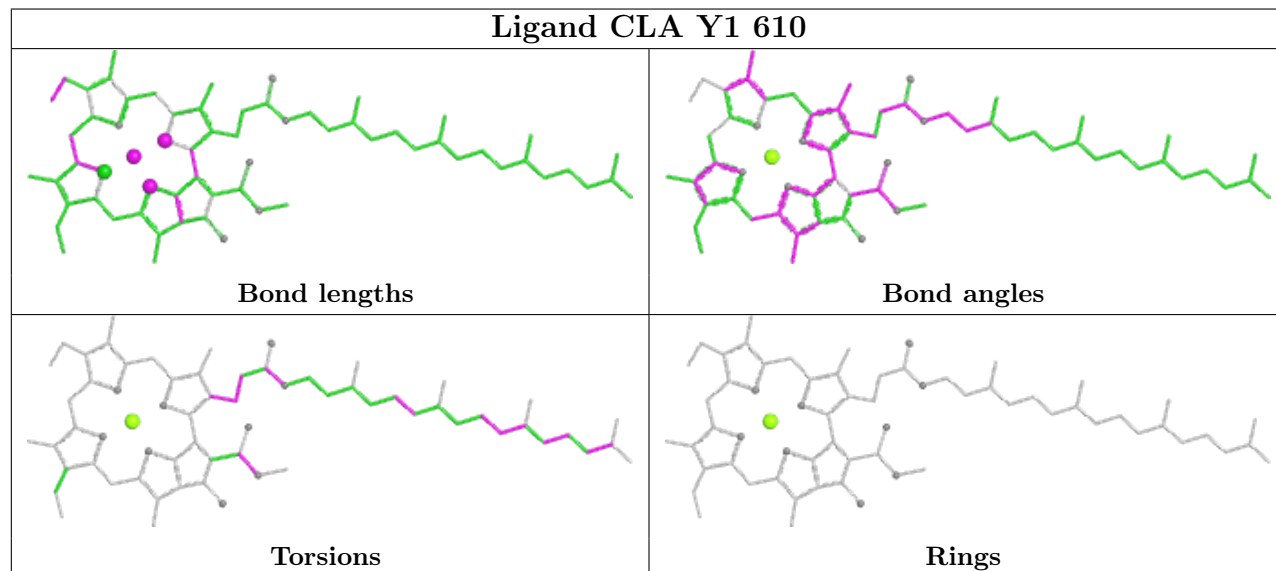
Bond angles

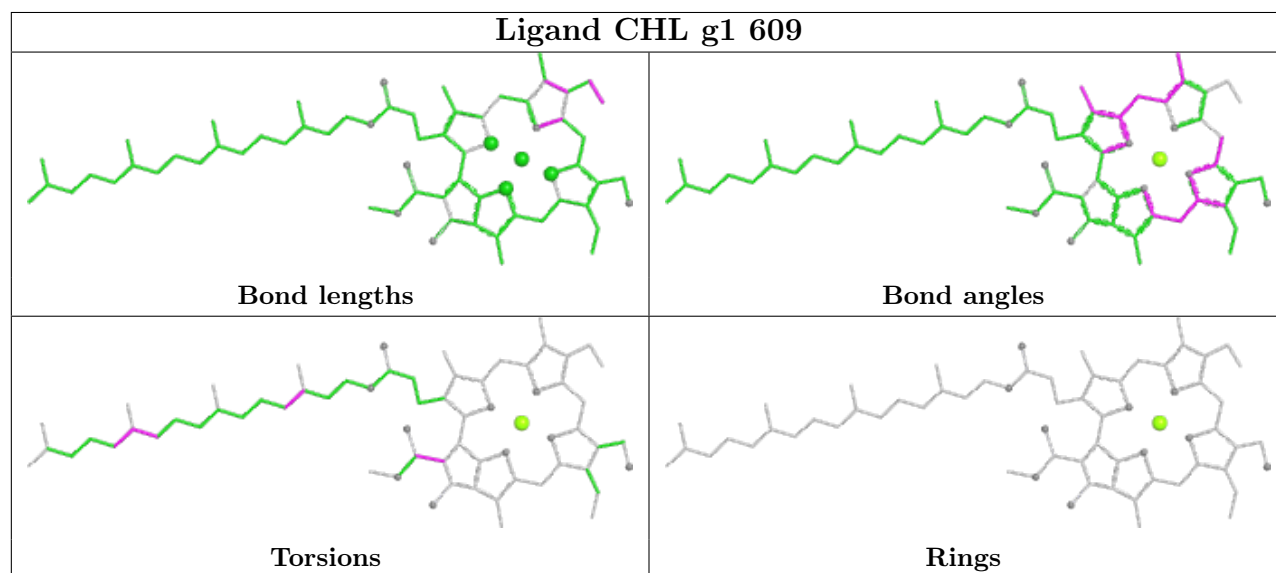
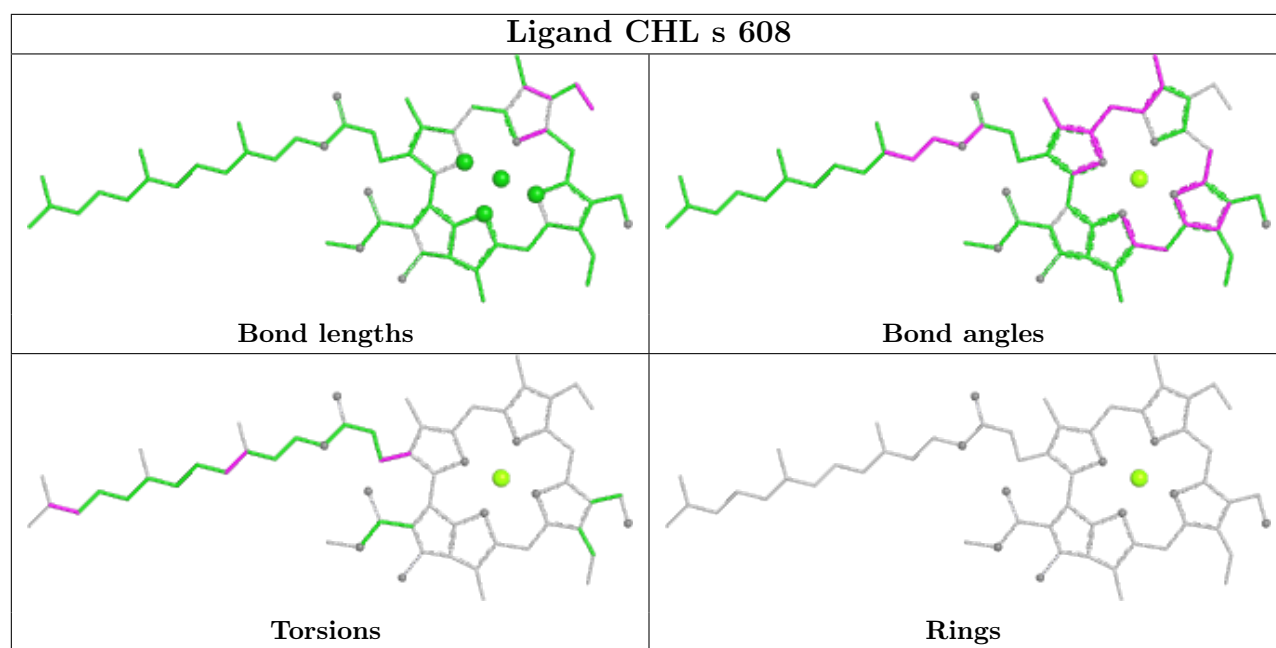


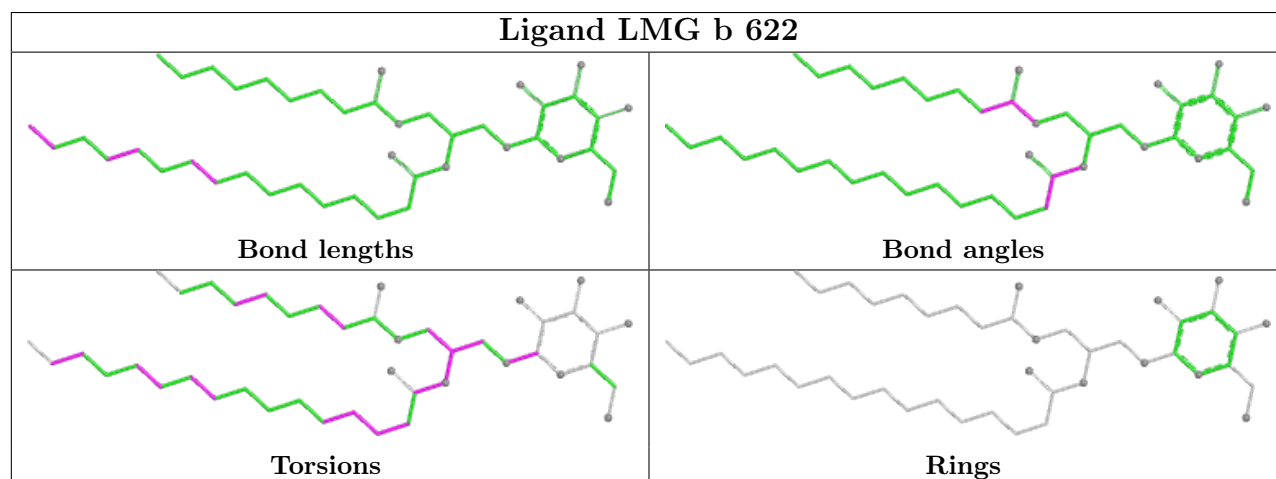
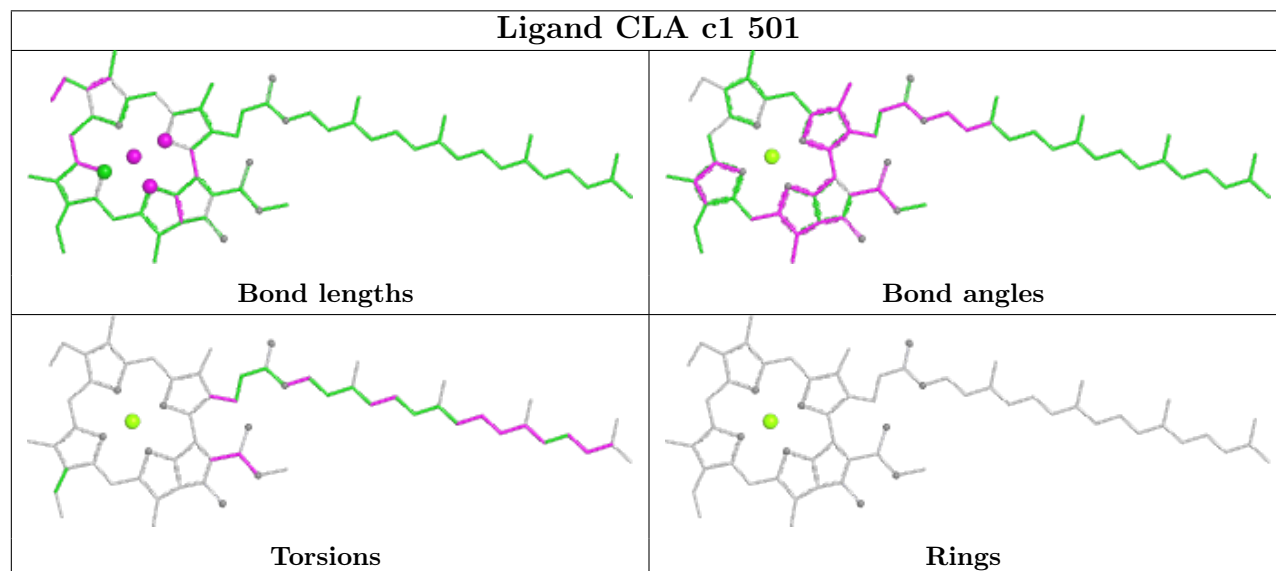
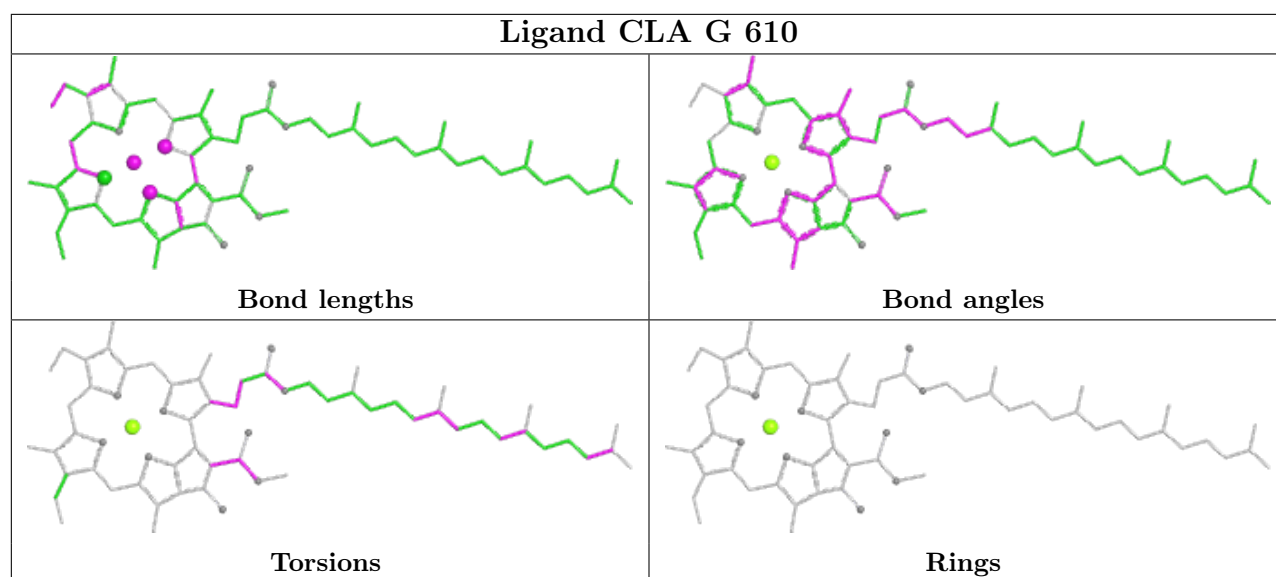
Torsions

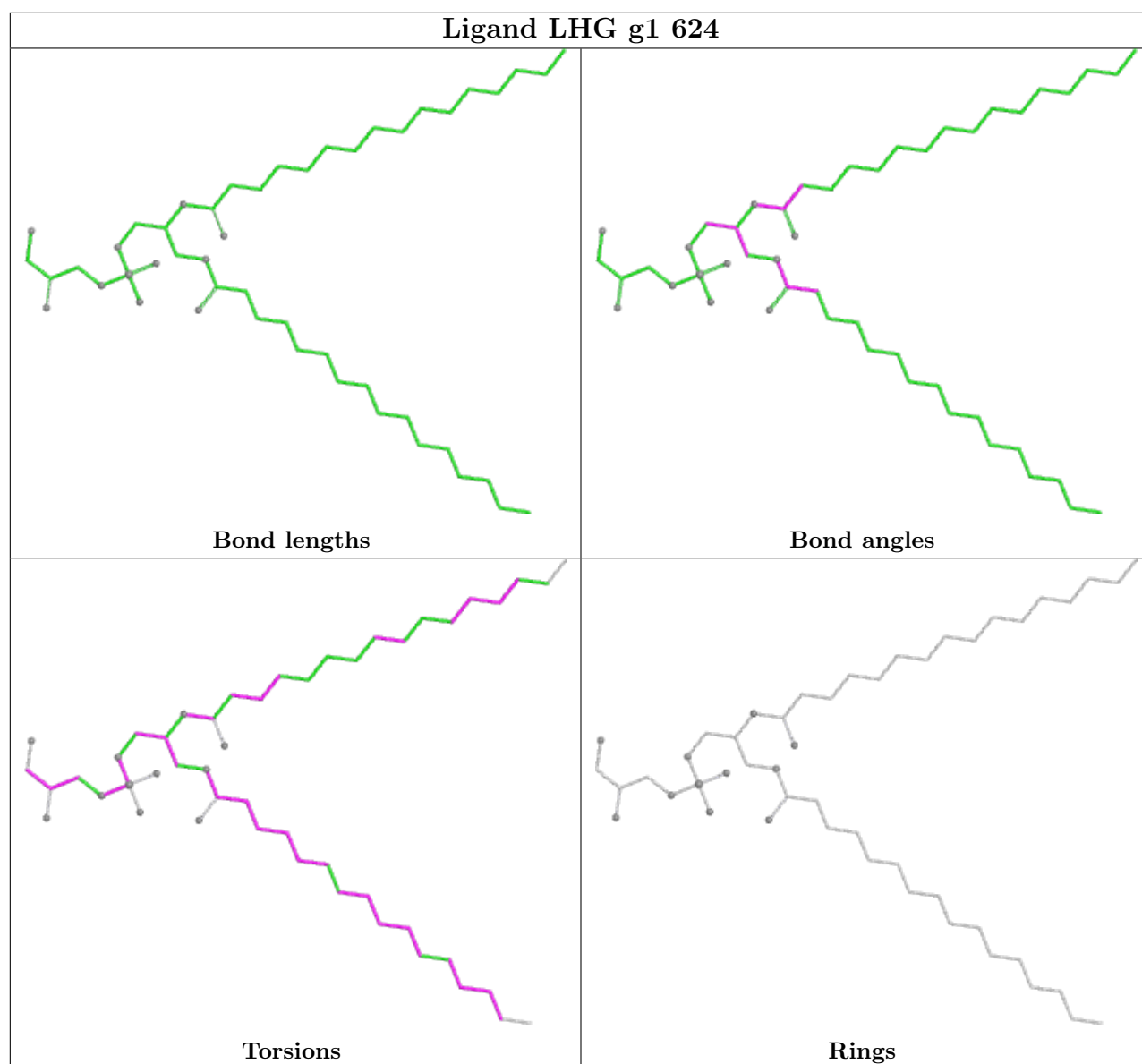


Rings

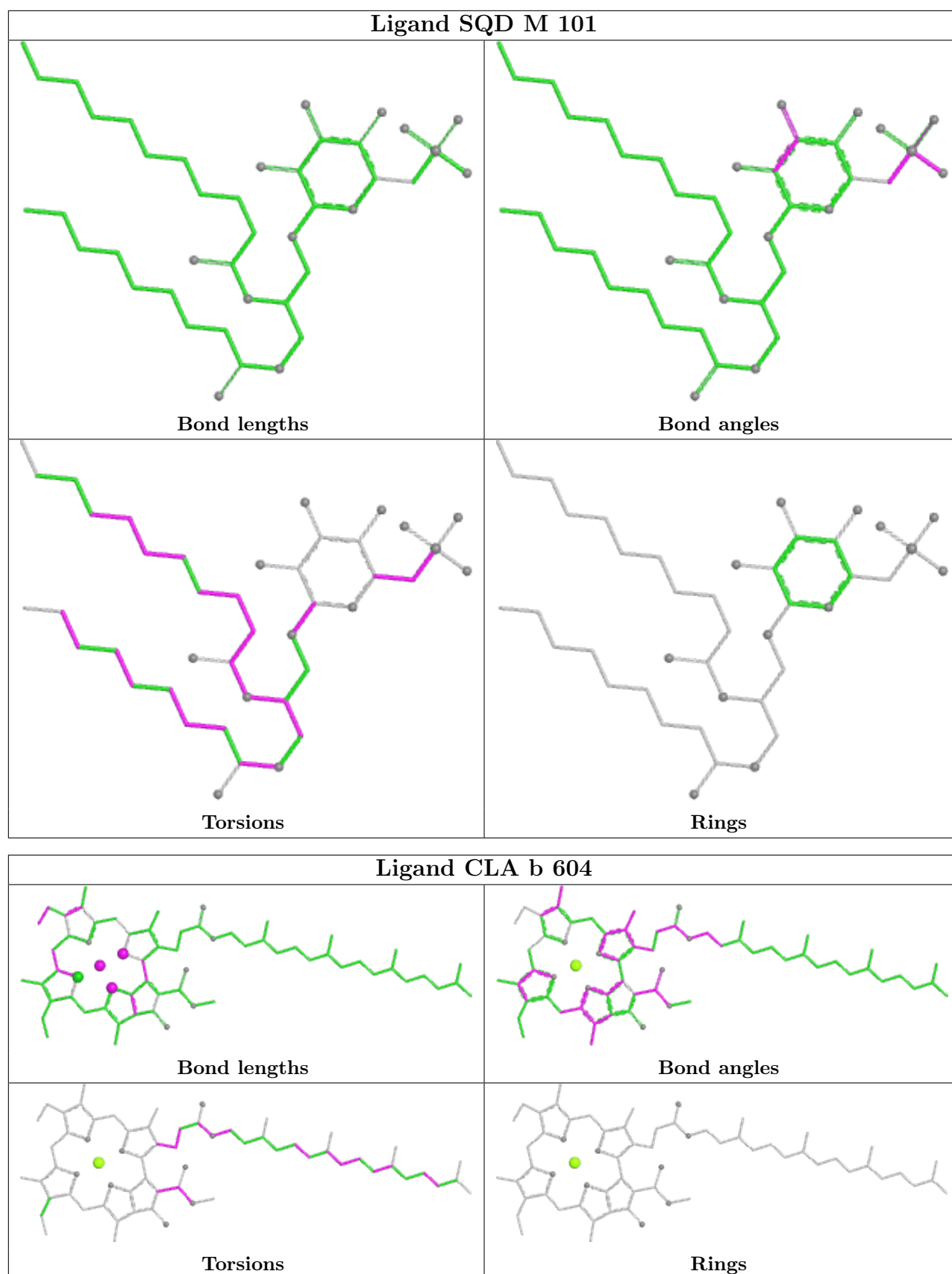
**Ligand CLA N1 603****Ligand CLA Y1 610**

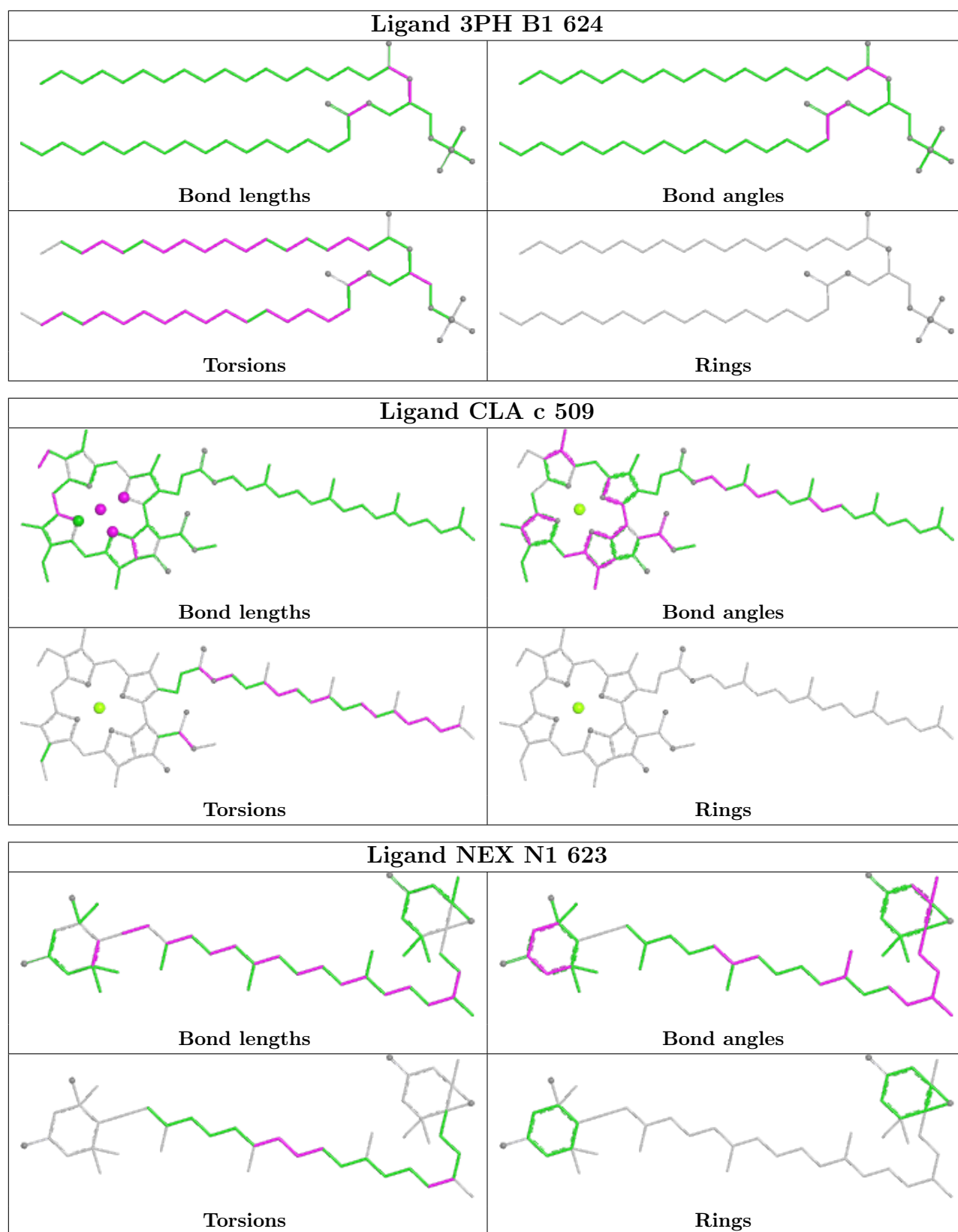




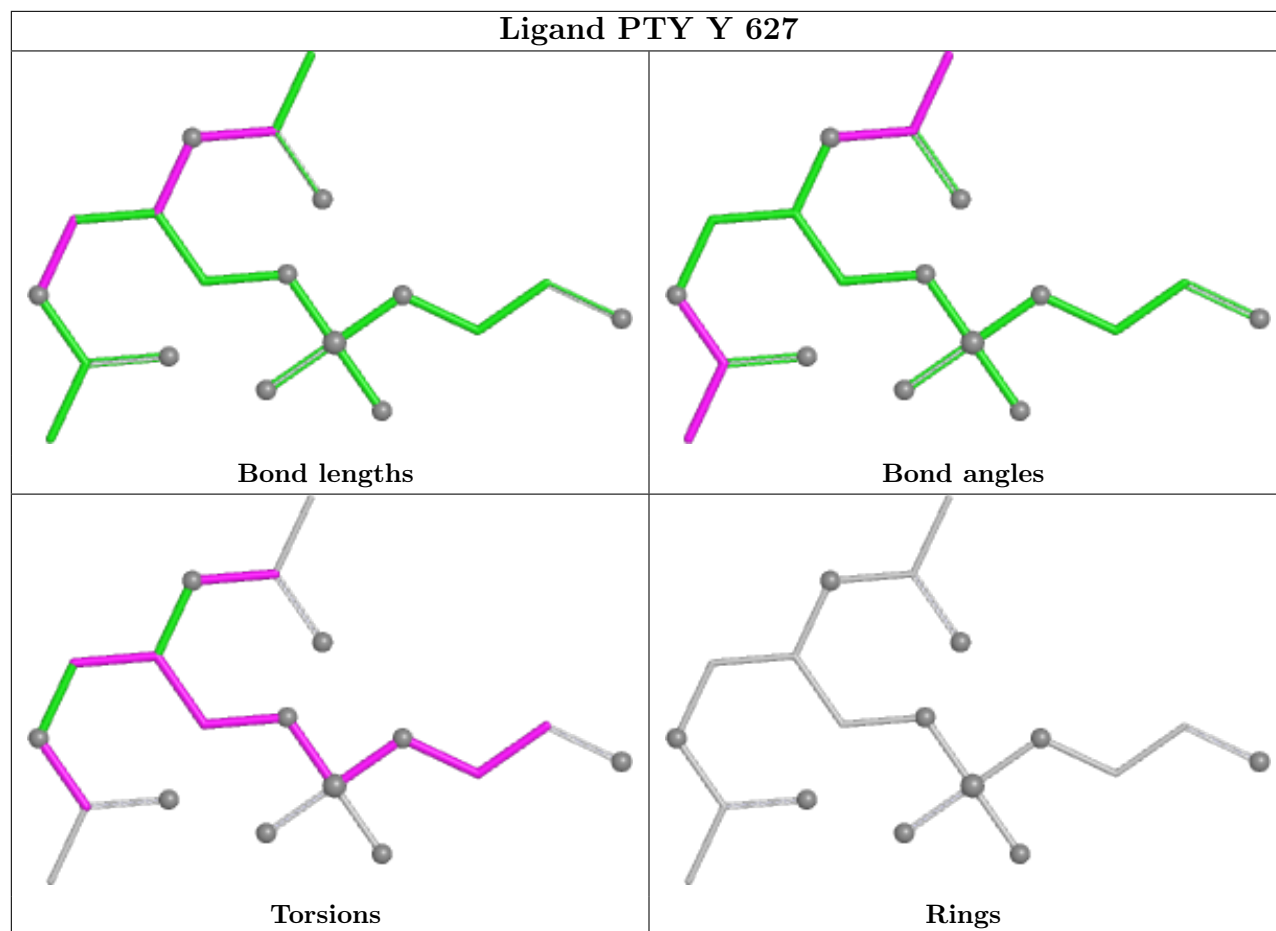




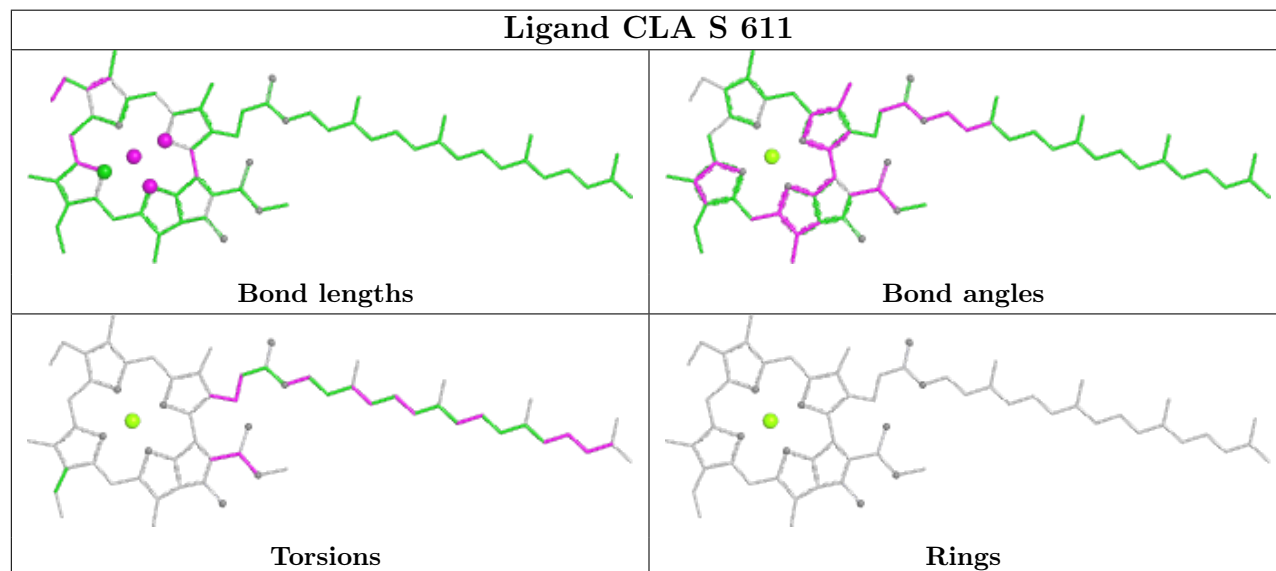




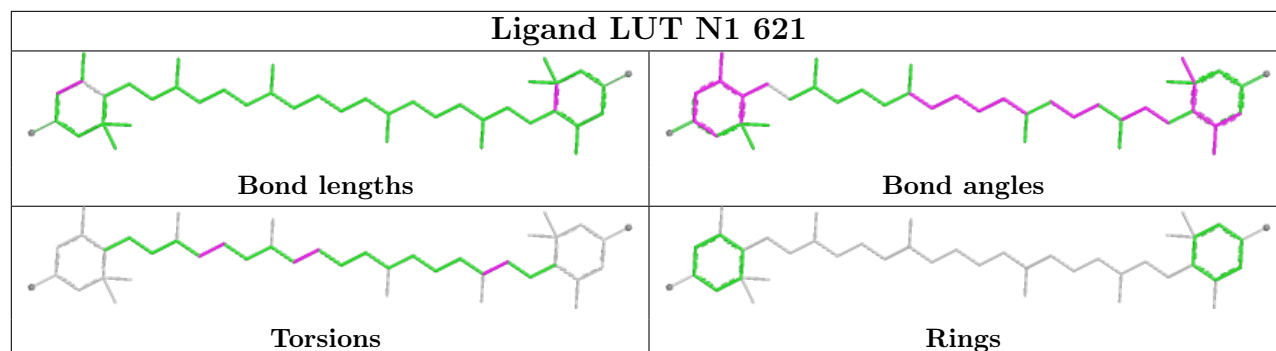
## Ligand PTY Y 627



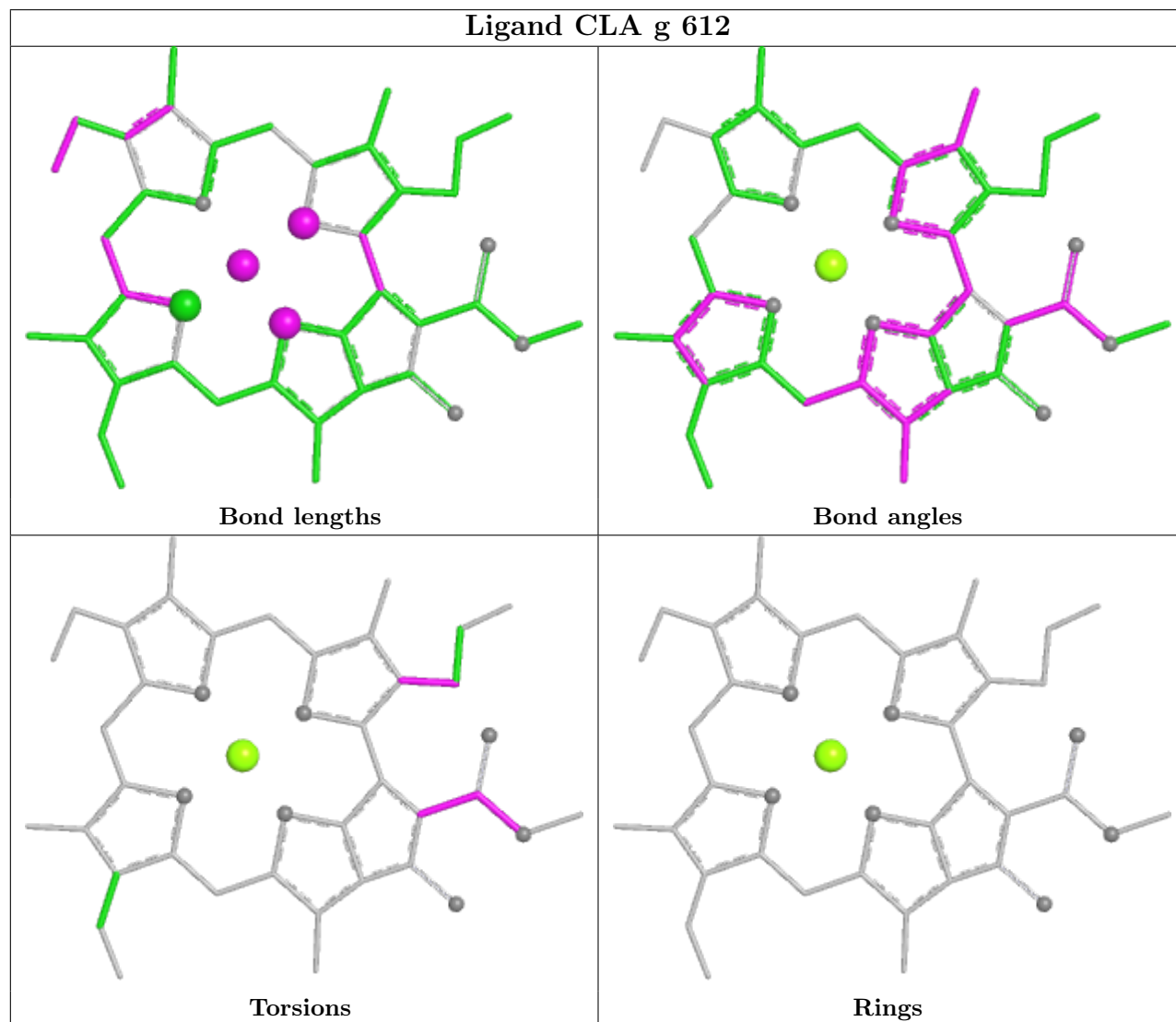
## Ligand CLA S 611

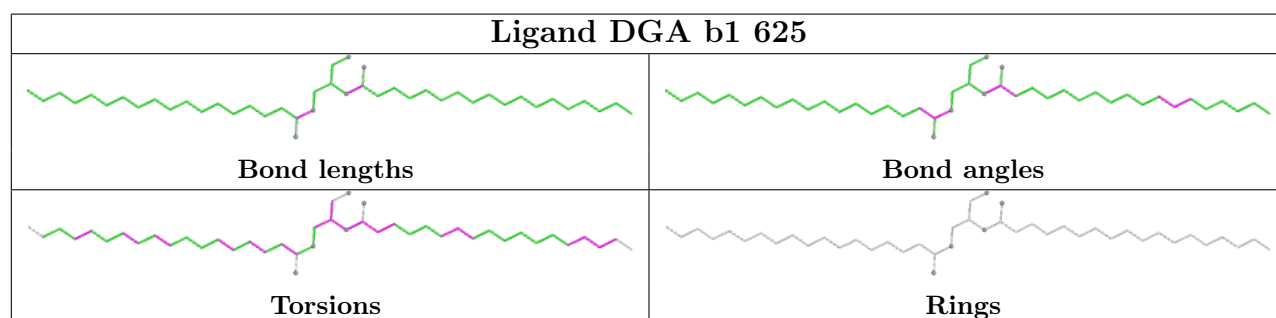
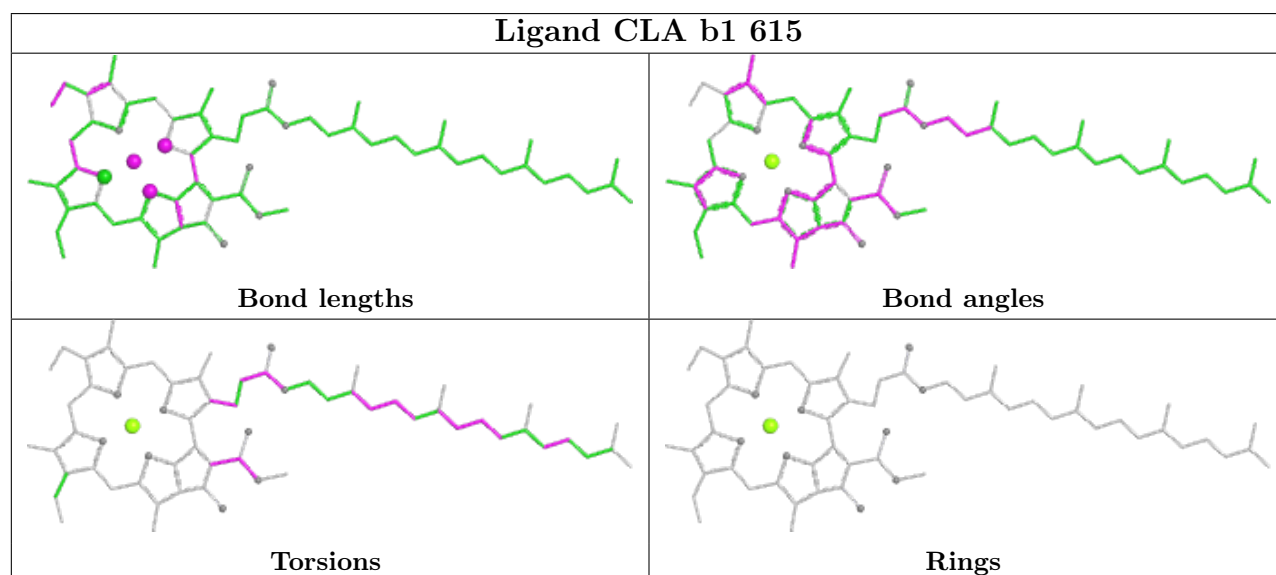
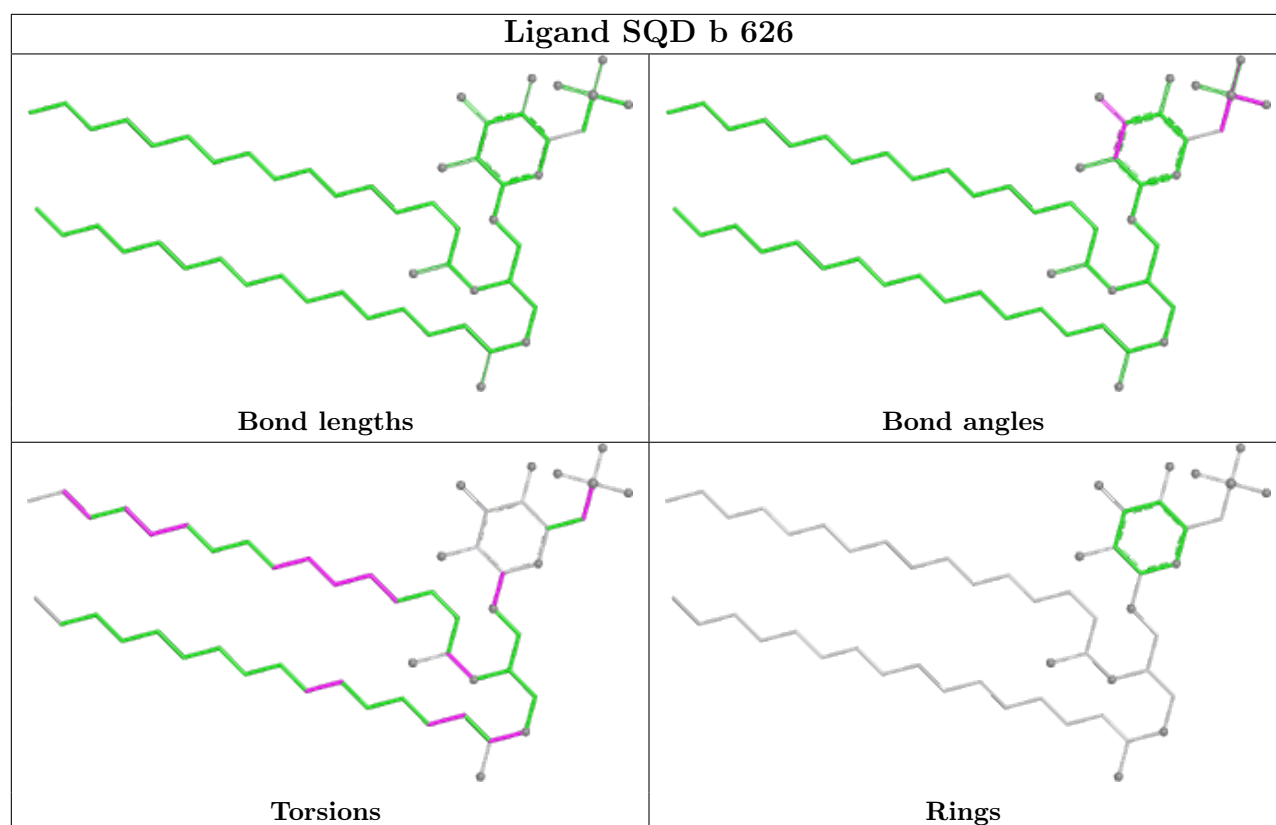


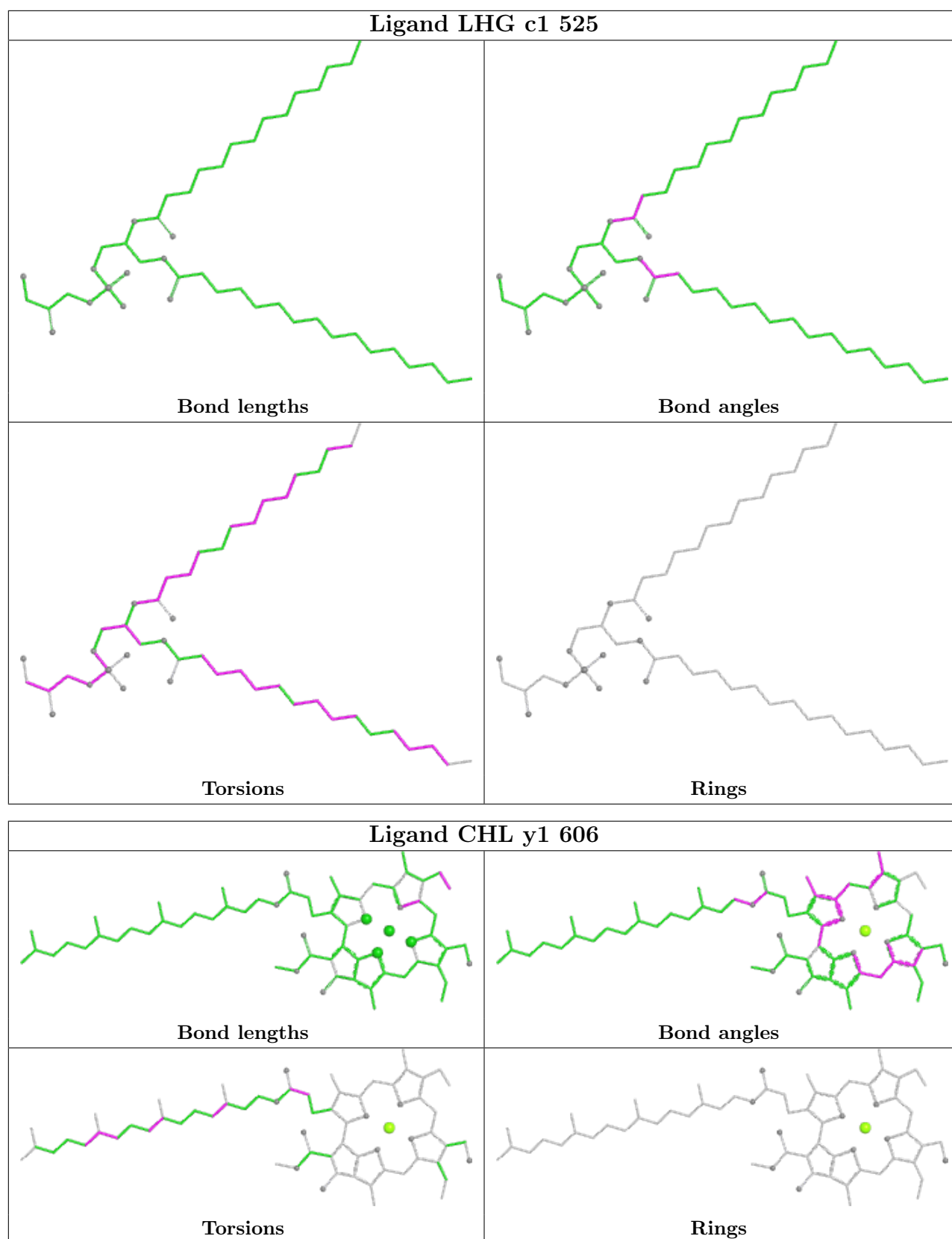
## Ligand LUT N1 621

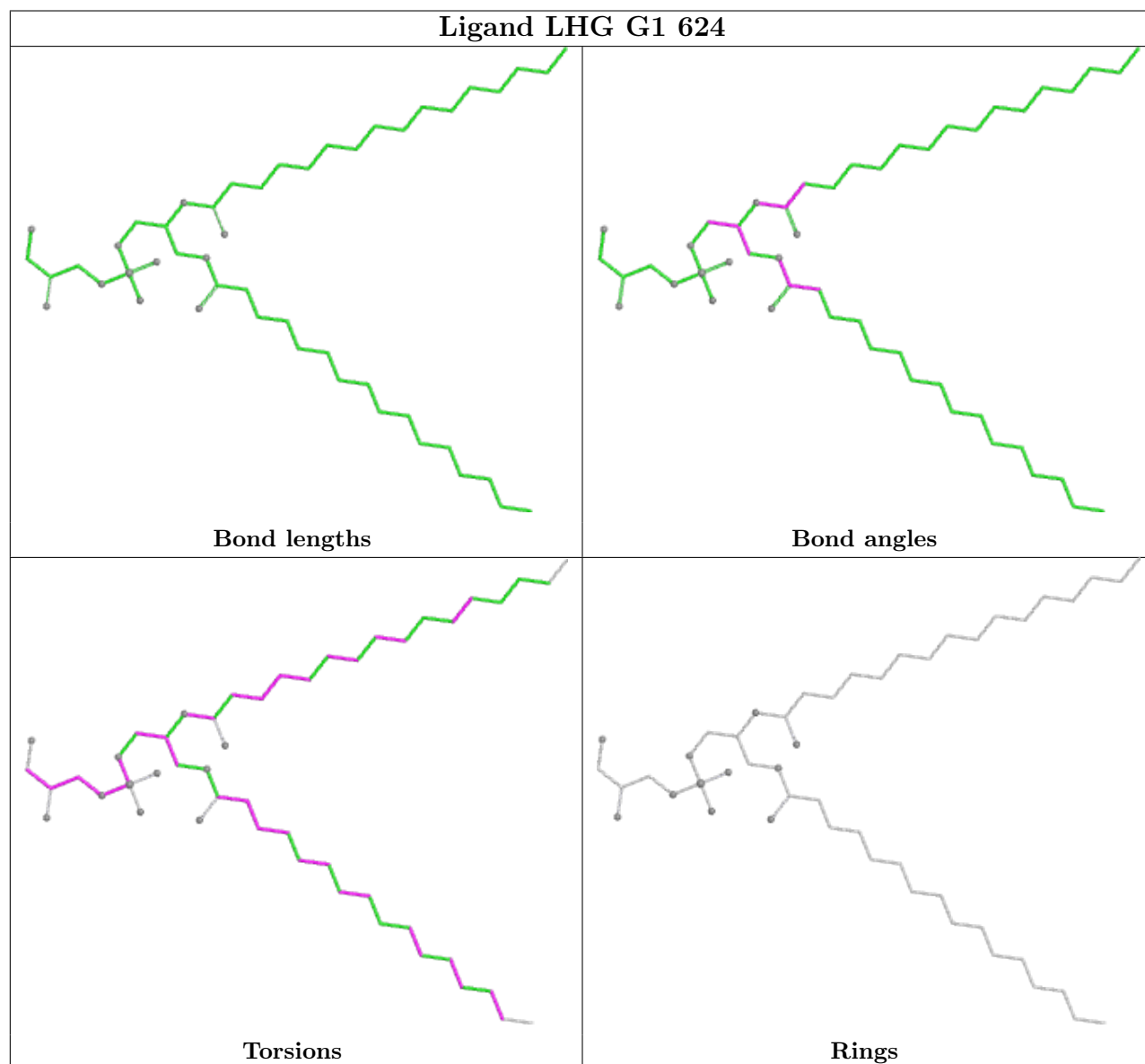
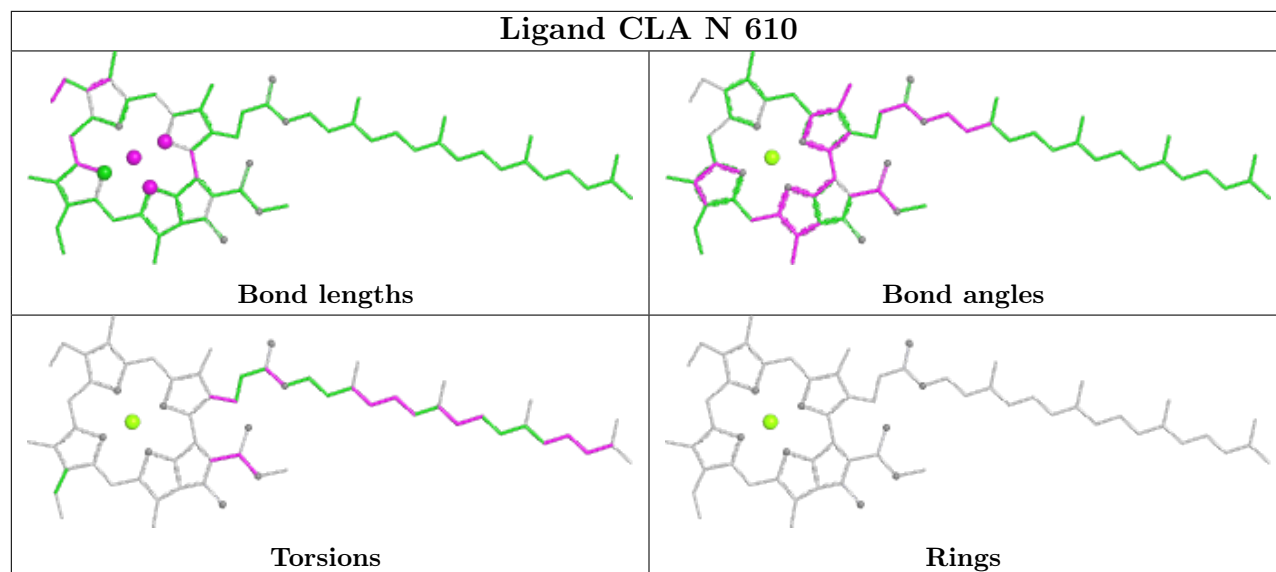


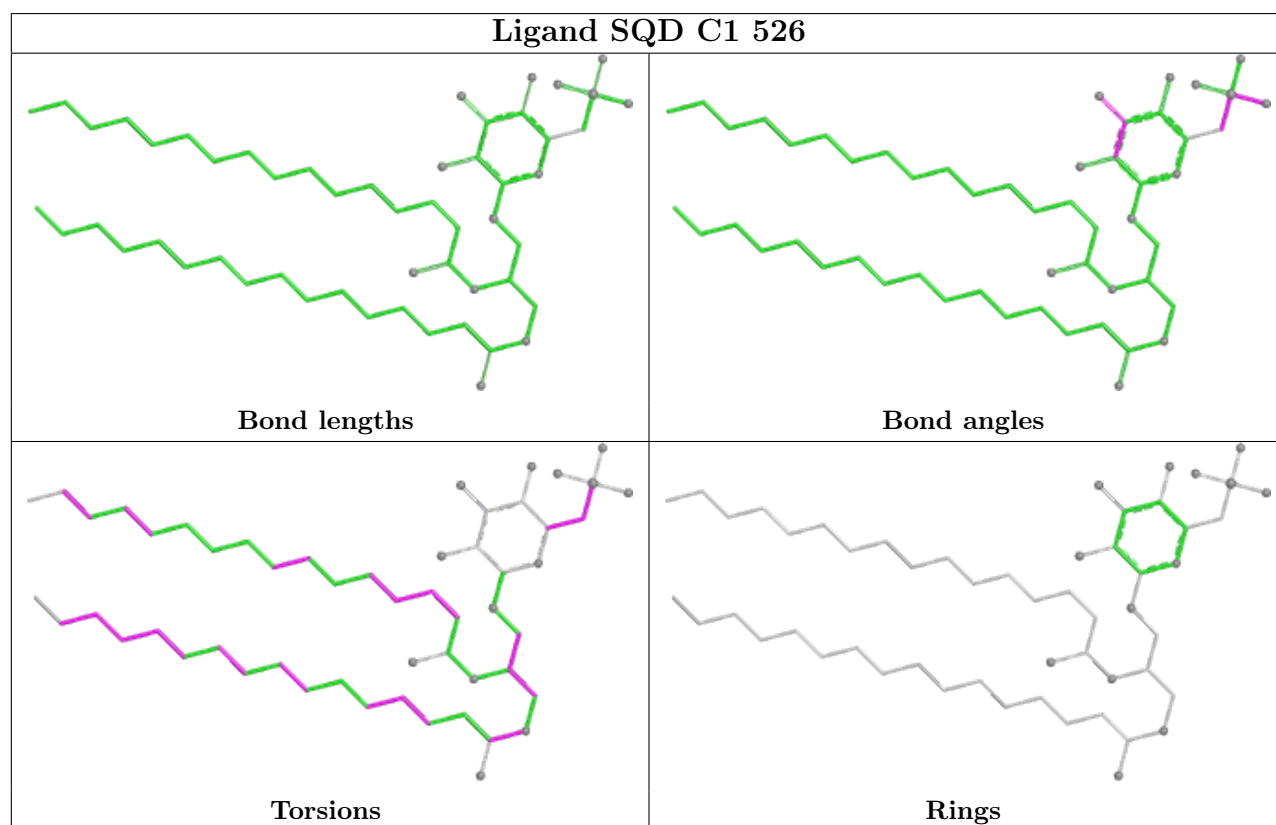
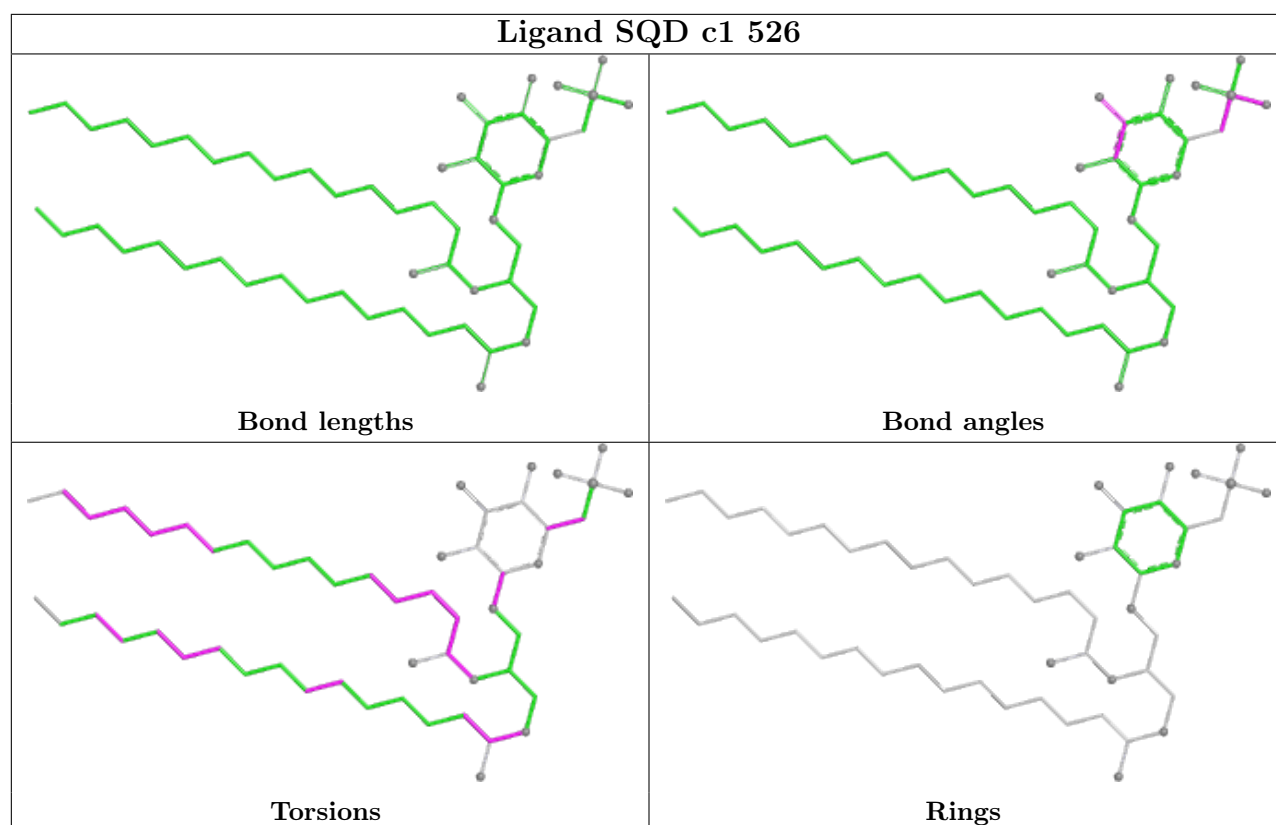
## Ligand CLA g 612



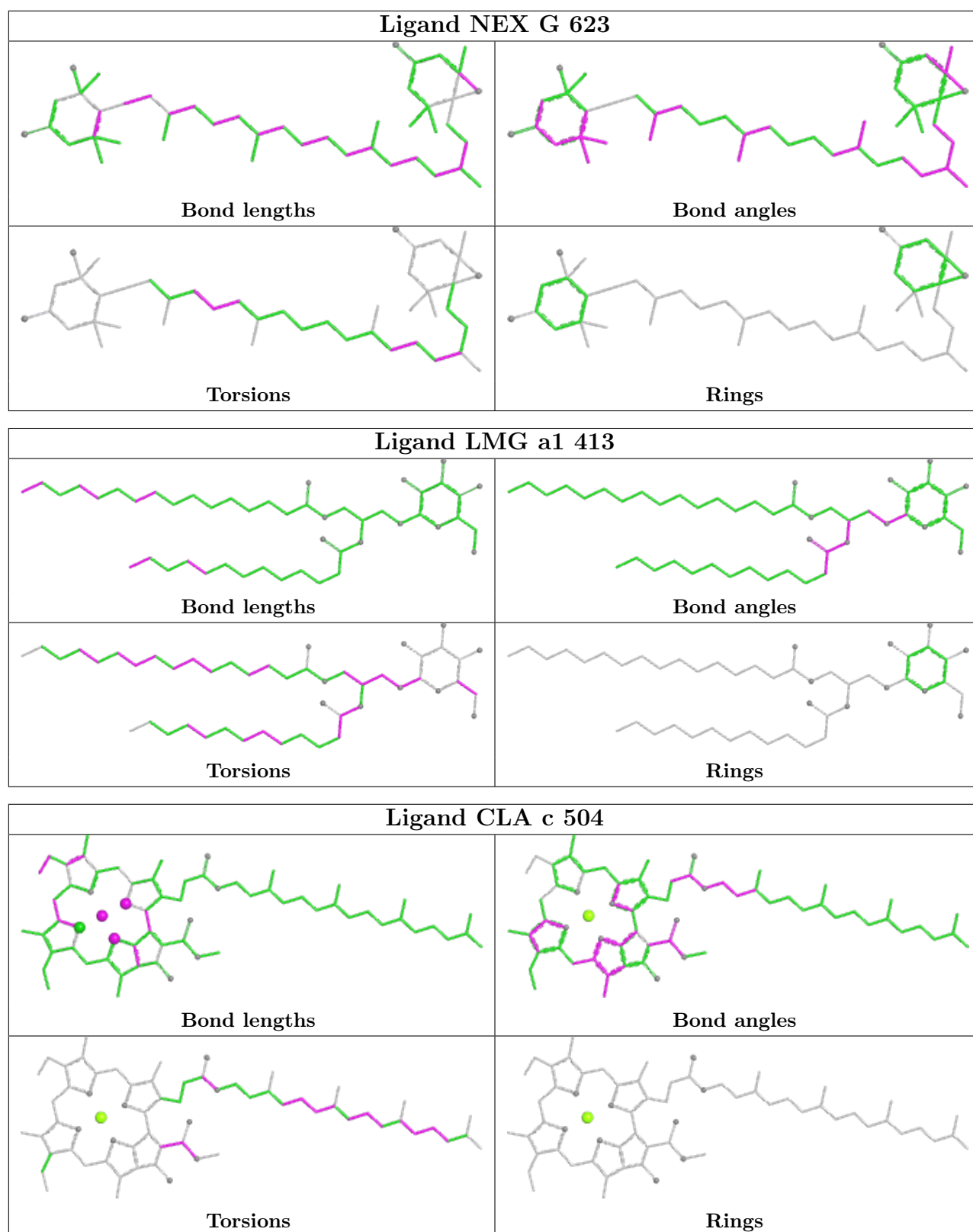


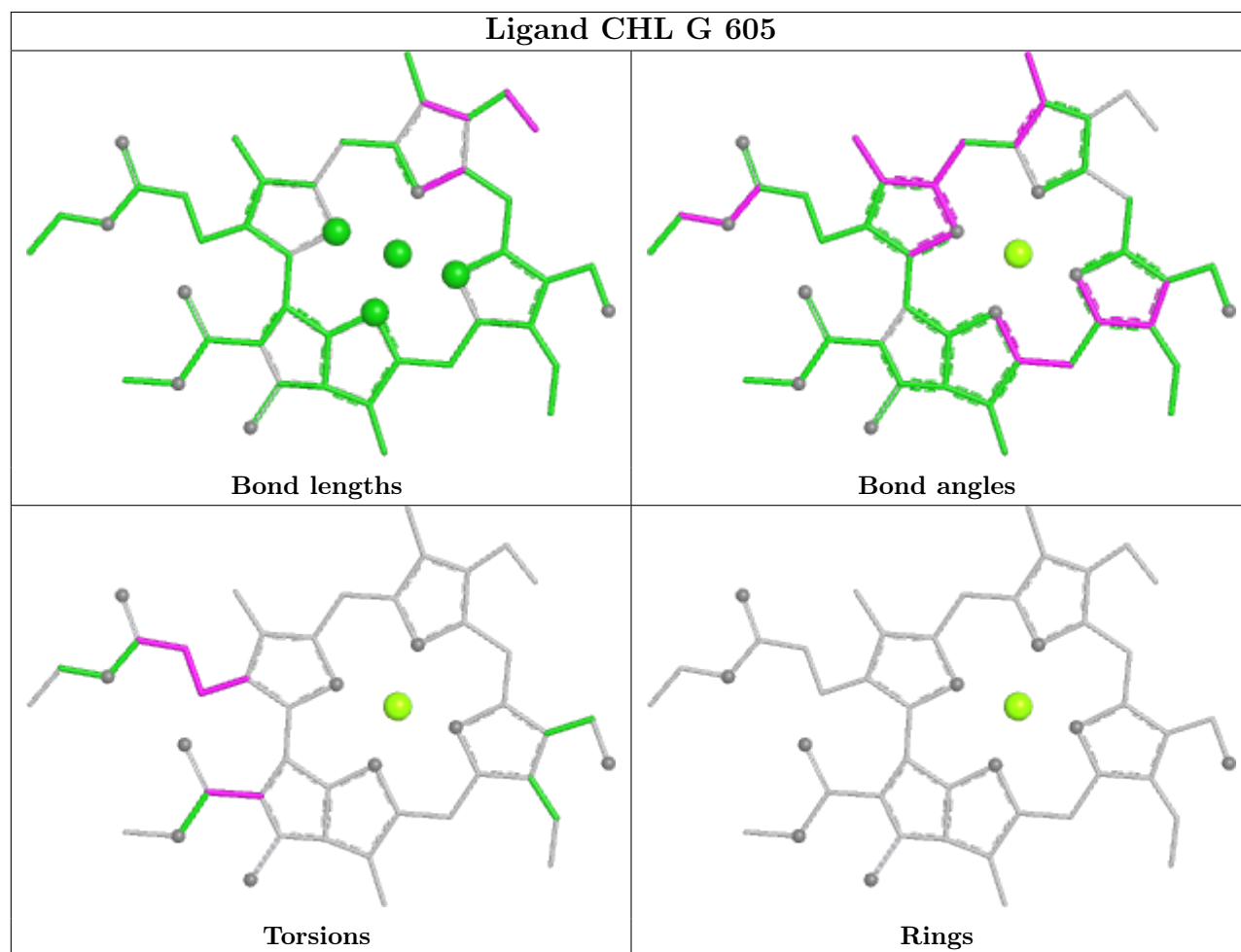
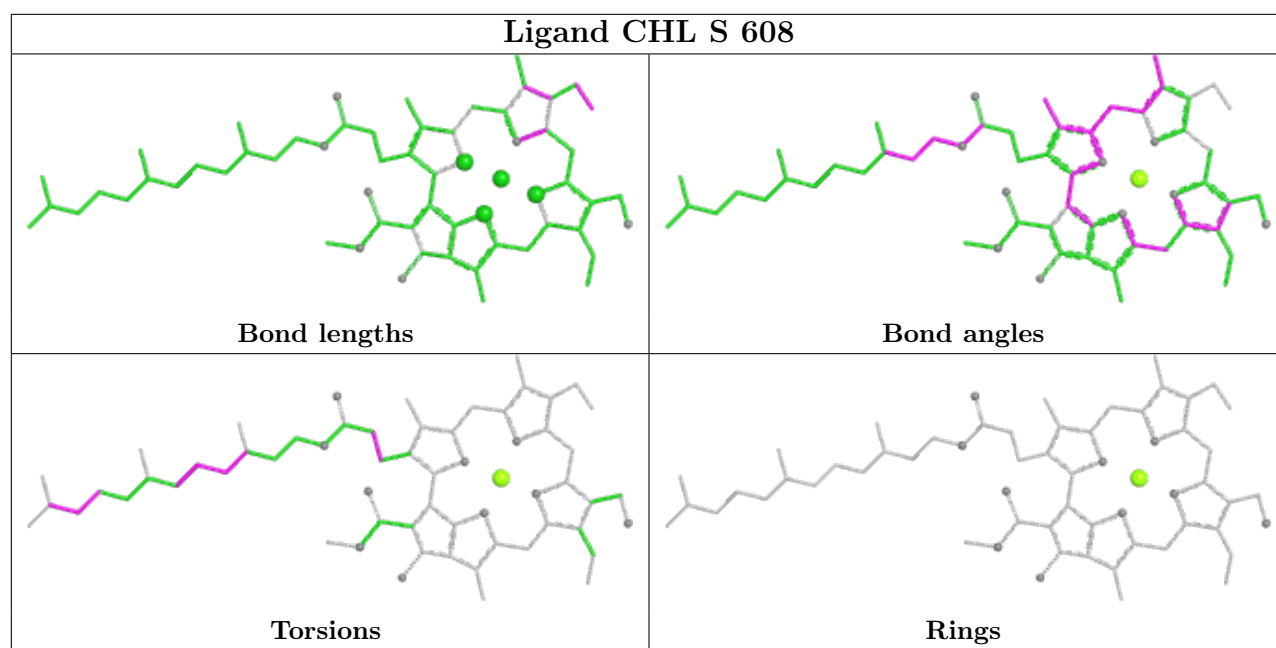


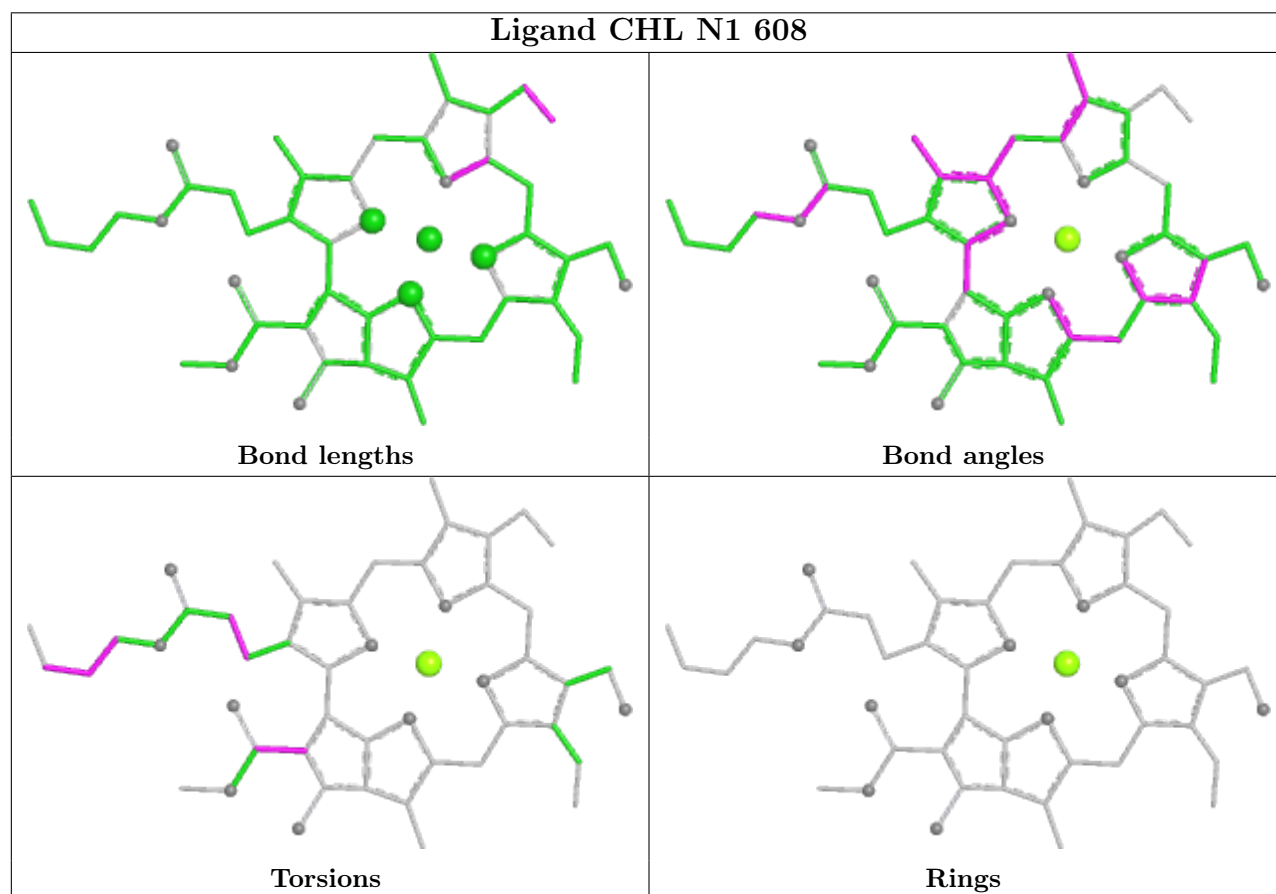
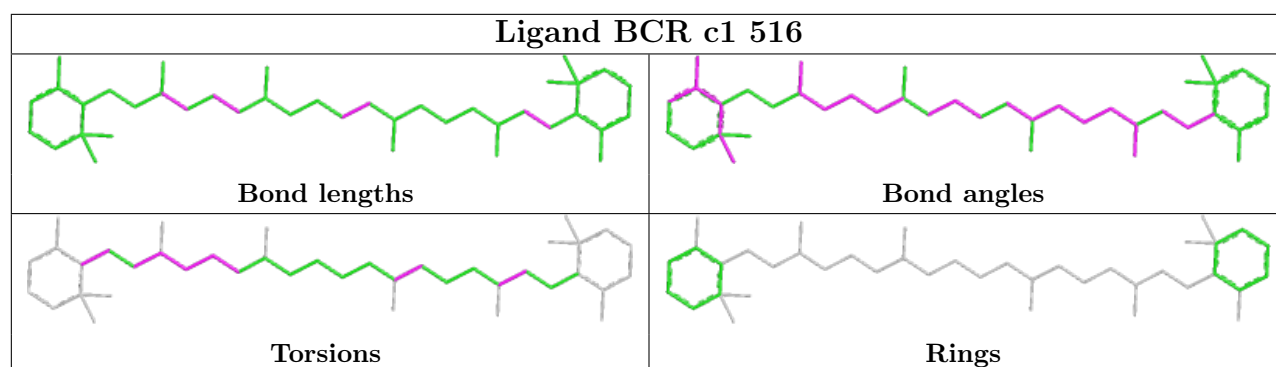


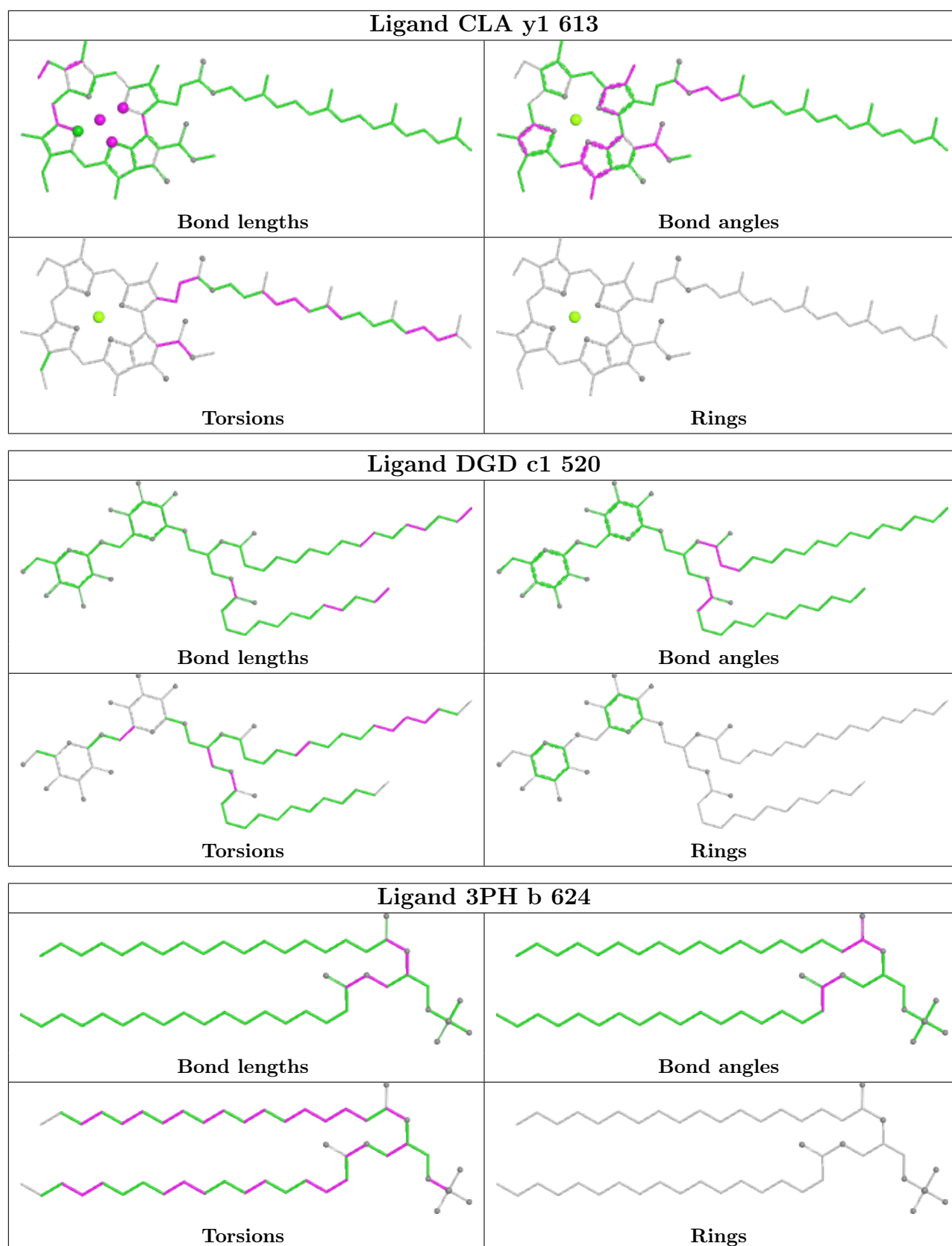


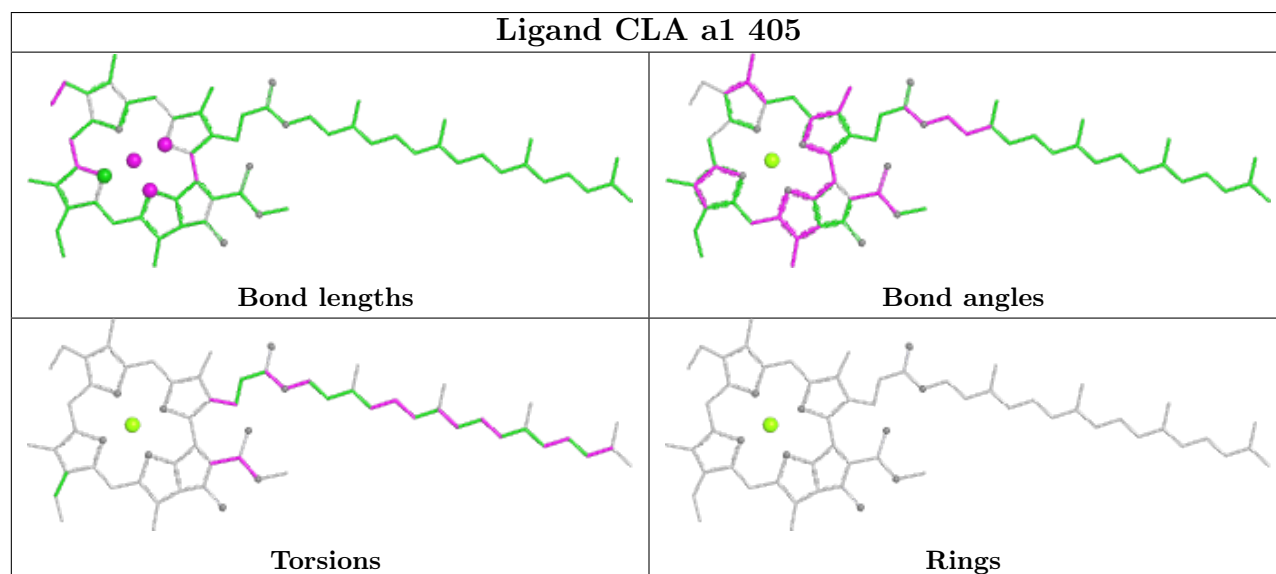
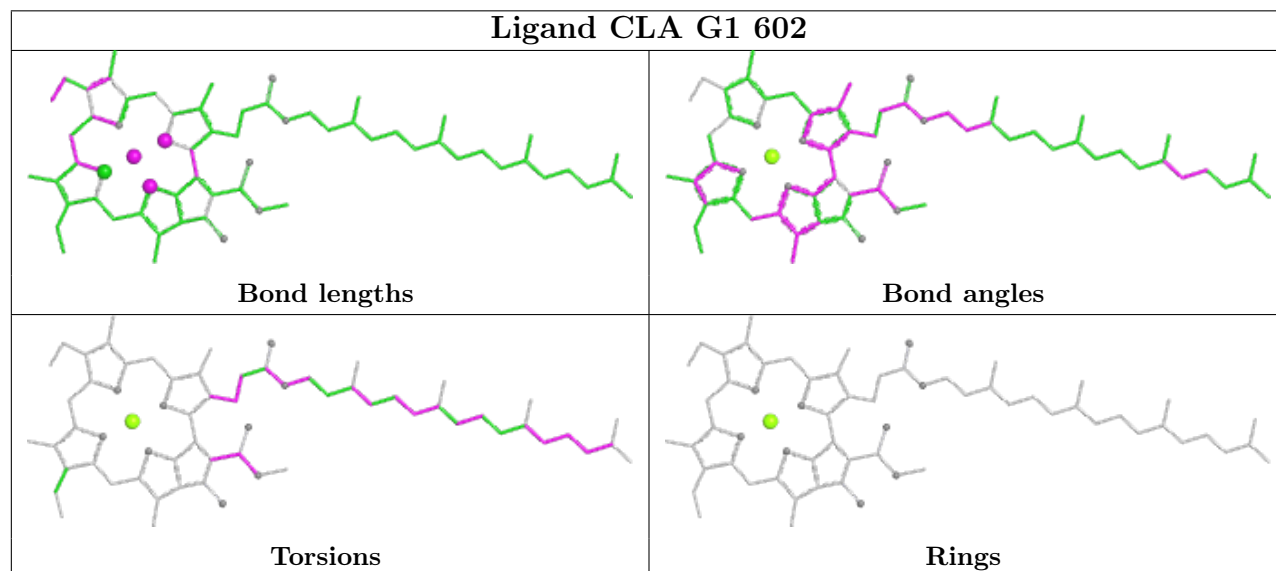
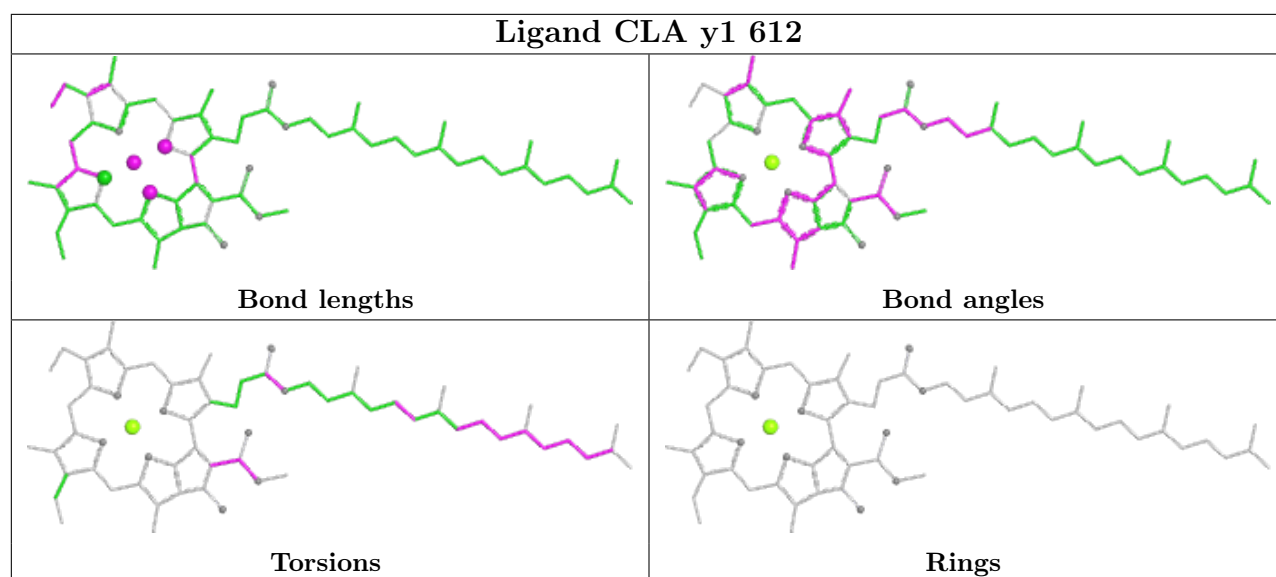


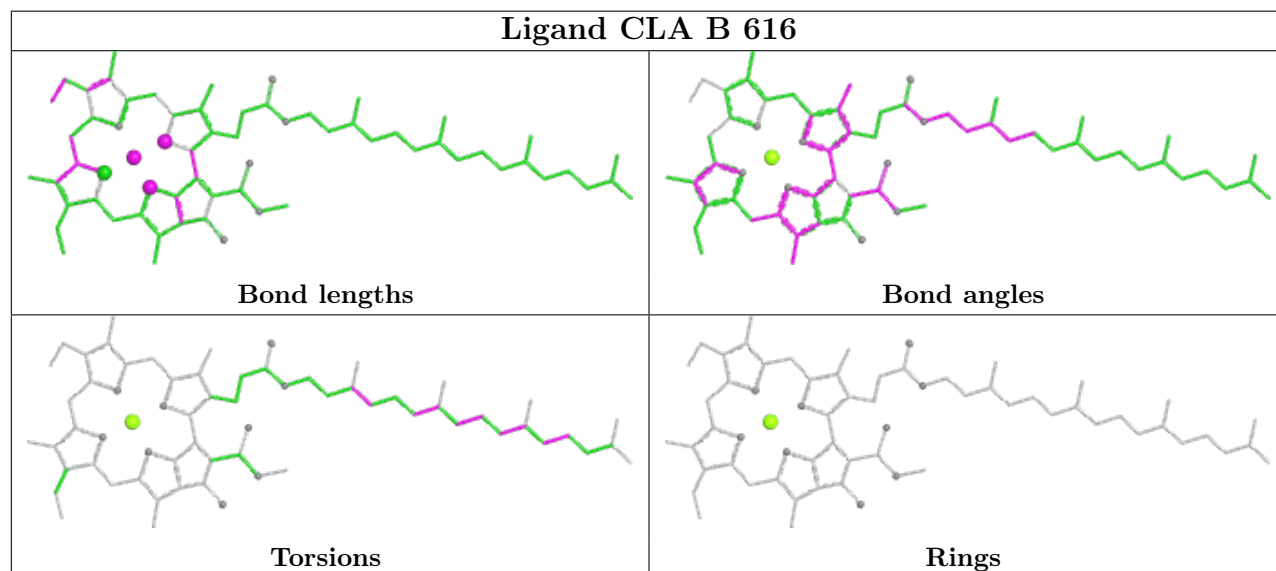
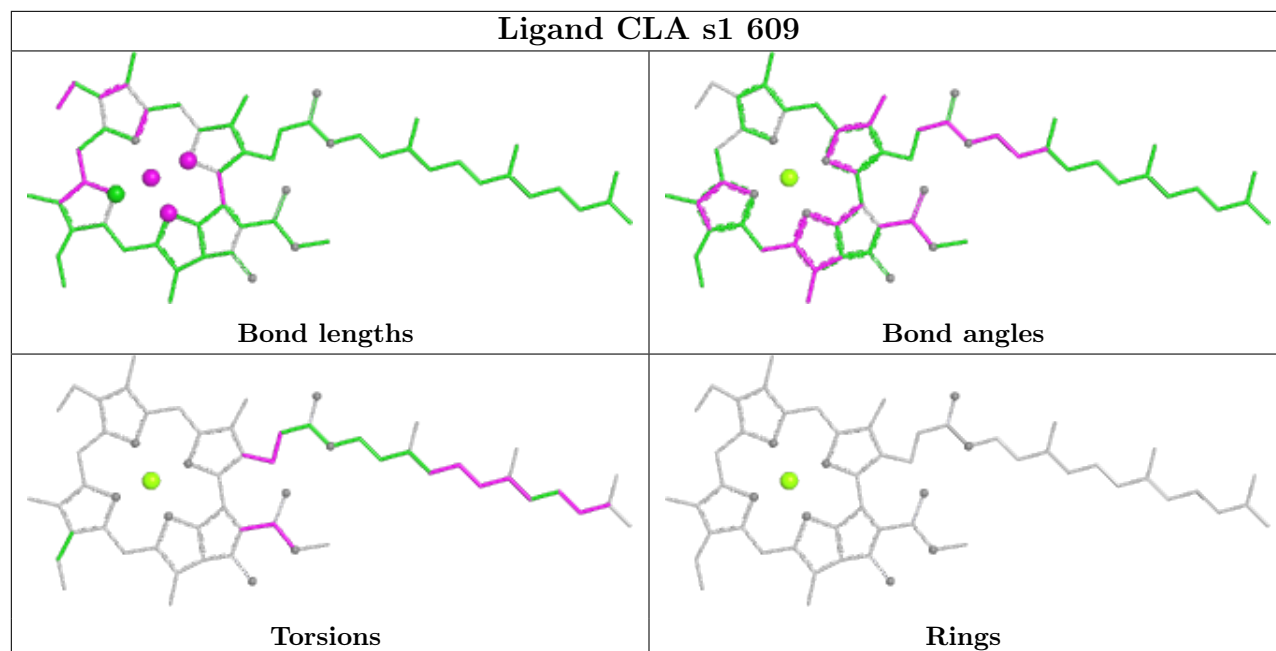


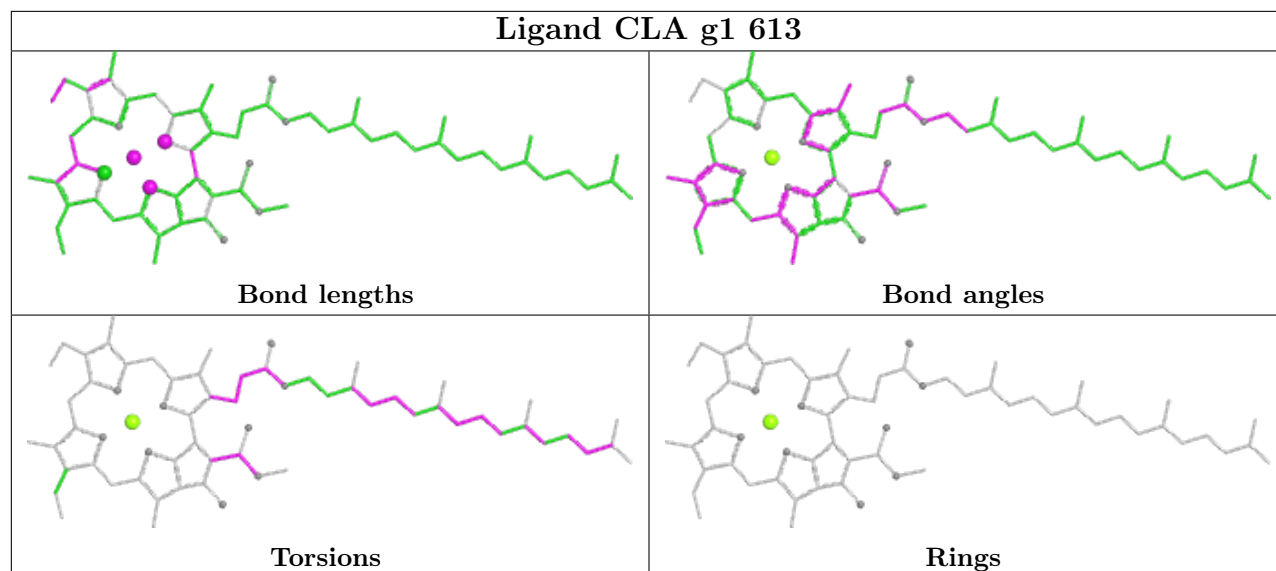
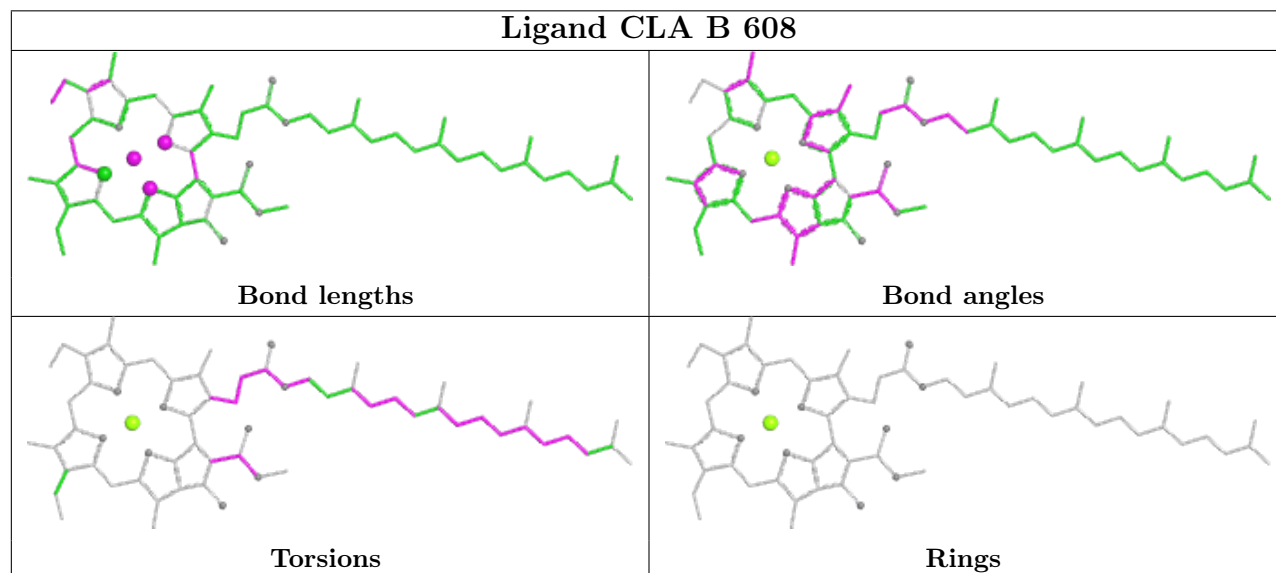
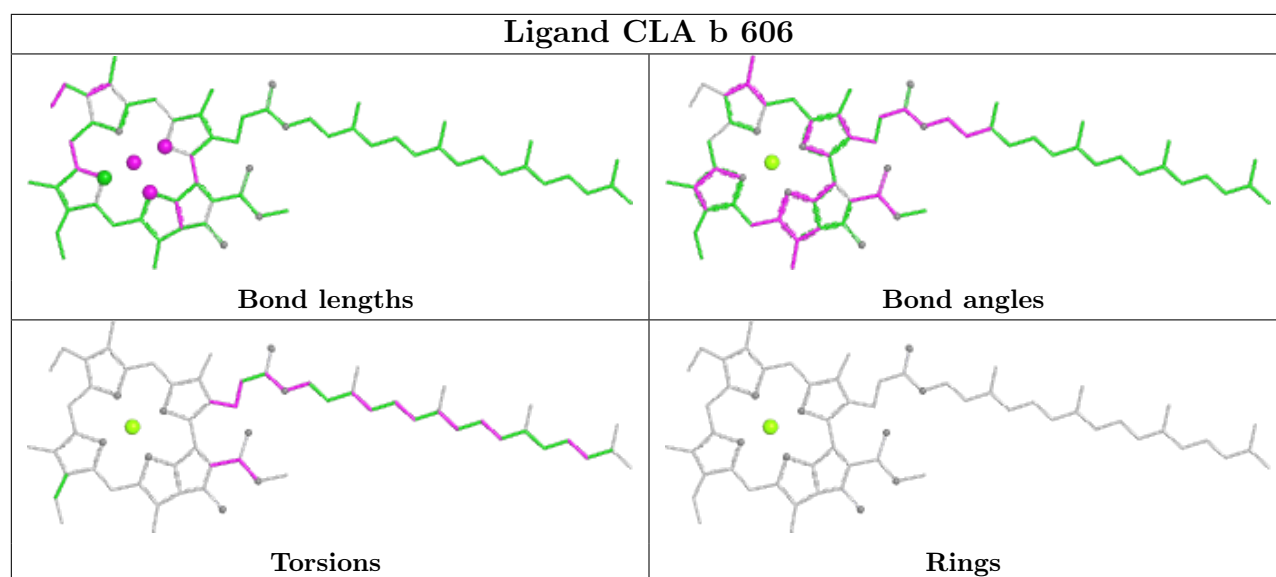


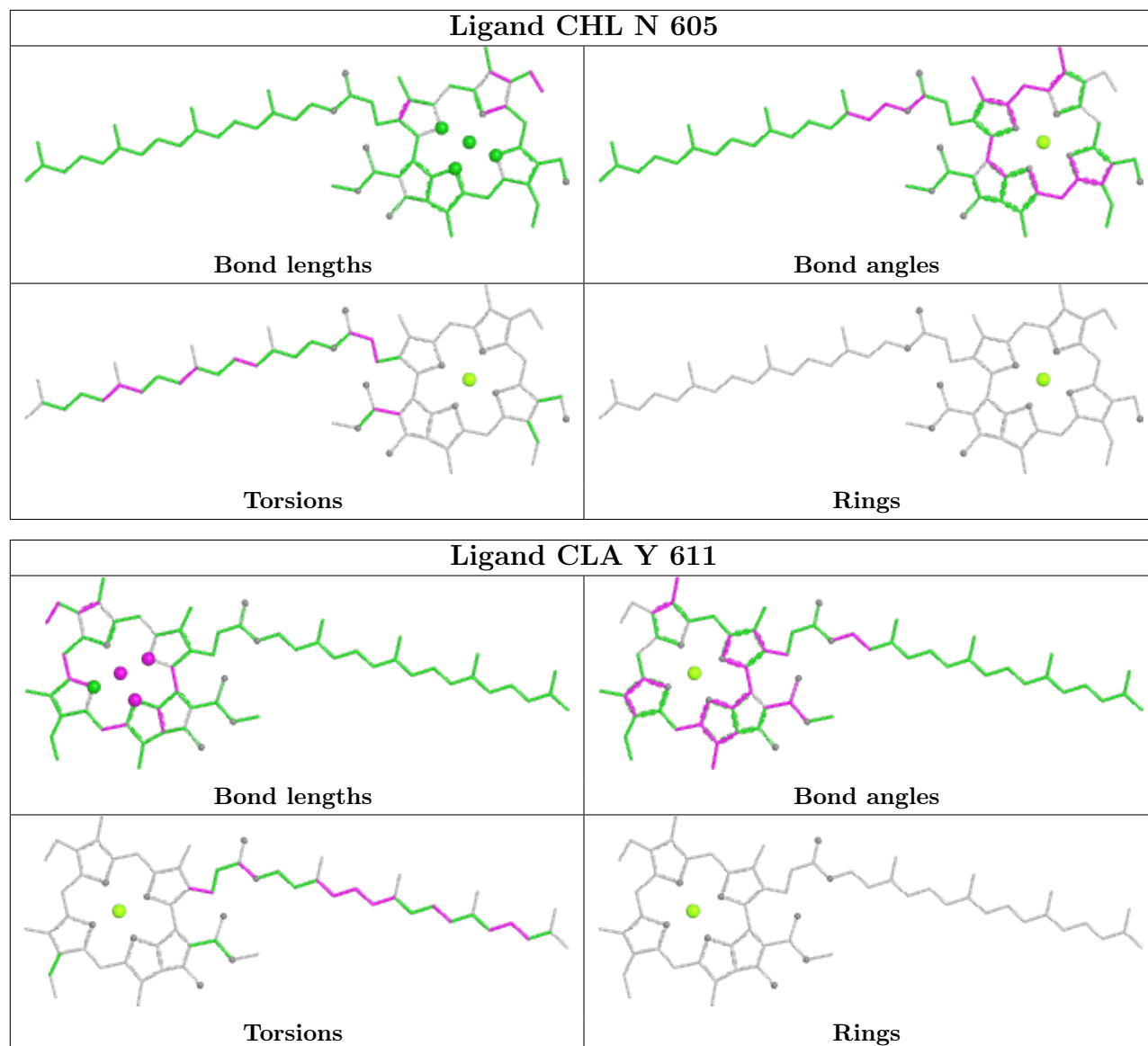




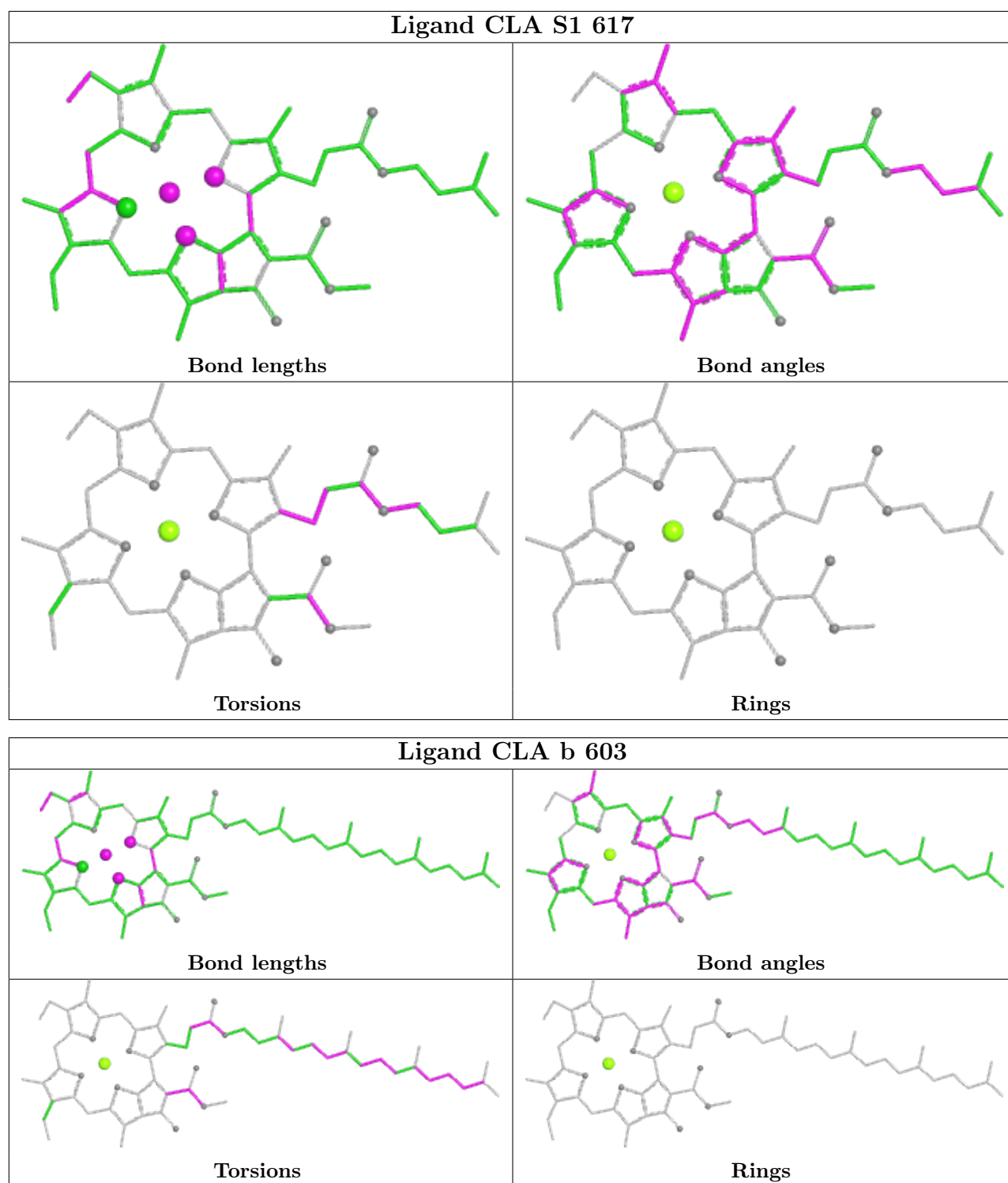


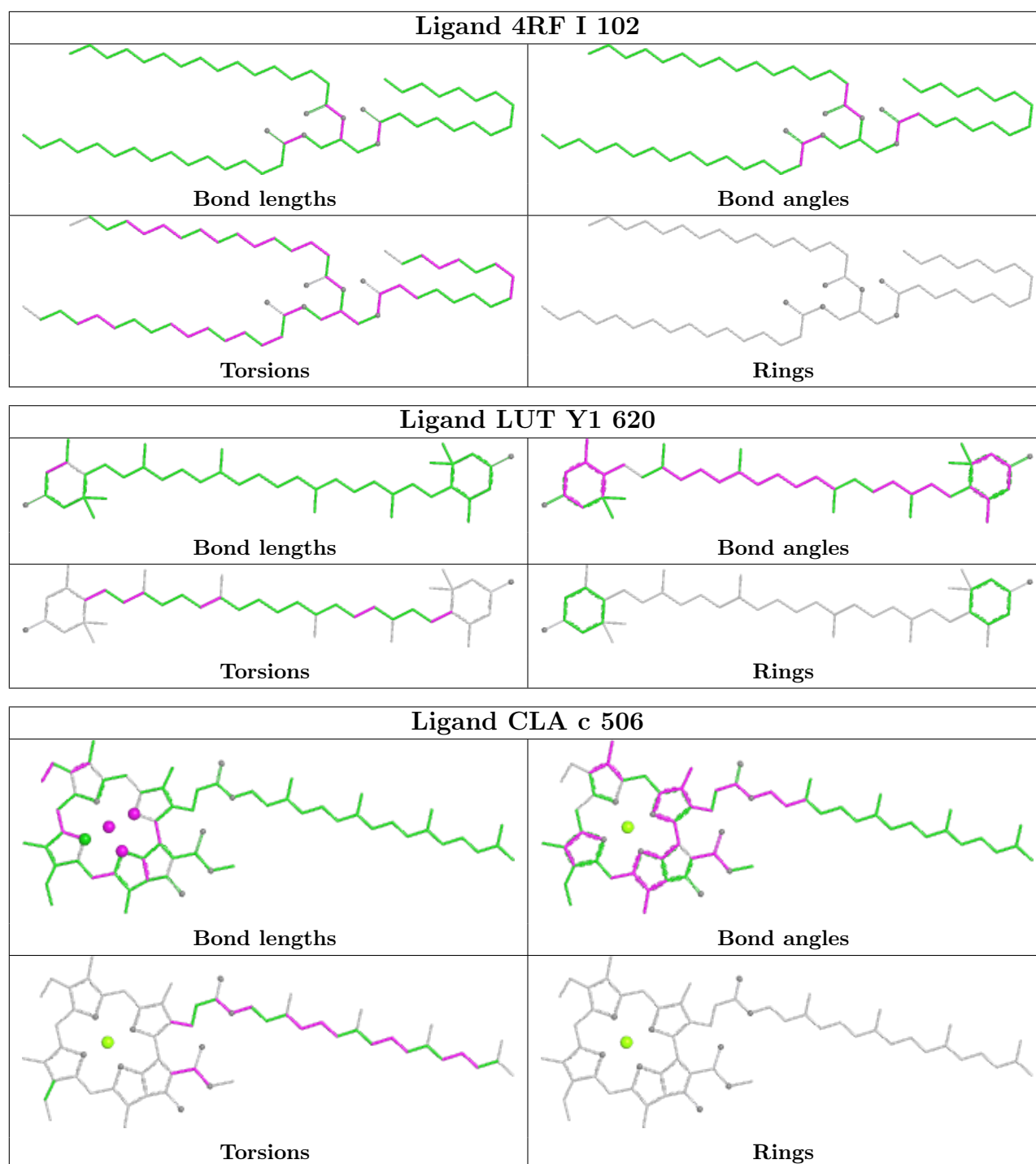


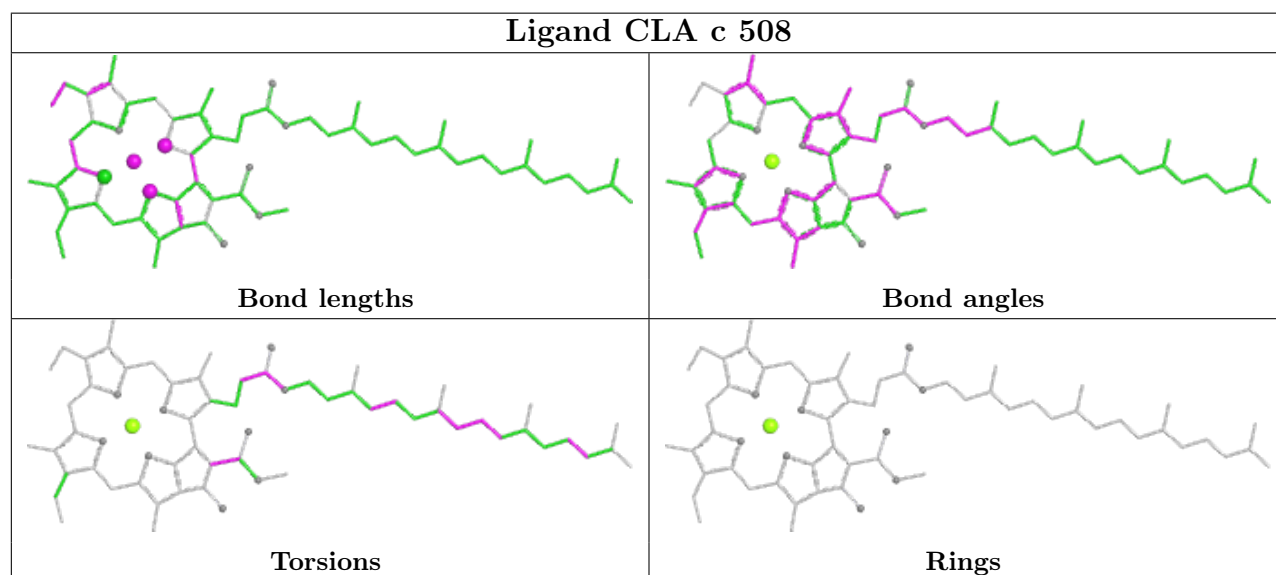
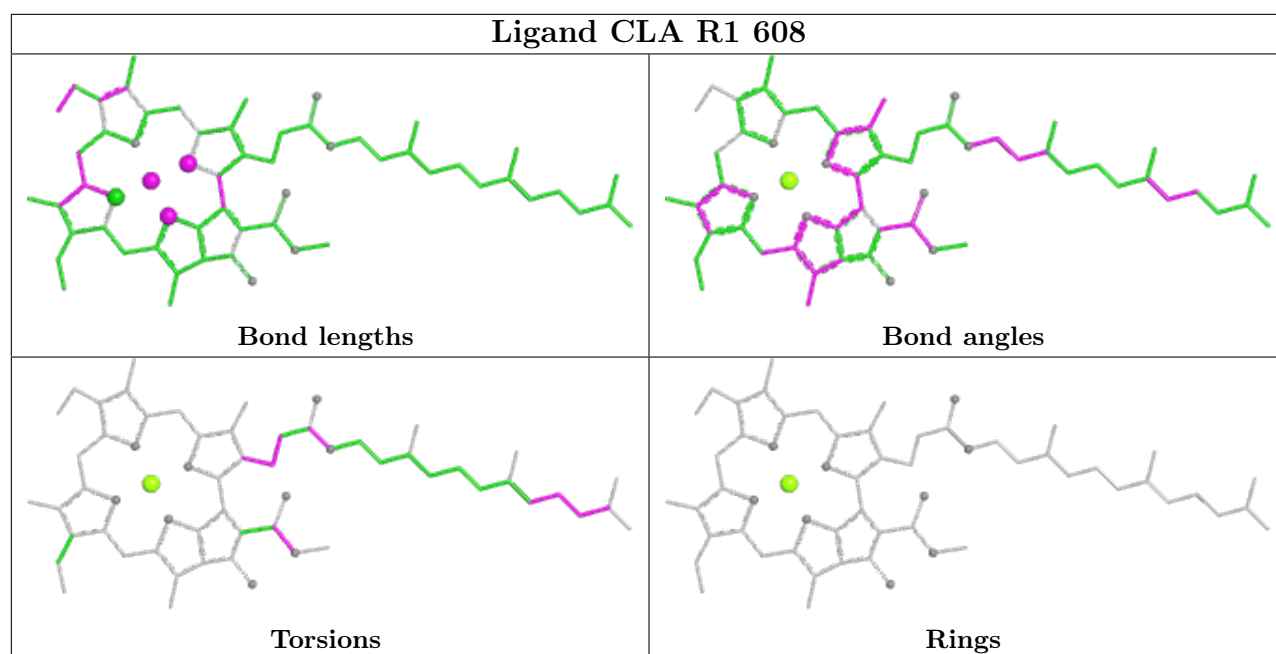


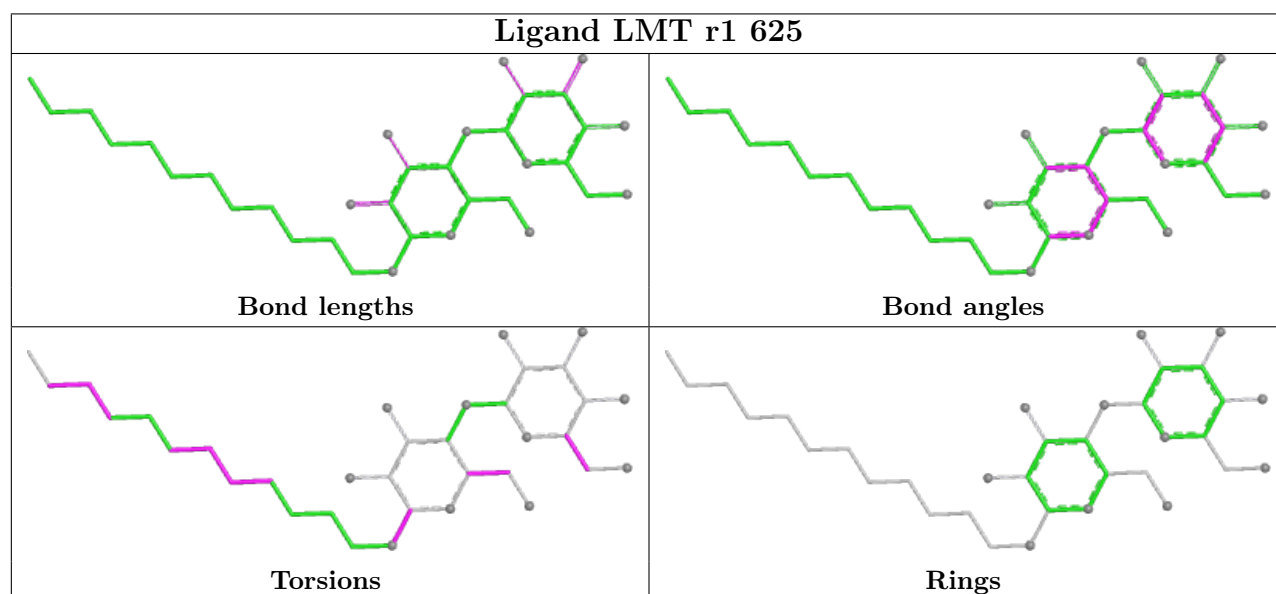
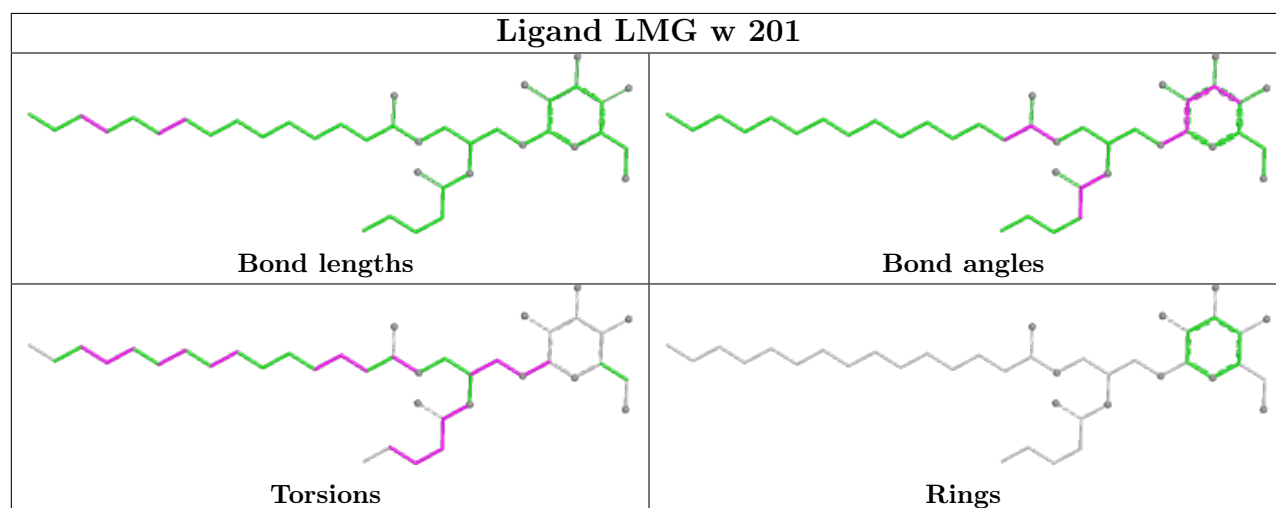
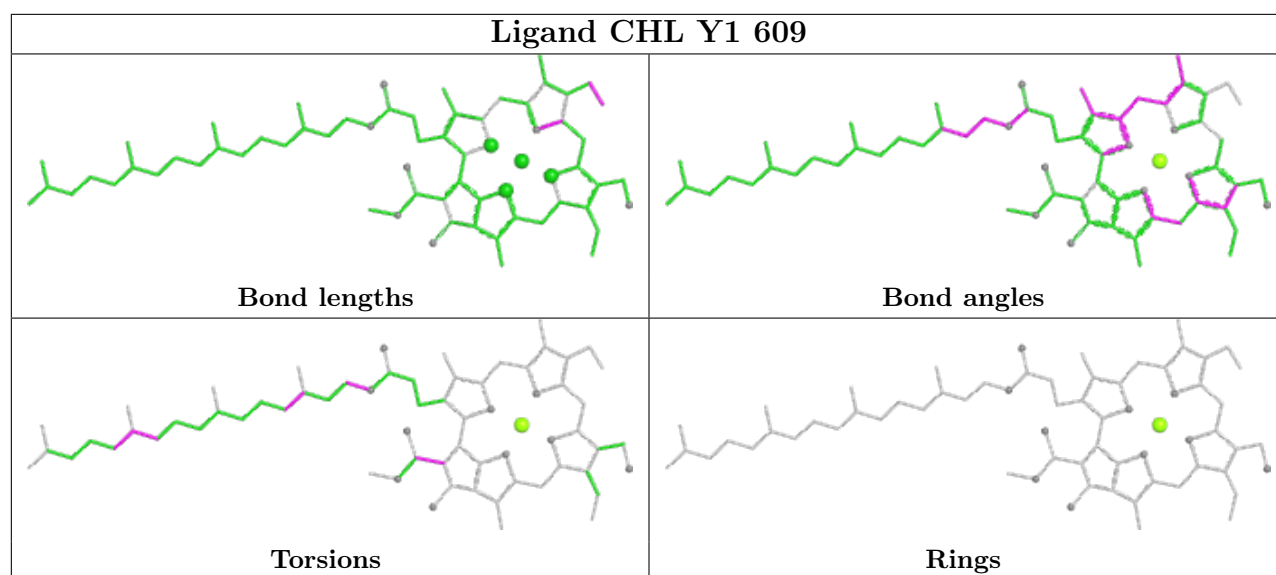


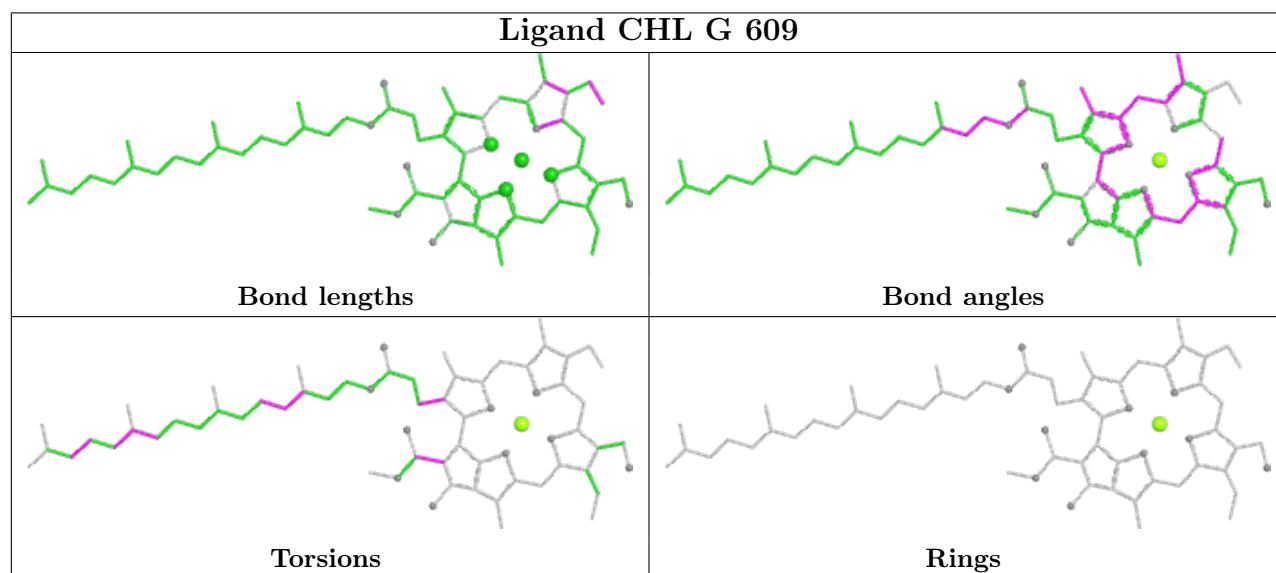
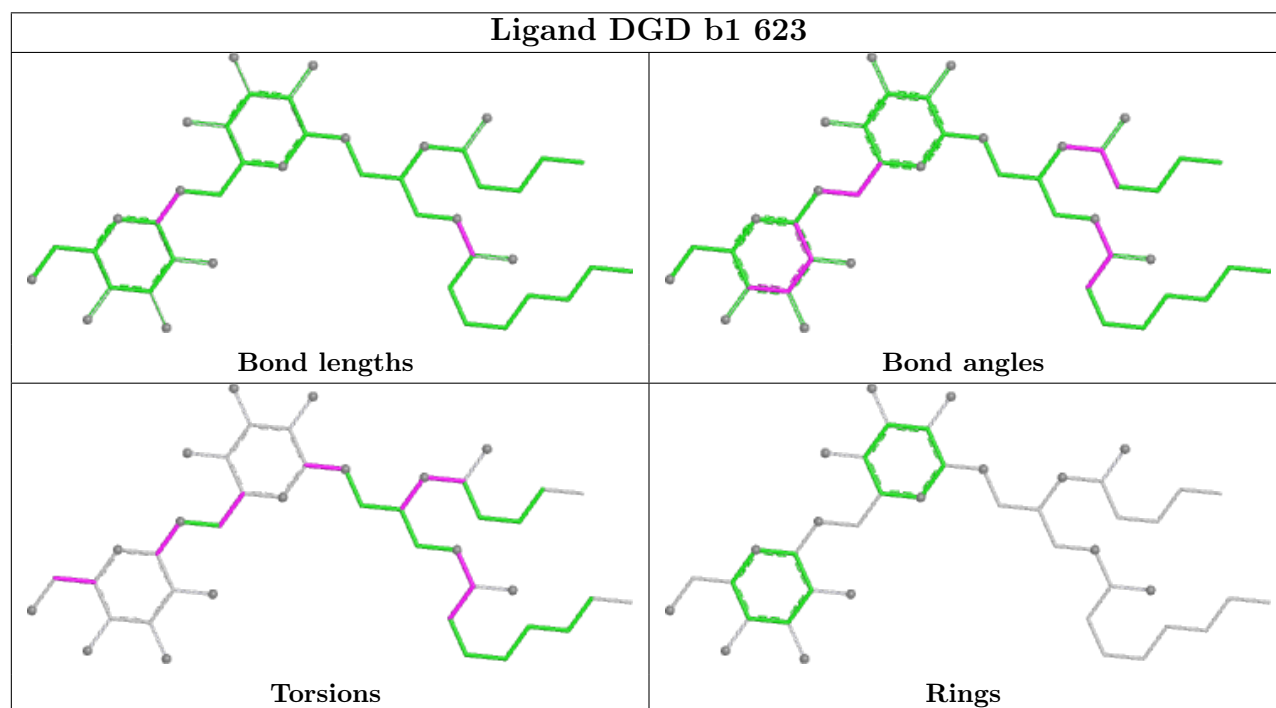
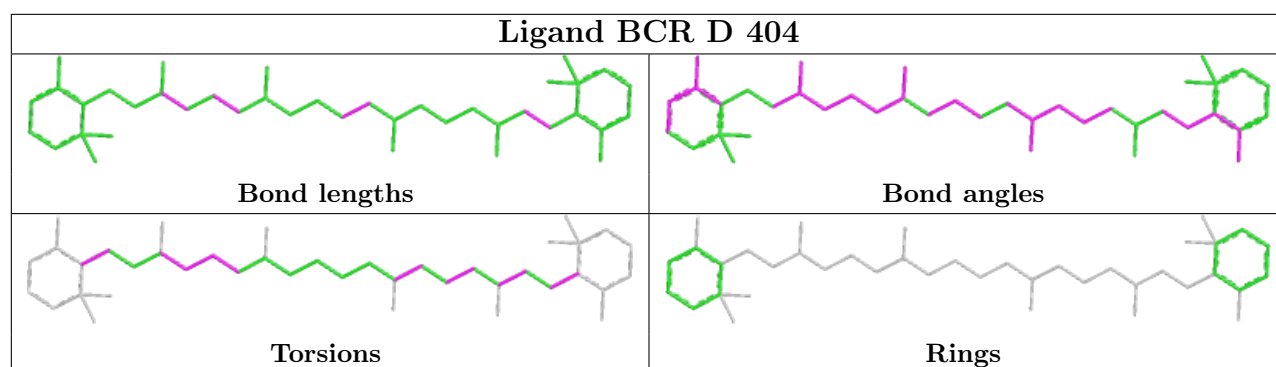


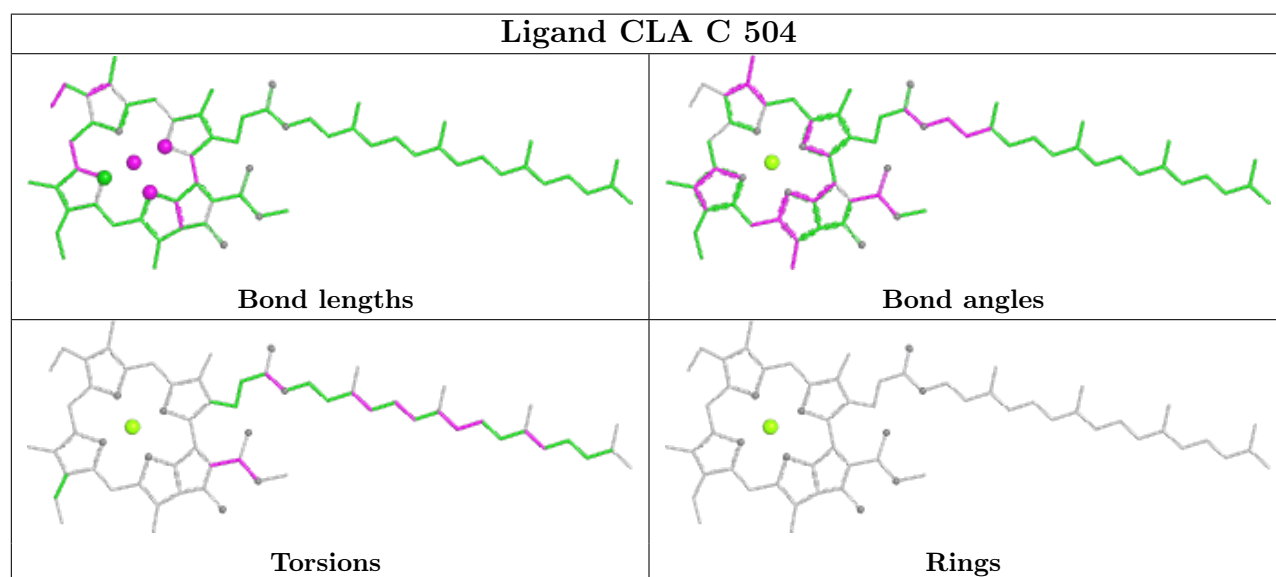
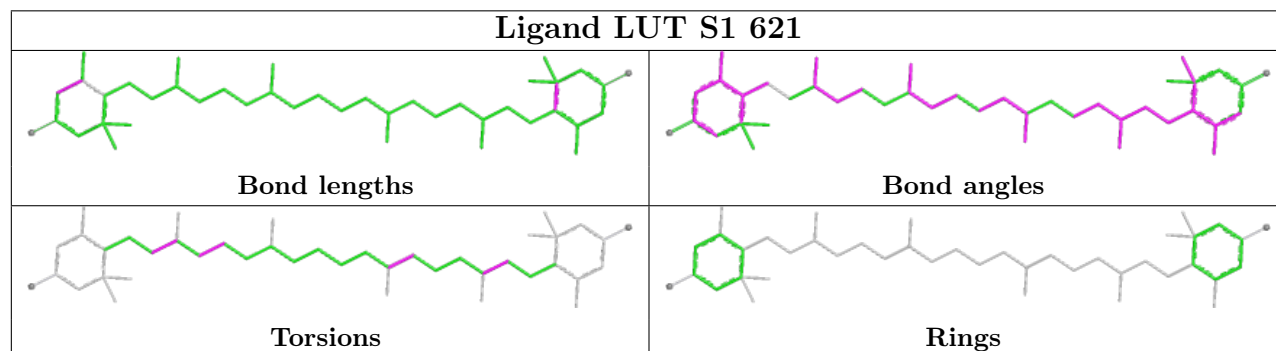
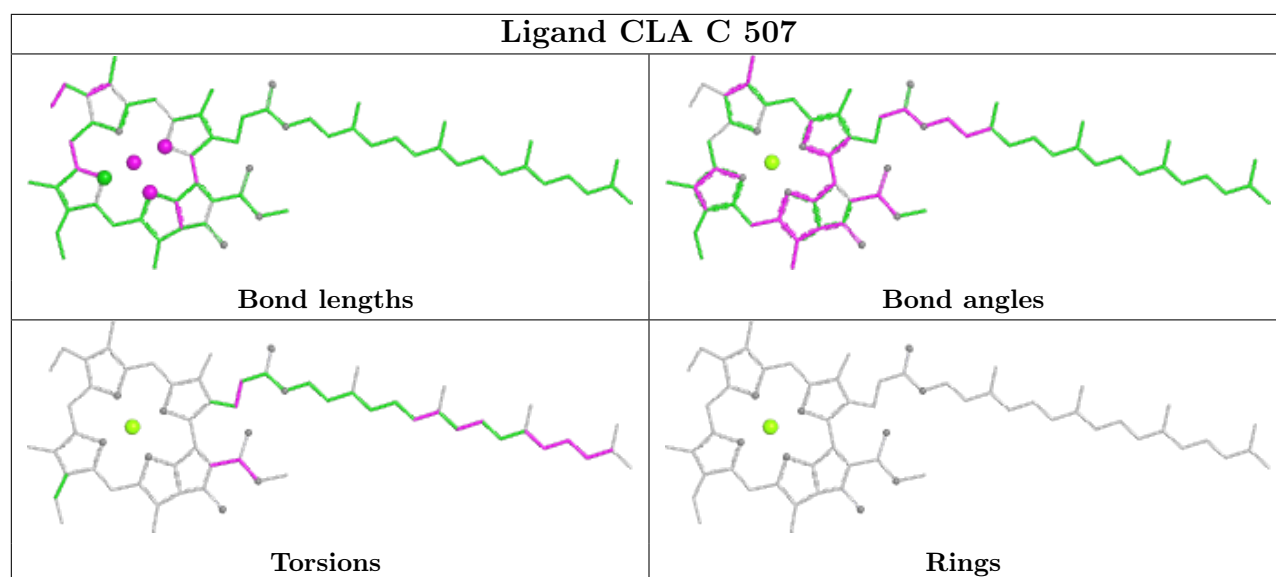


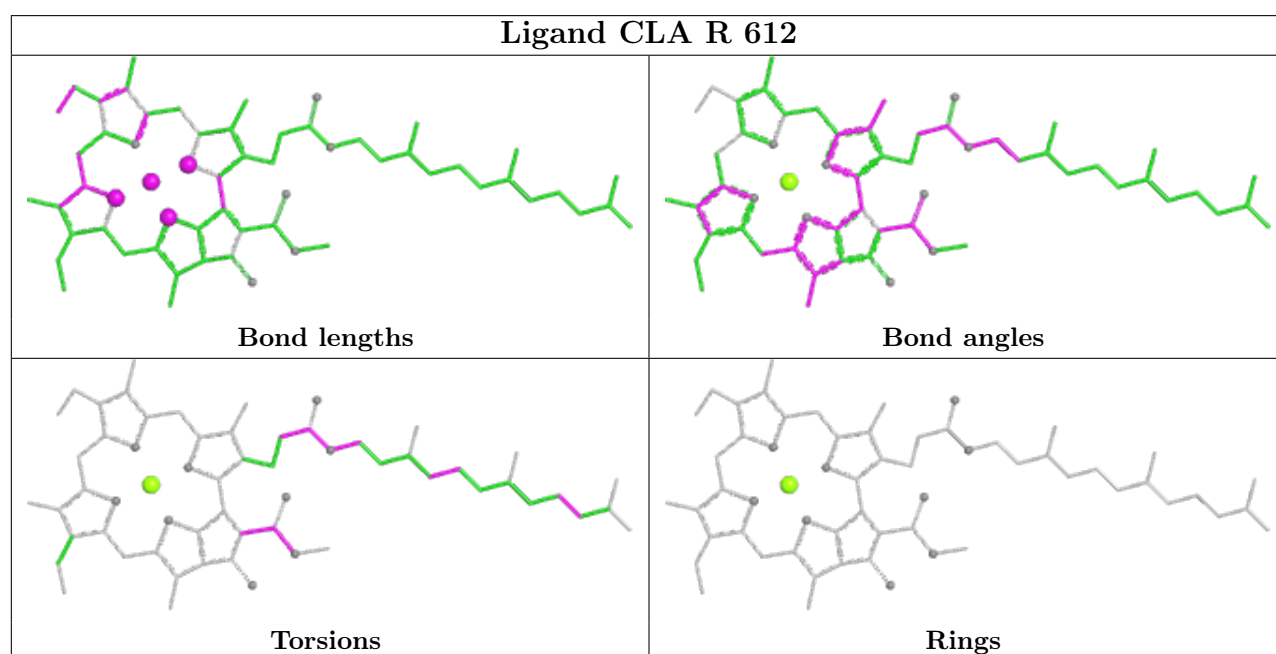
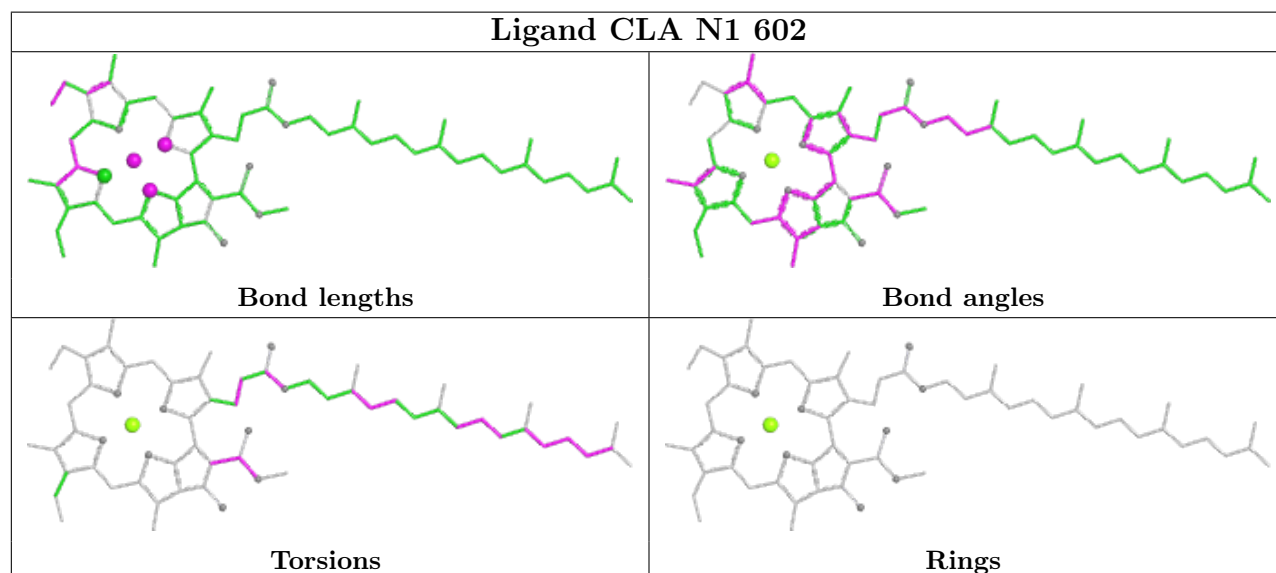
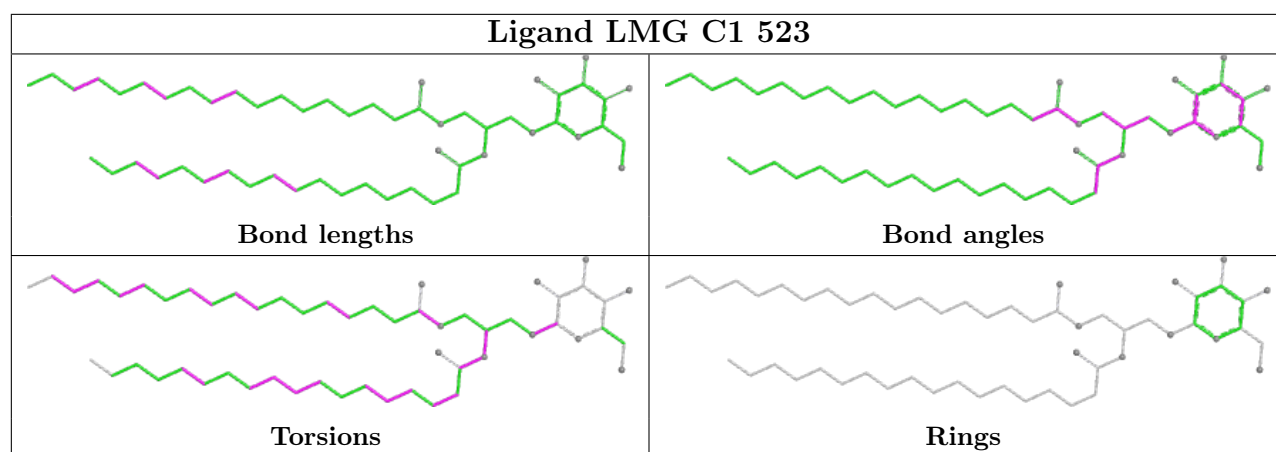


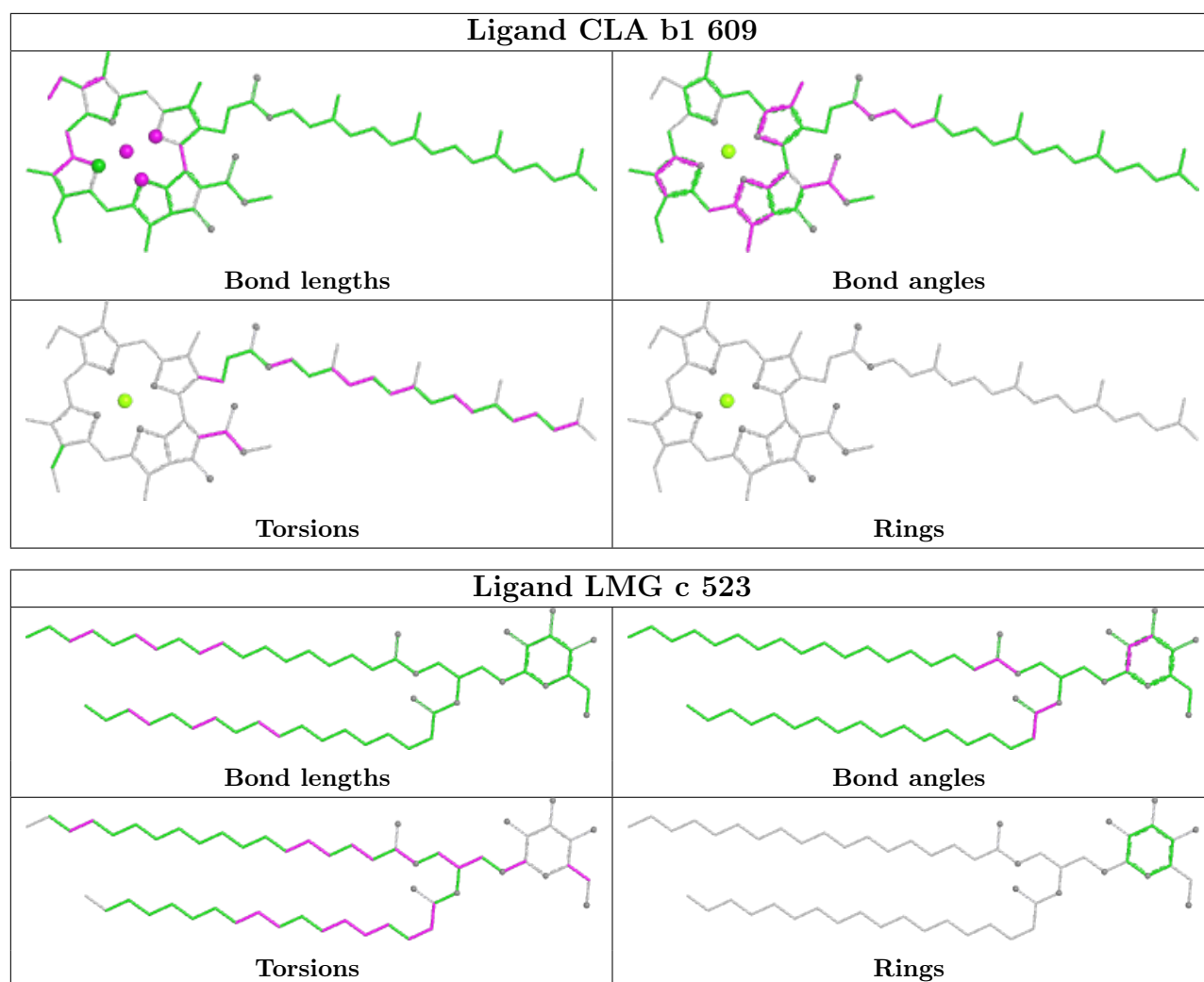




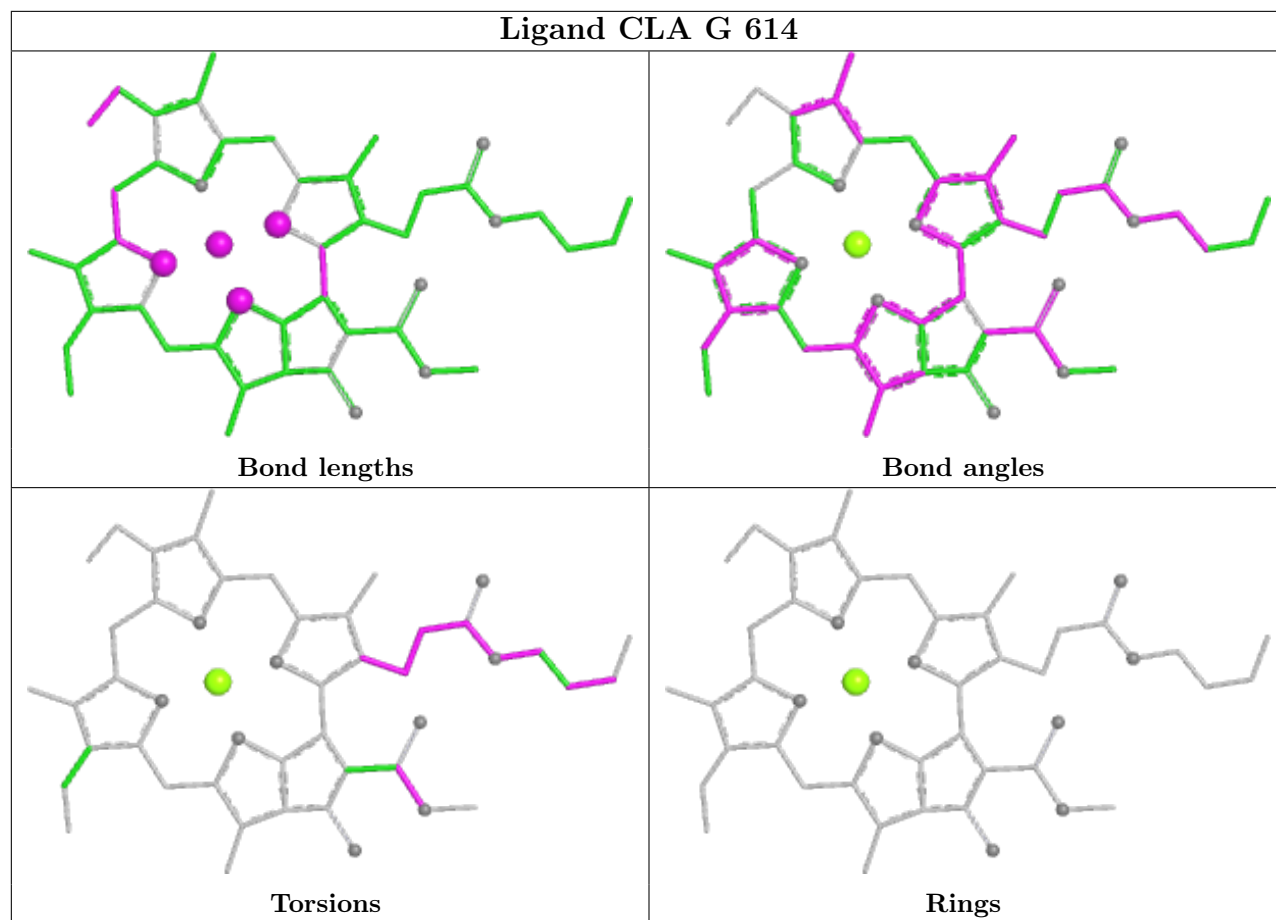


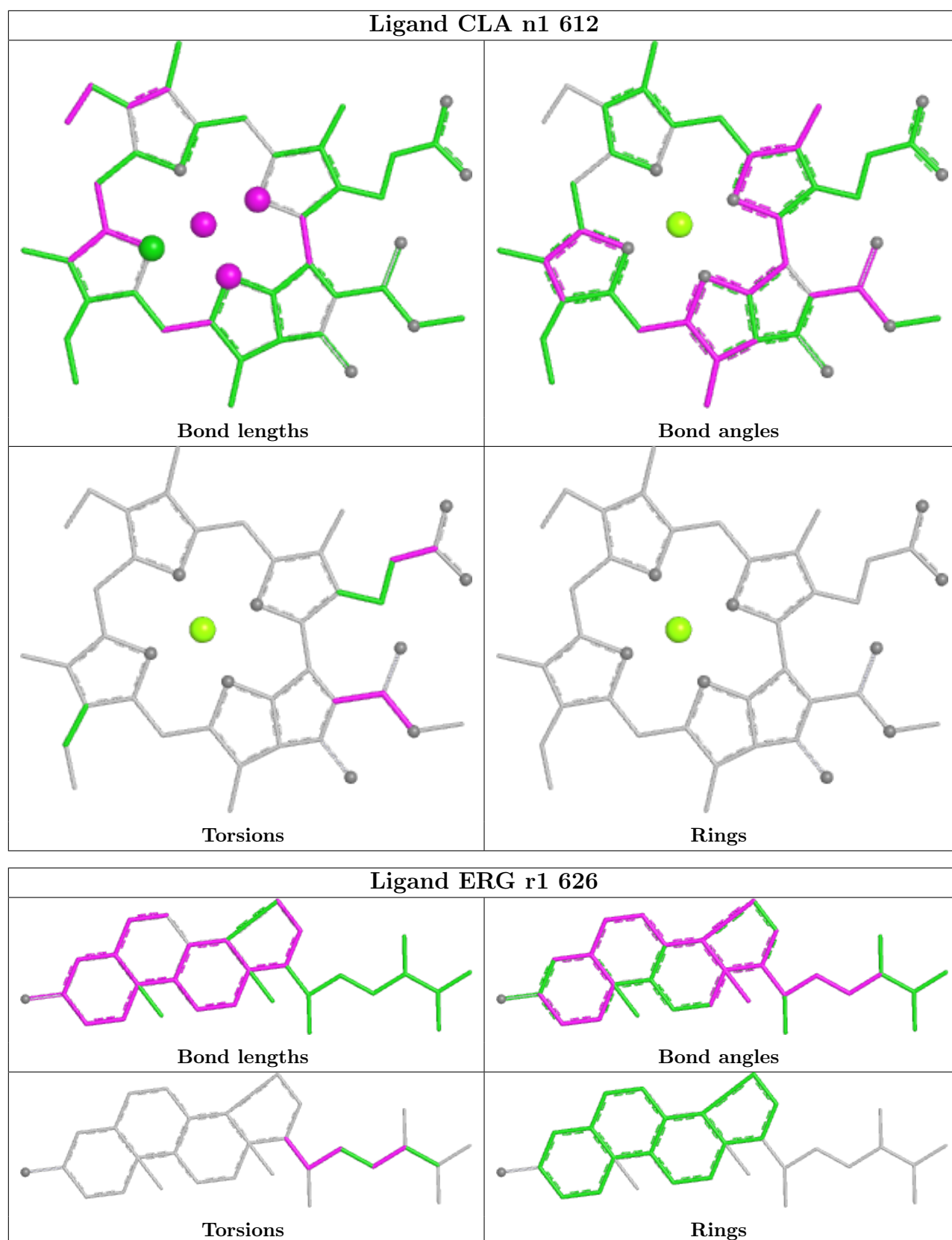


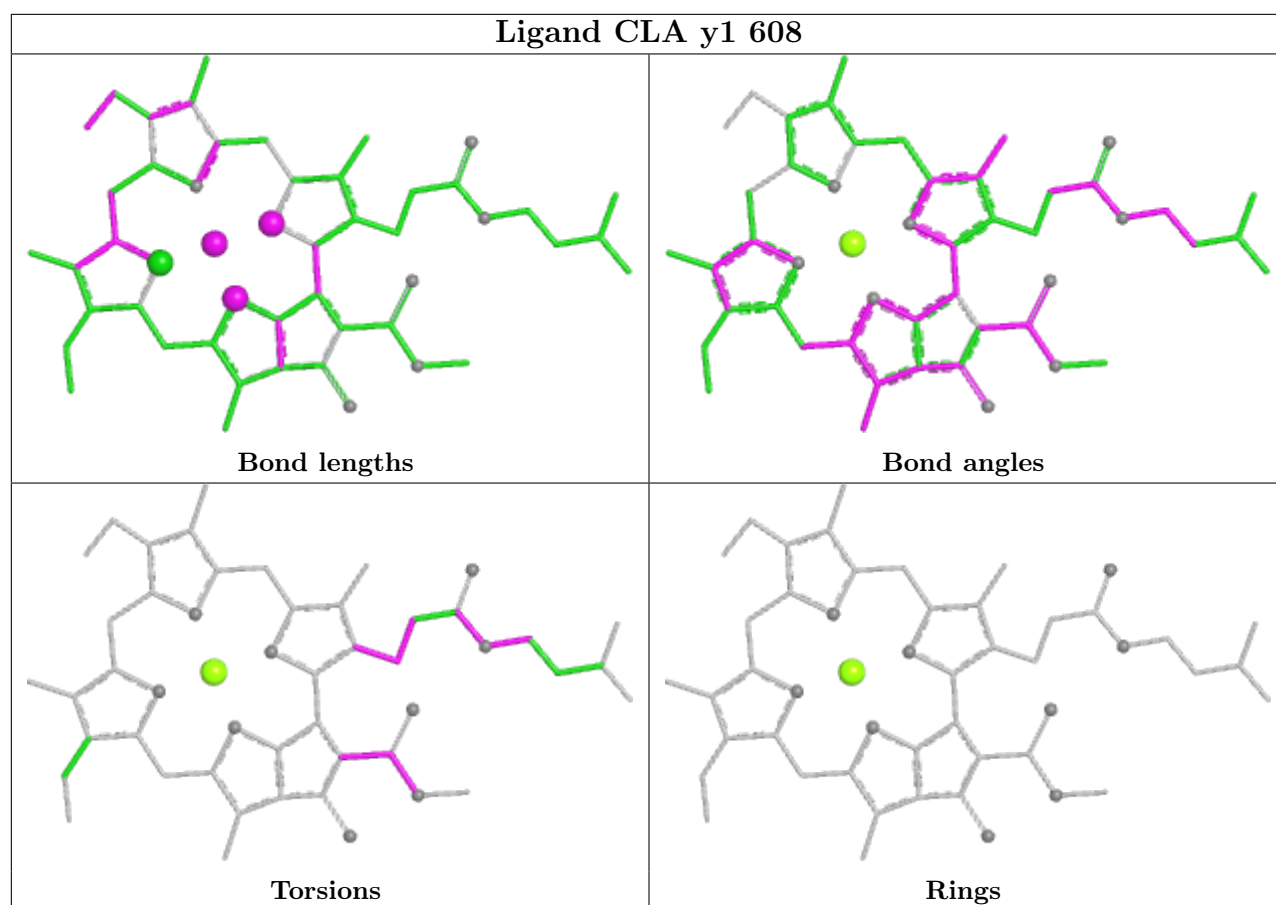




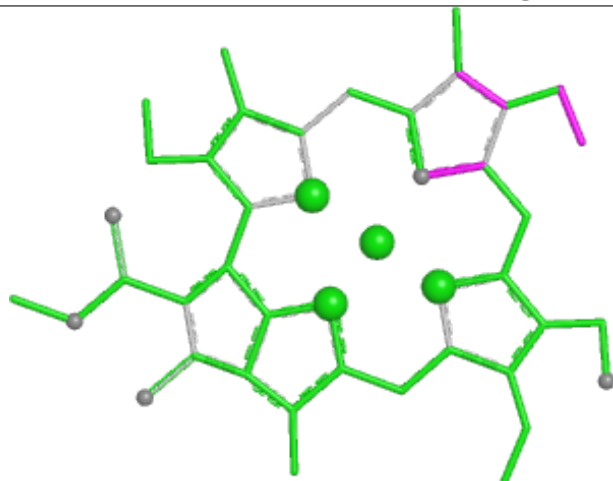




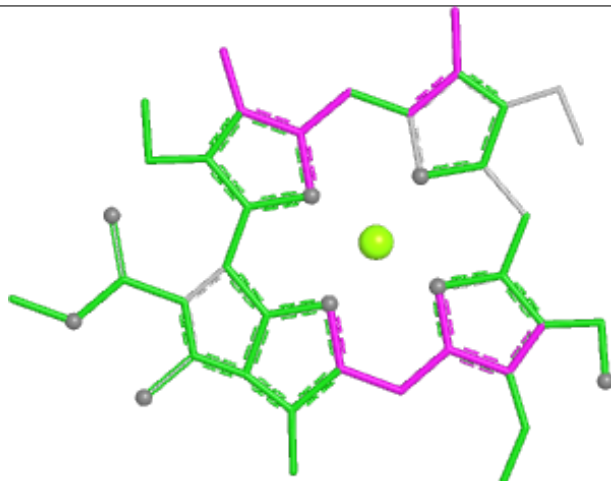




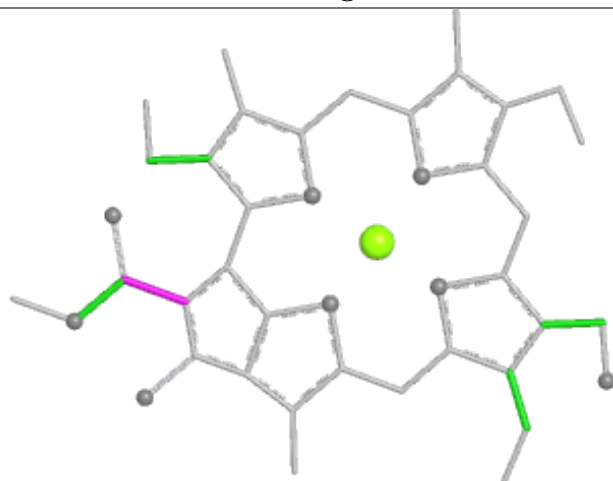
## Ligand CHL S 607



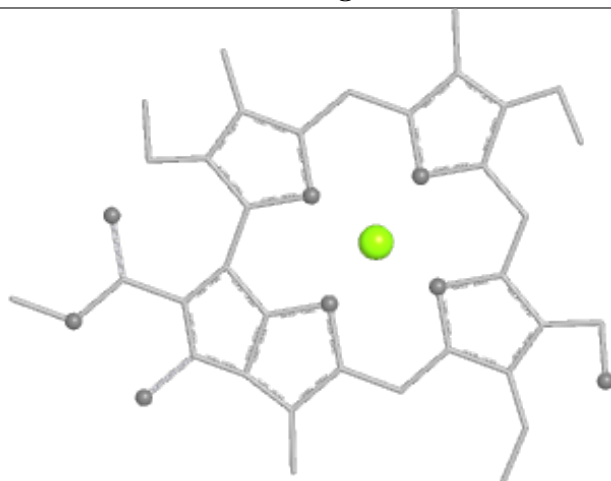
Bond lengths



Bond angles

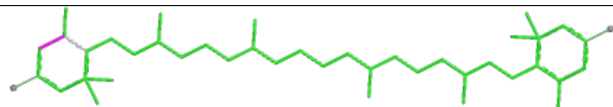


Torsions

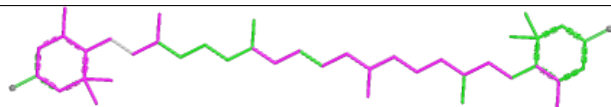


Rings

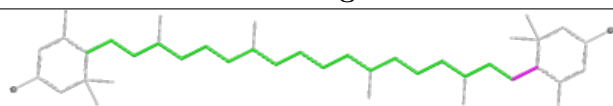
## Ligand LUT N 620



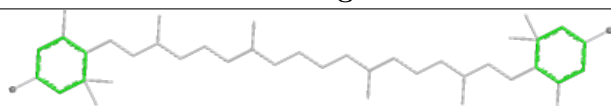
Bond lengths



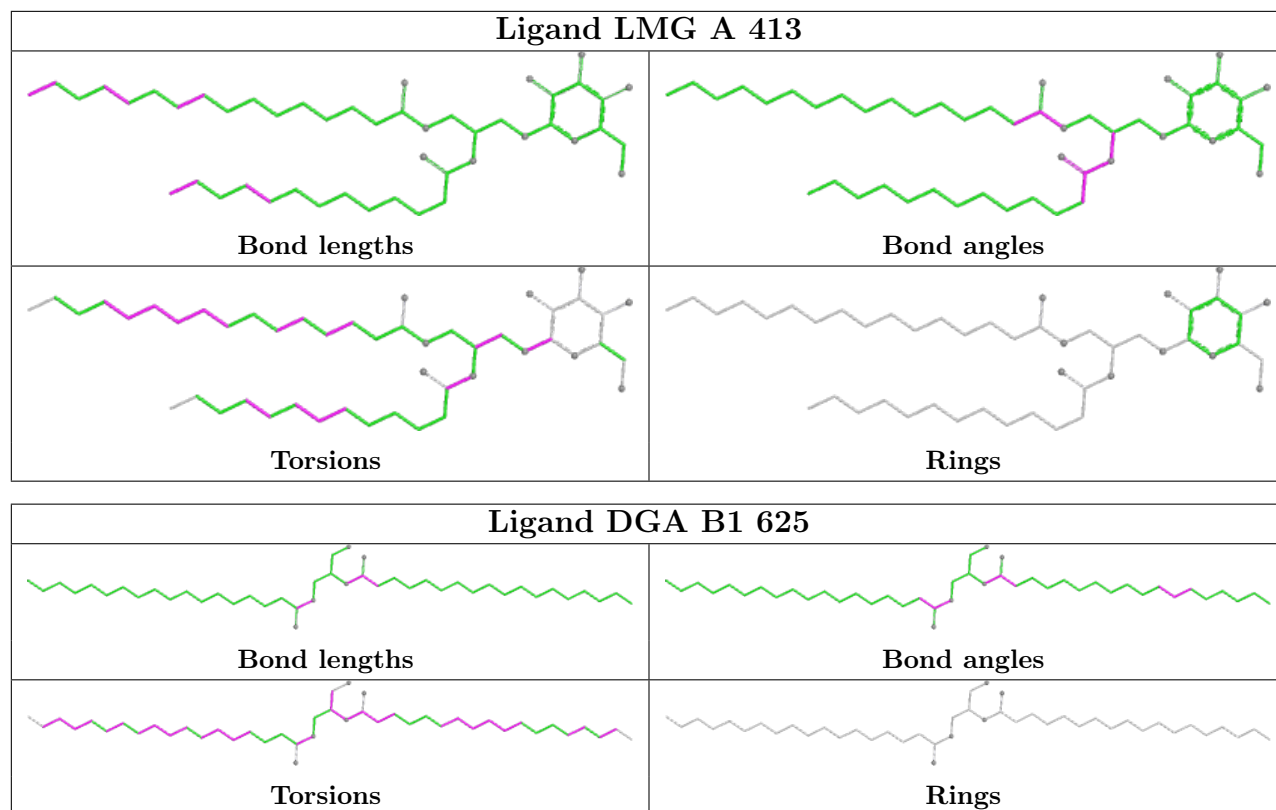
Bond angles

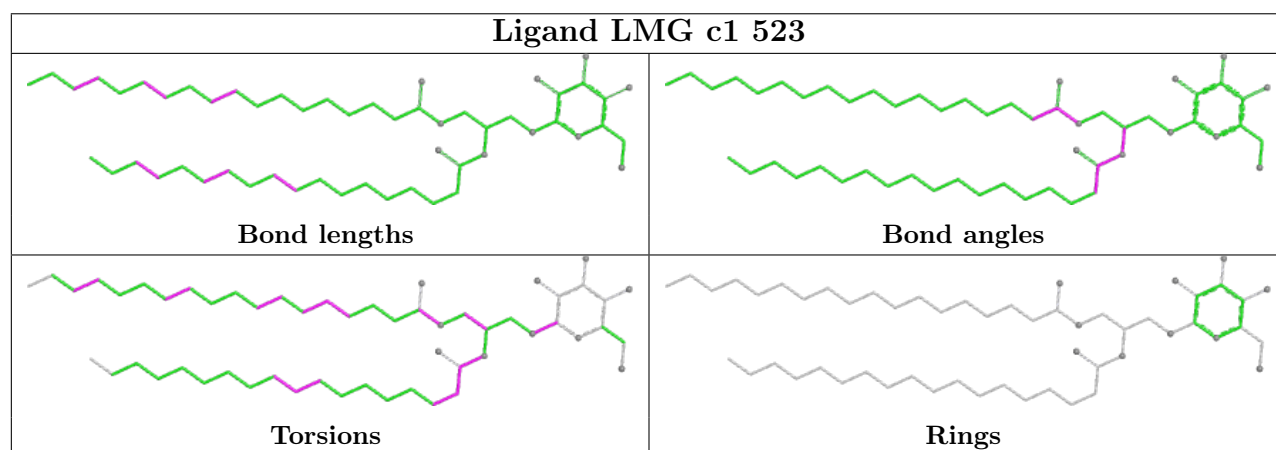
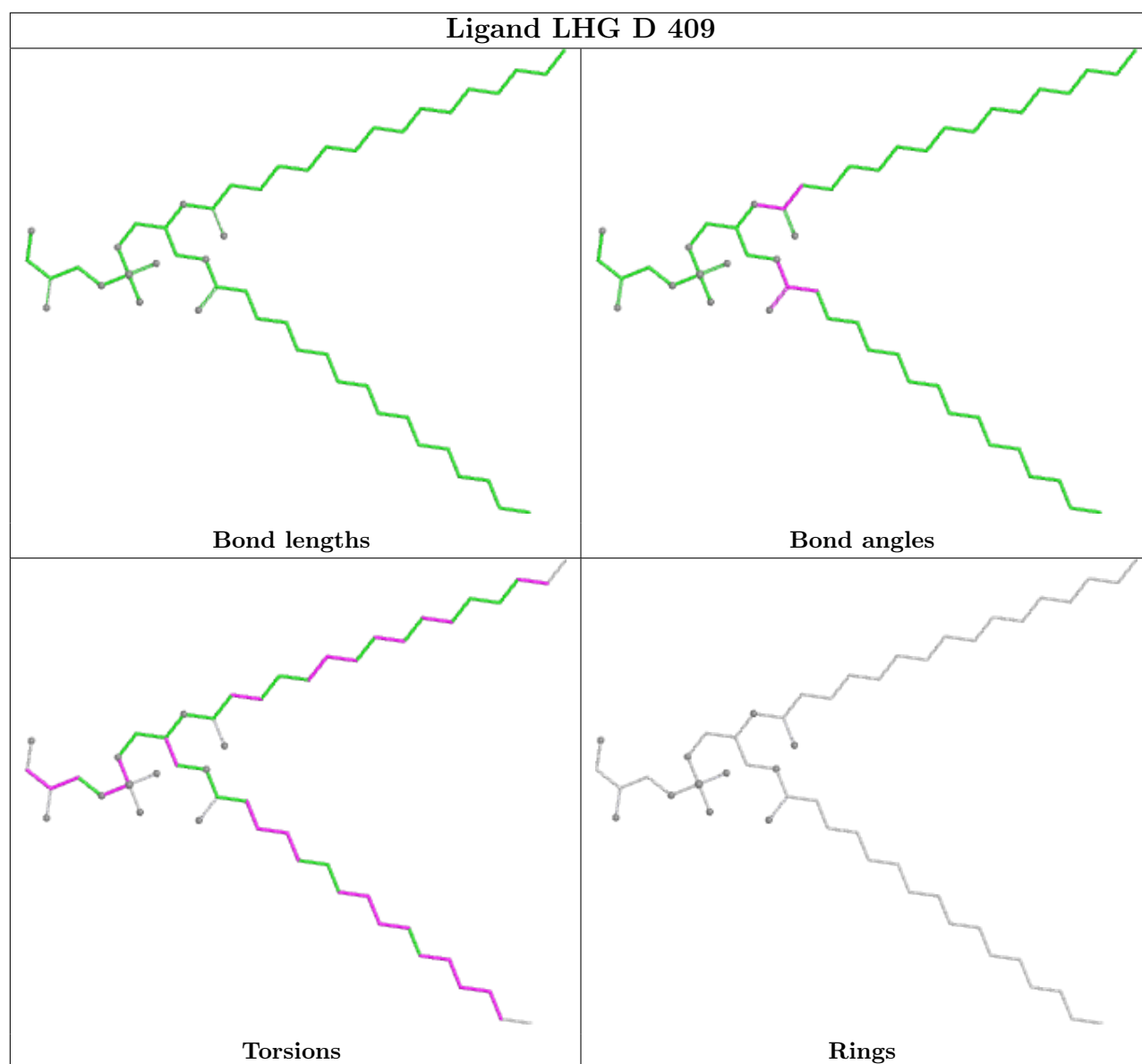


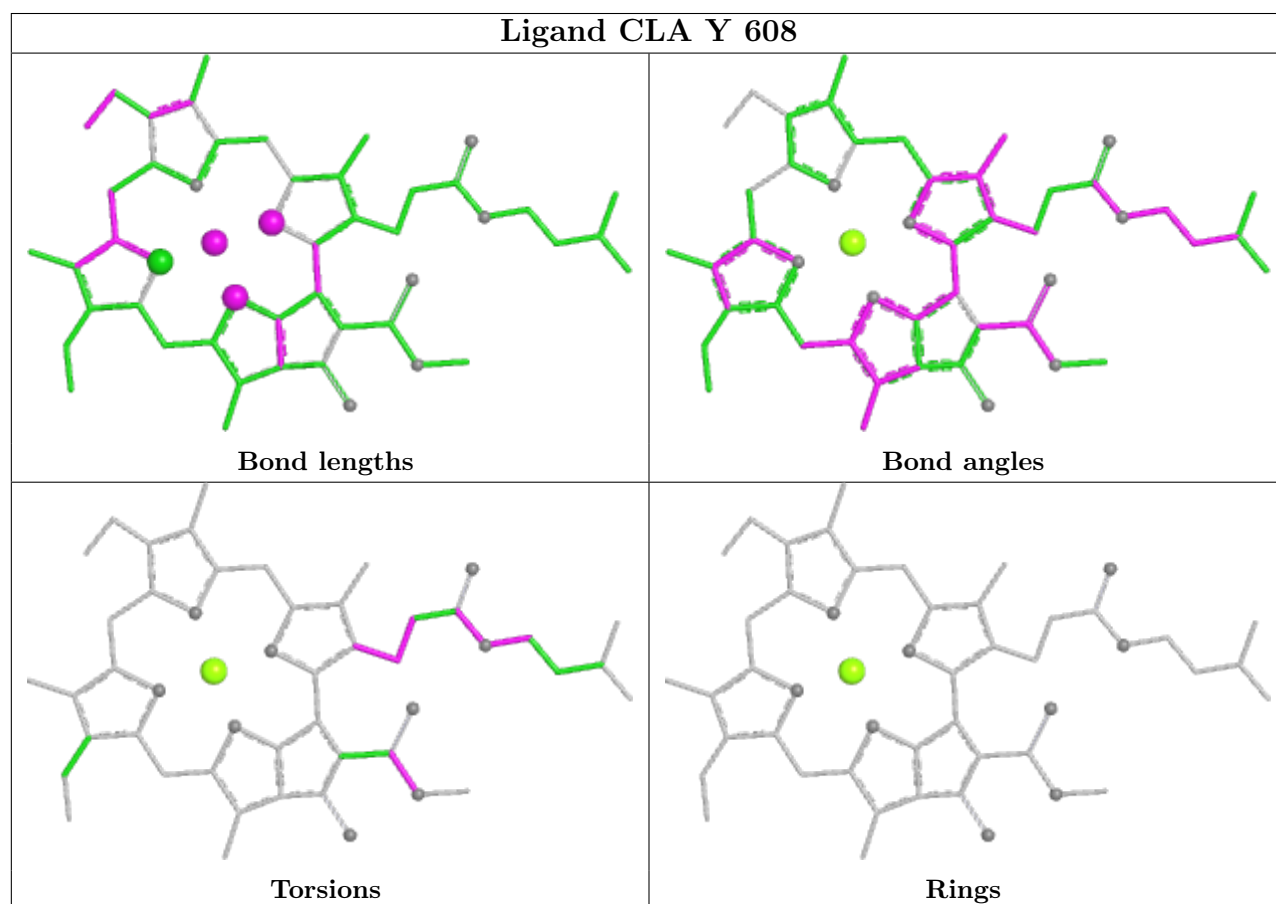
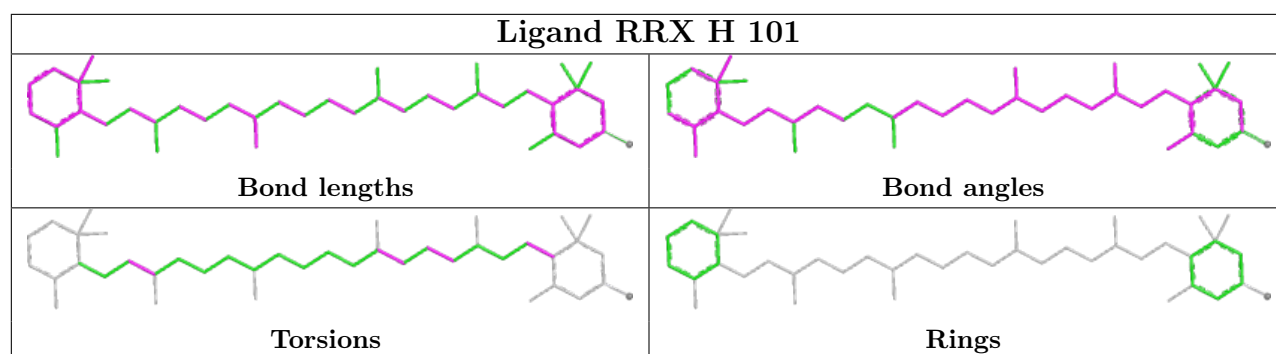
Torsions

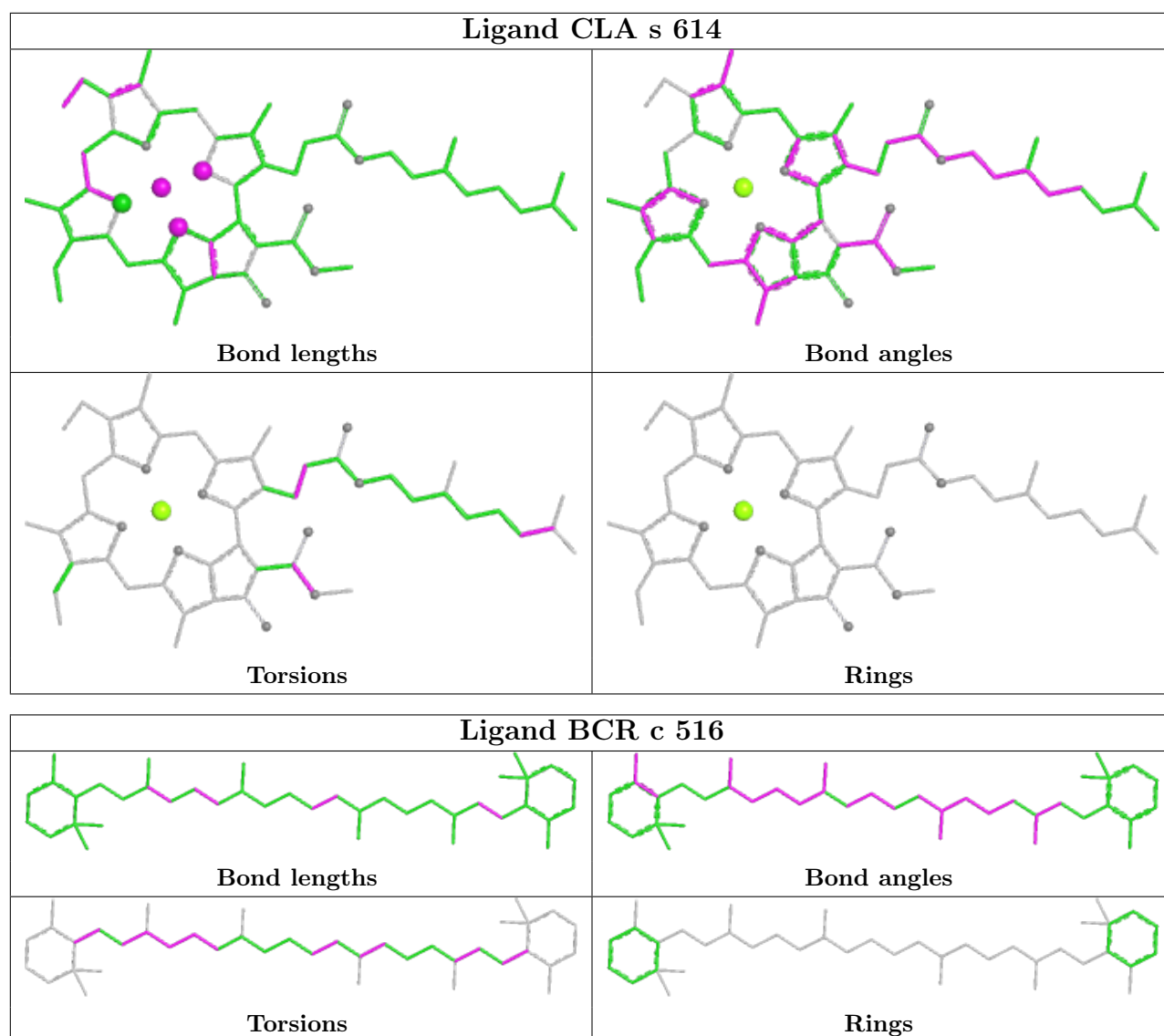


Rings



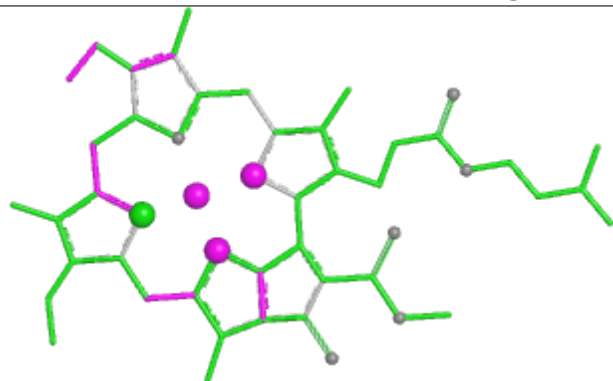




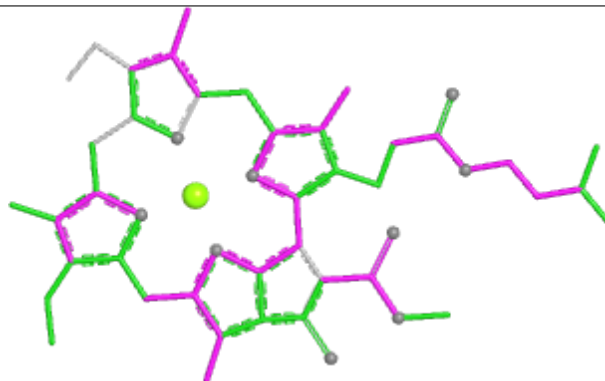




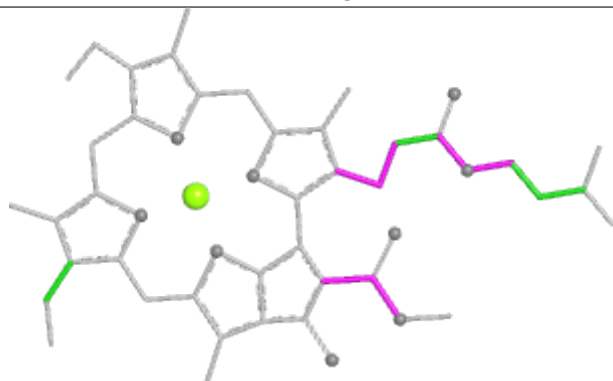
## Ligand CLA A1 407



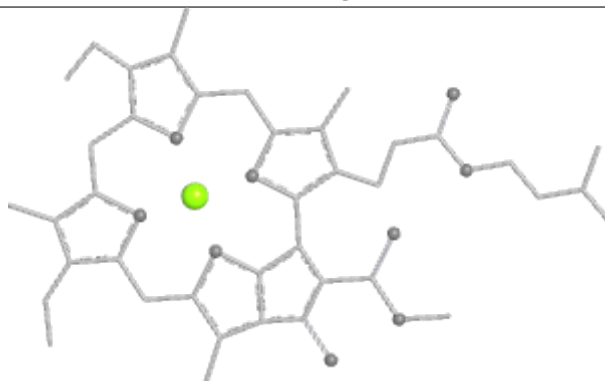
Bond lengths



Bond angles

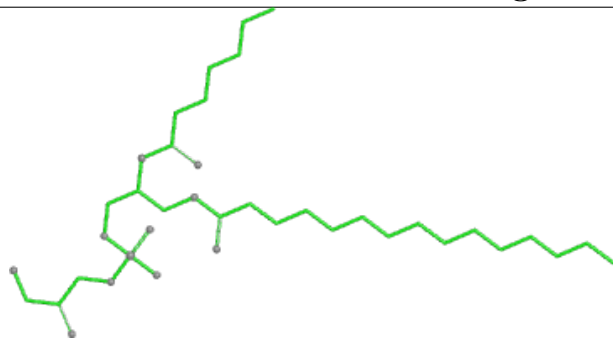


Torsions

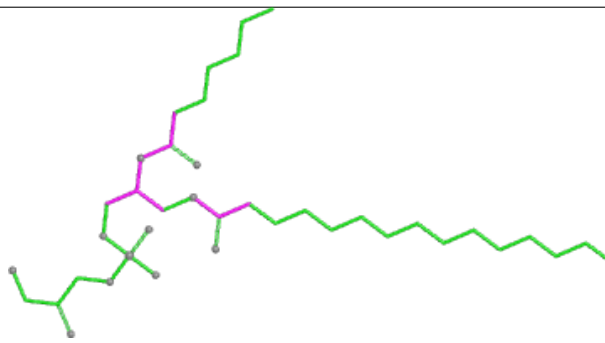


Rings

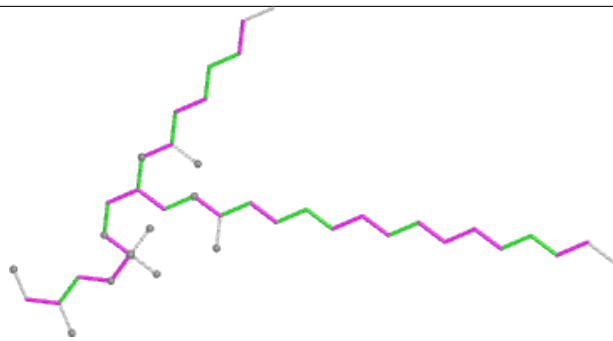
## Ligand LHG D 410



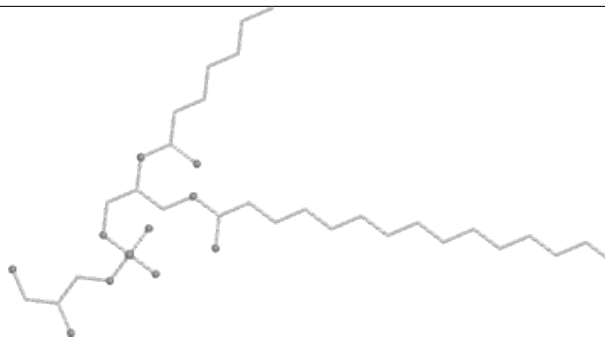
Bond lengths



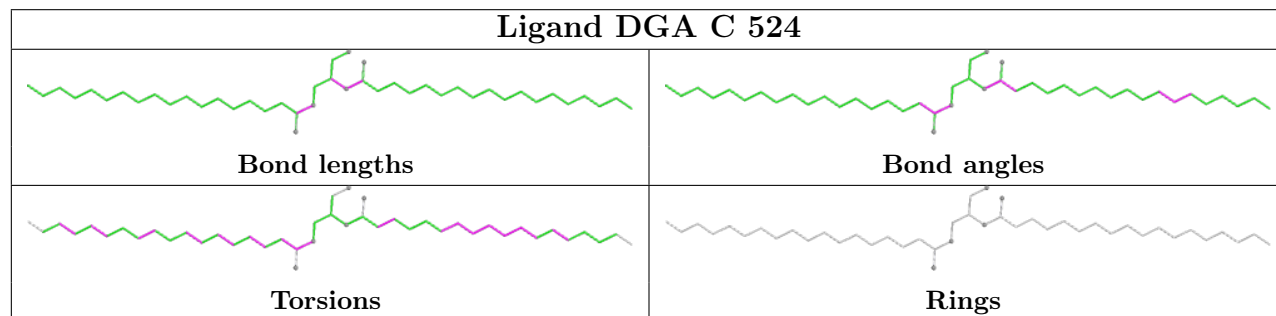
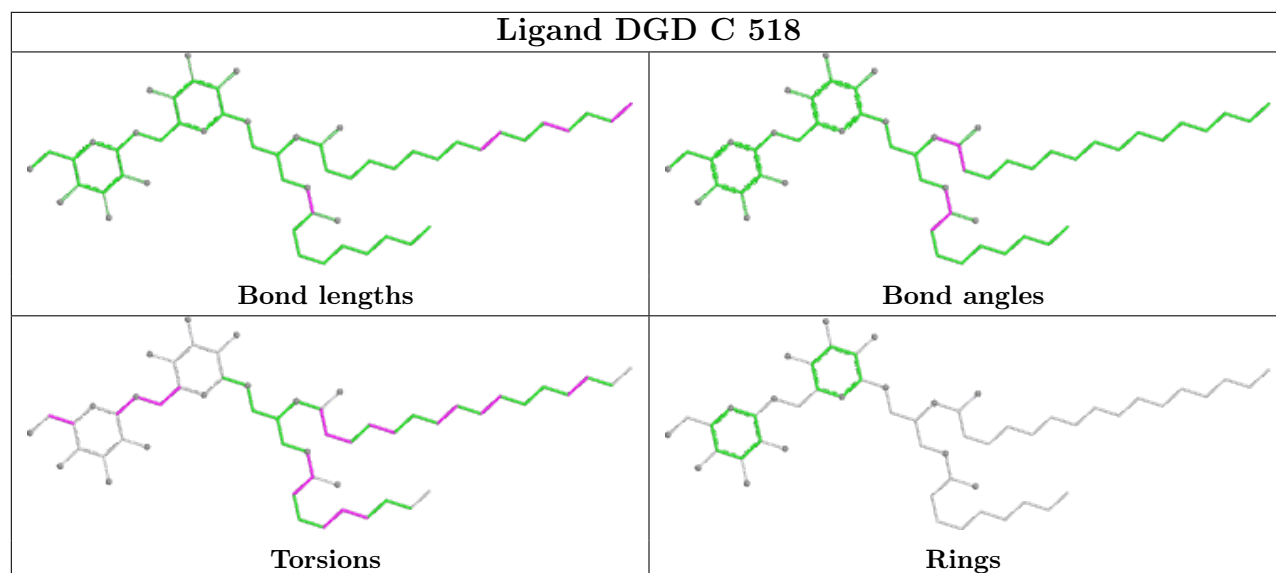
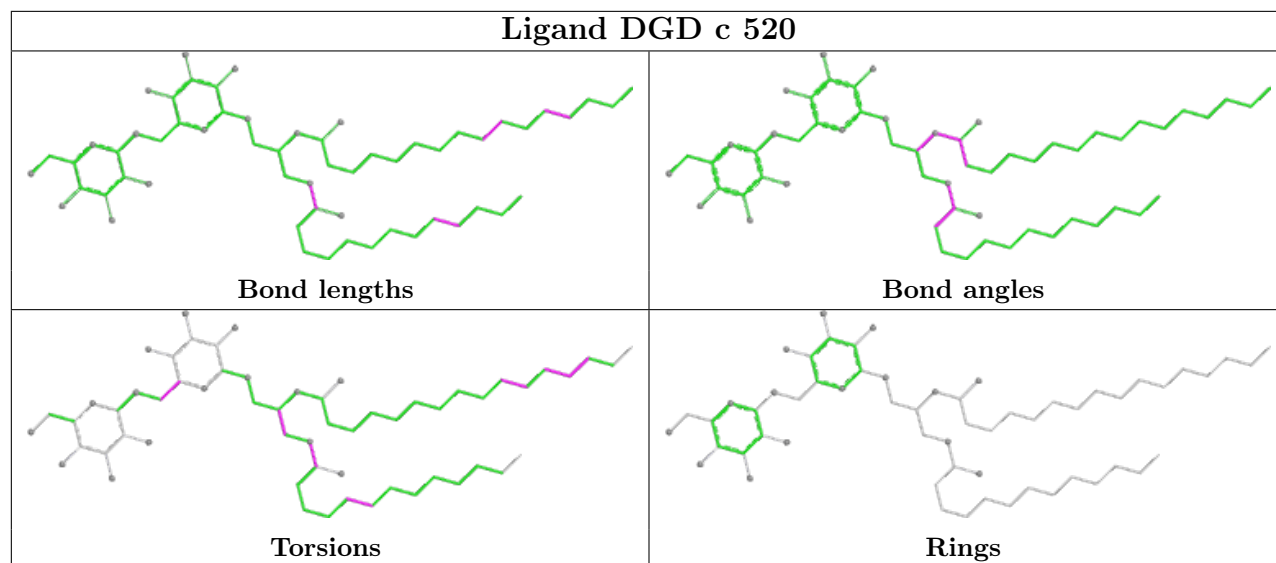
Bond angles

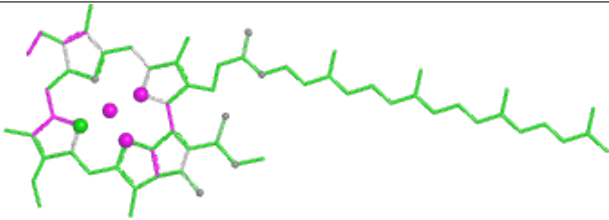
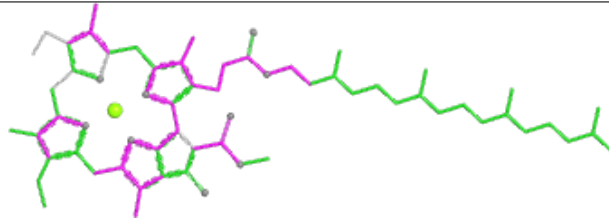
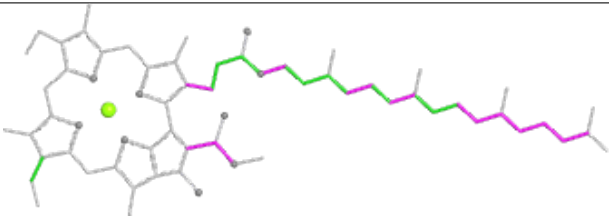
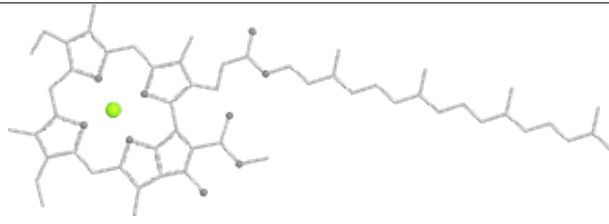


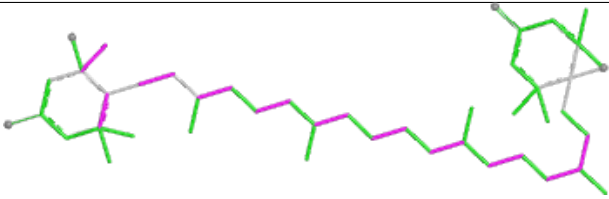
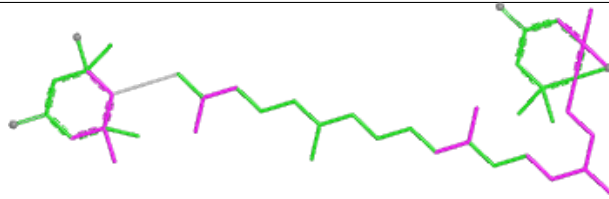
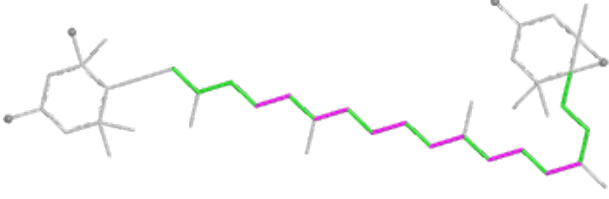
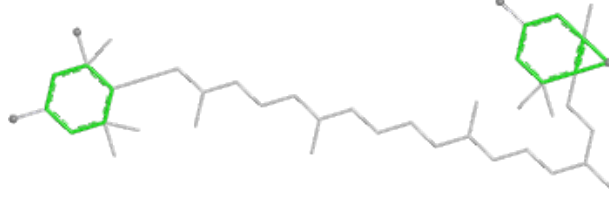
Torsions

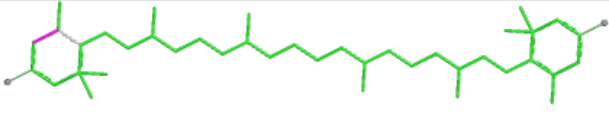
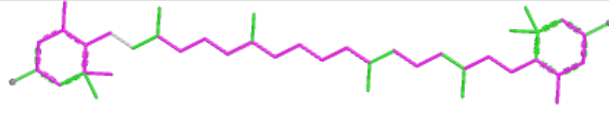
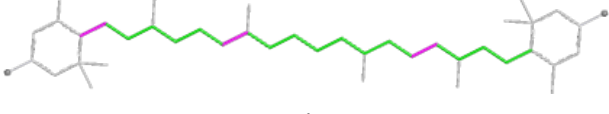
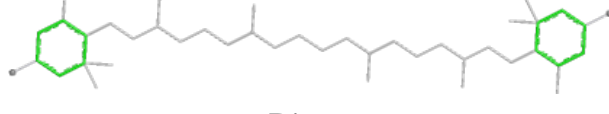


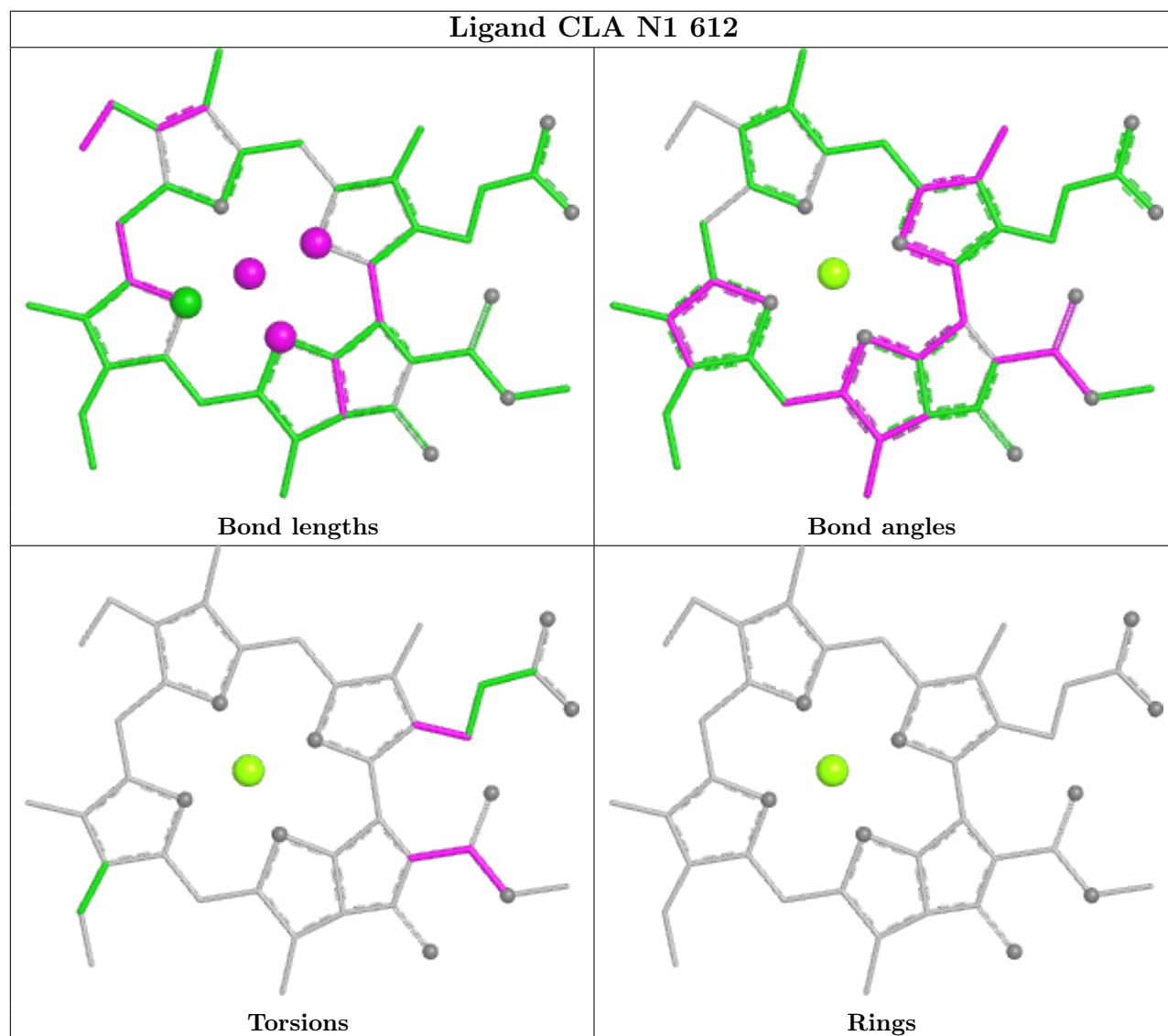
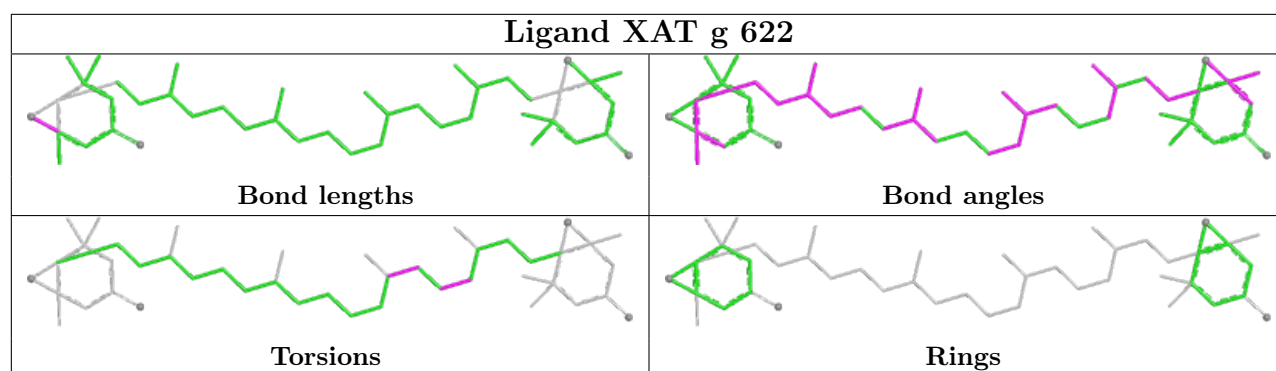
Rings

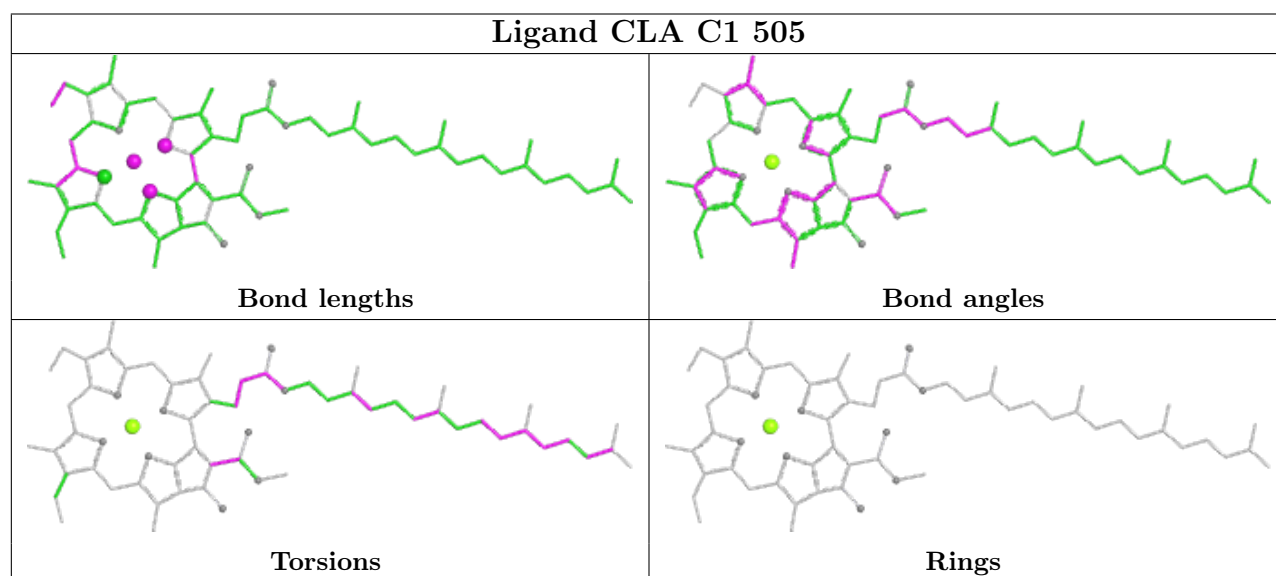
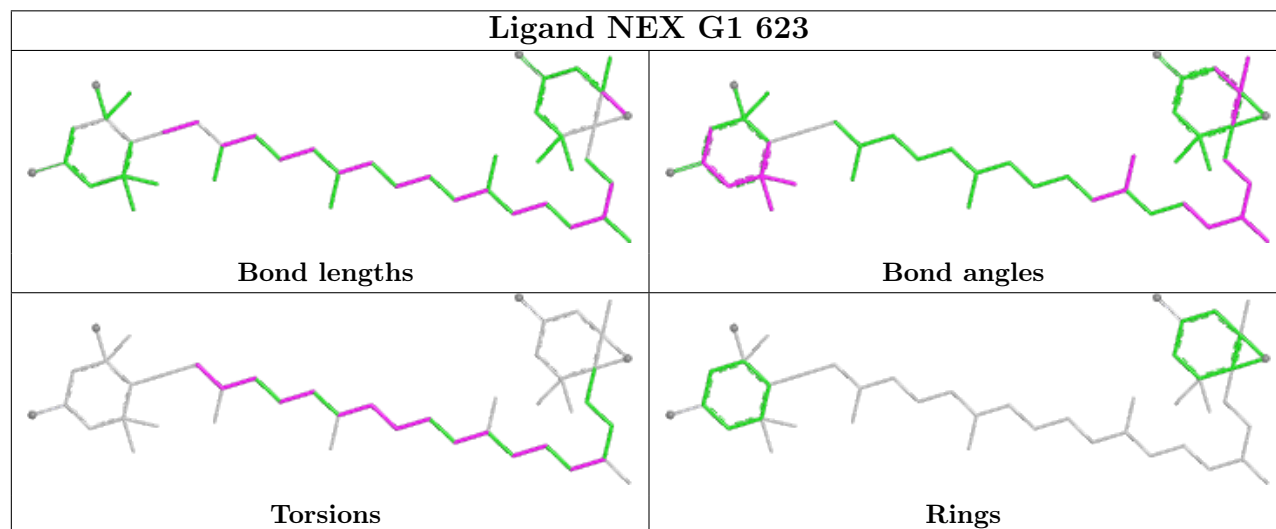
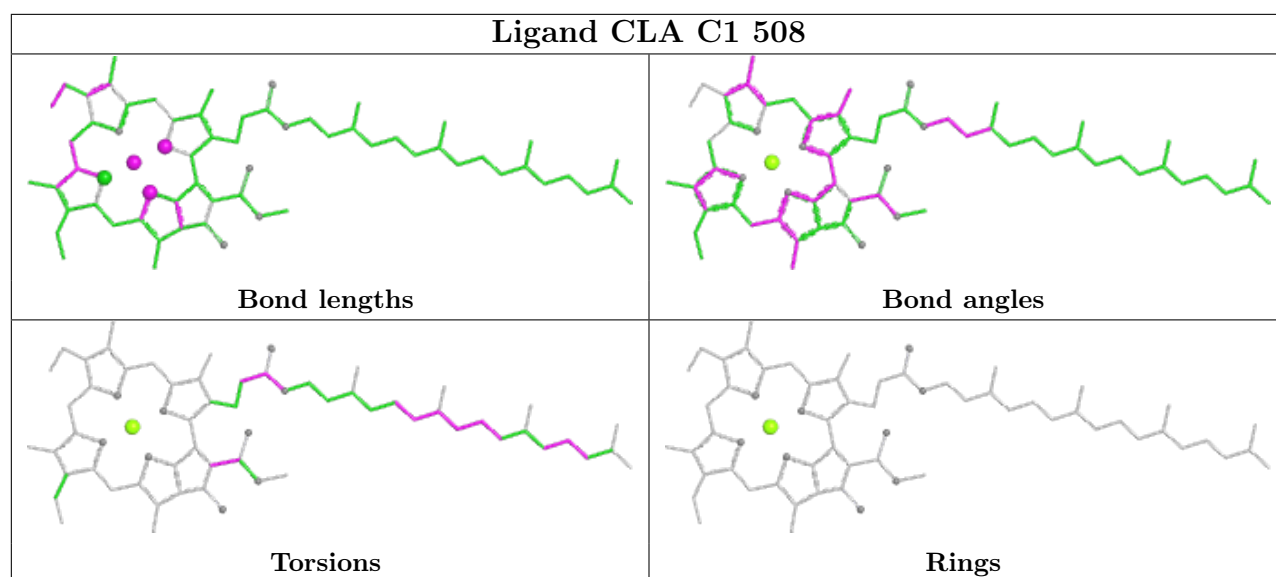


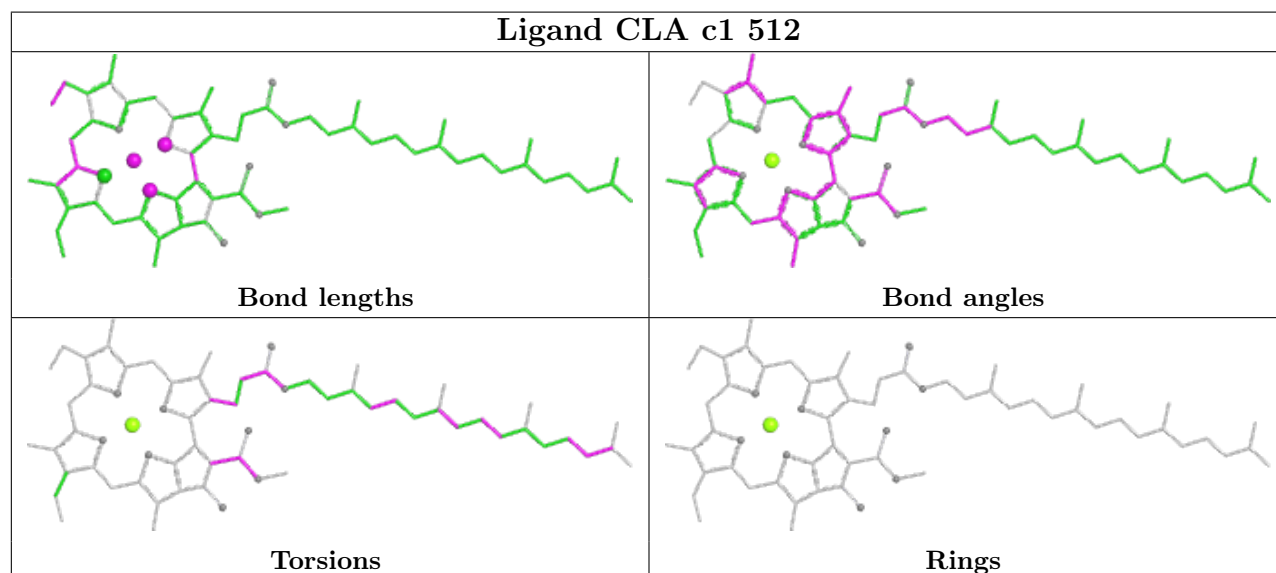
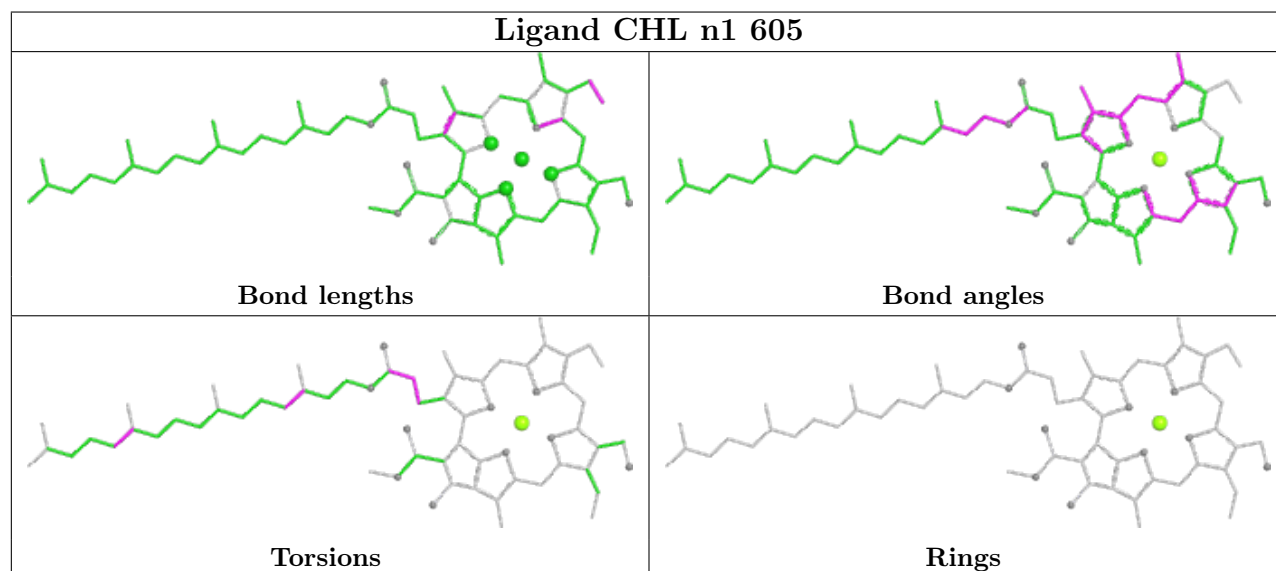
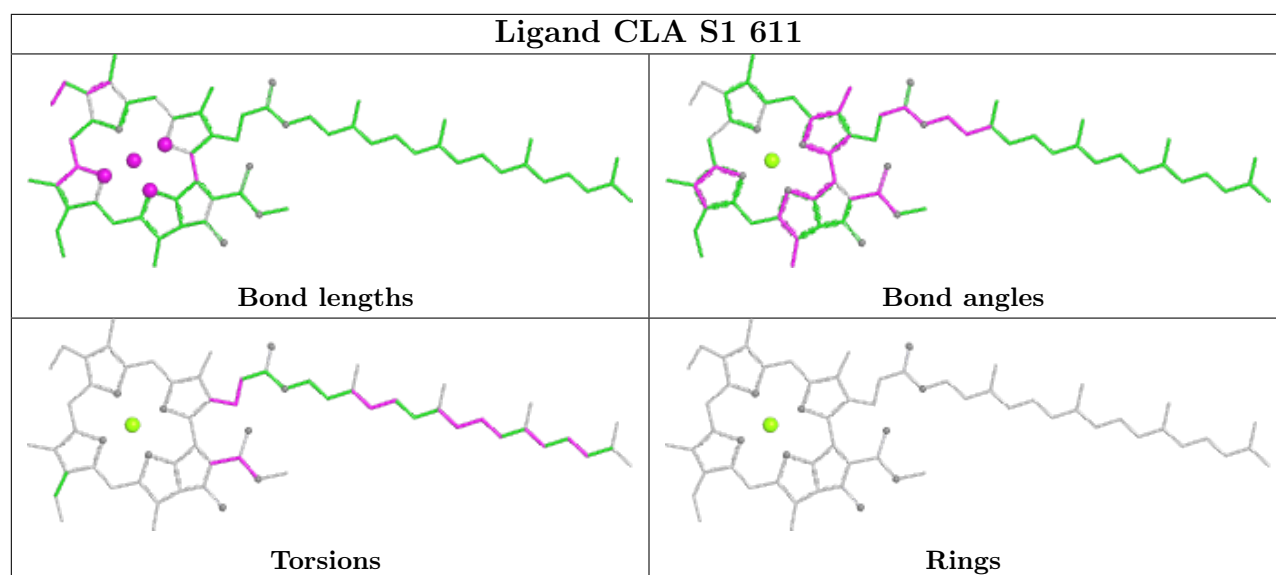
Ligand CLA n 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand NEX R 622	
	
Bond lengths	Bond angles
	
Torsions	Rings

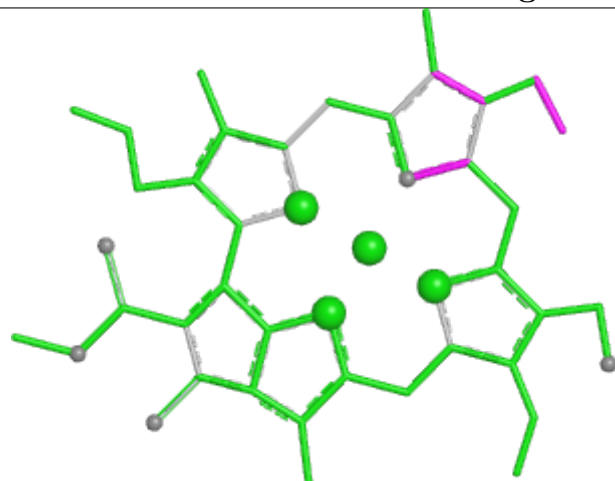
Ligand LUT g 620	
	
Bond lengths	Bond angles
	
Torsions	Rings



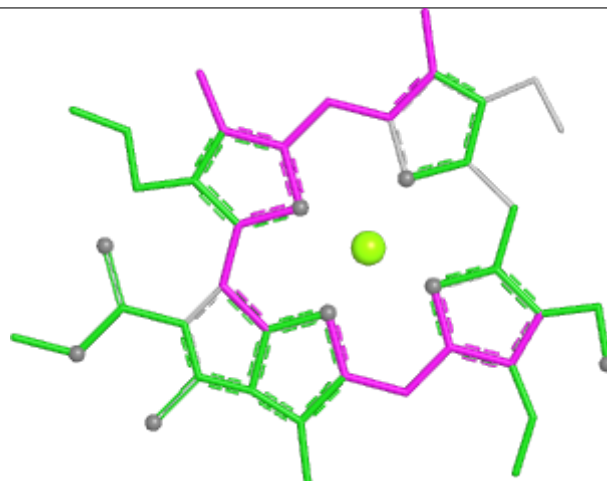




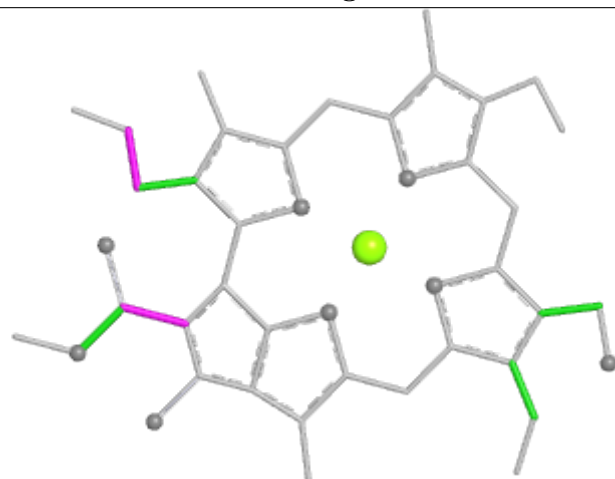
## Ligand CHL S 606



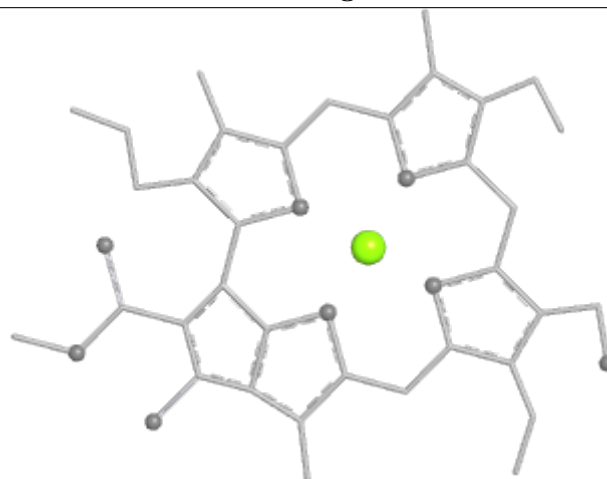
Bond lengths



Bond angles

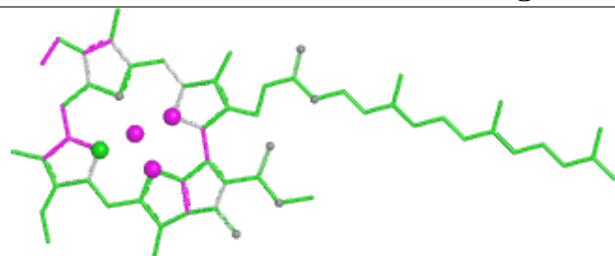


Torsions

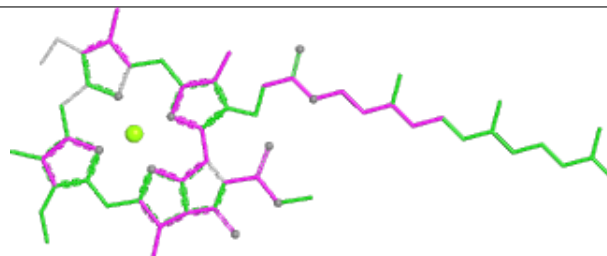


Rings

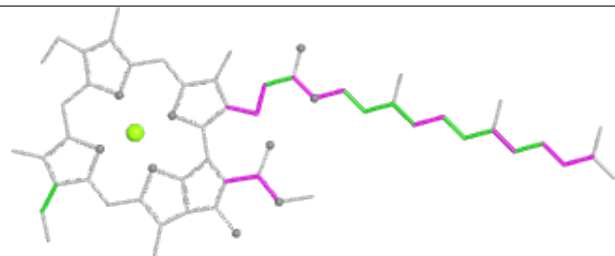
## Ligand CLA R 603



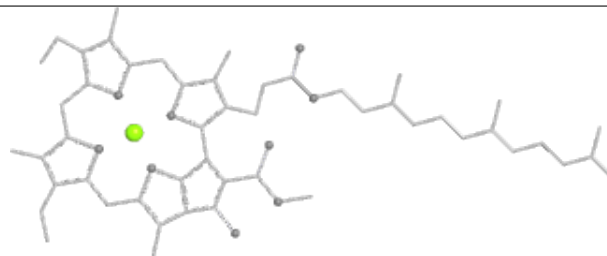
Bond lengths



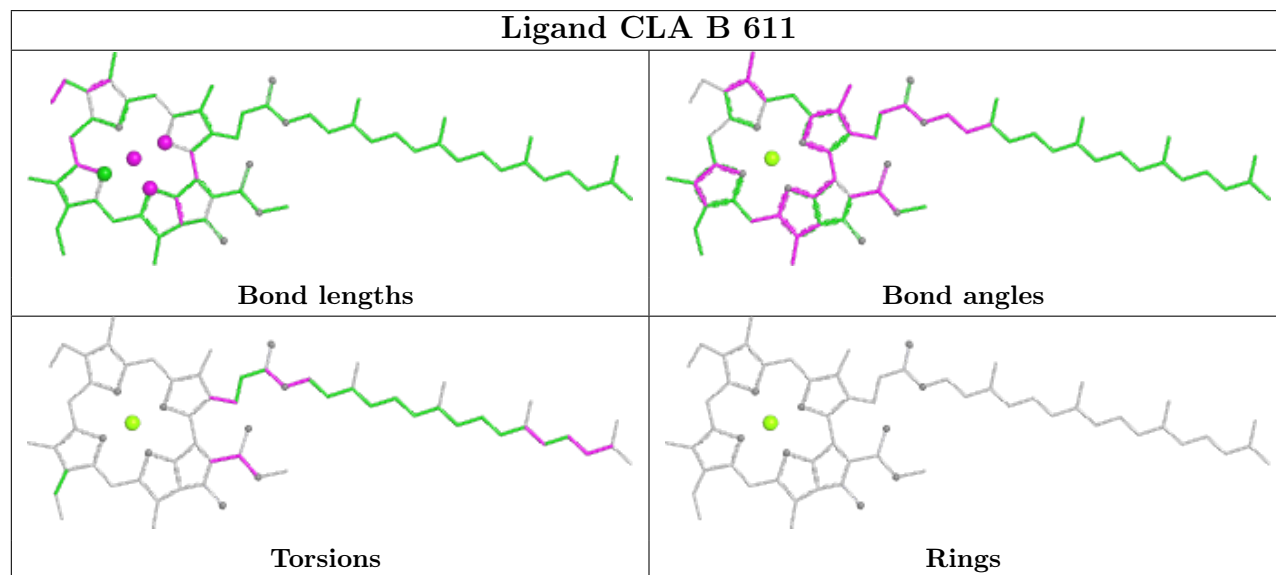
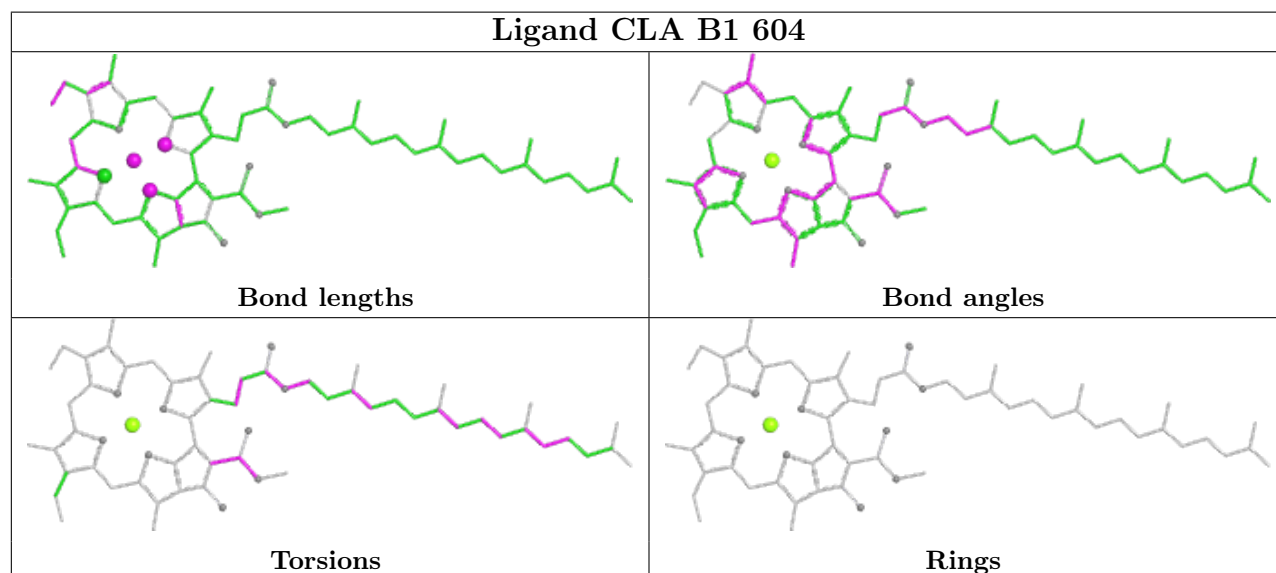
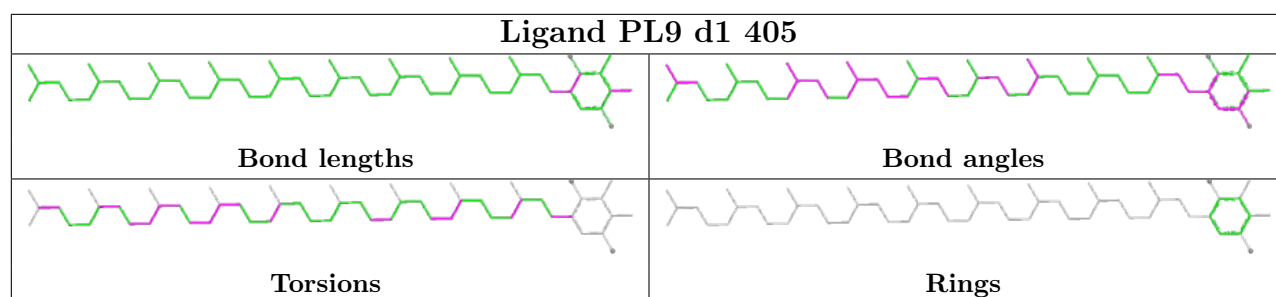
Bond angles



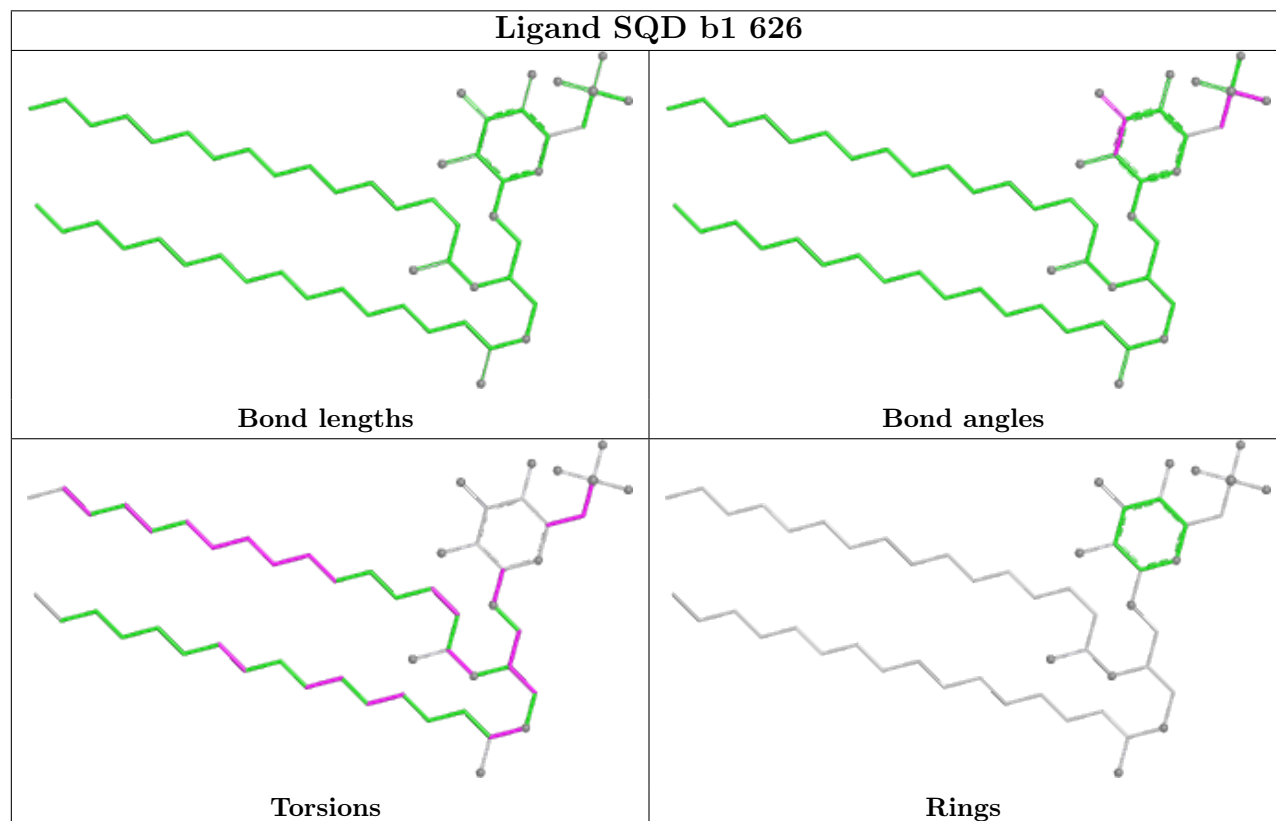
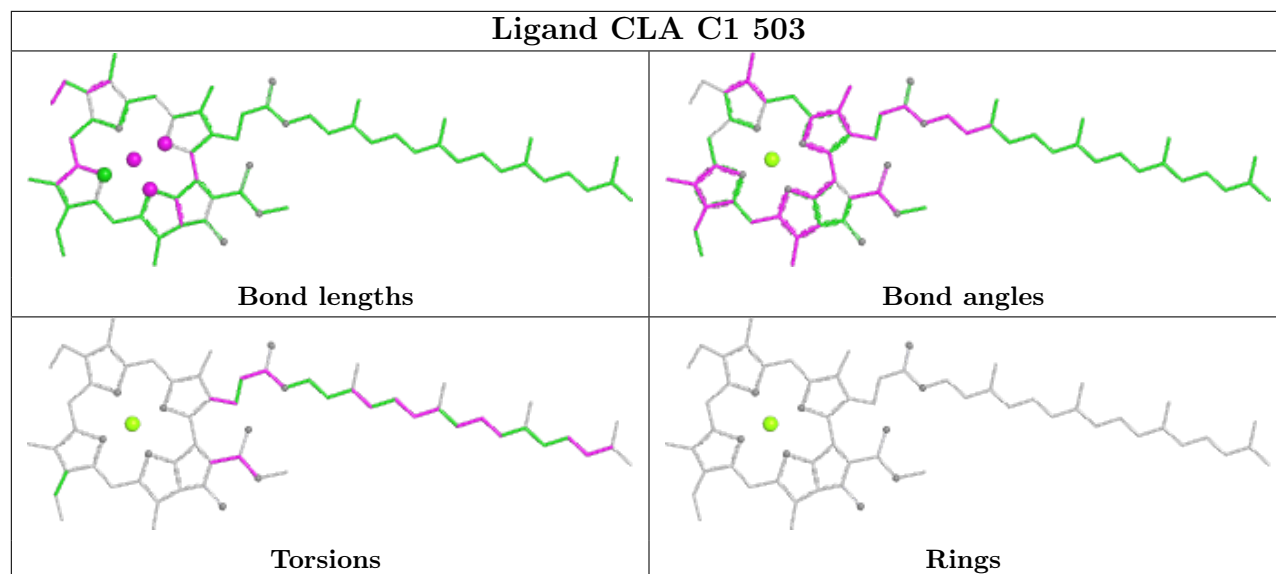
Torsions

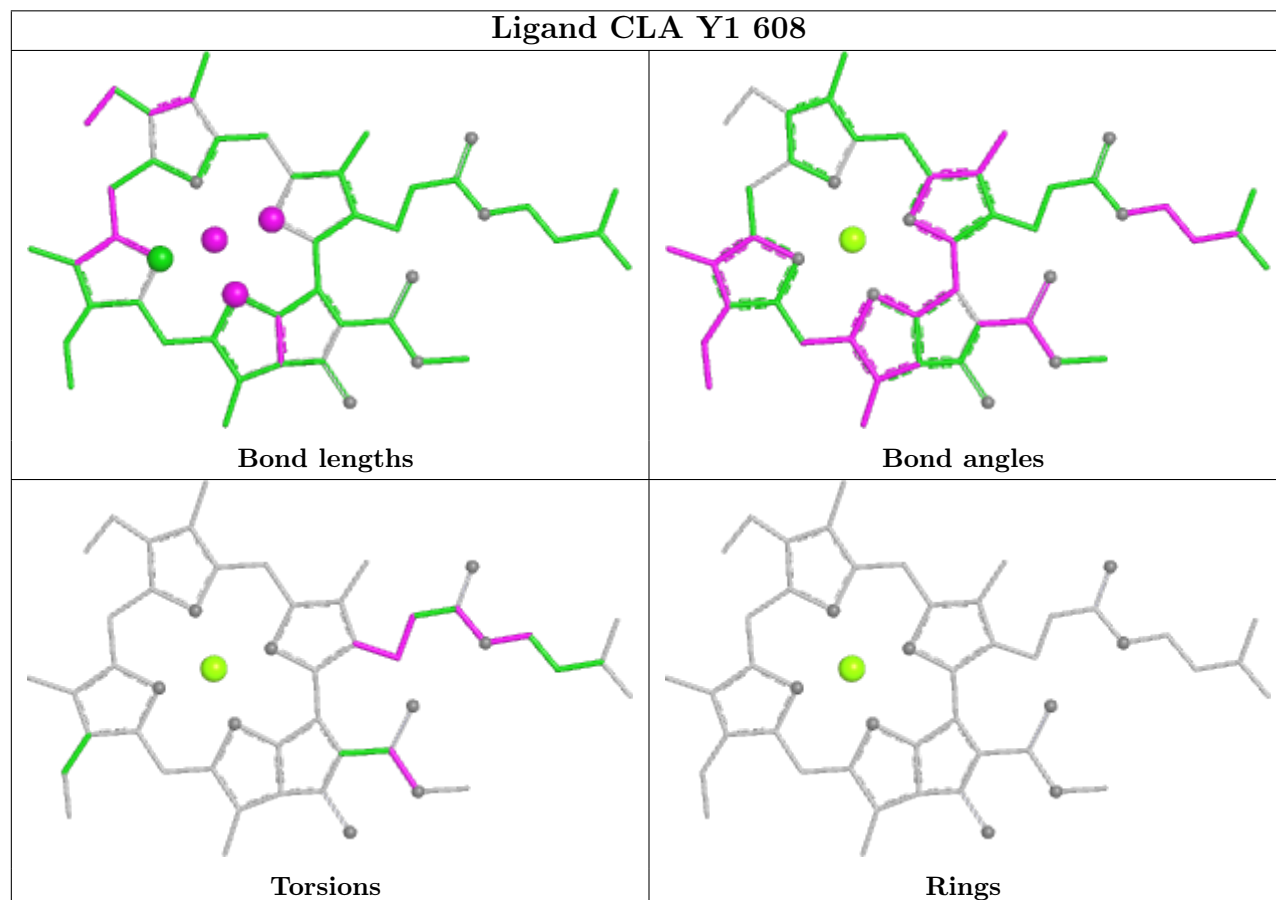
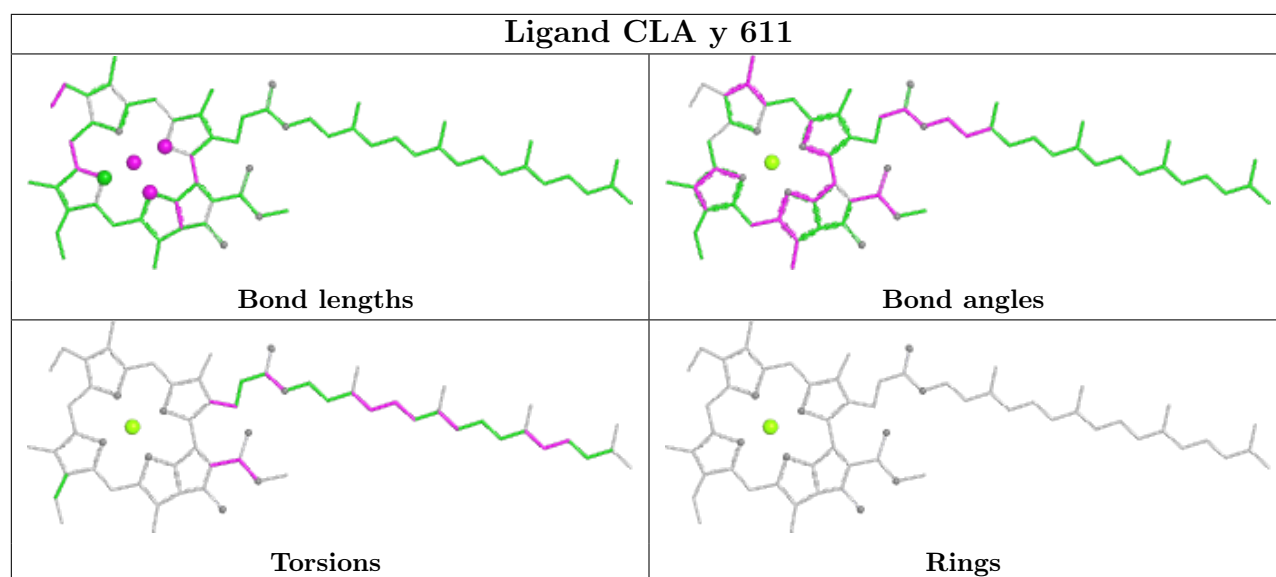


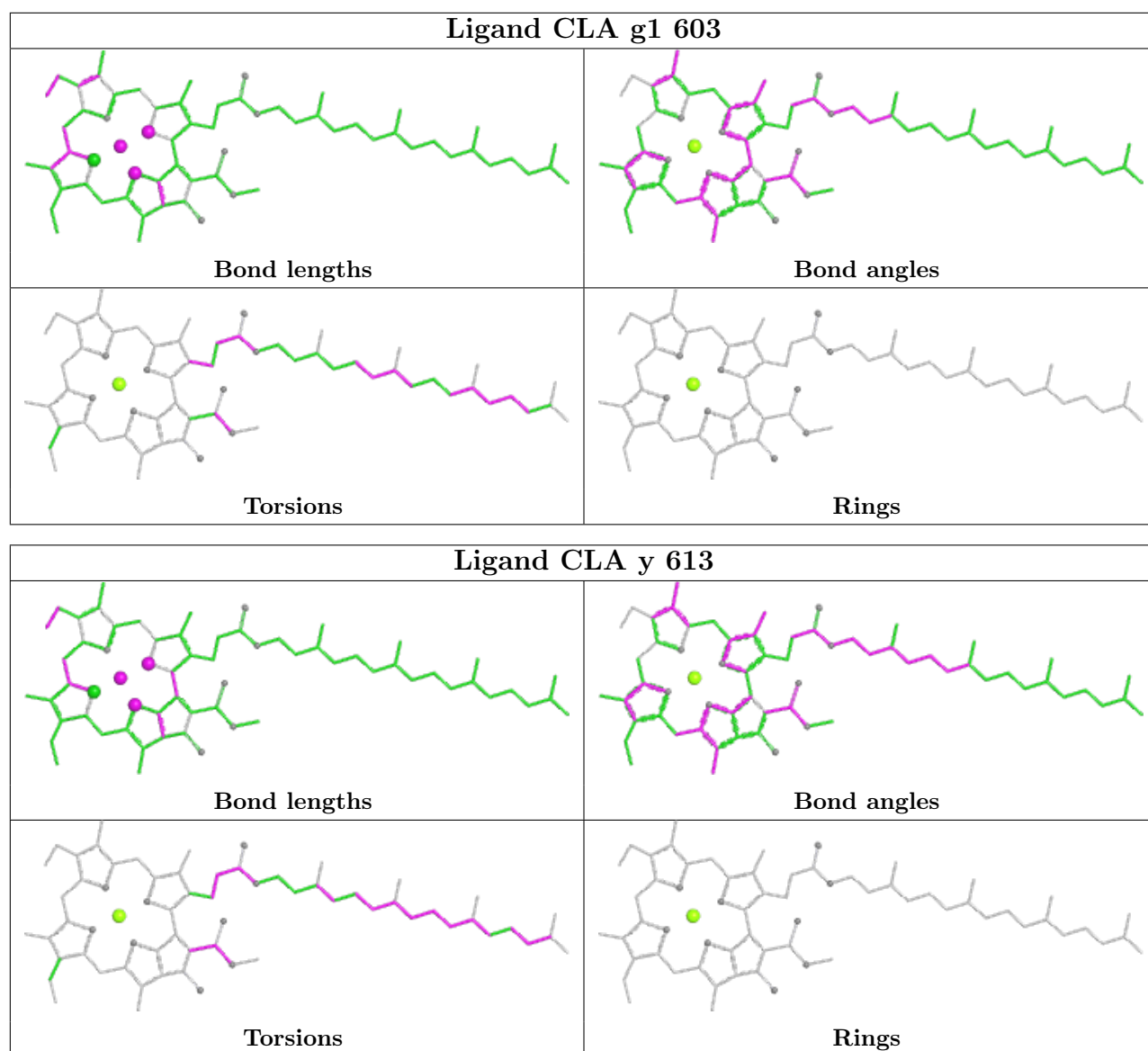
Rings

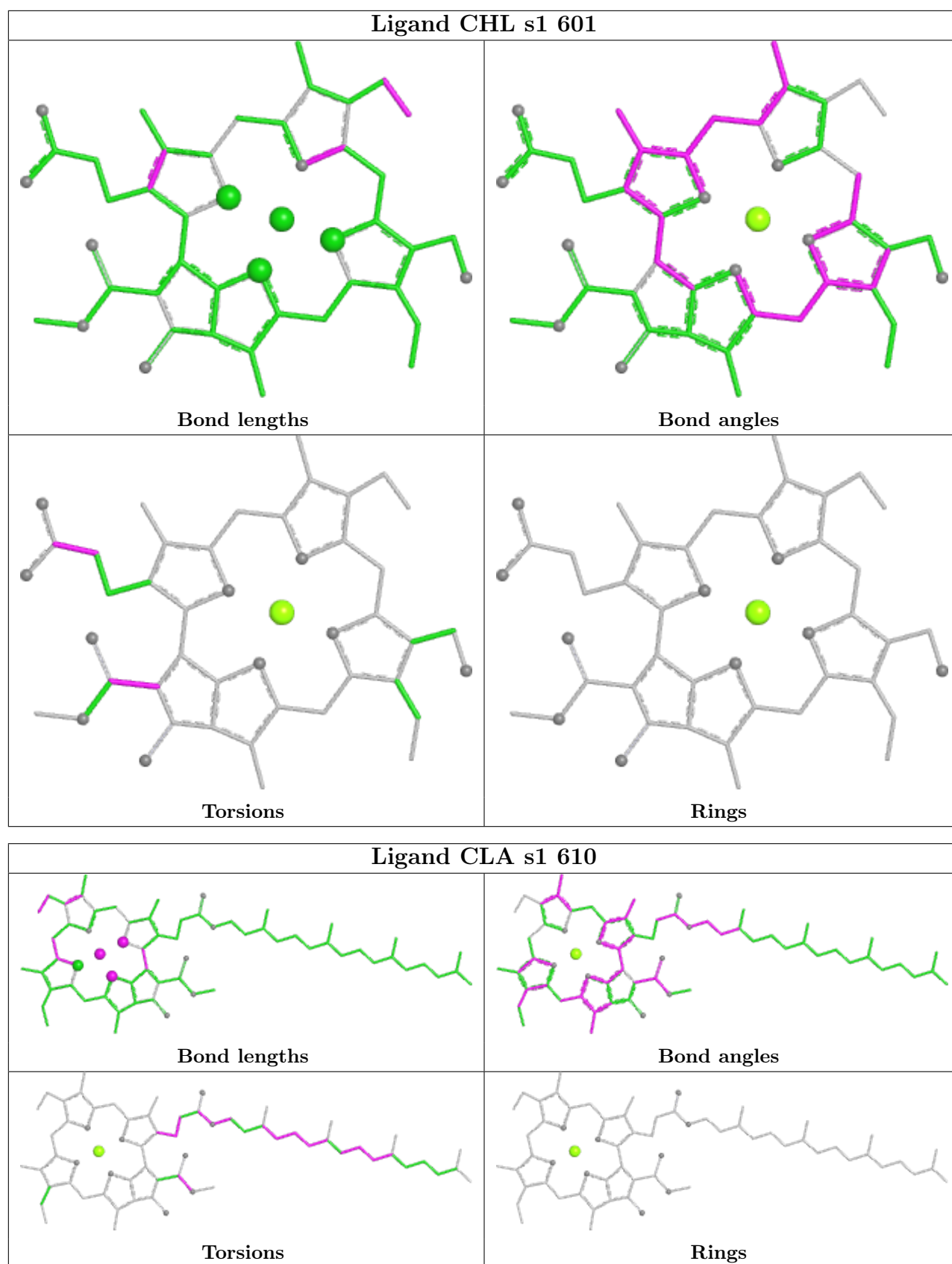


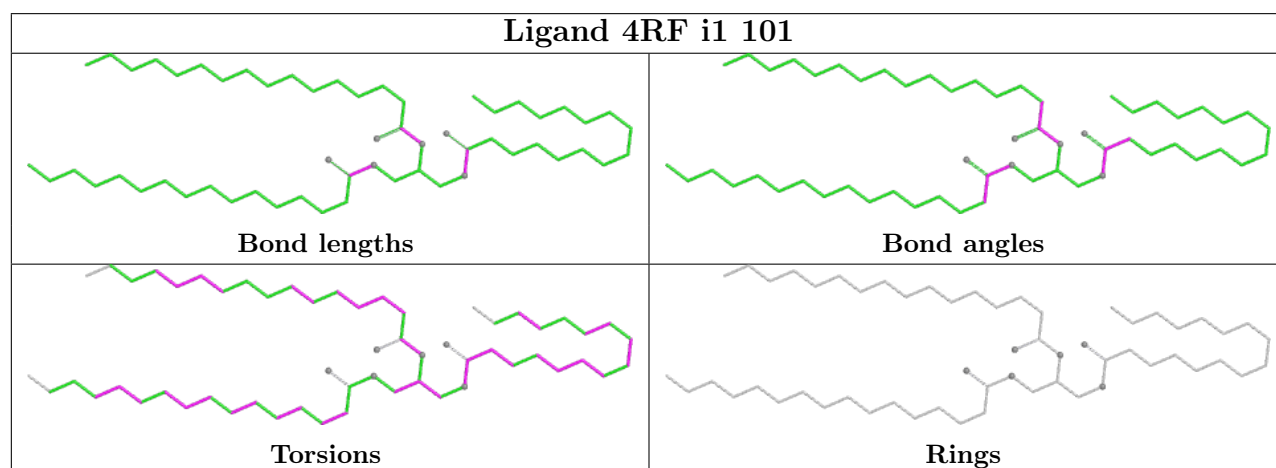
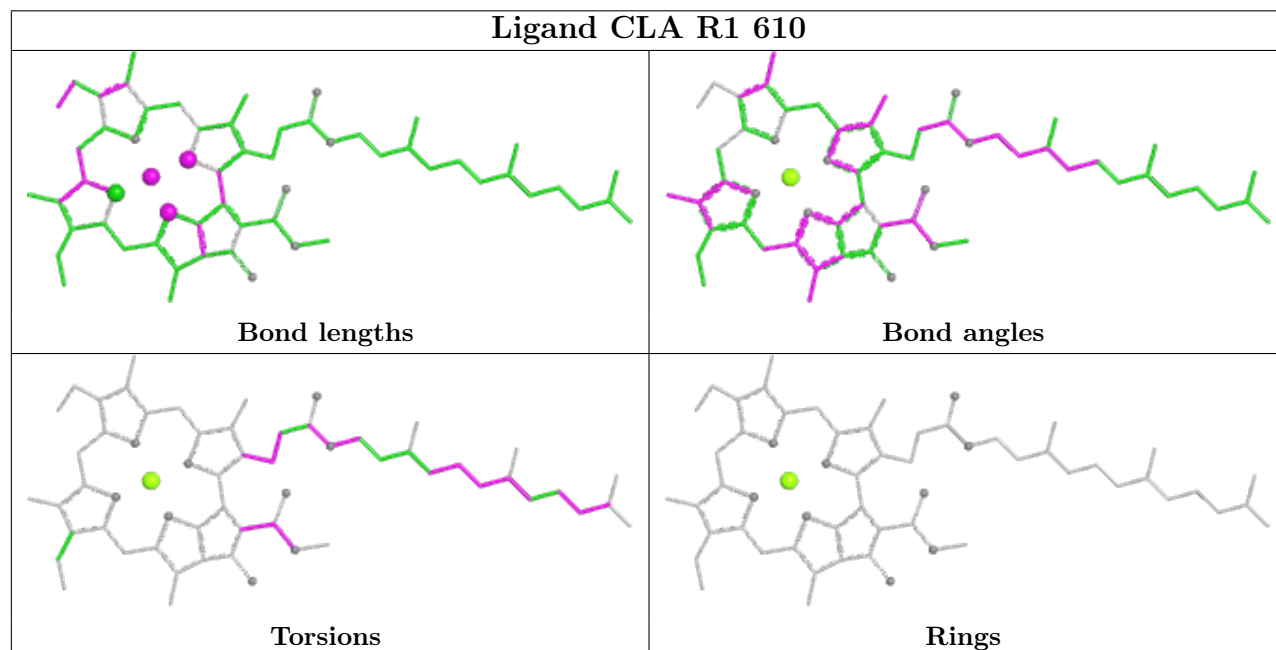
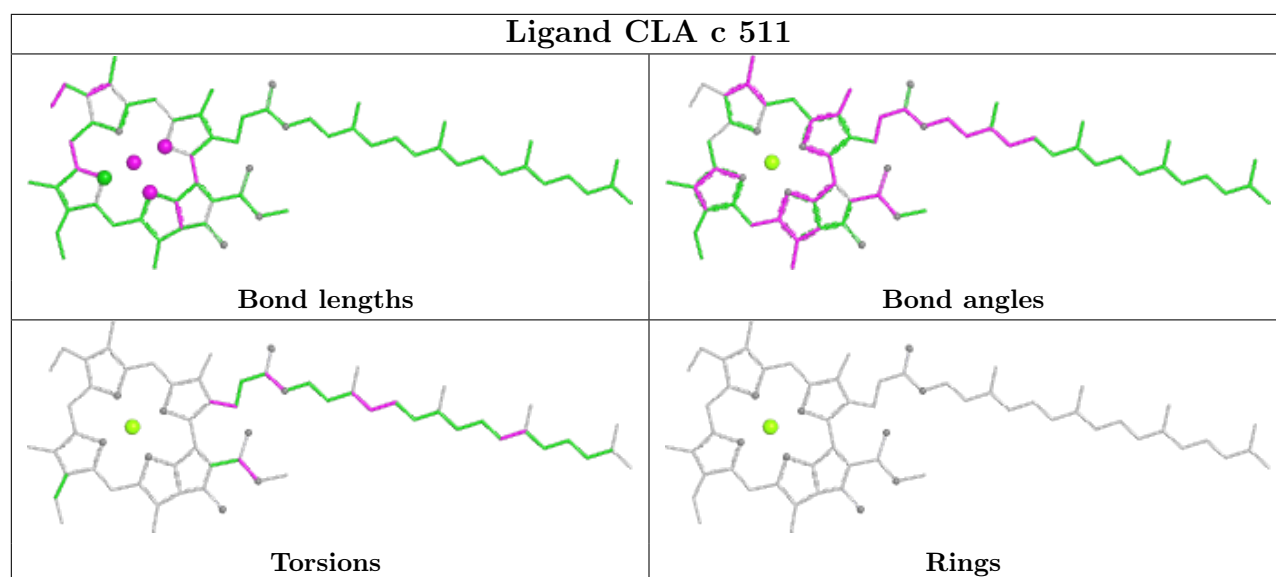


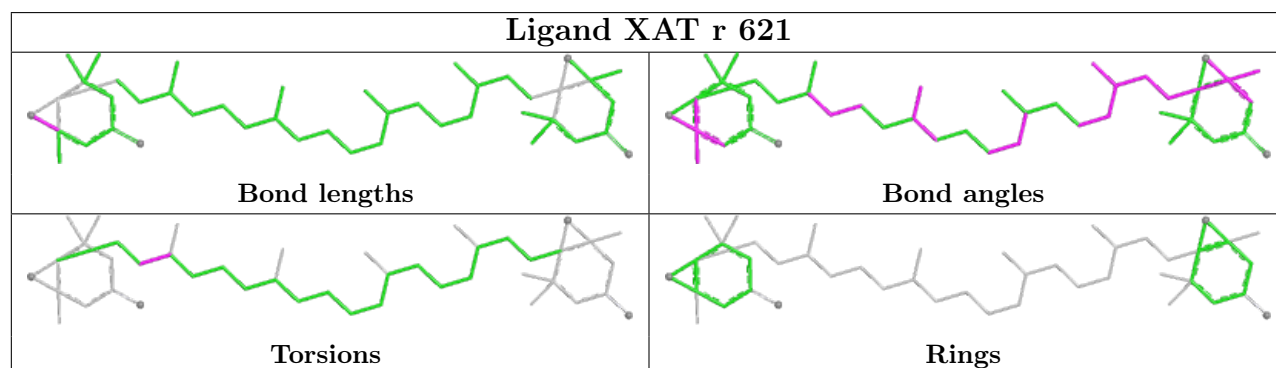
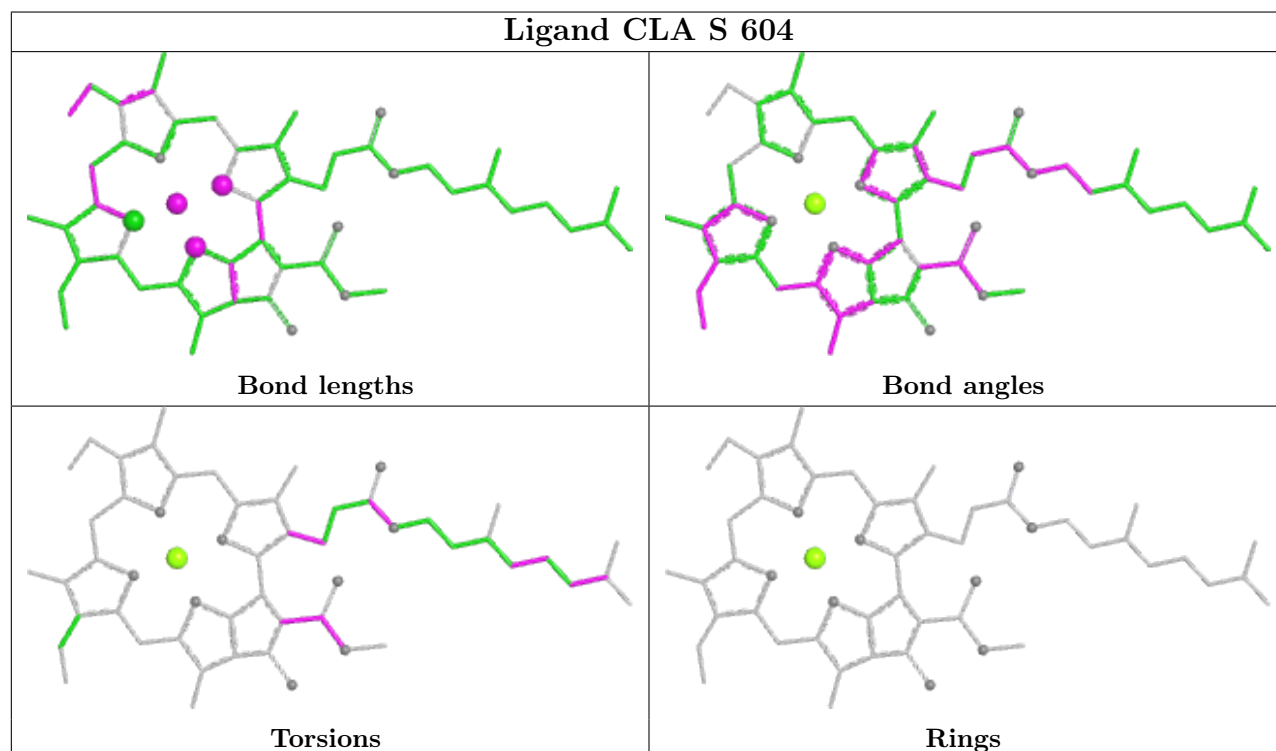
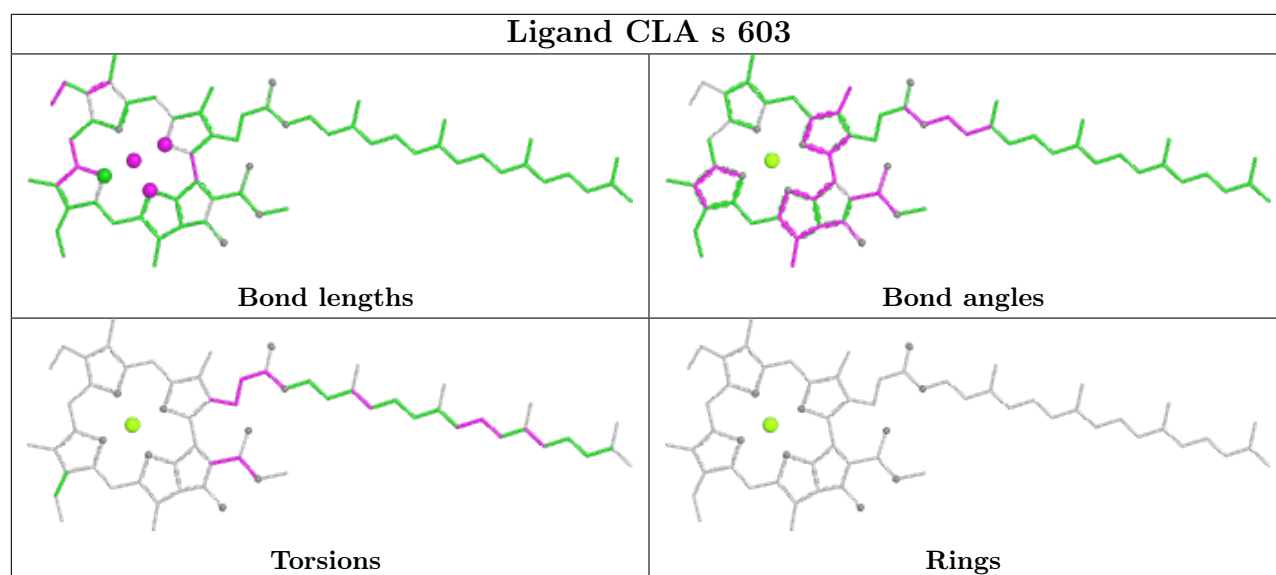


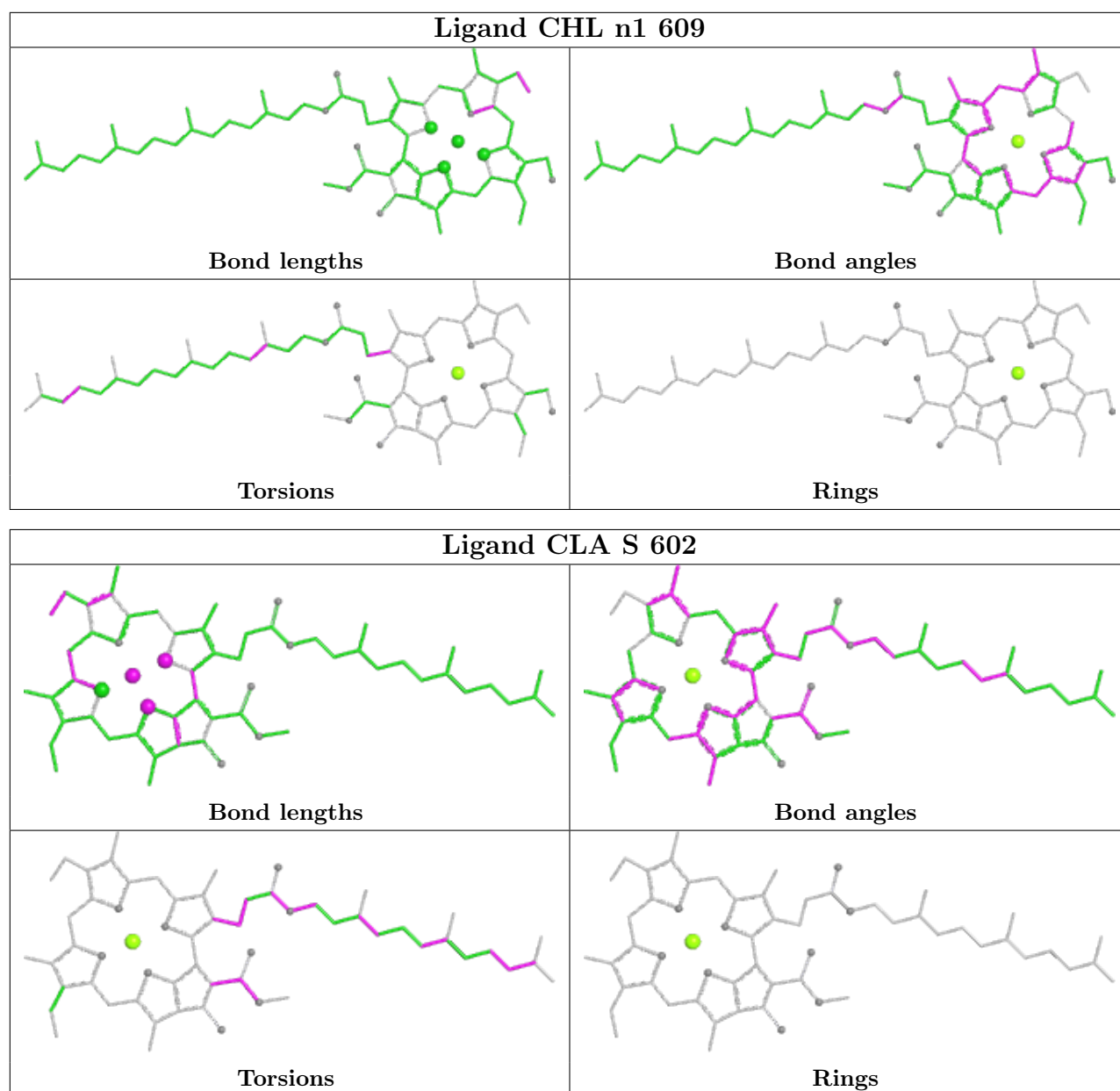


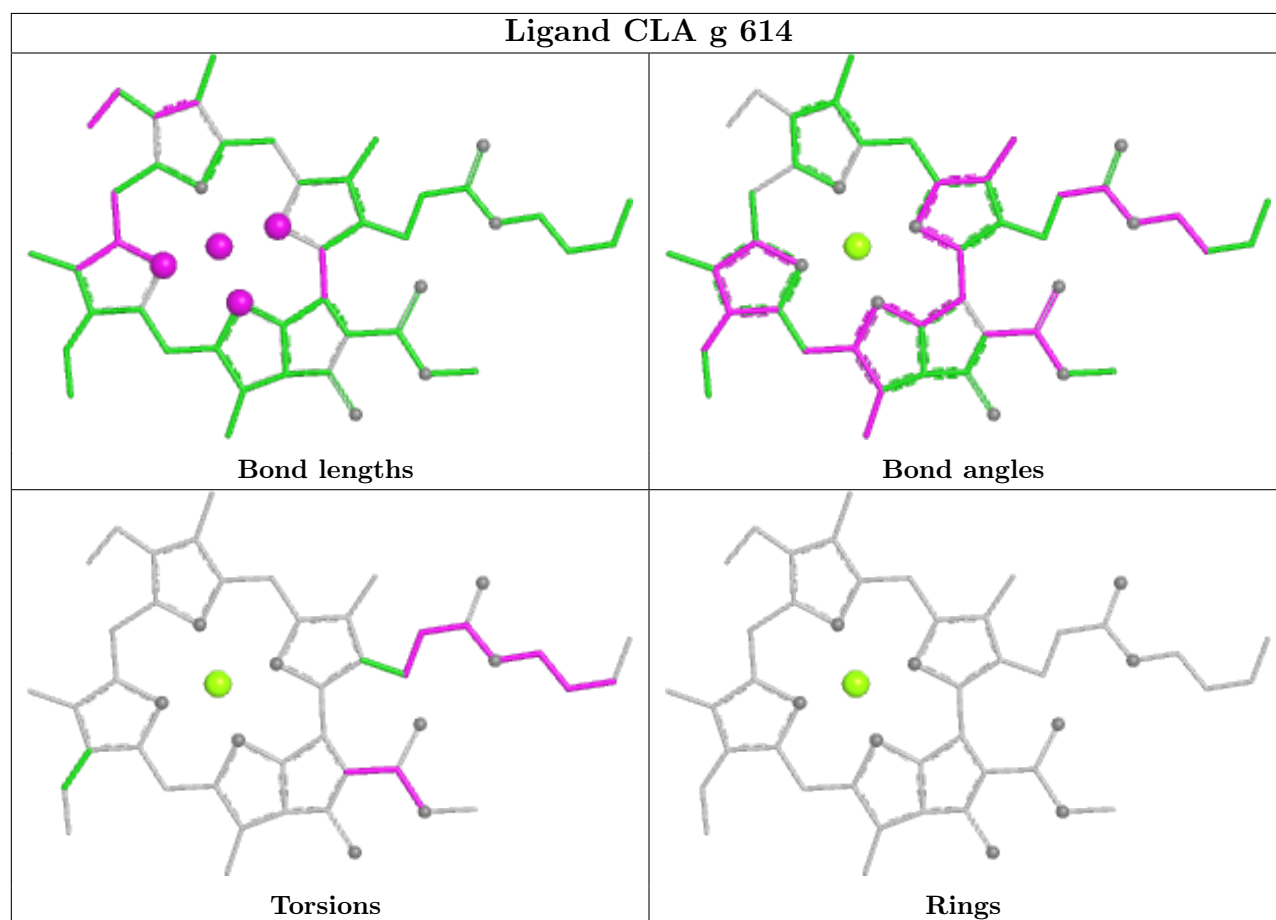
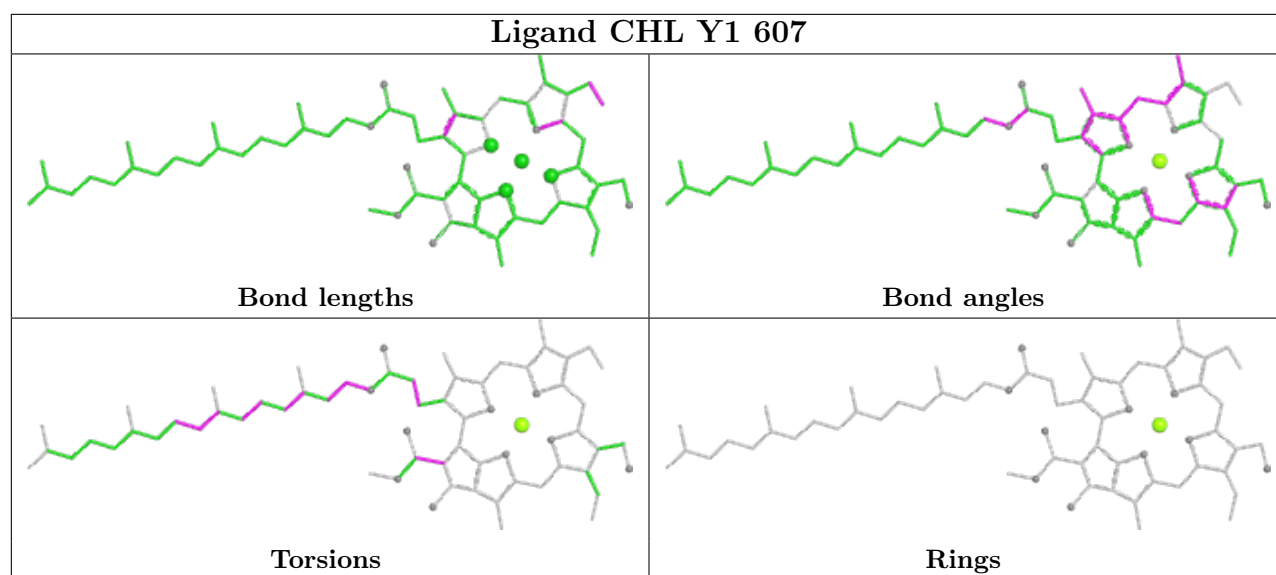




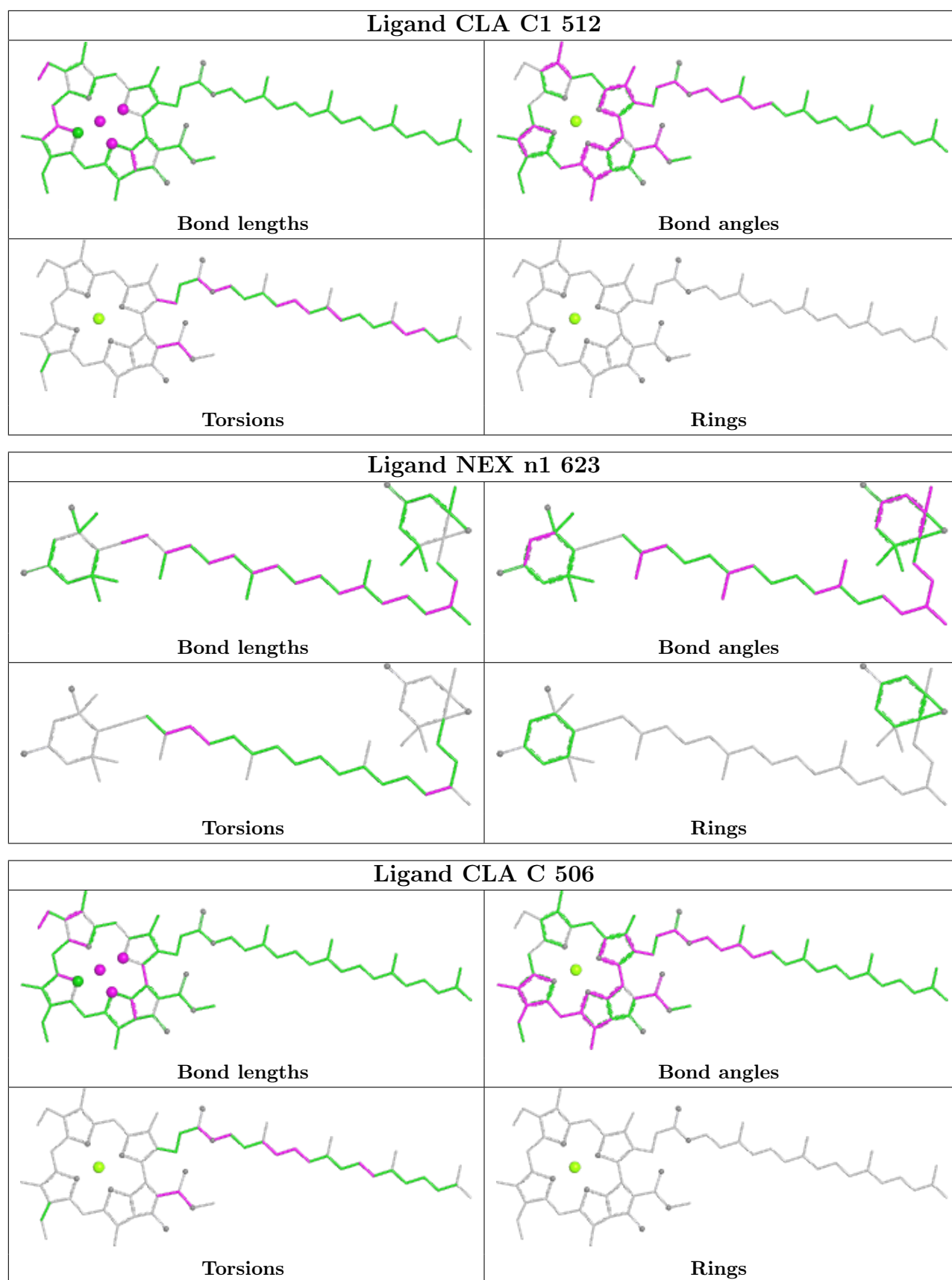


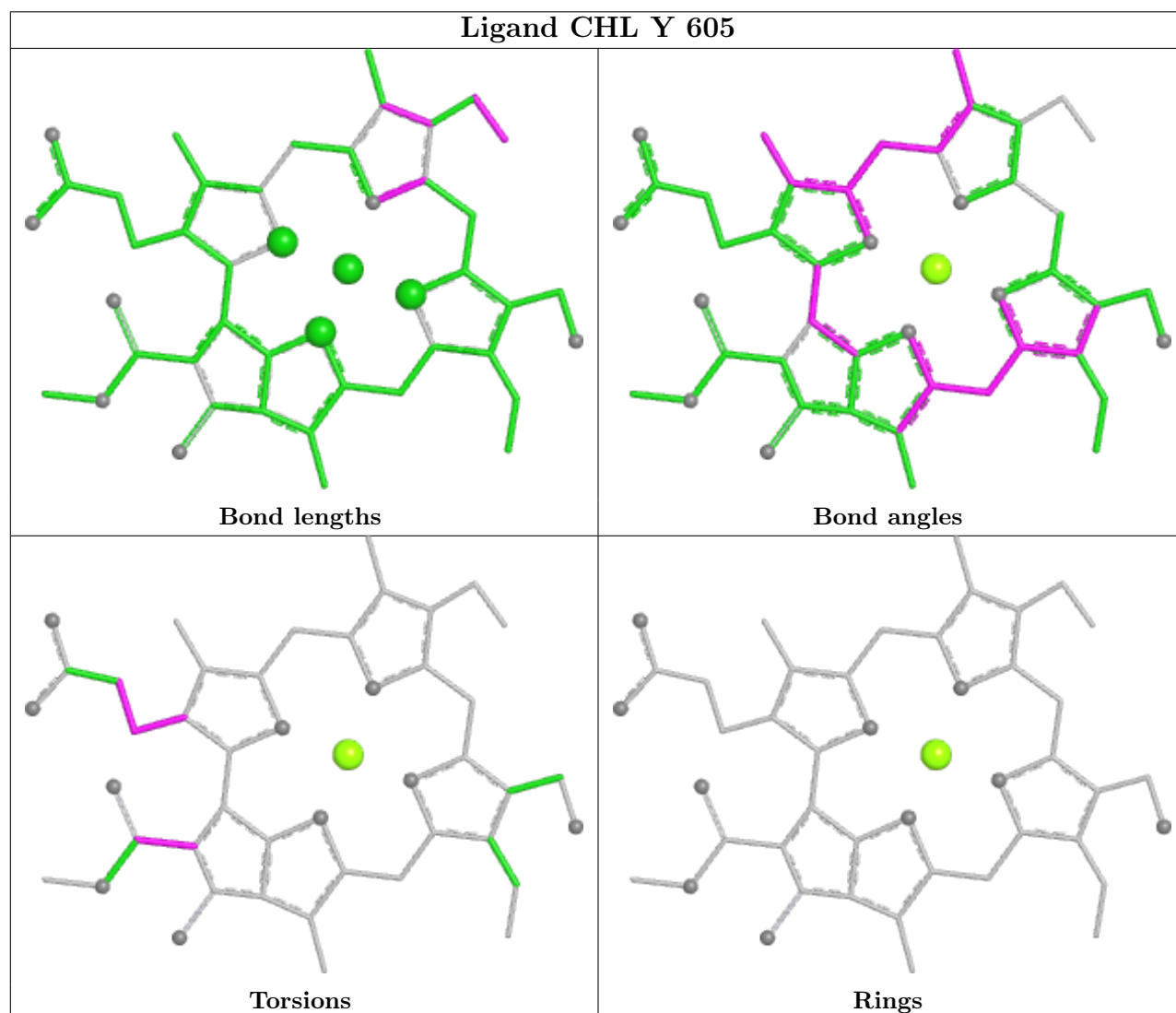
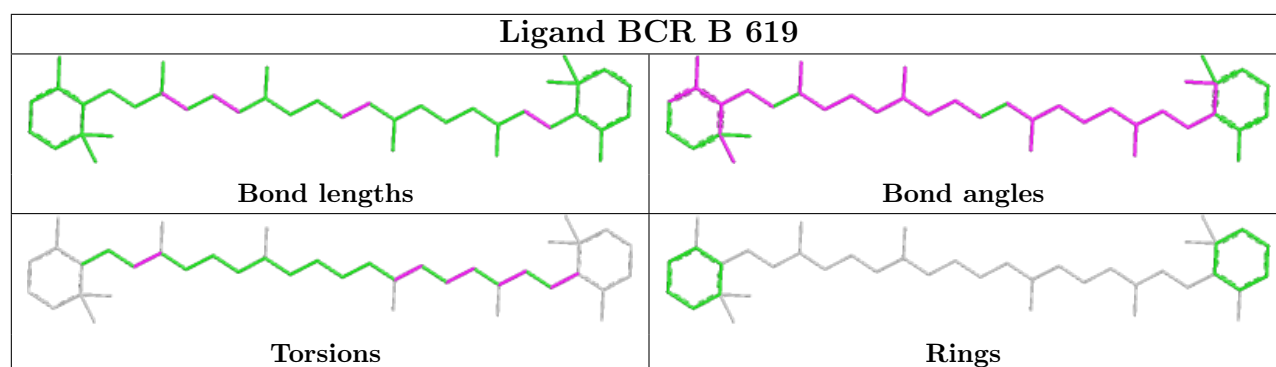


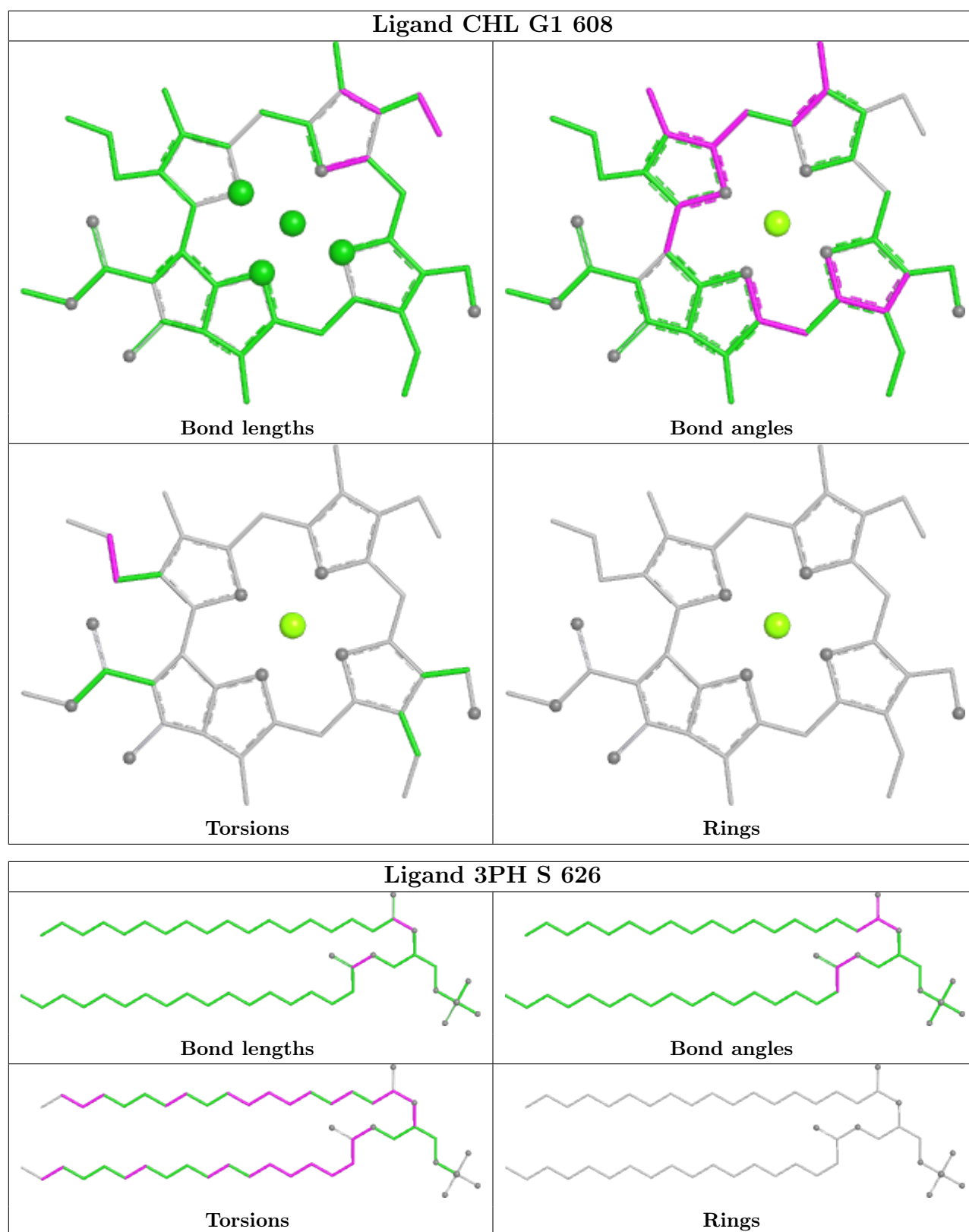


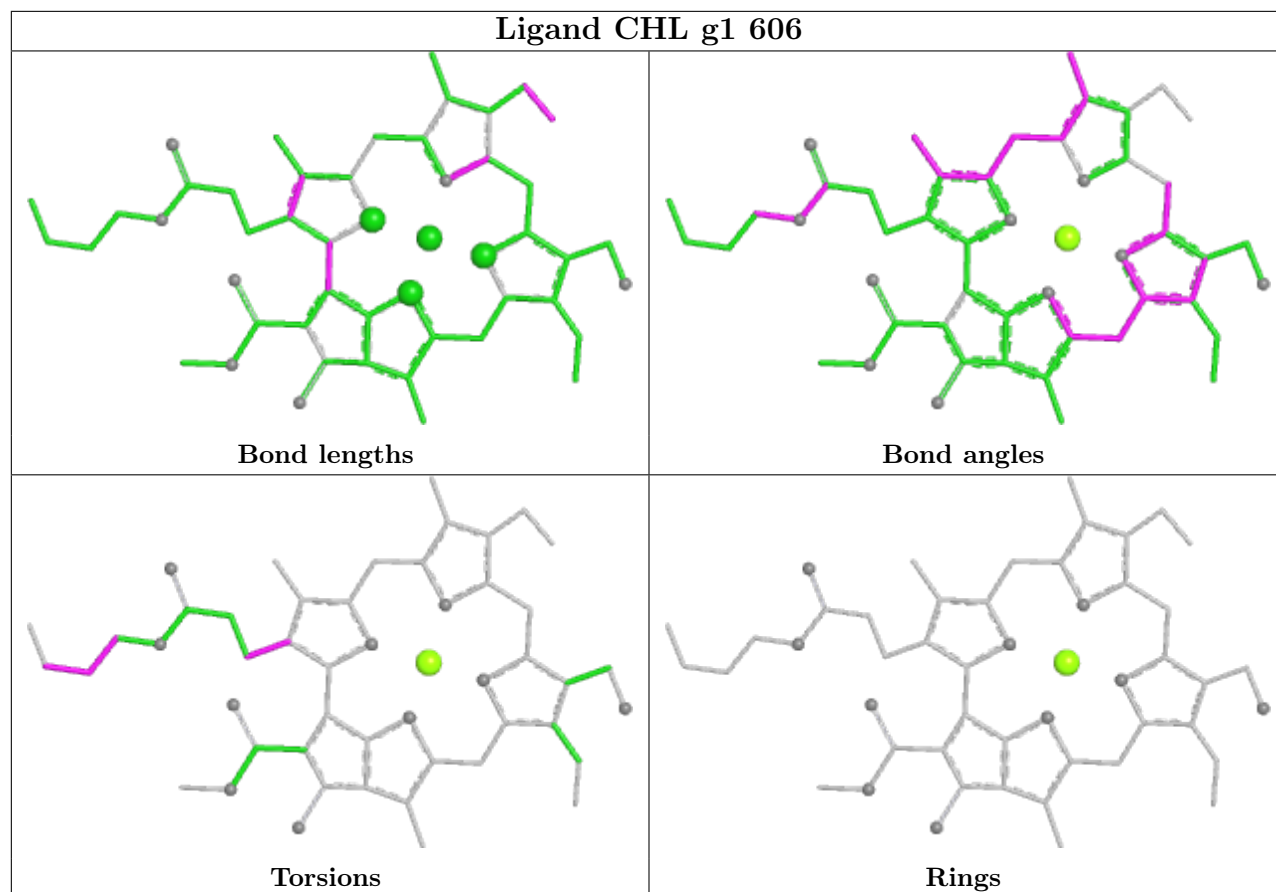




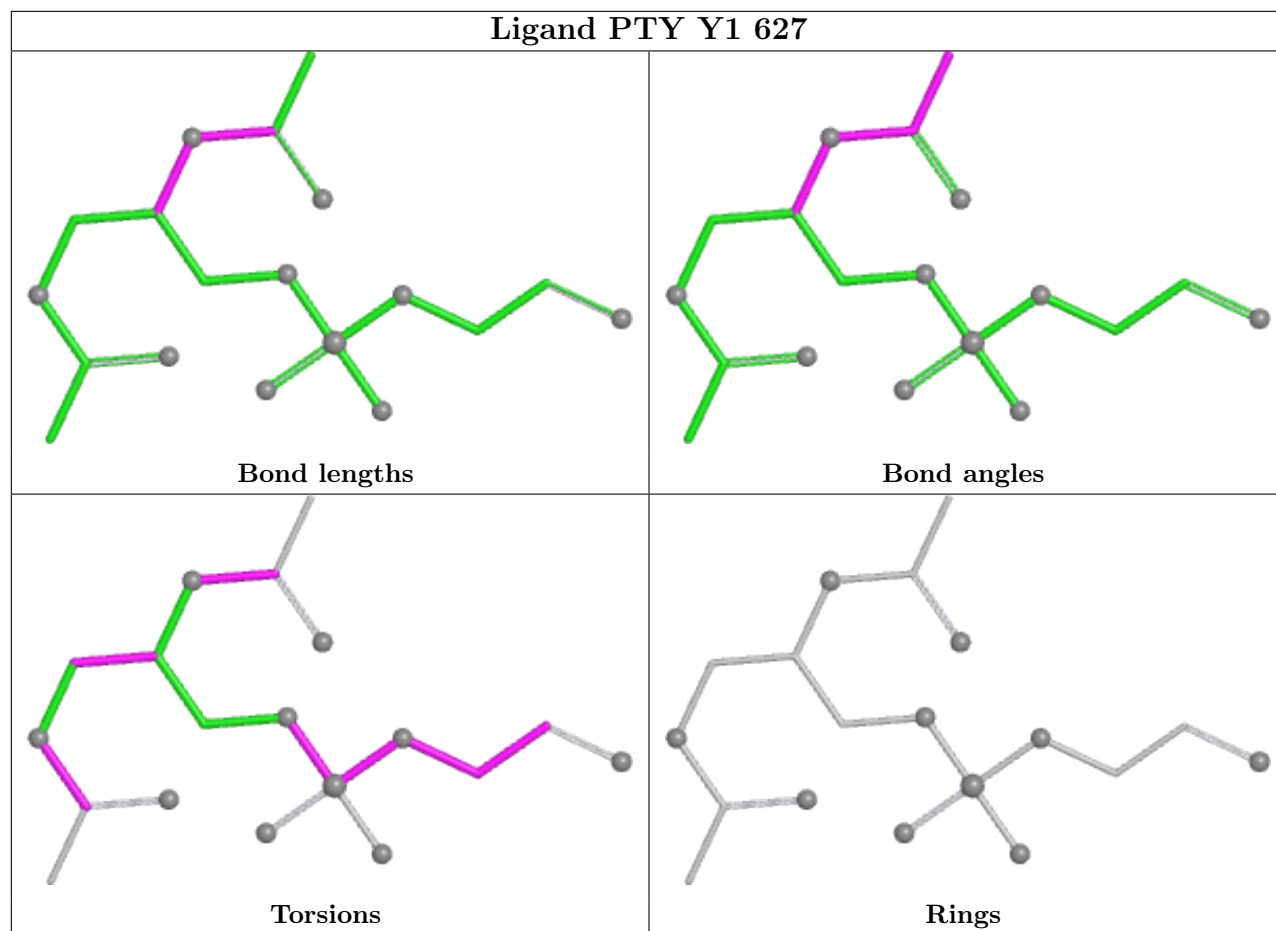




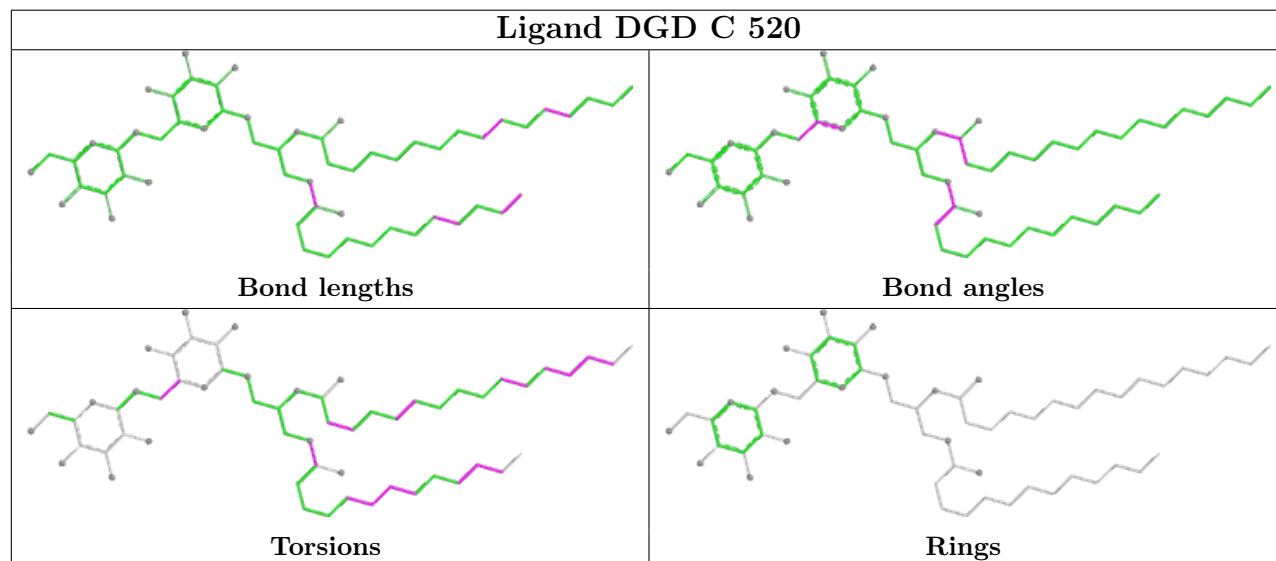


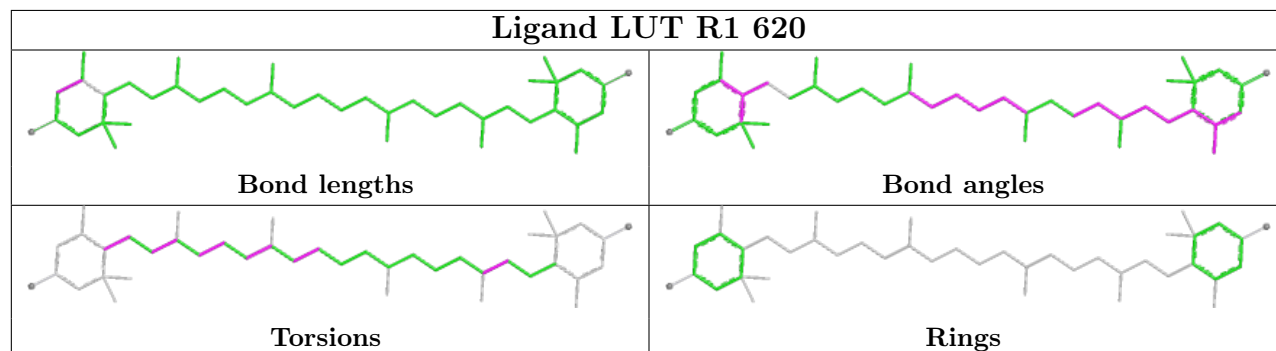
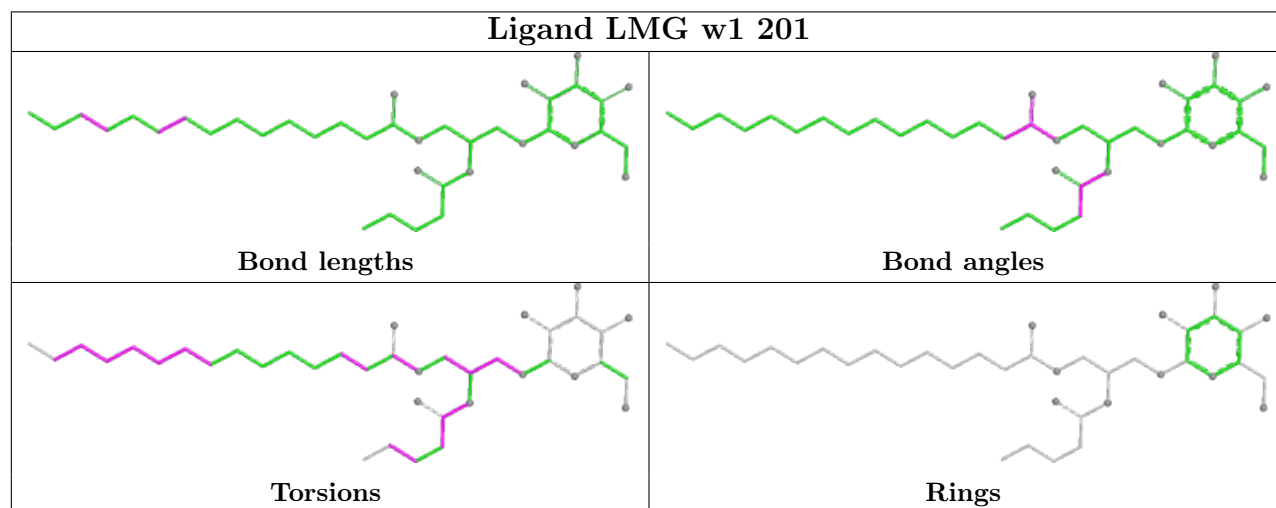
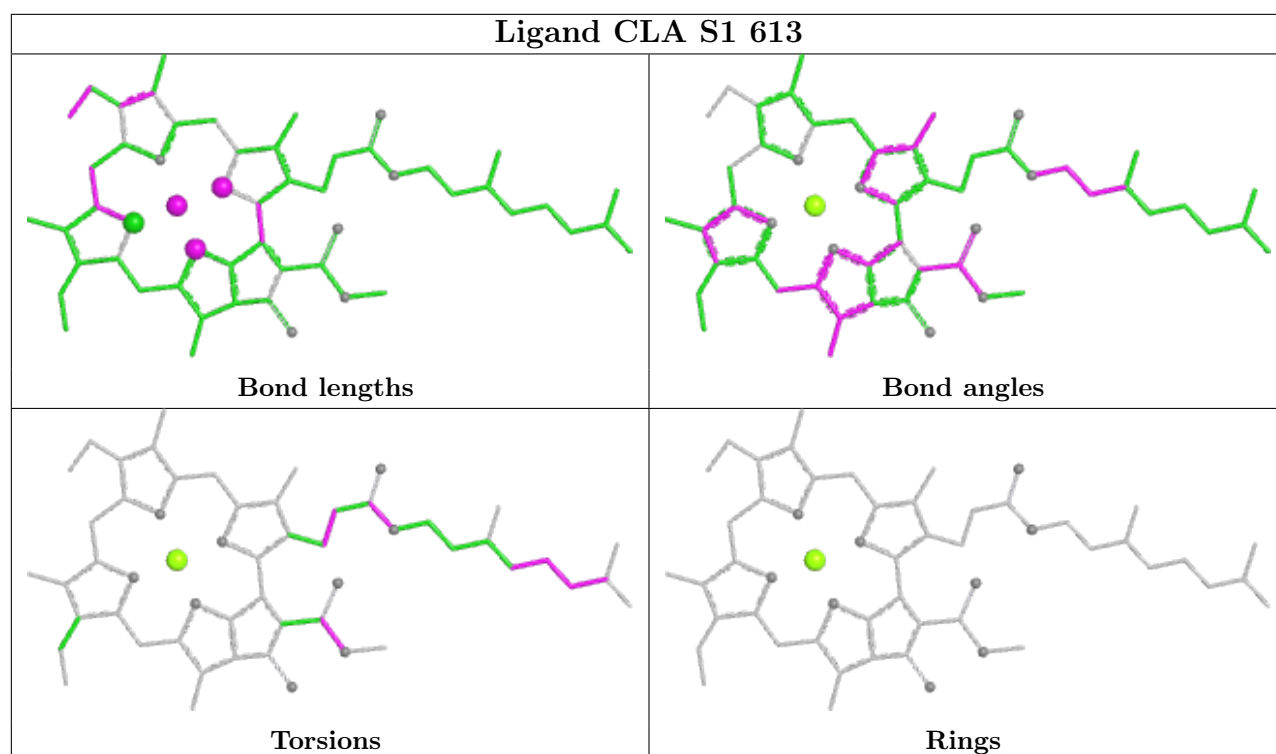


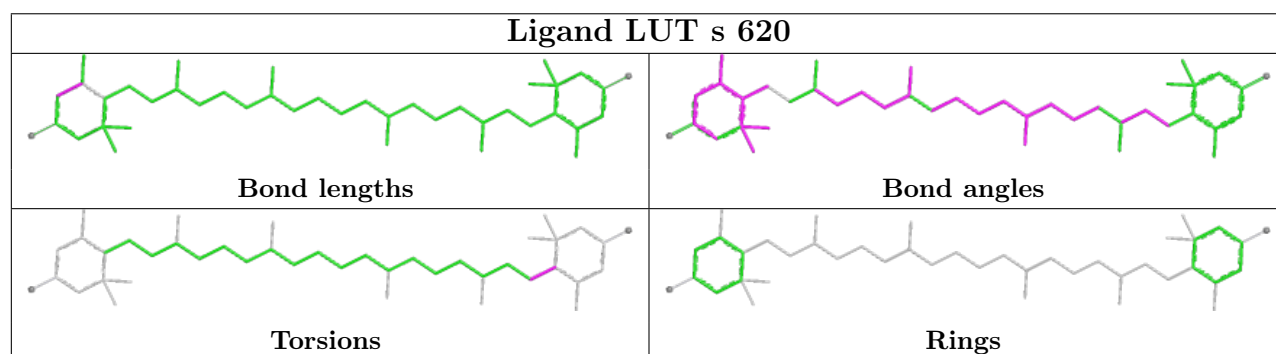
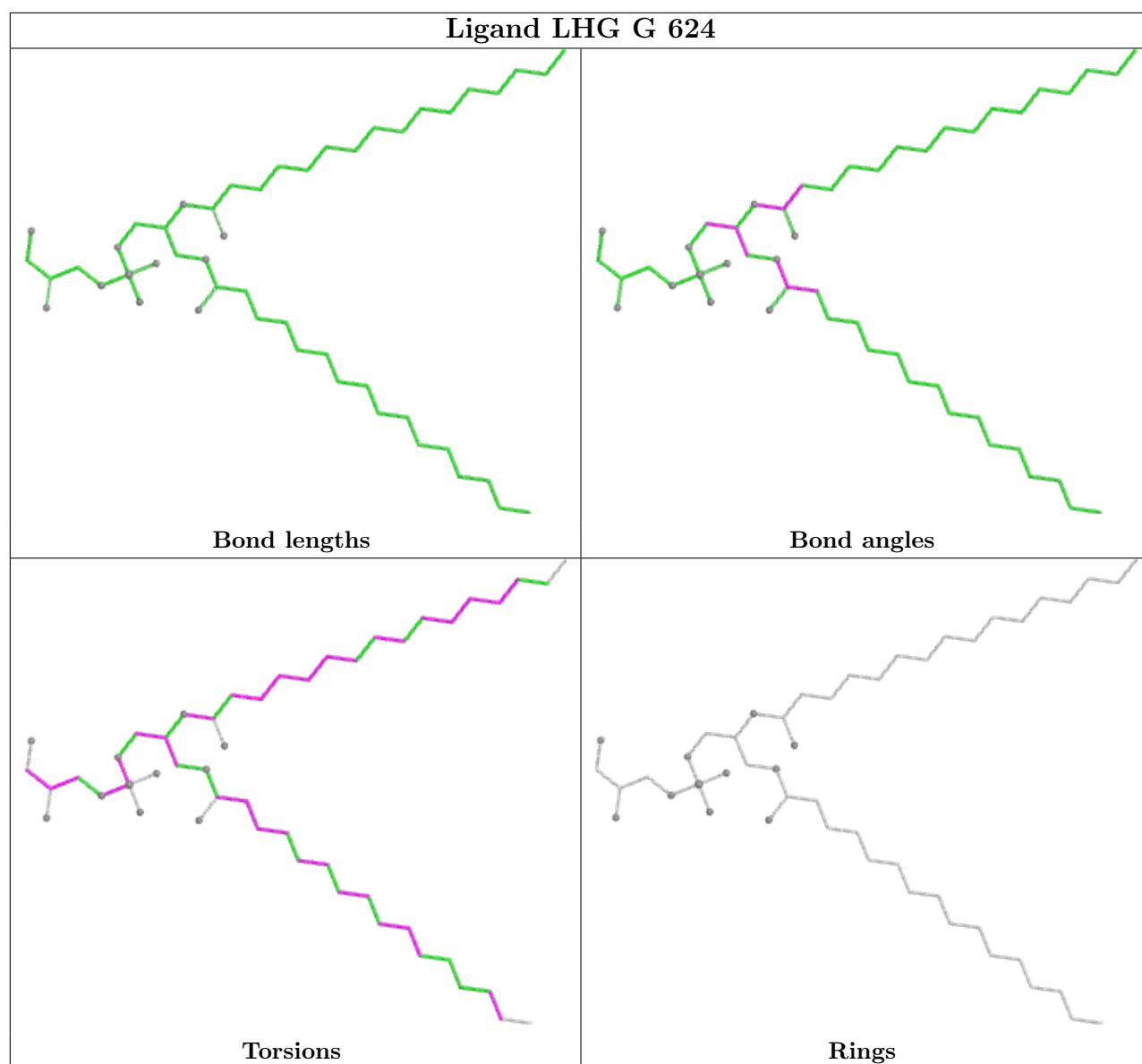
## Ligand PTY Y1 627

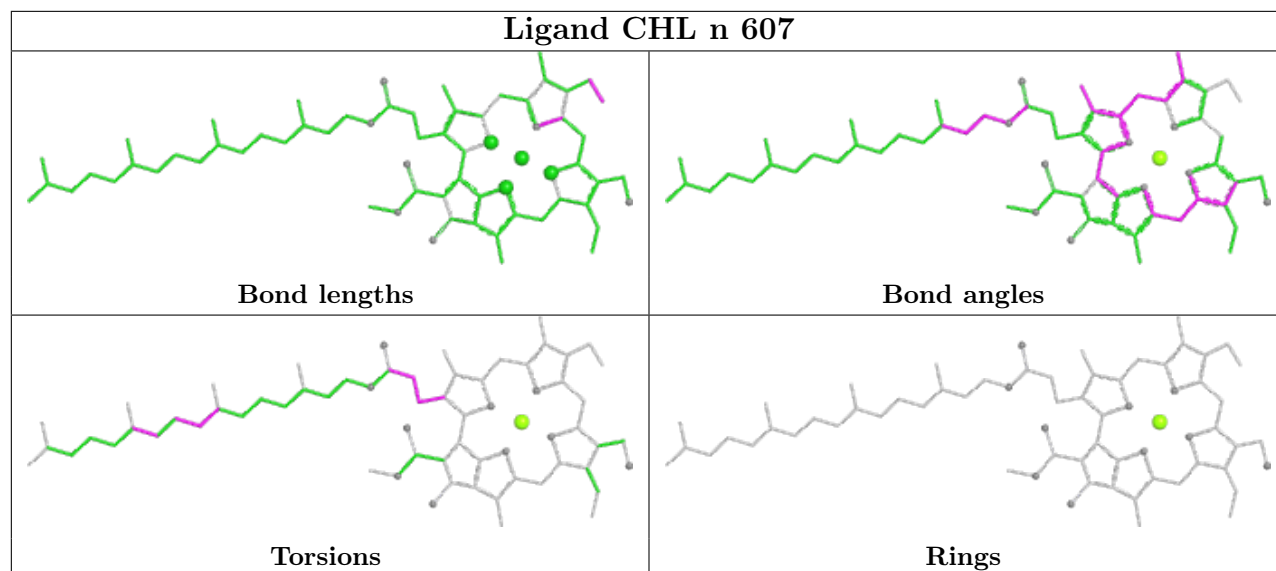
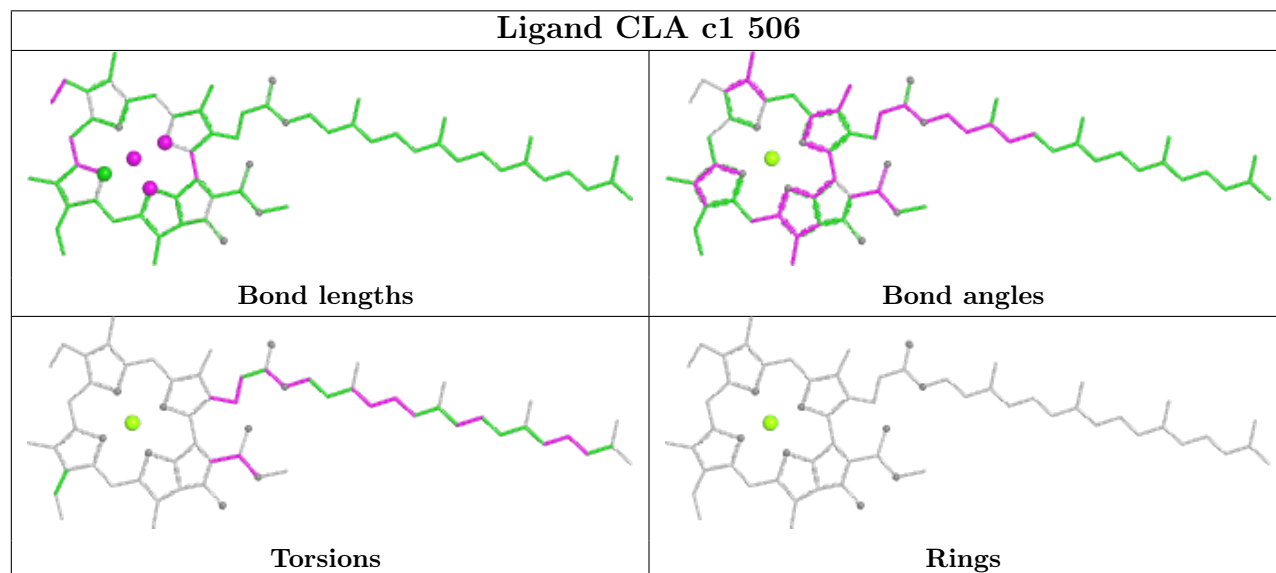
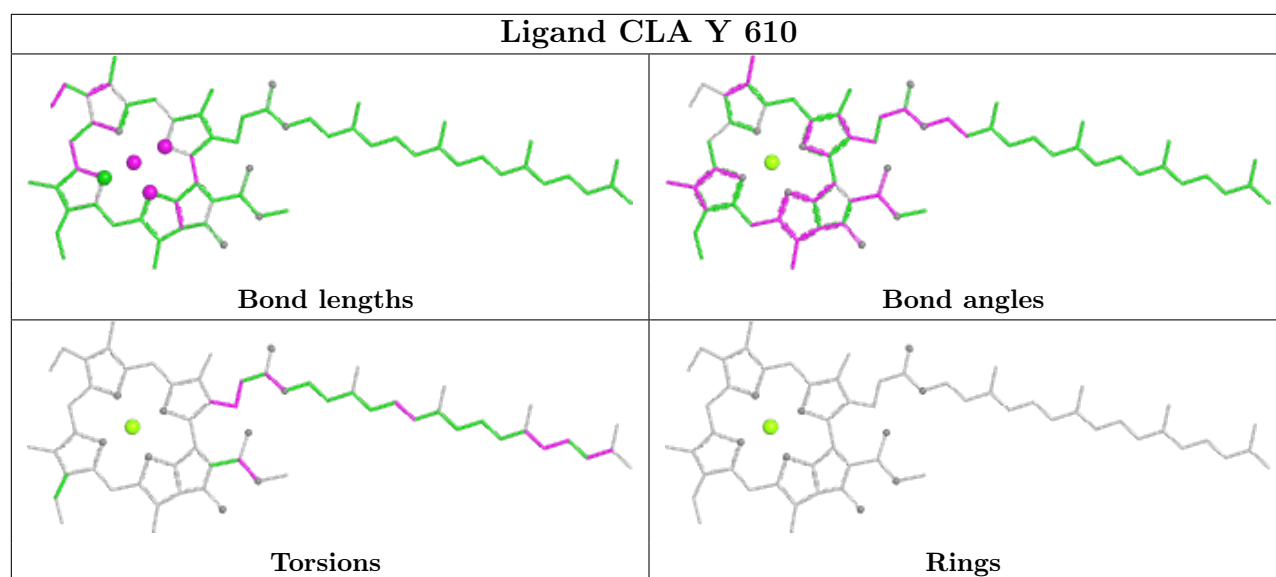


## Ligand DGD C 520



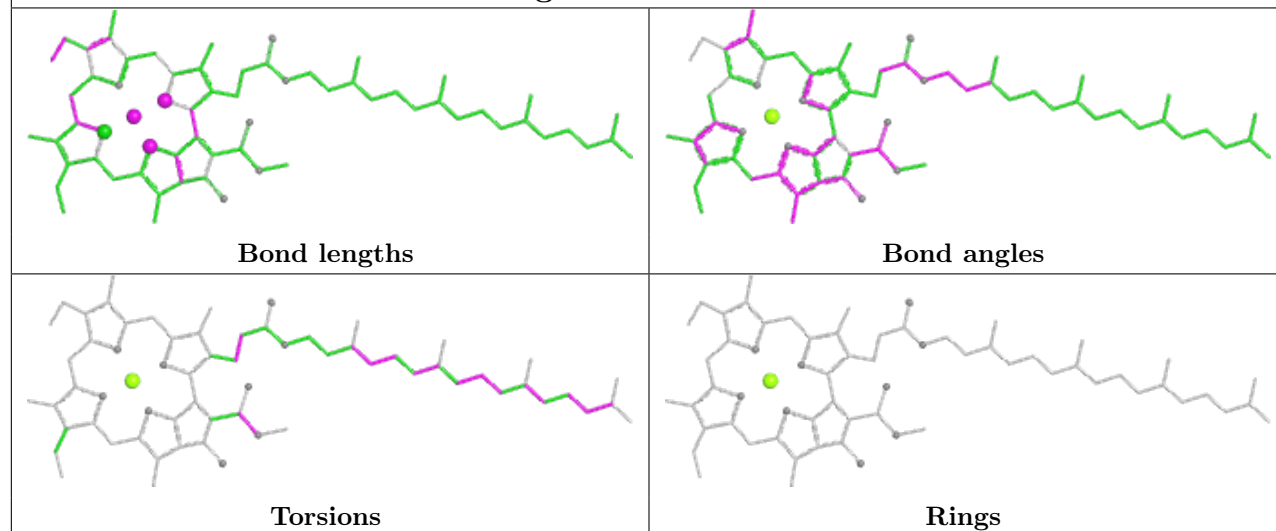




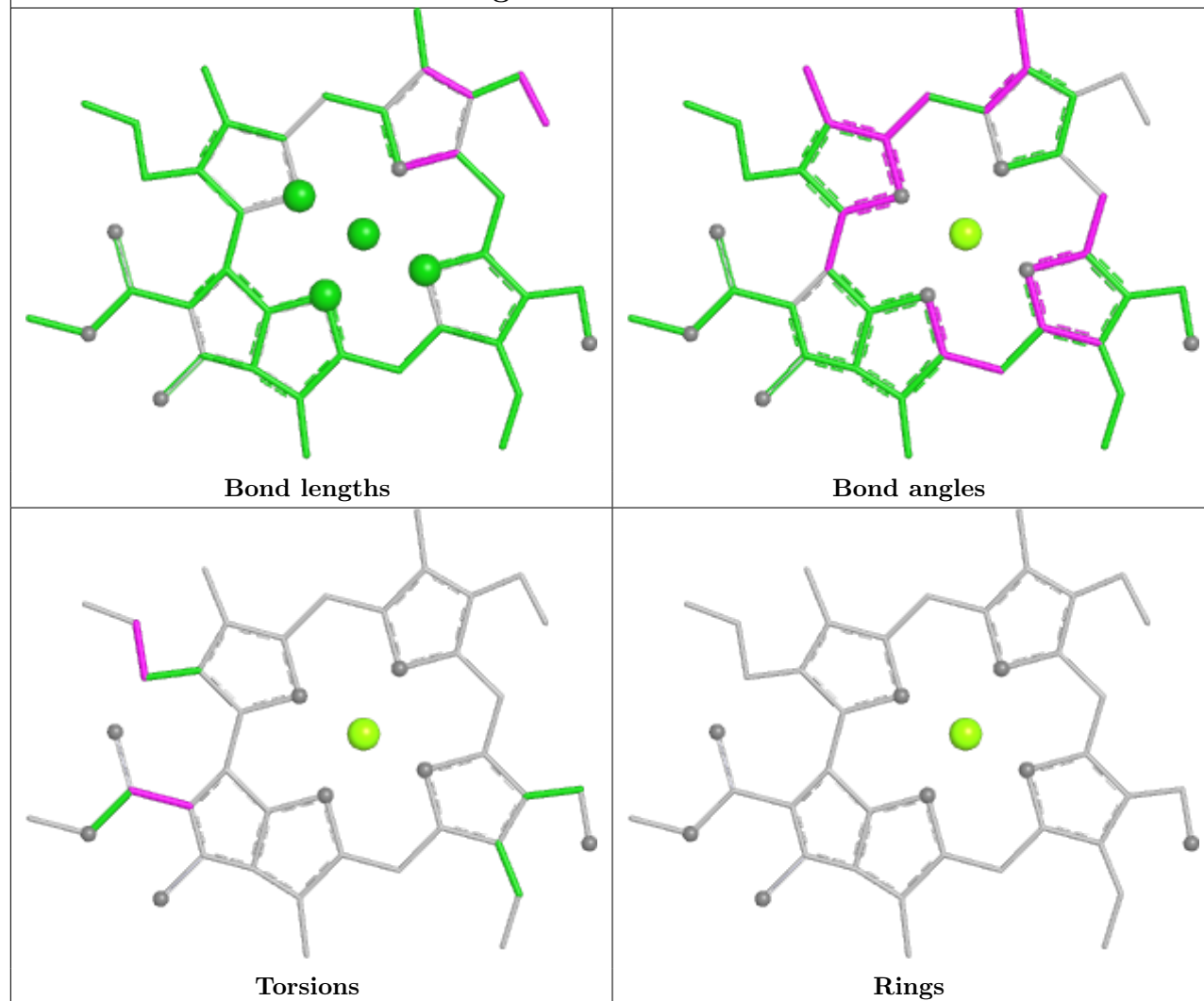


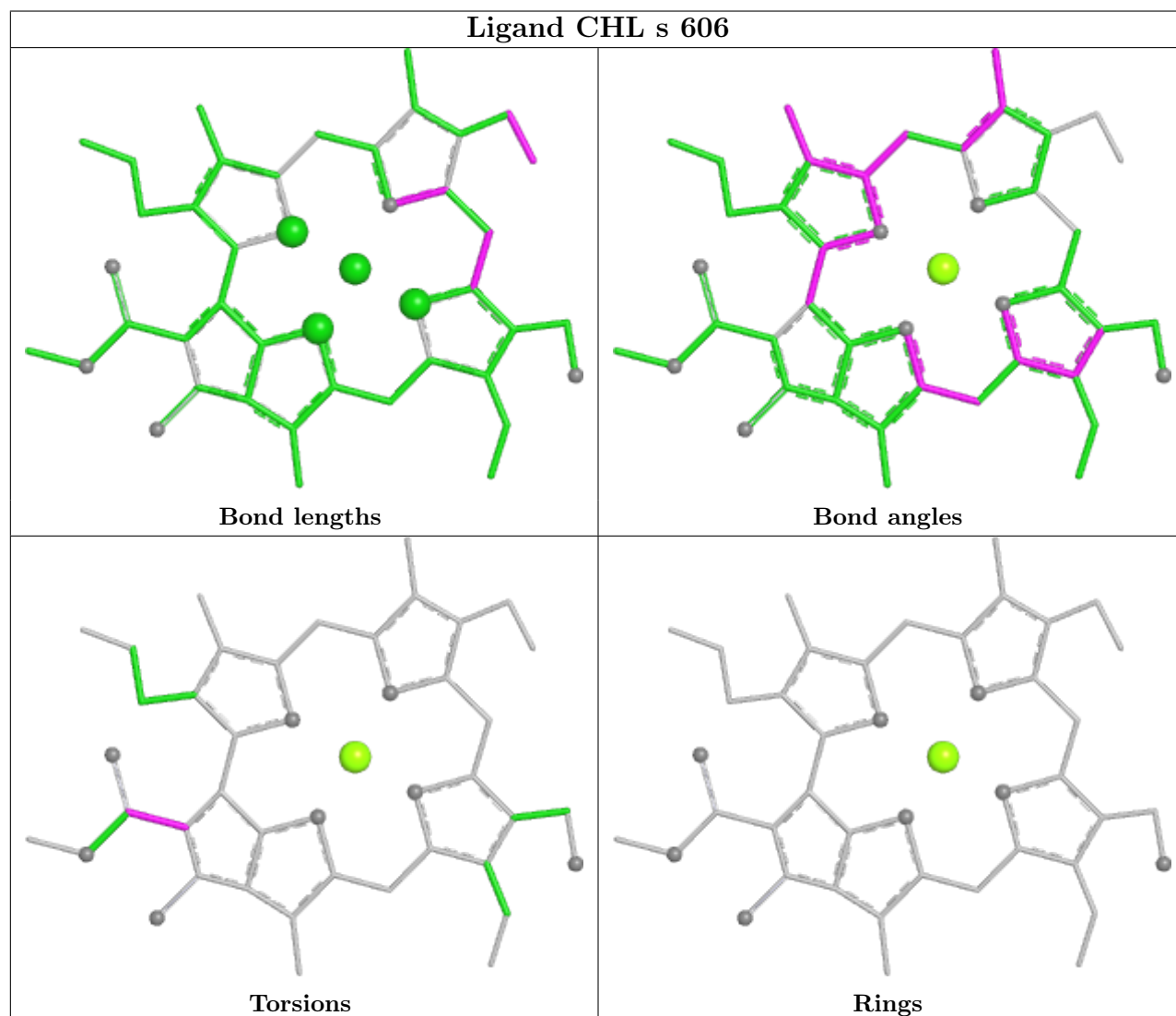
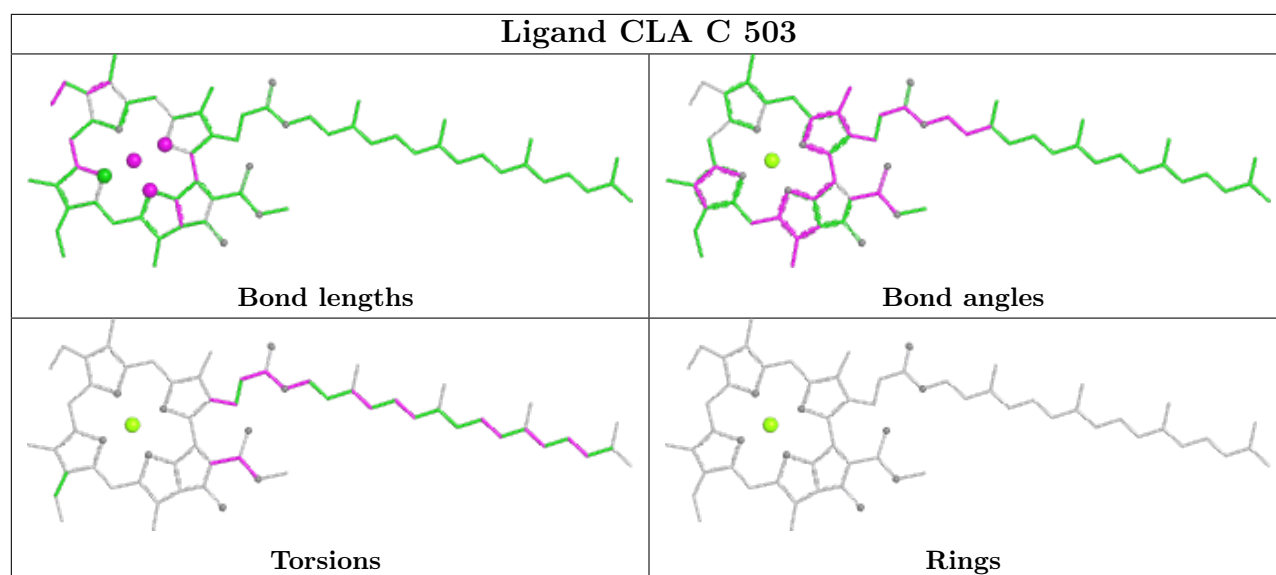


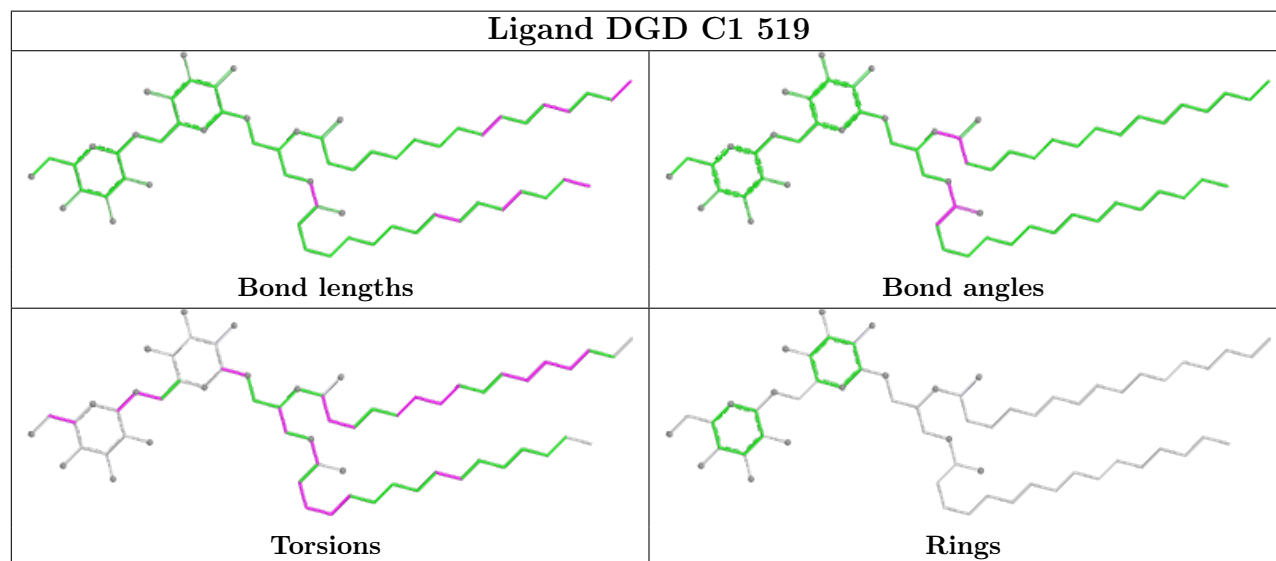
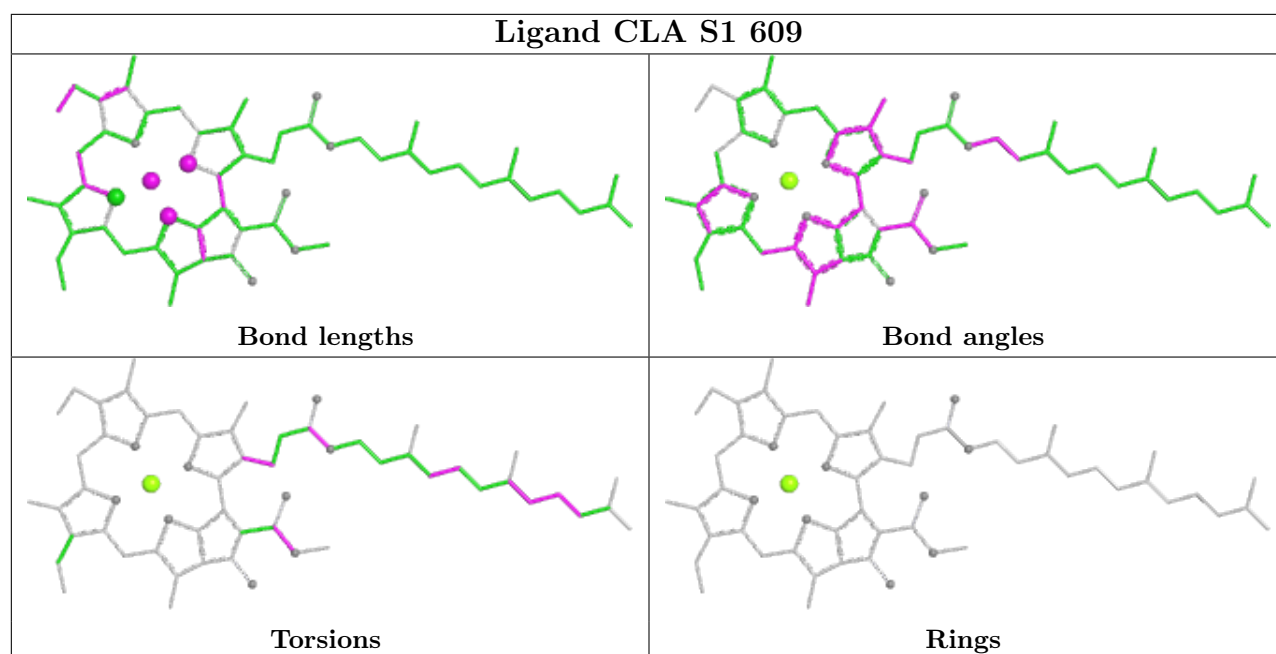
## Ligand CLA n 604

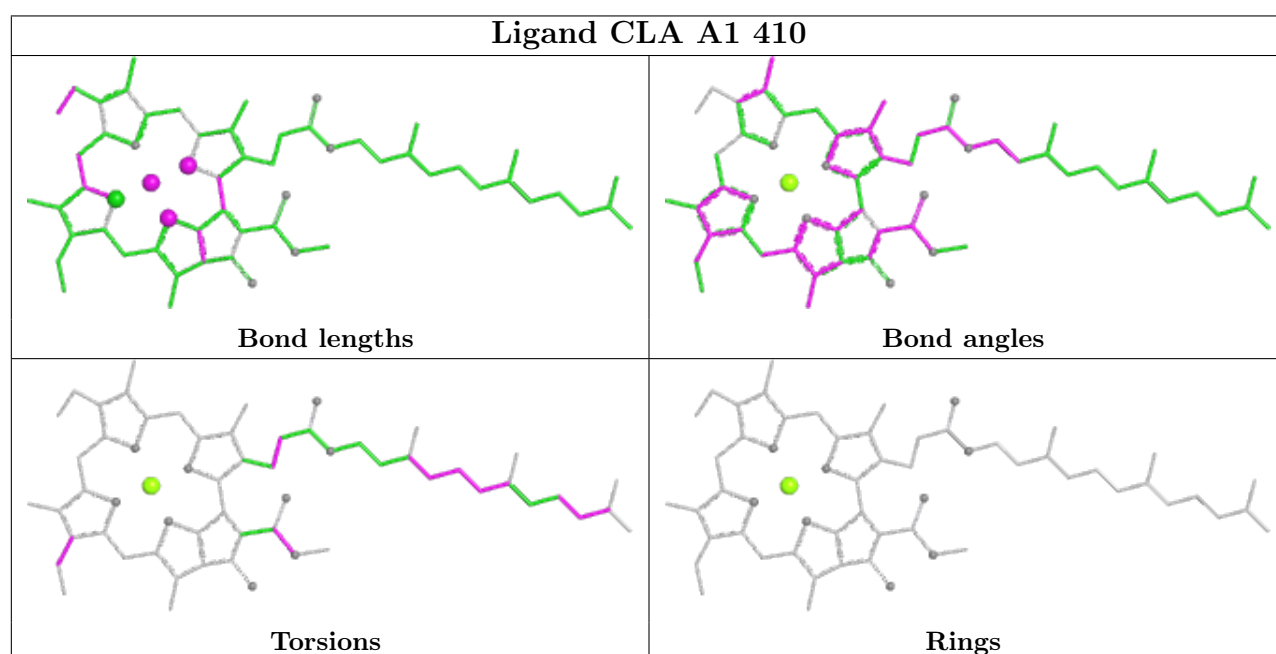
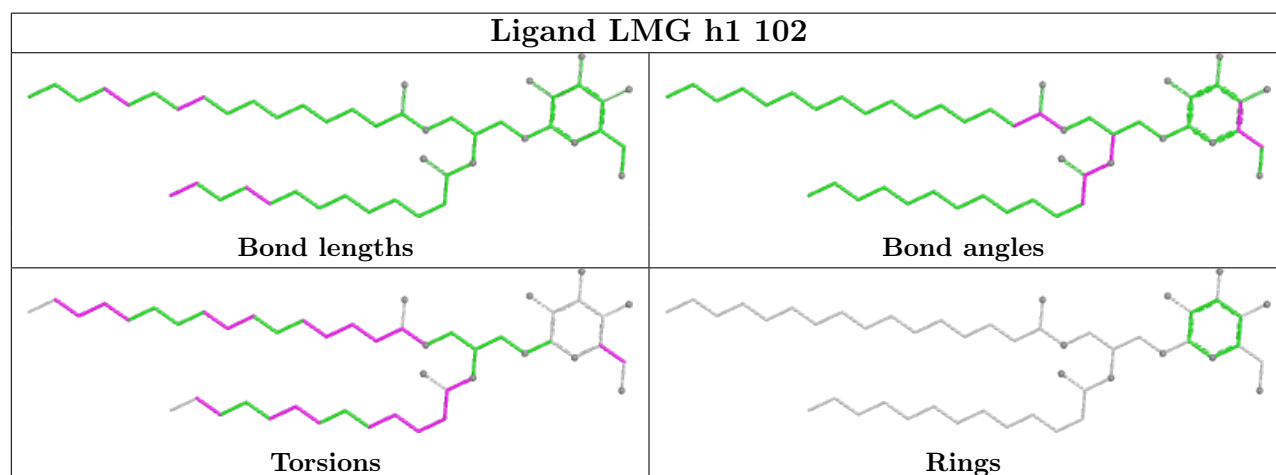
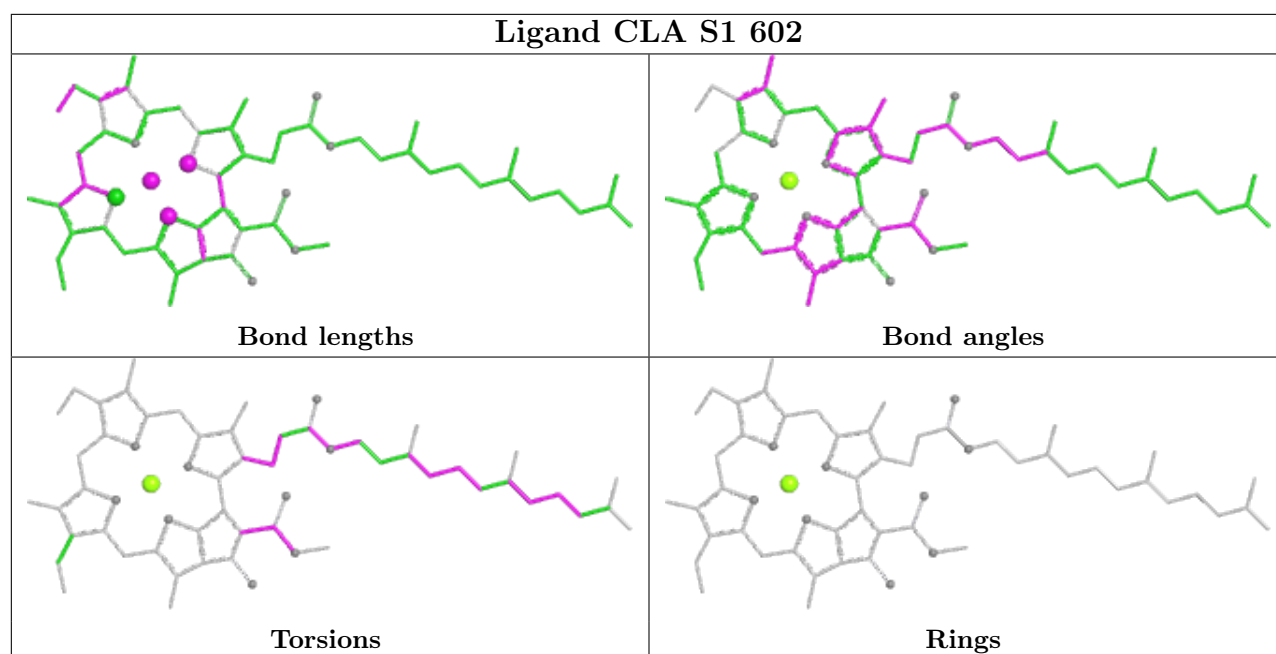


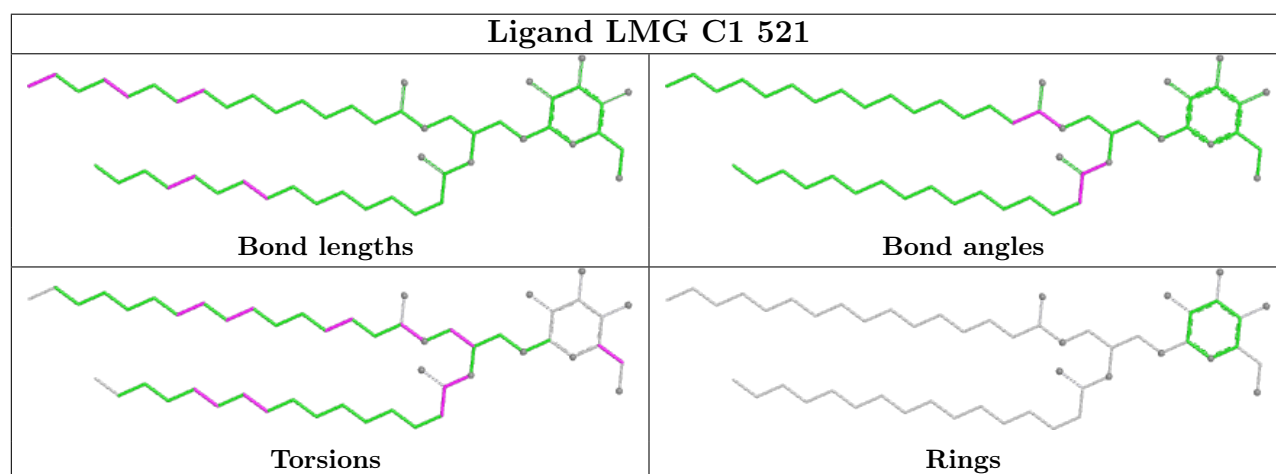
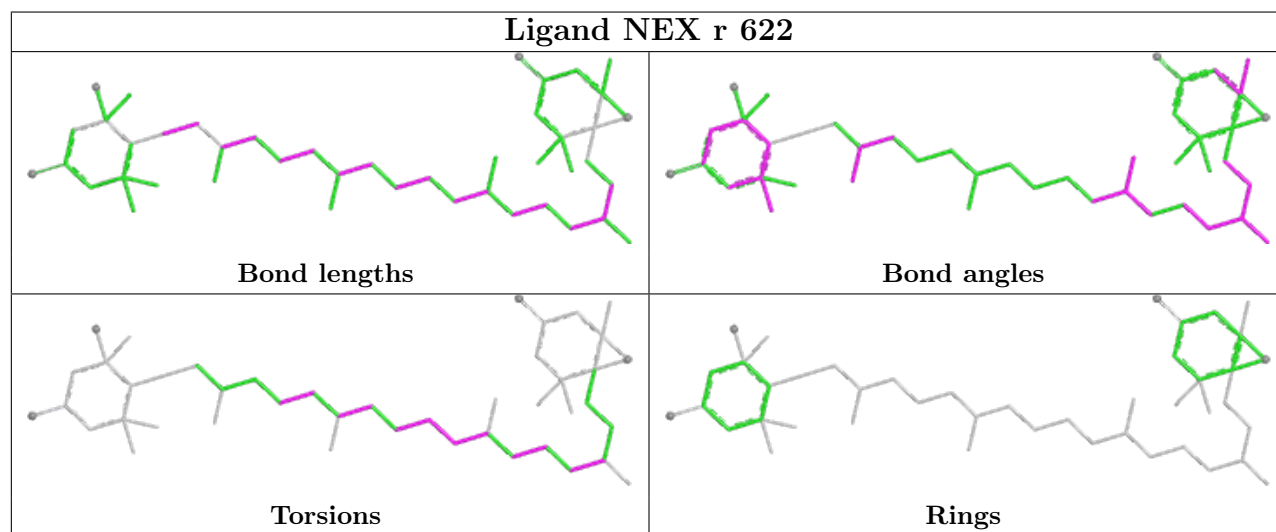
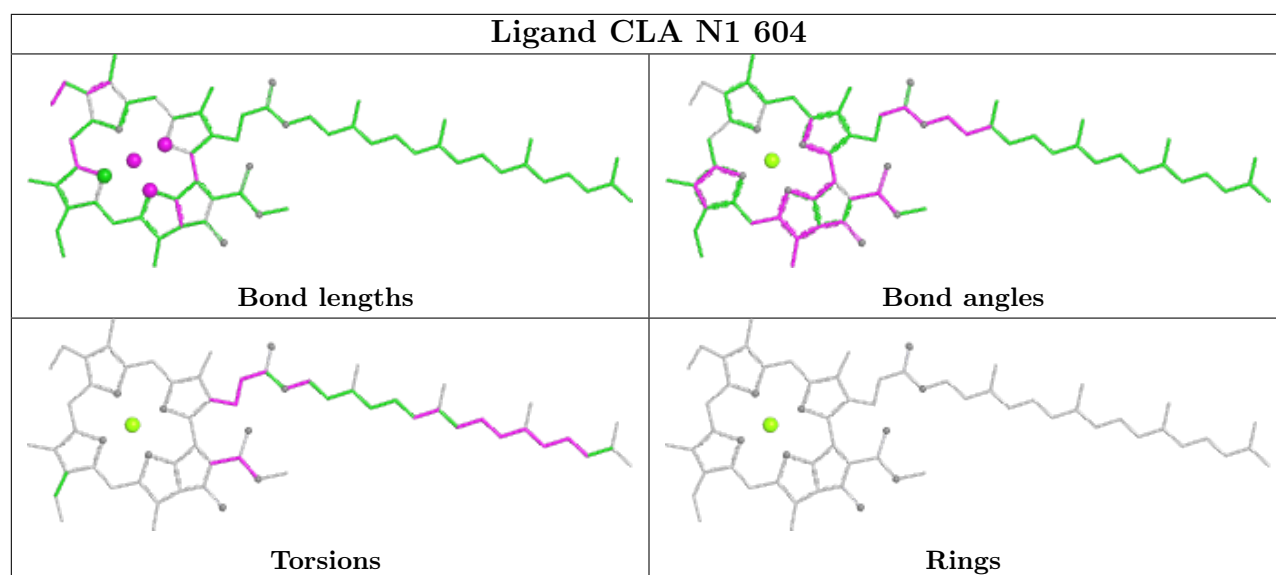
## Ligand CHL R1 606

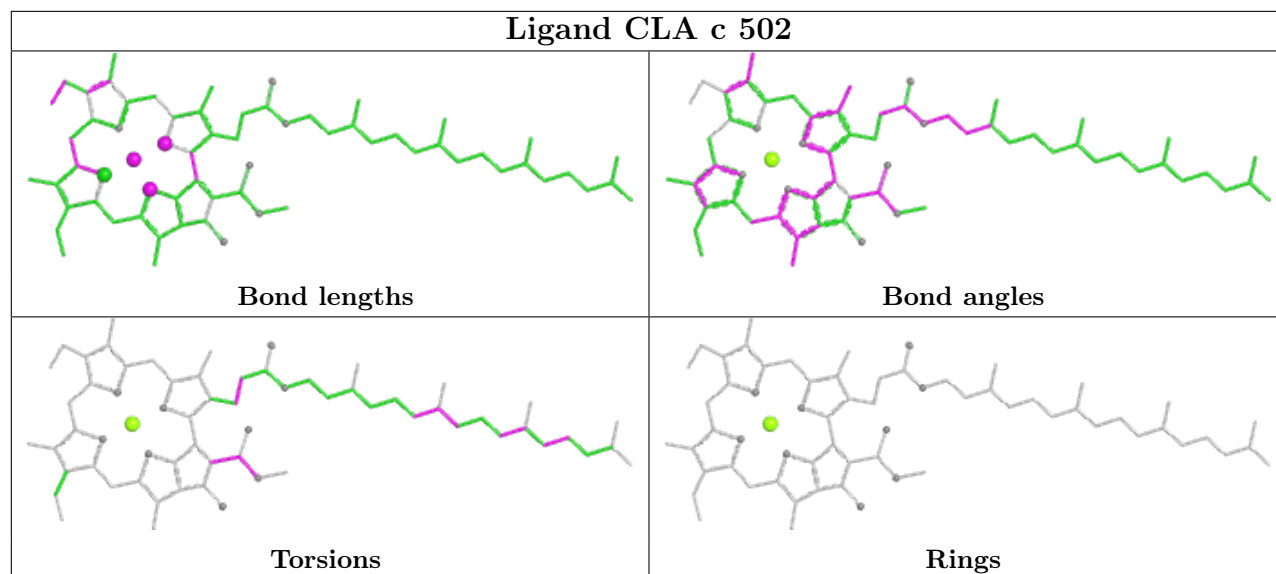
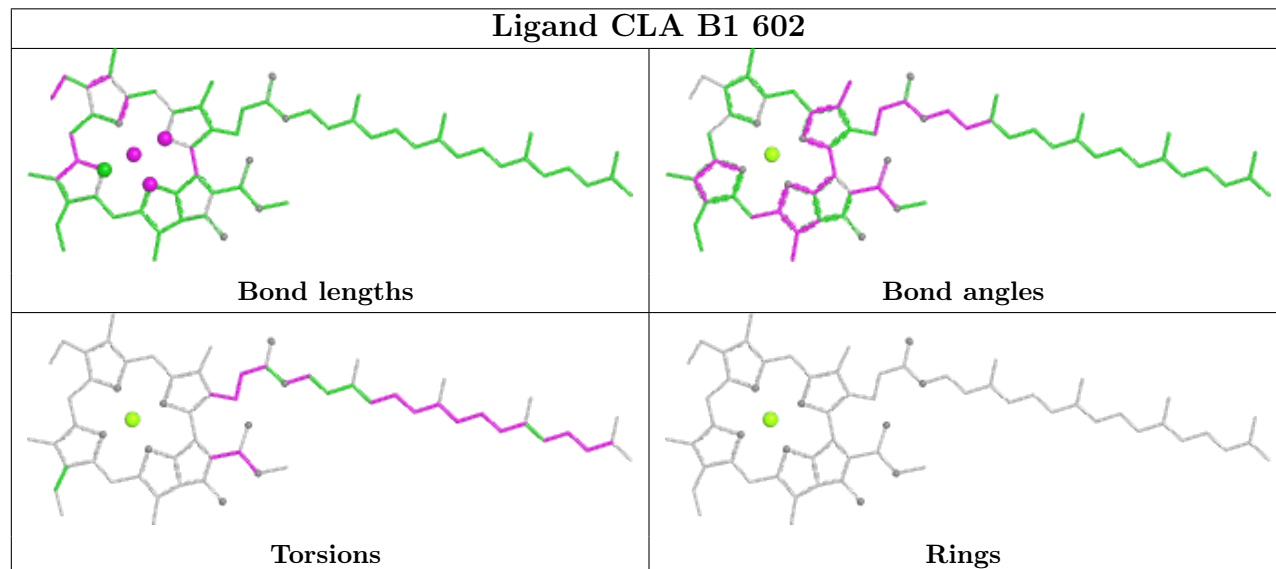


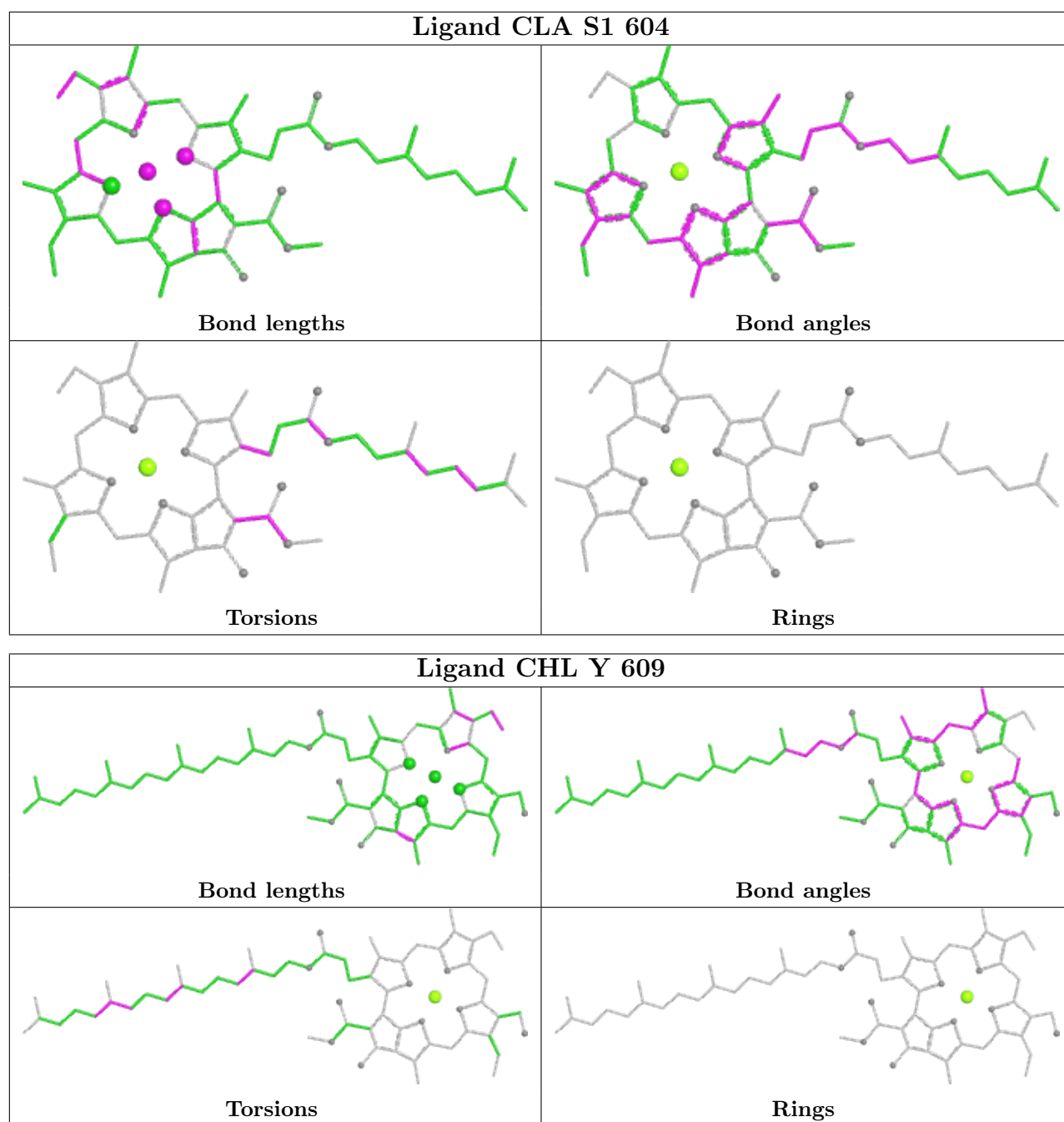


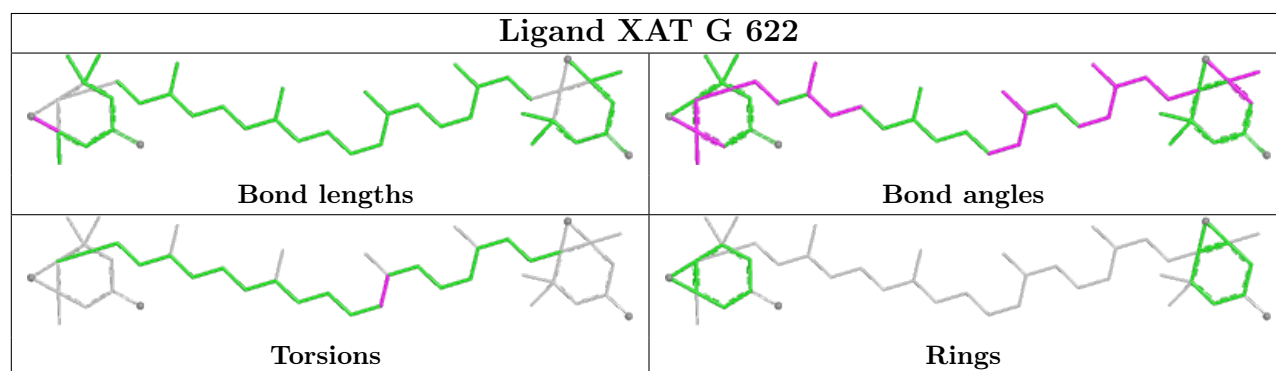
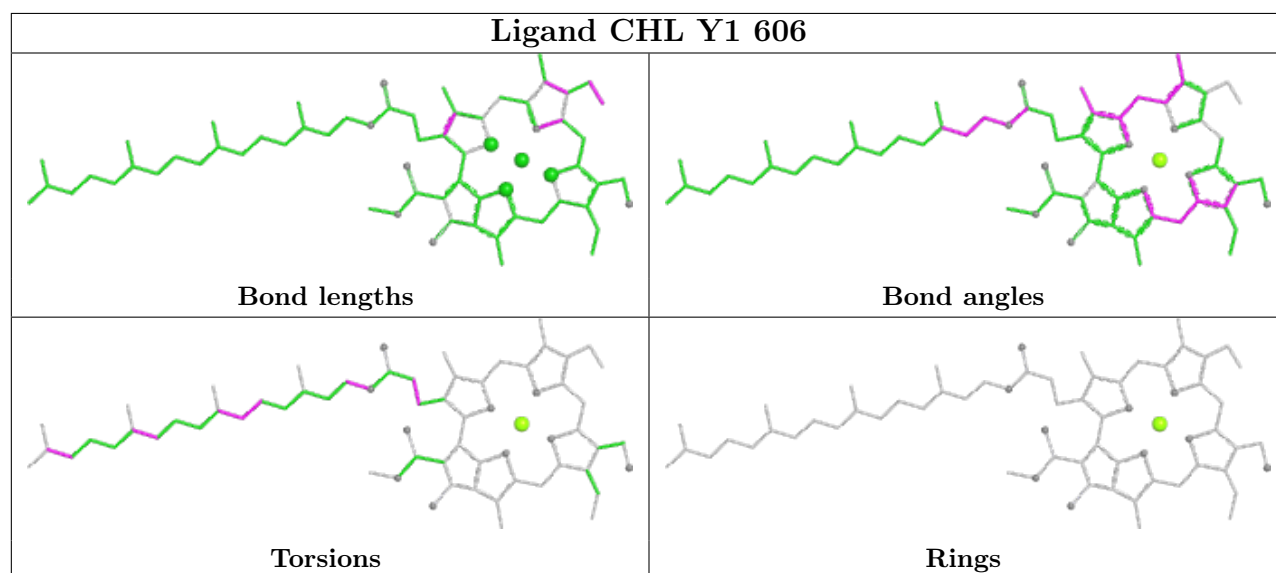
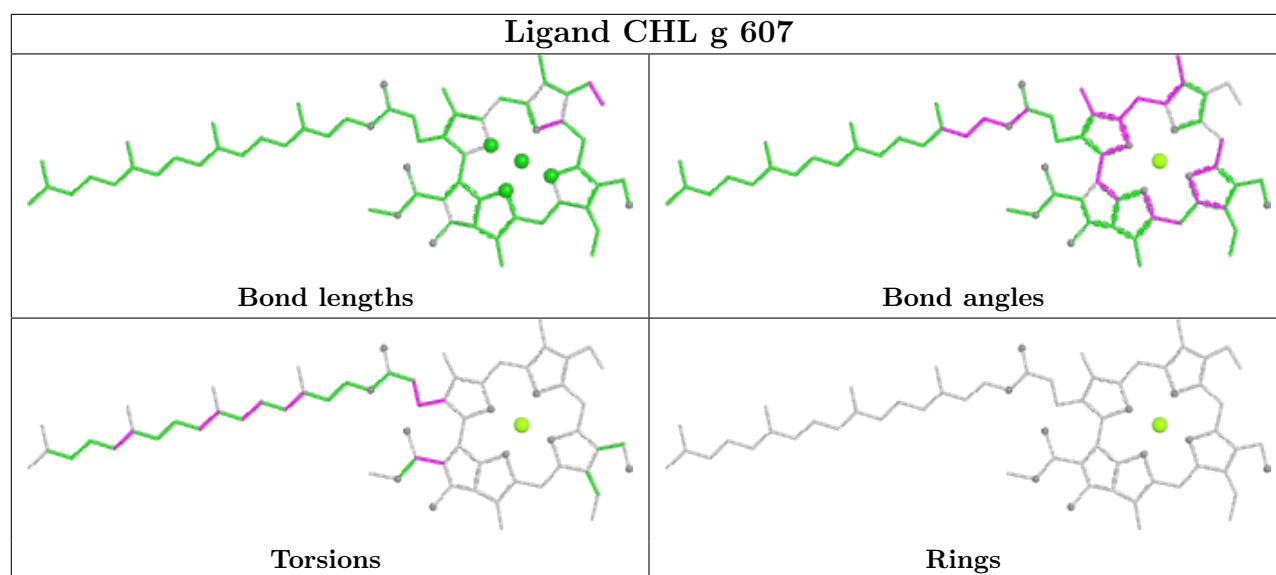






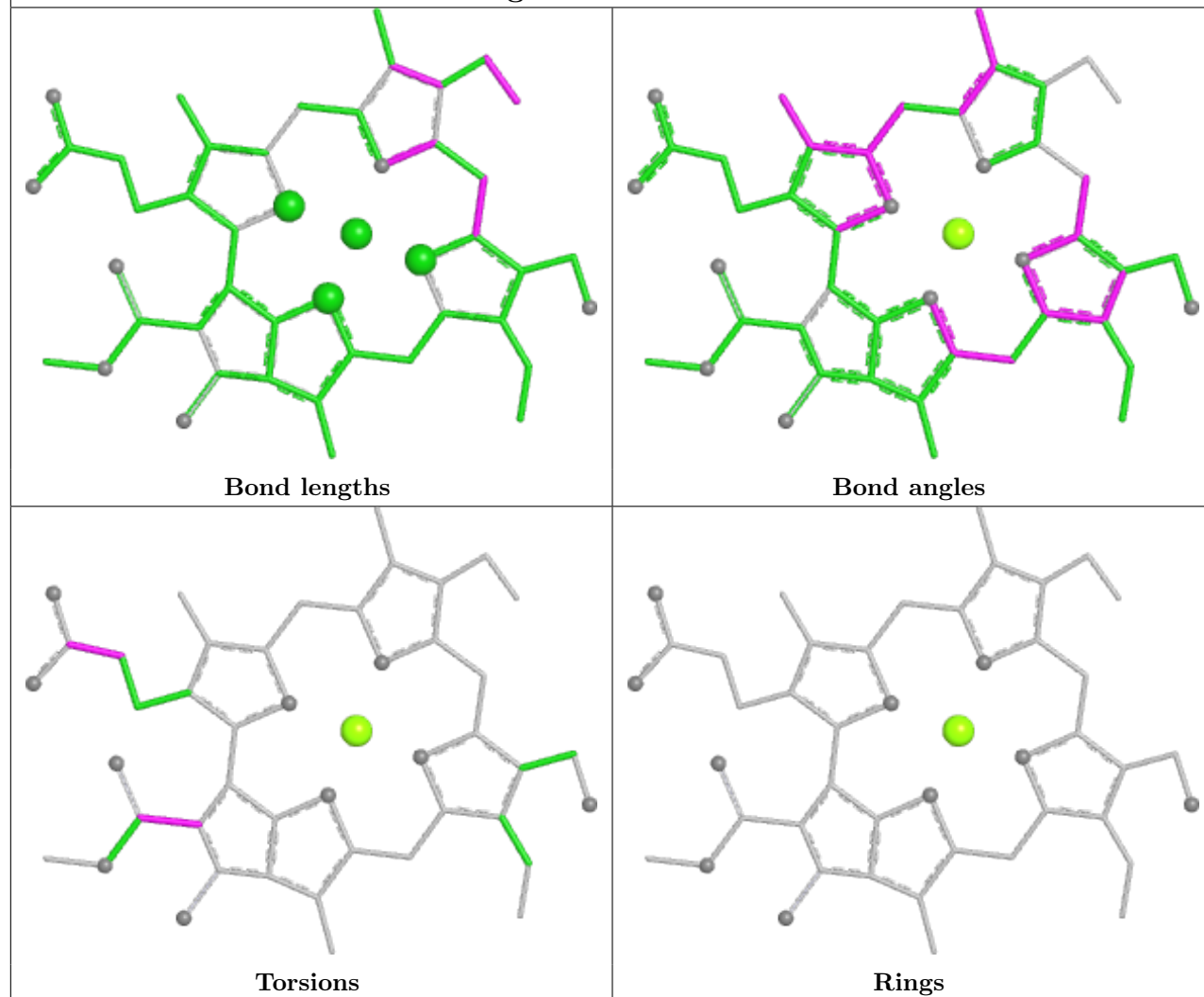
**Ligand CLA c 502****Ligand CLA B1 602**



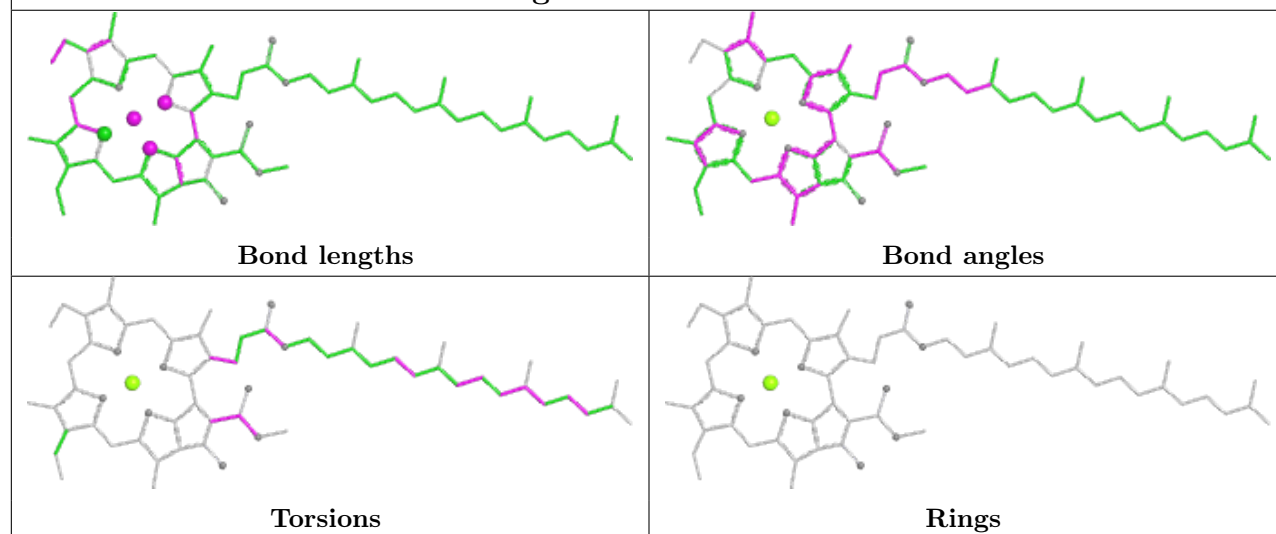


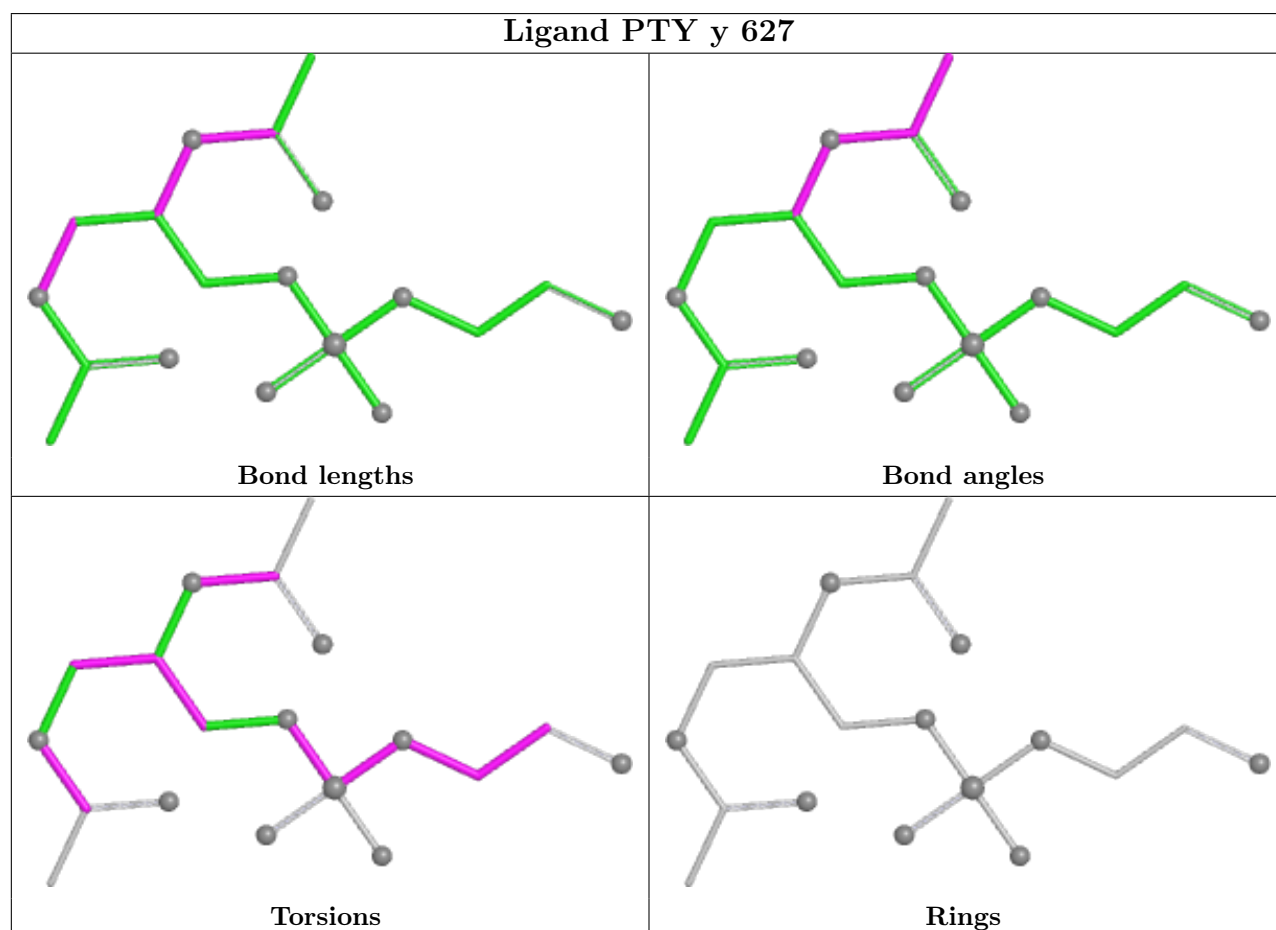
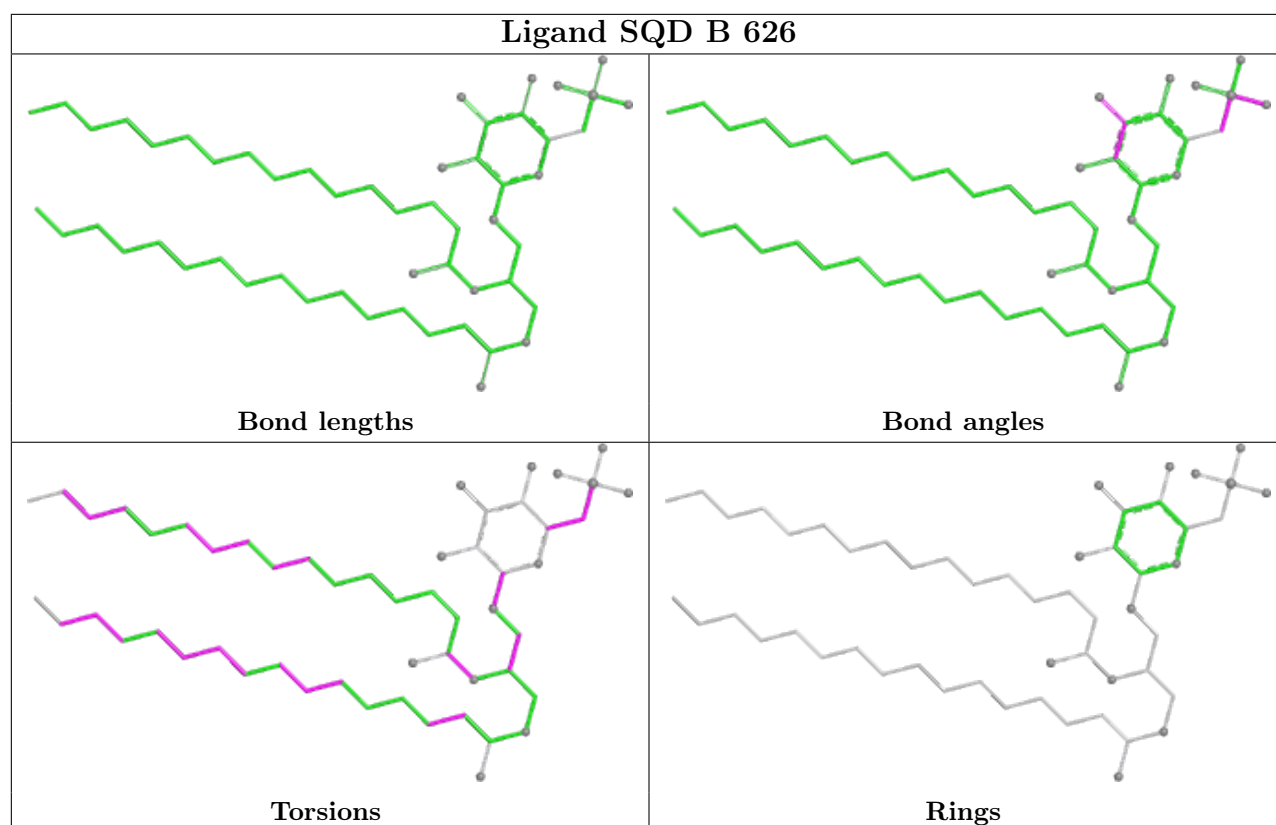


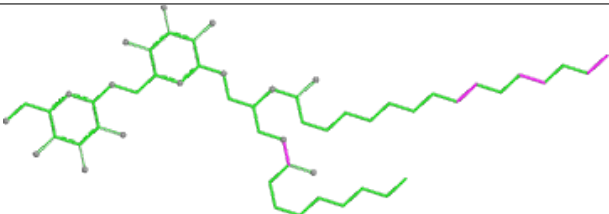
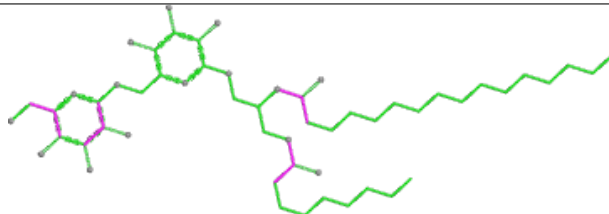
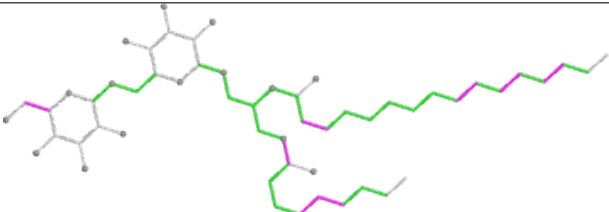
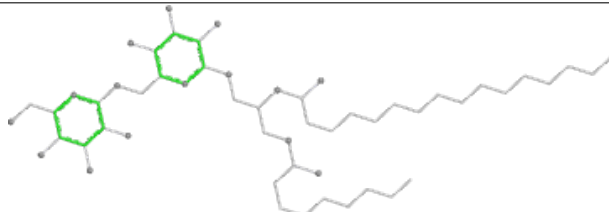
## Ligand CHL s 601

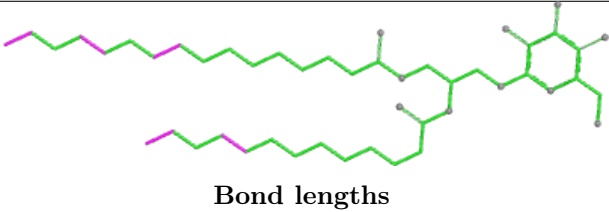
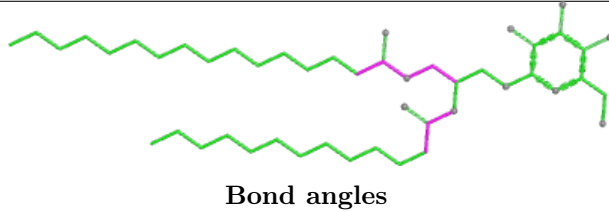
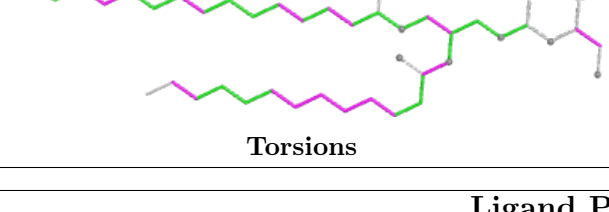



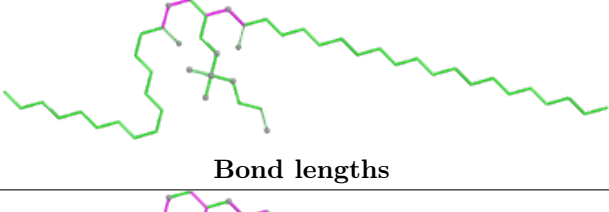
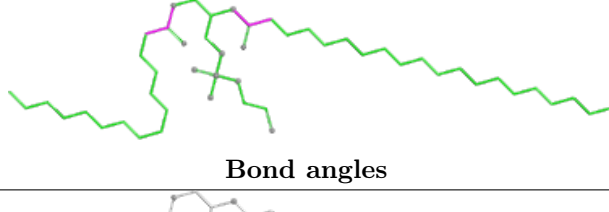


## Ligand CLA C 511

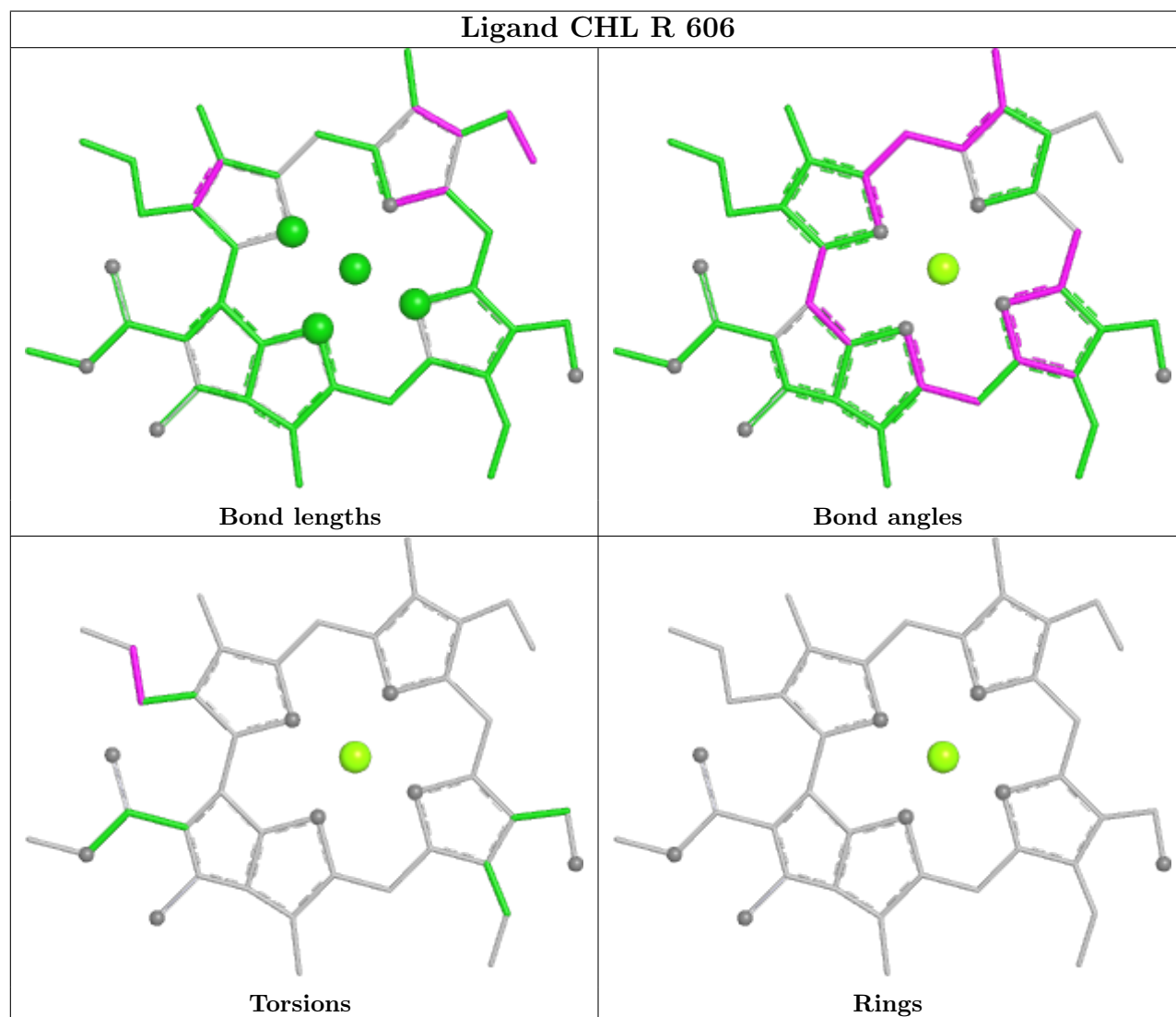
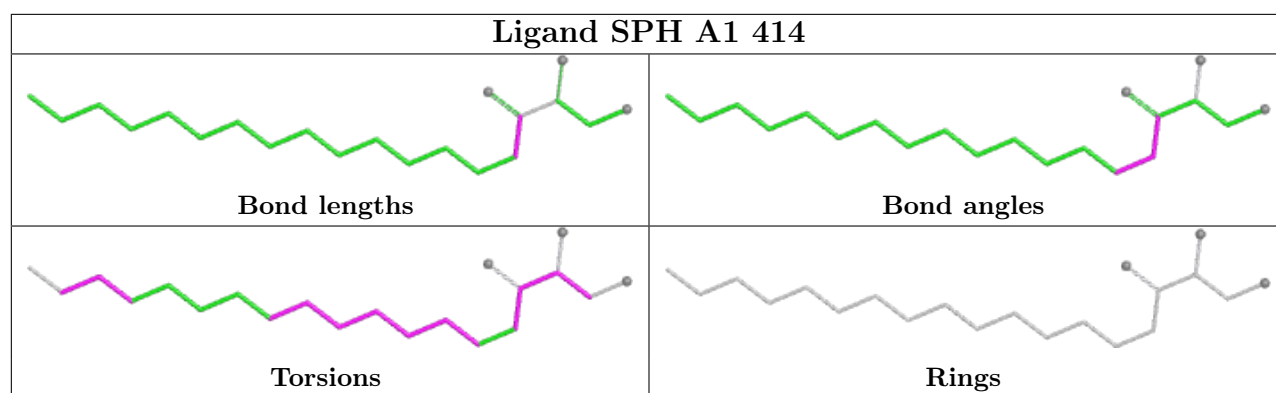


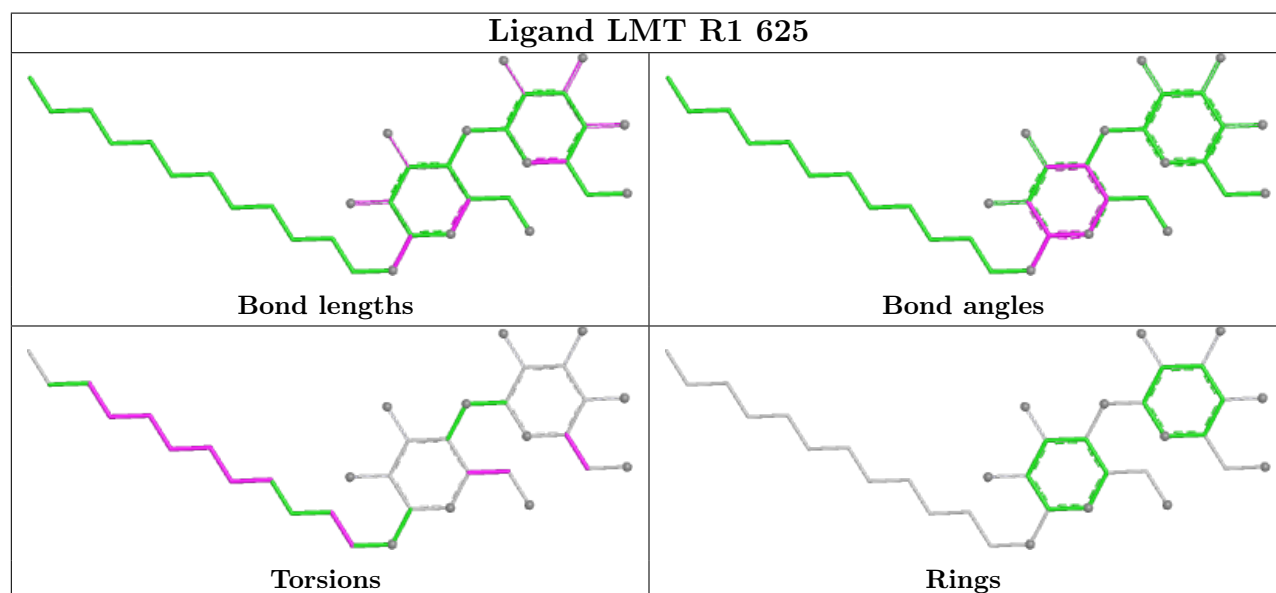
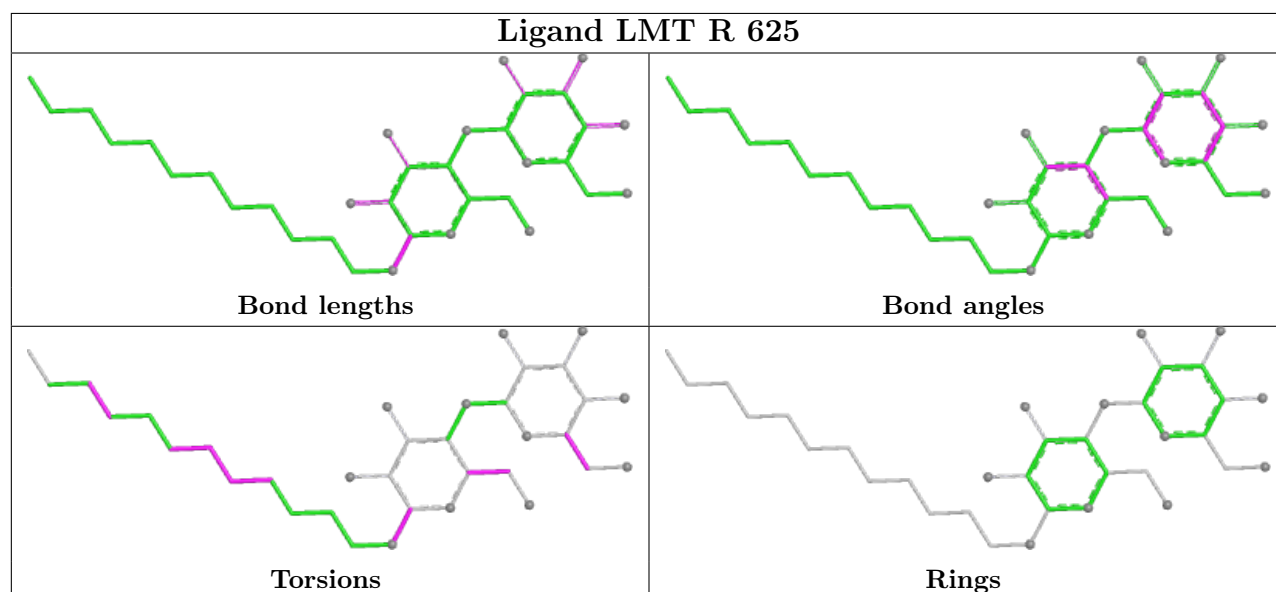
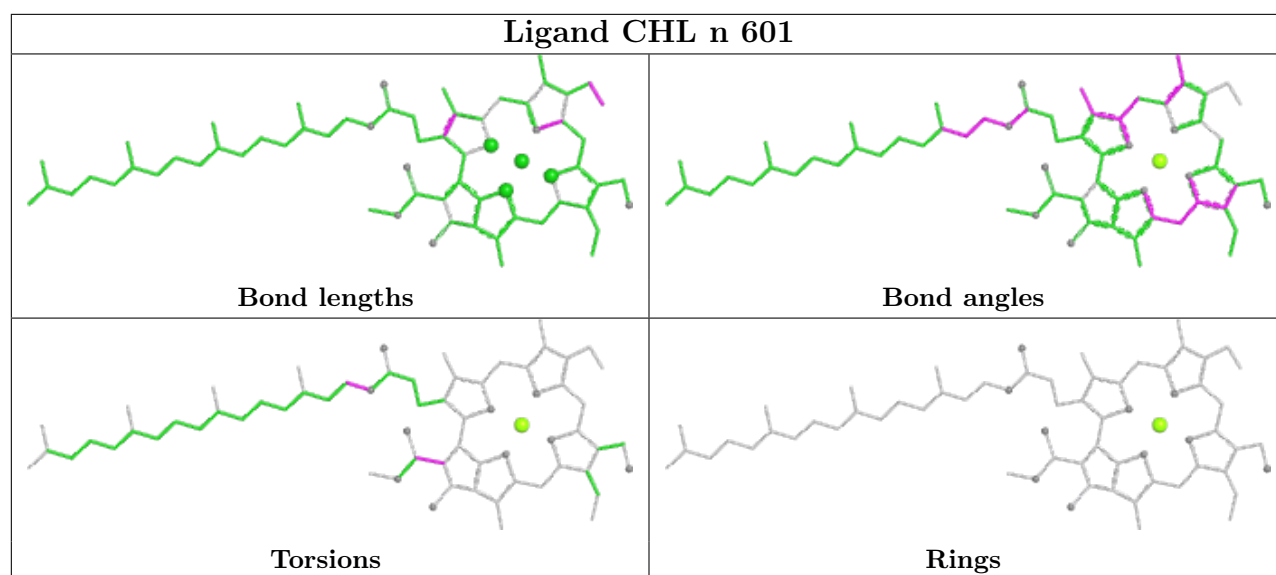


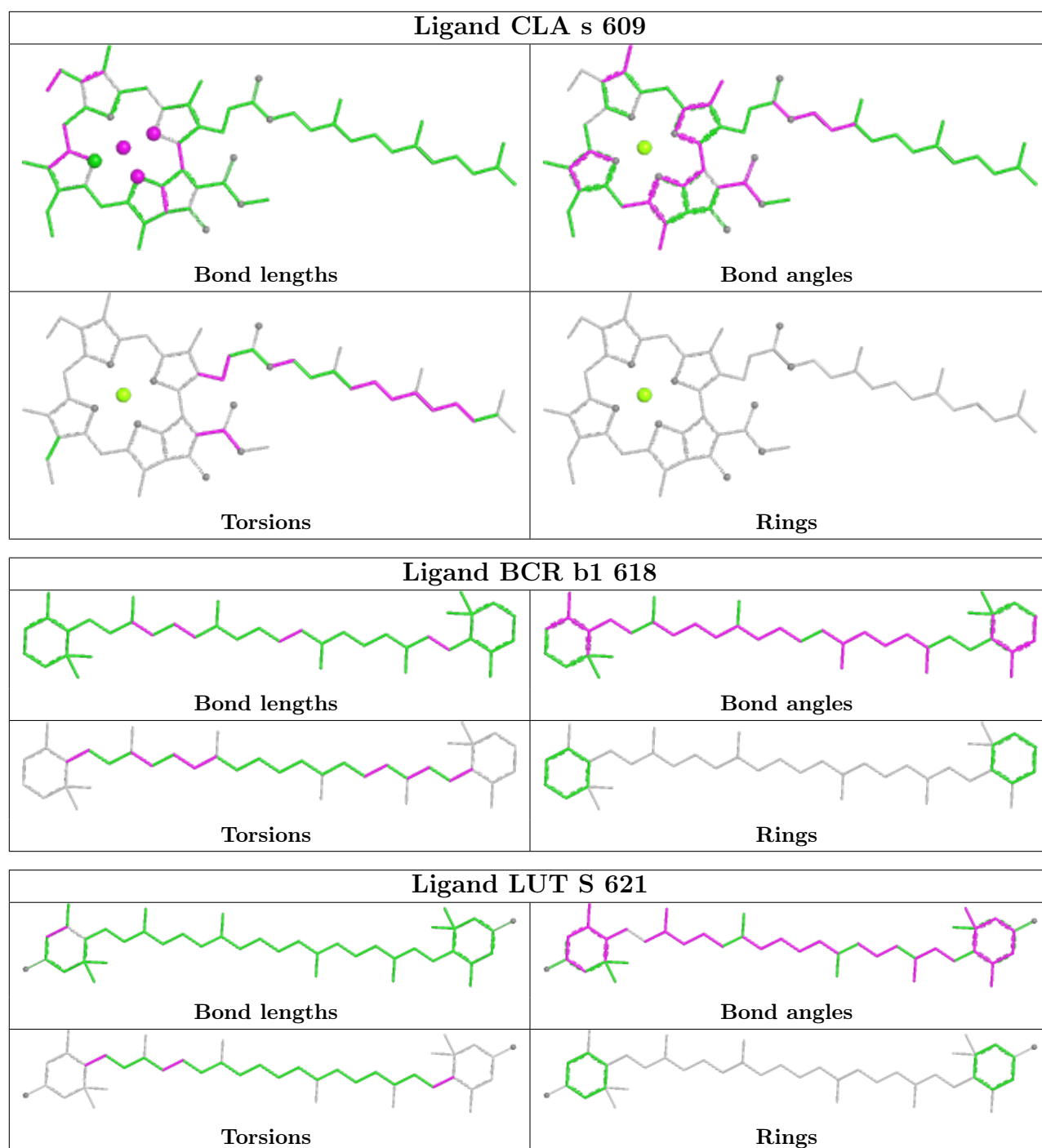
Ligand DGD c 518	
	
Bond lengths	Bond angles
	
Torsions	Rings

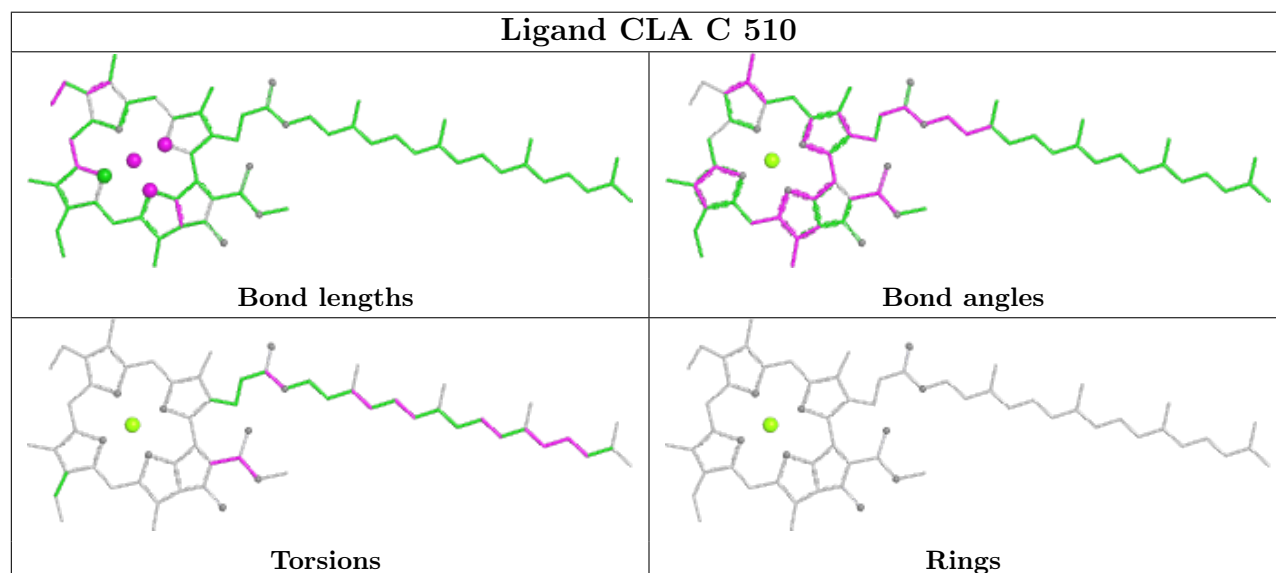
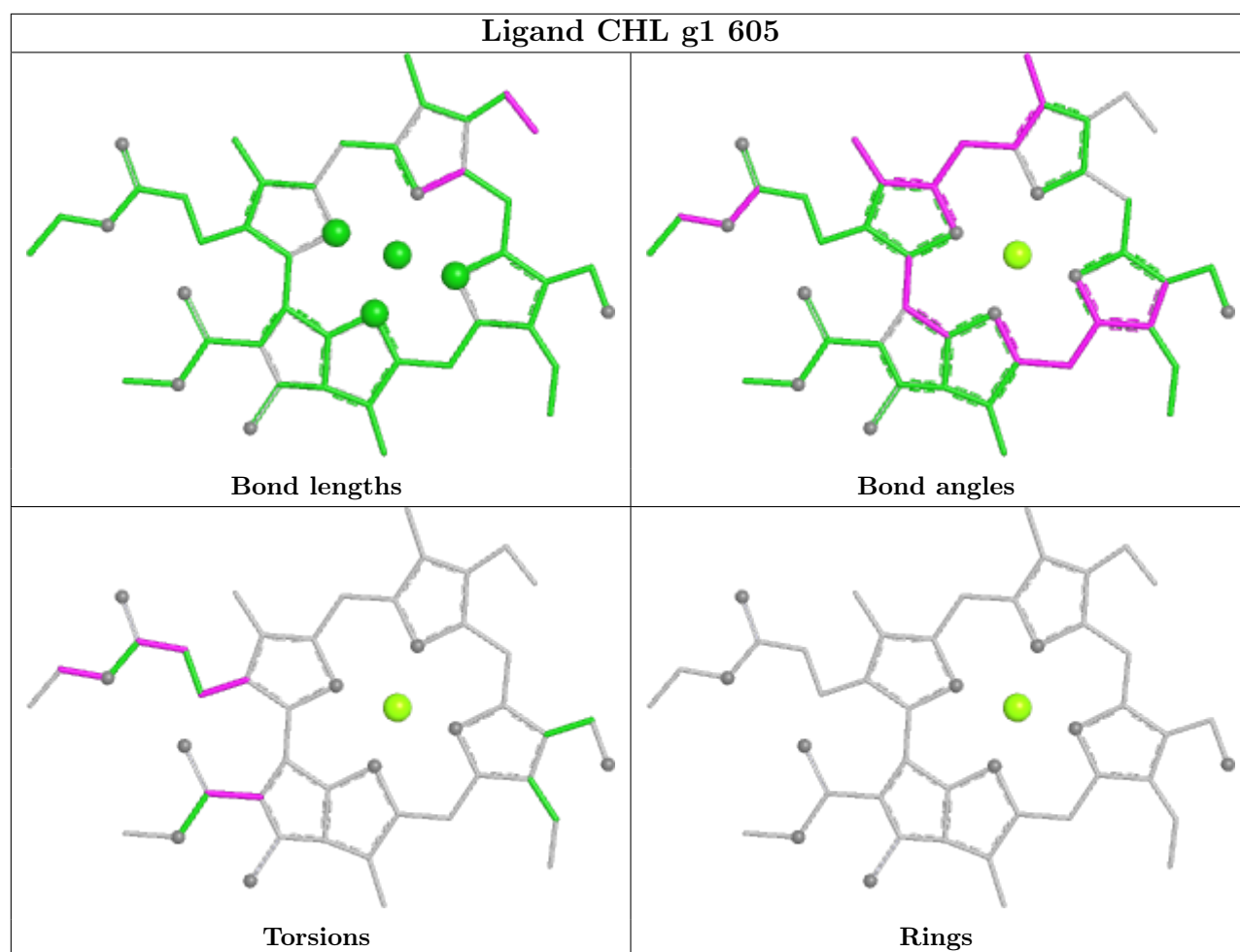
Ligand LMG H1 102	
	
Bond lengths	Bond angles
	
Torsions	Rings

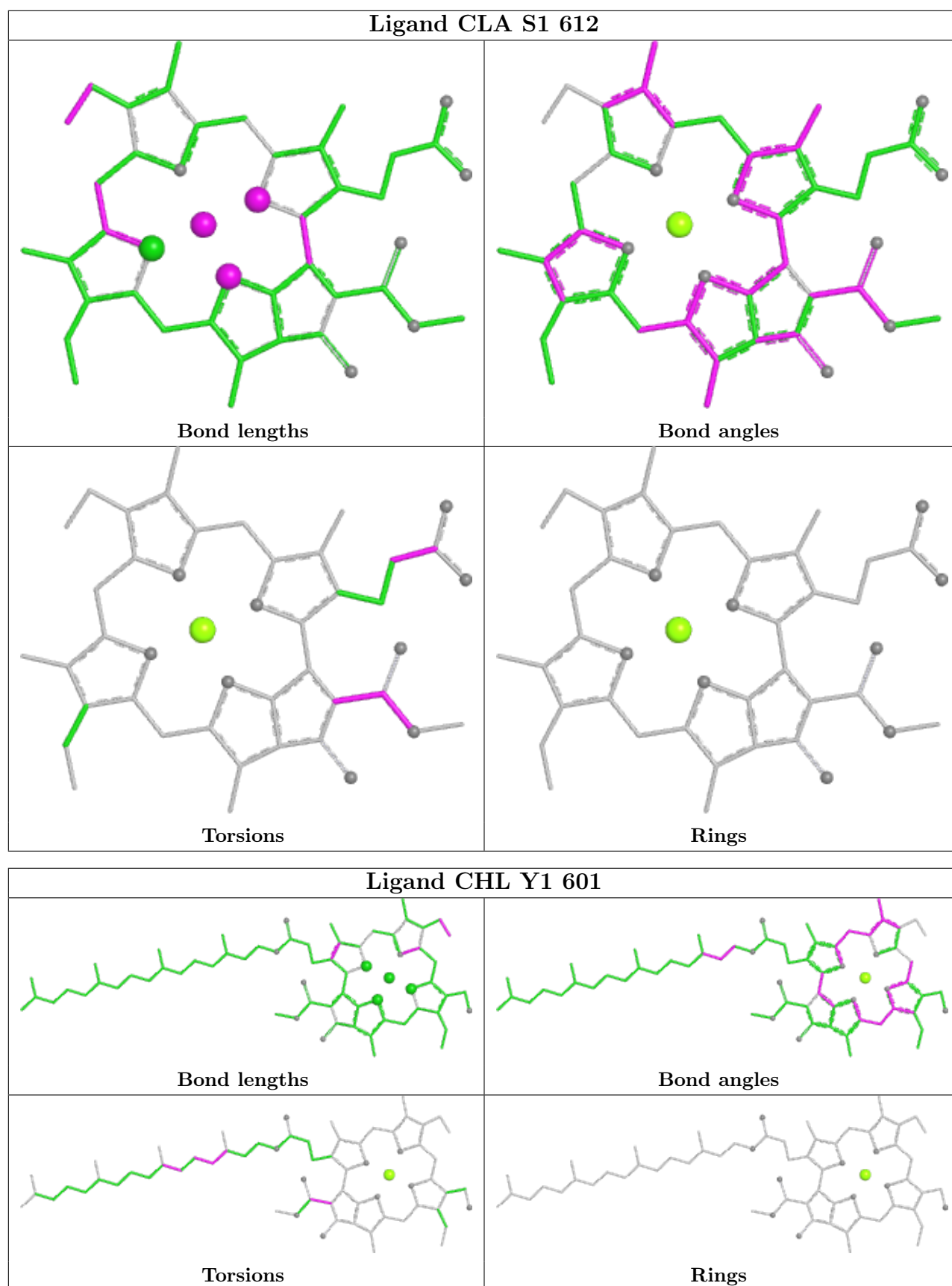
Ligand PTY y1 626	
	
Bond lengths	Bond angles
	
Torsions	Rings



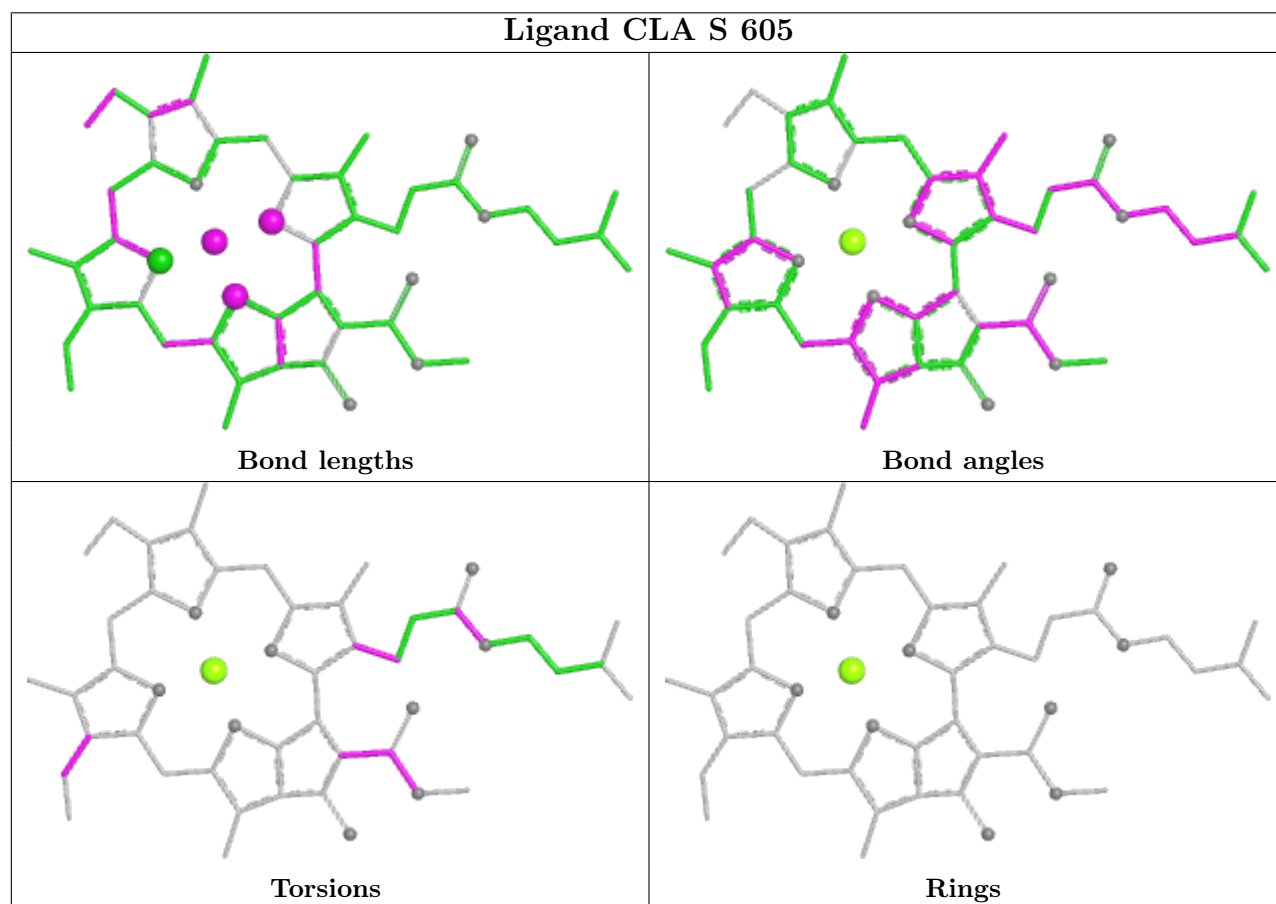
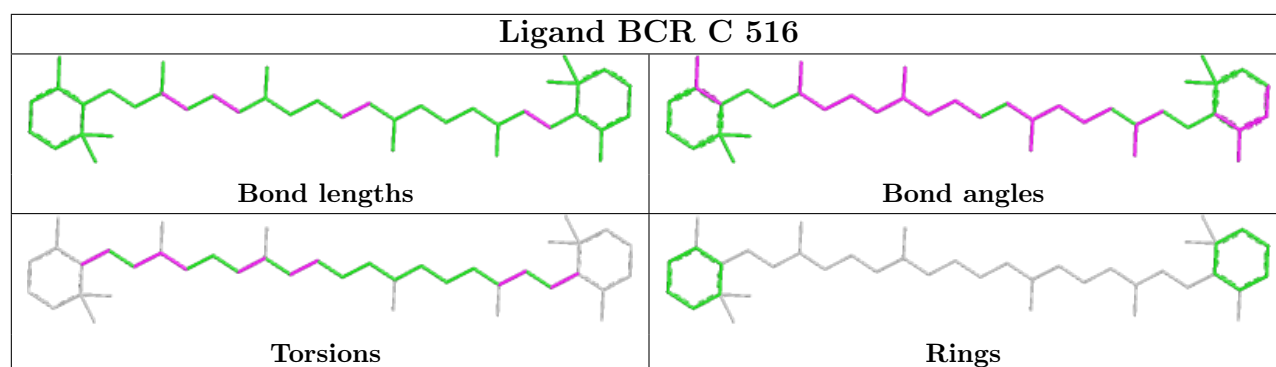


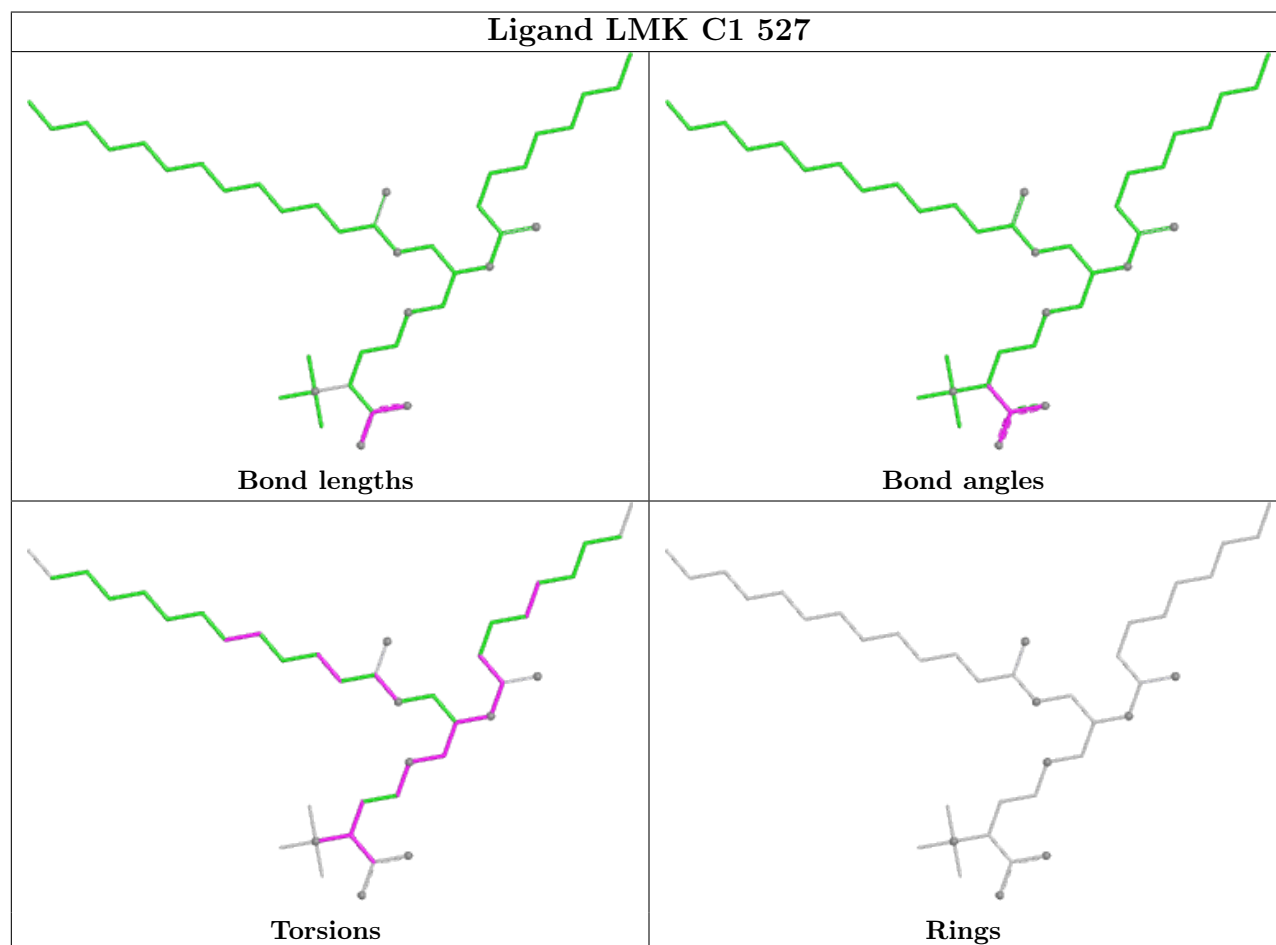
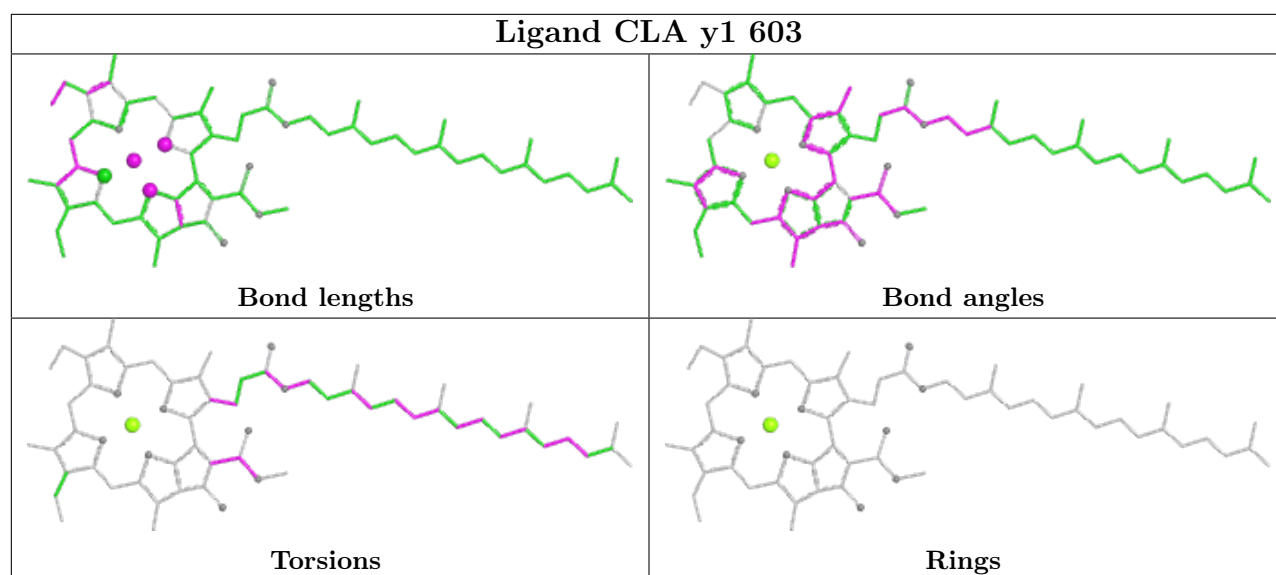


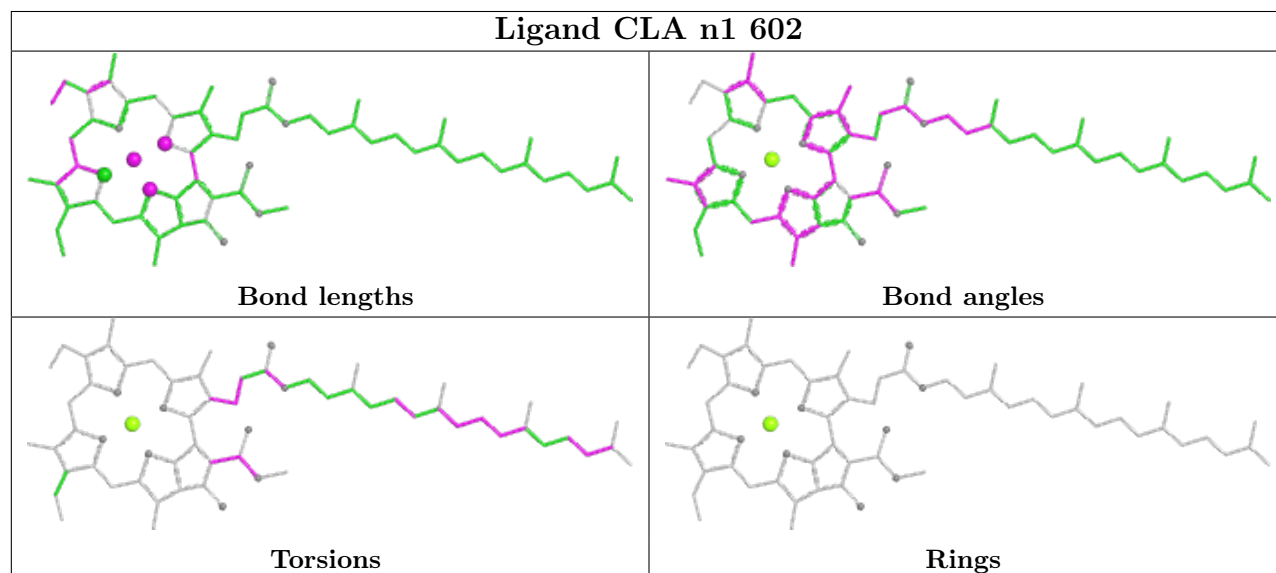
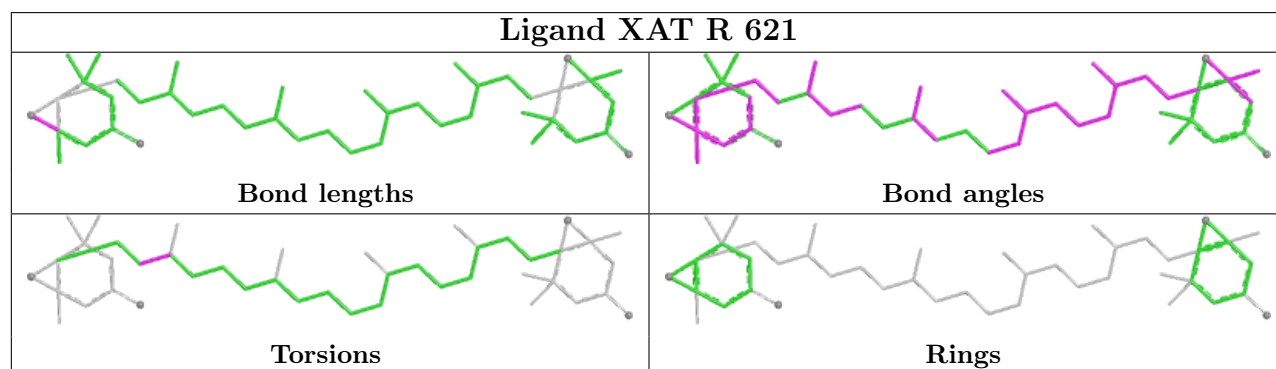
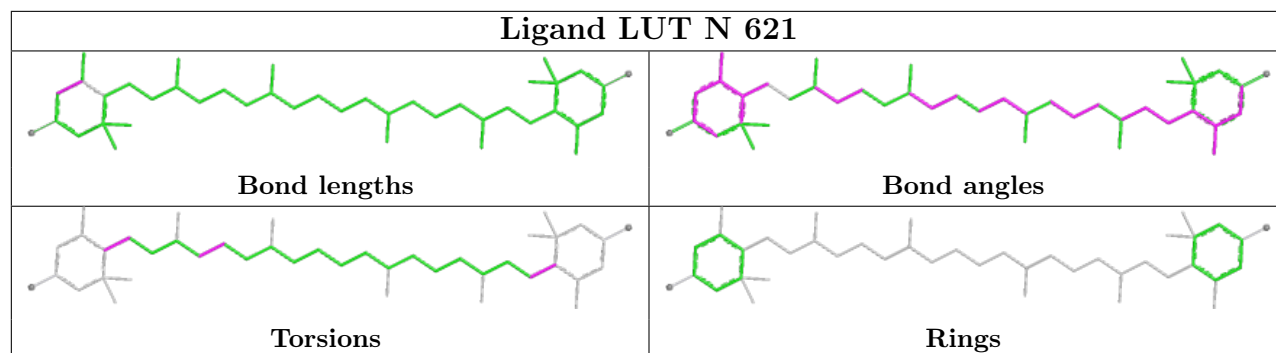


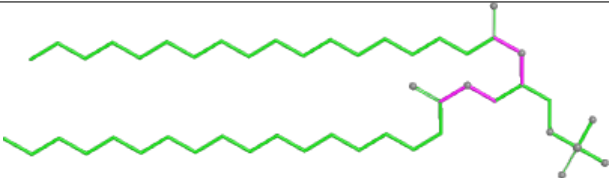
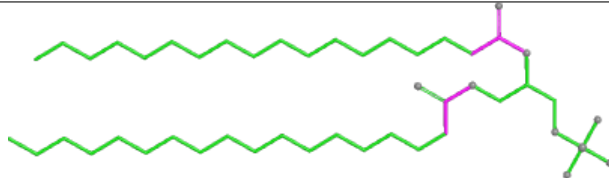
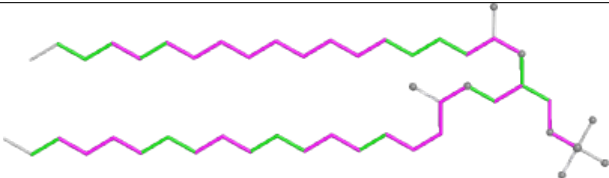
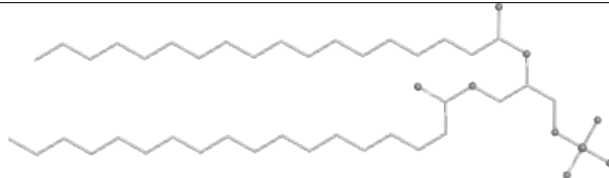


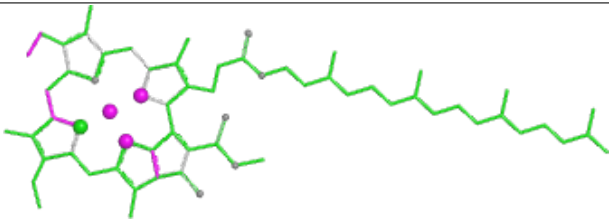
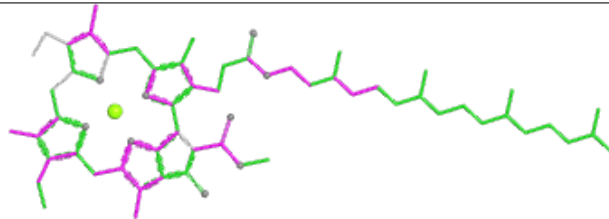
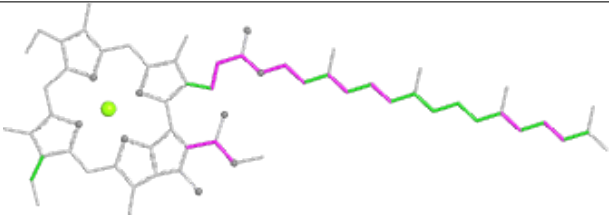
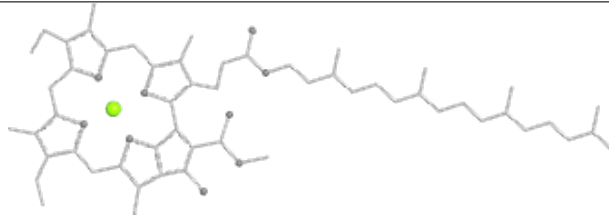


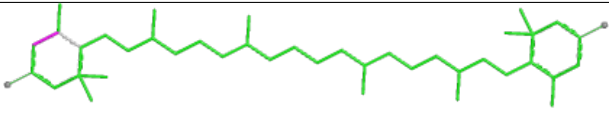
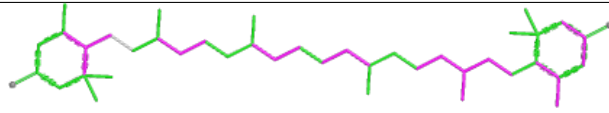
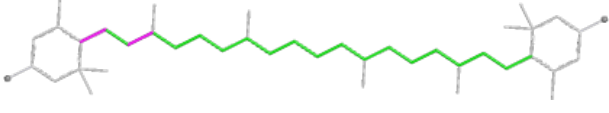
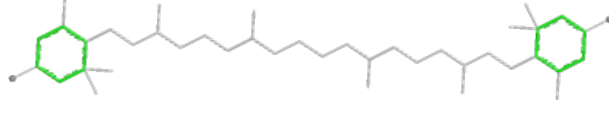


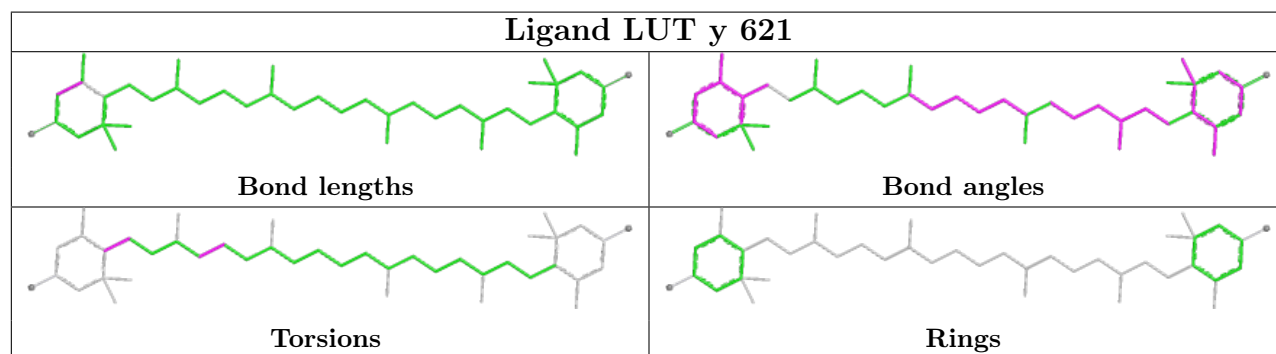
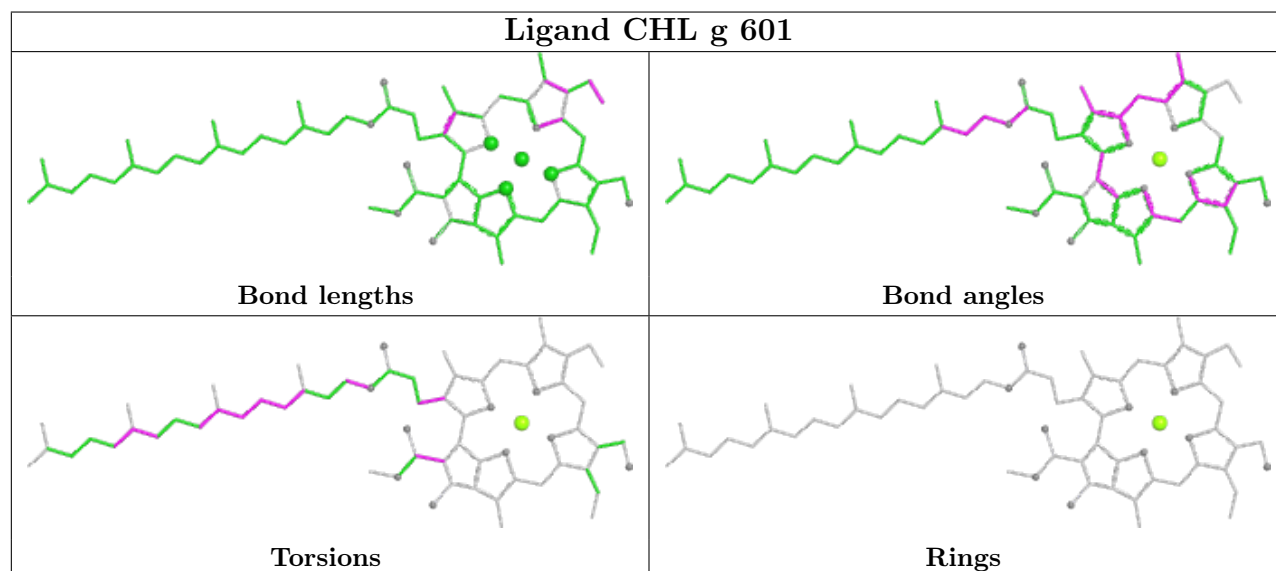
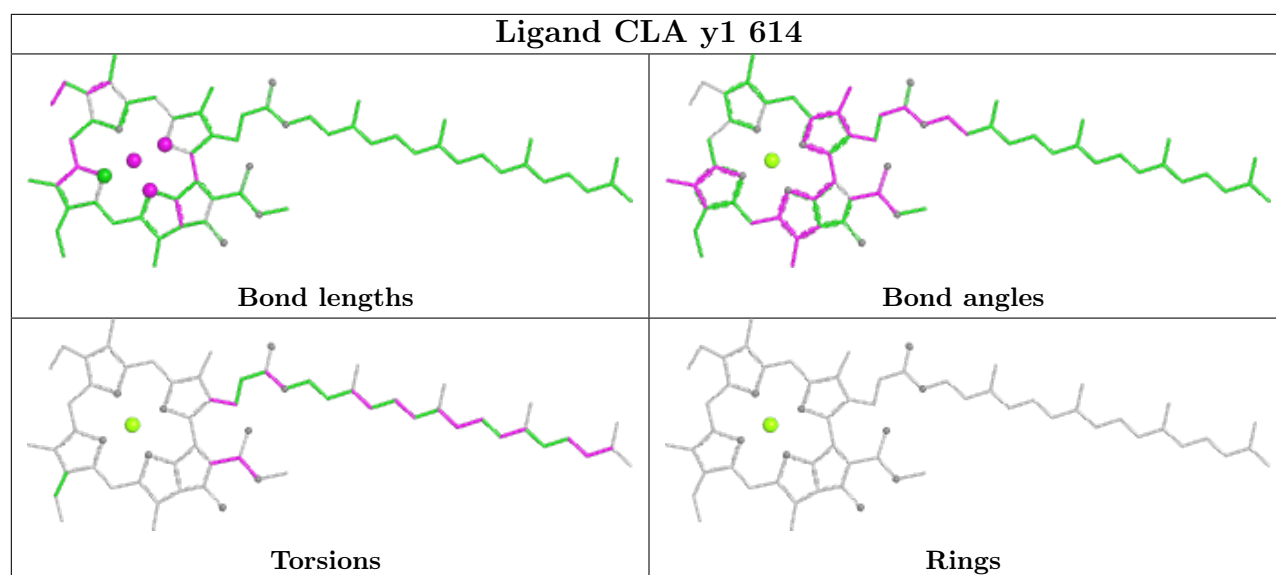


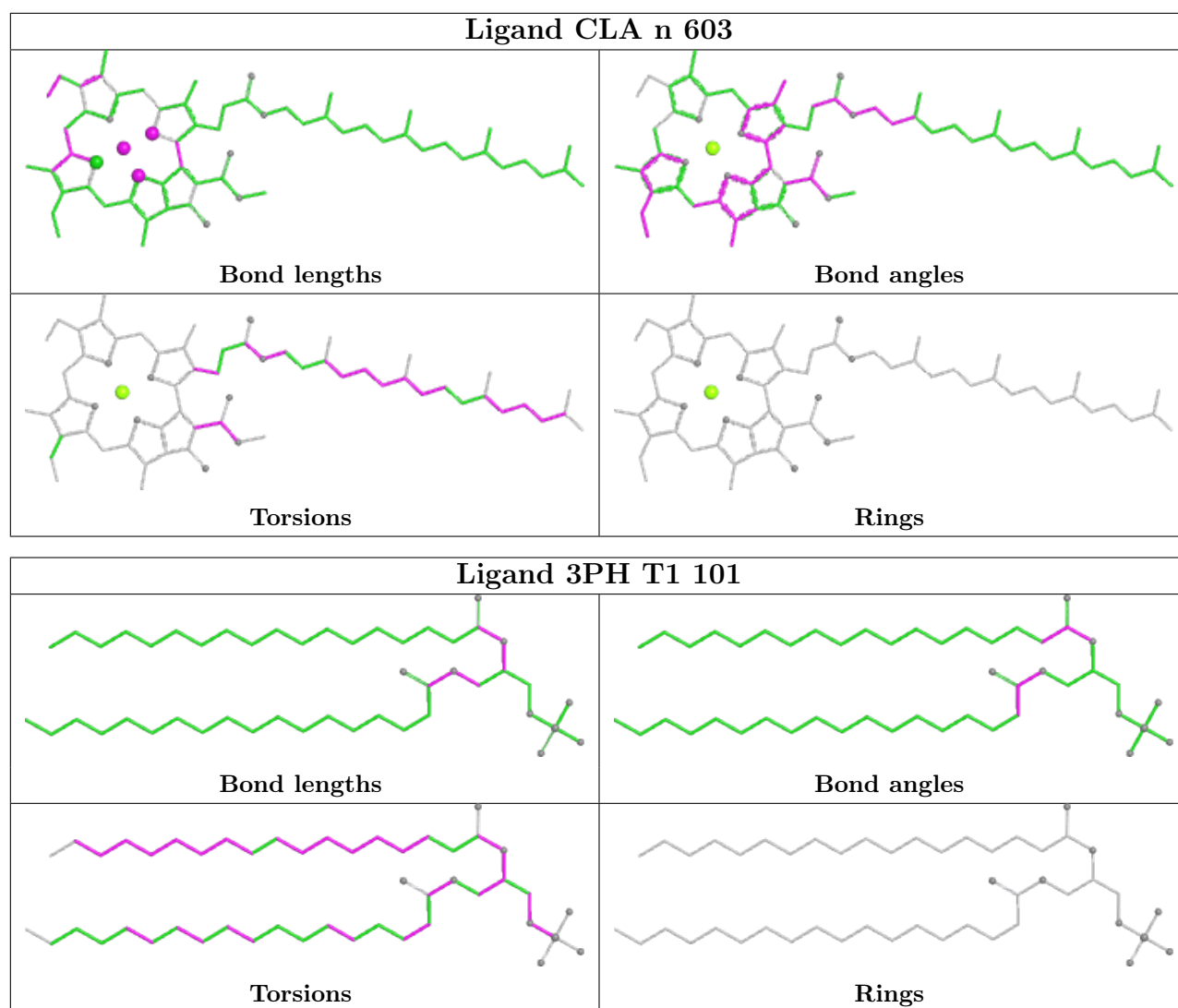


Ligand 3PH S1 626	
	
Bond lengths	Bond angles
	
Torsions	Rings

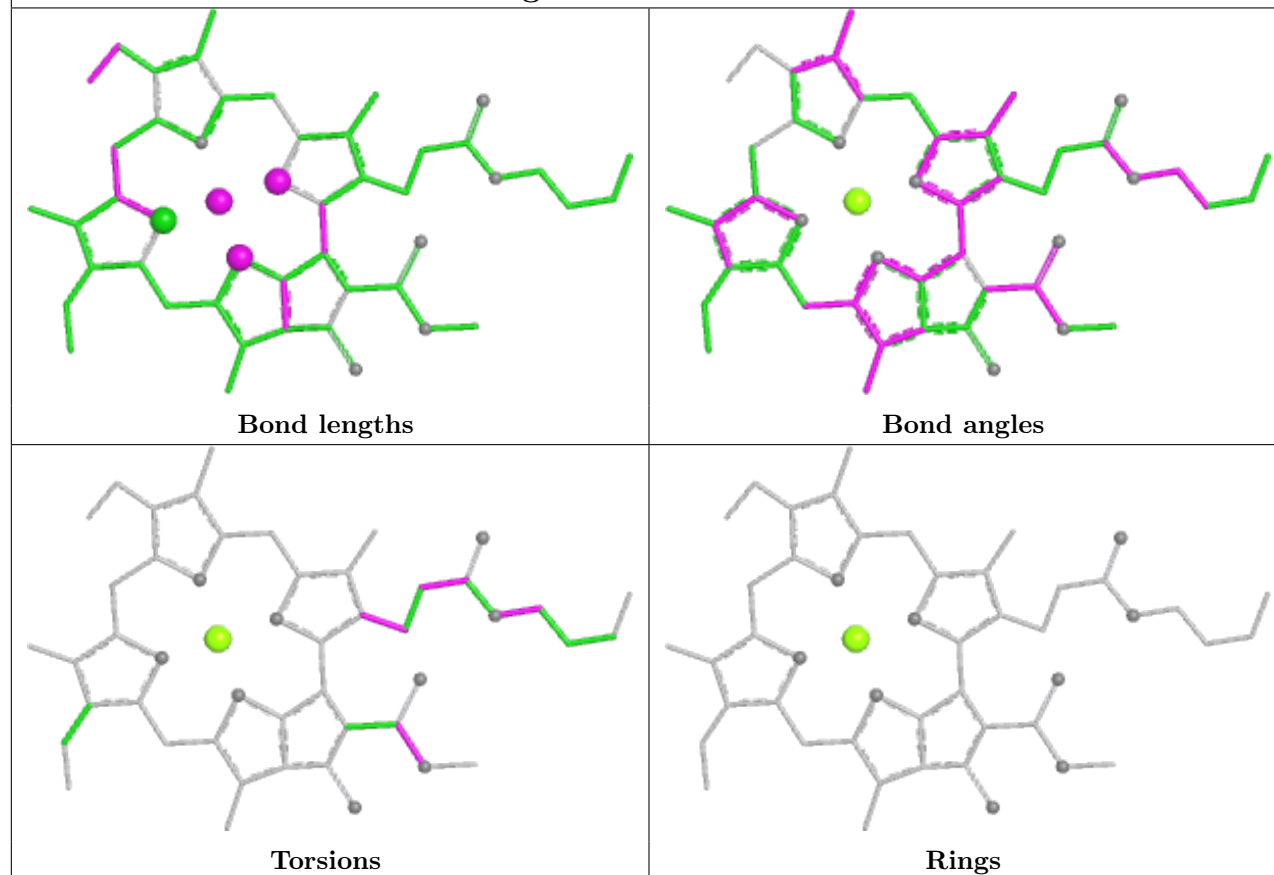
Ligand CLA A 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT y1 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

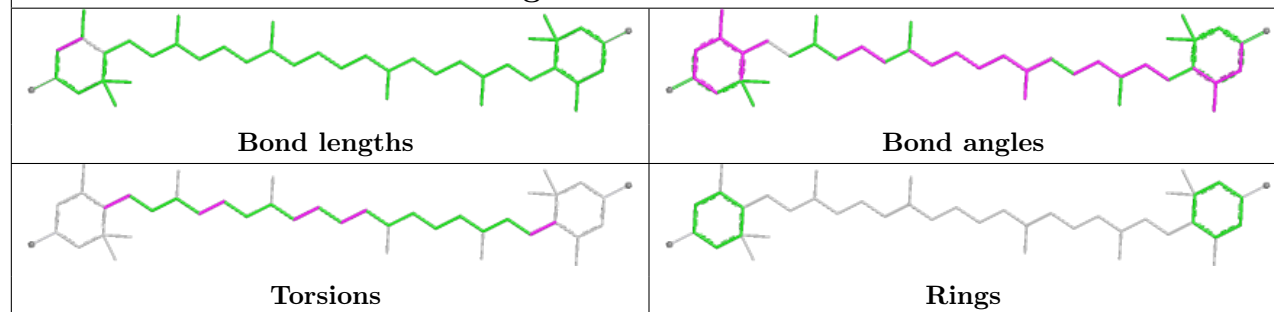


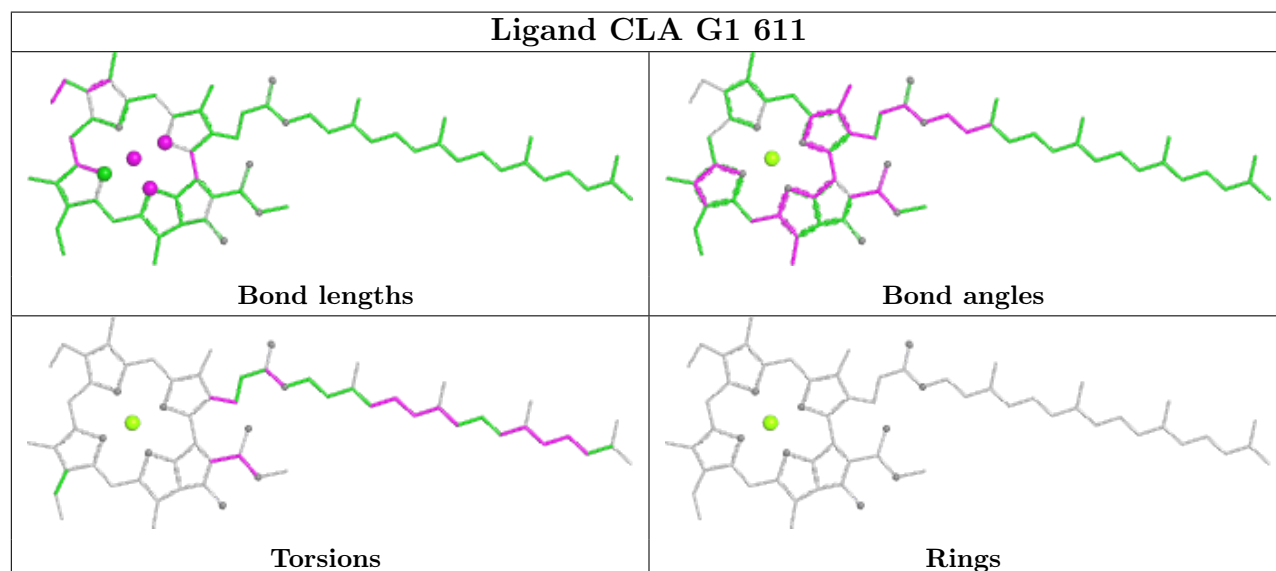
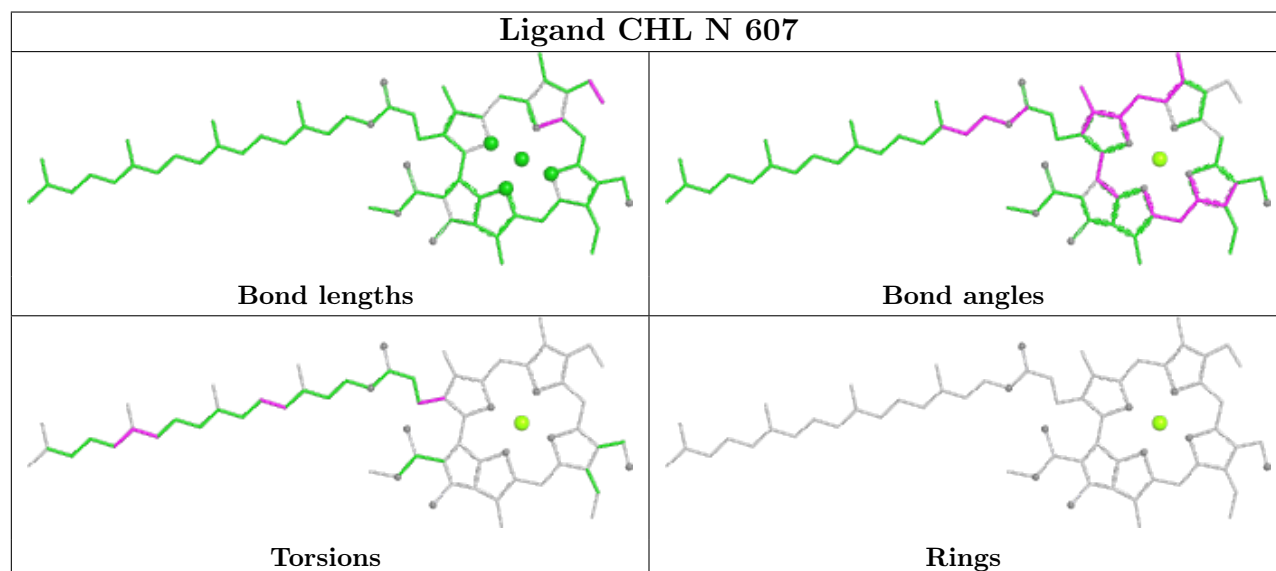
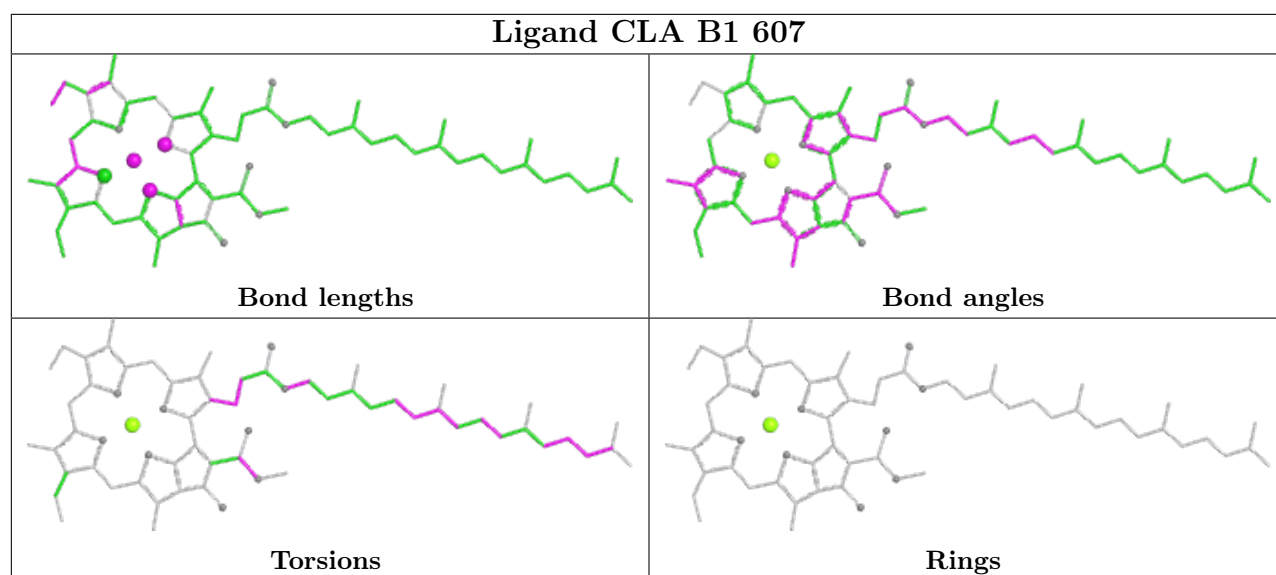


## Ligand CLA N1 614

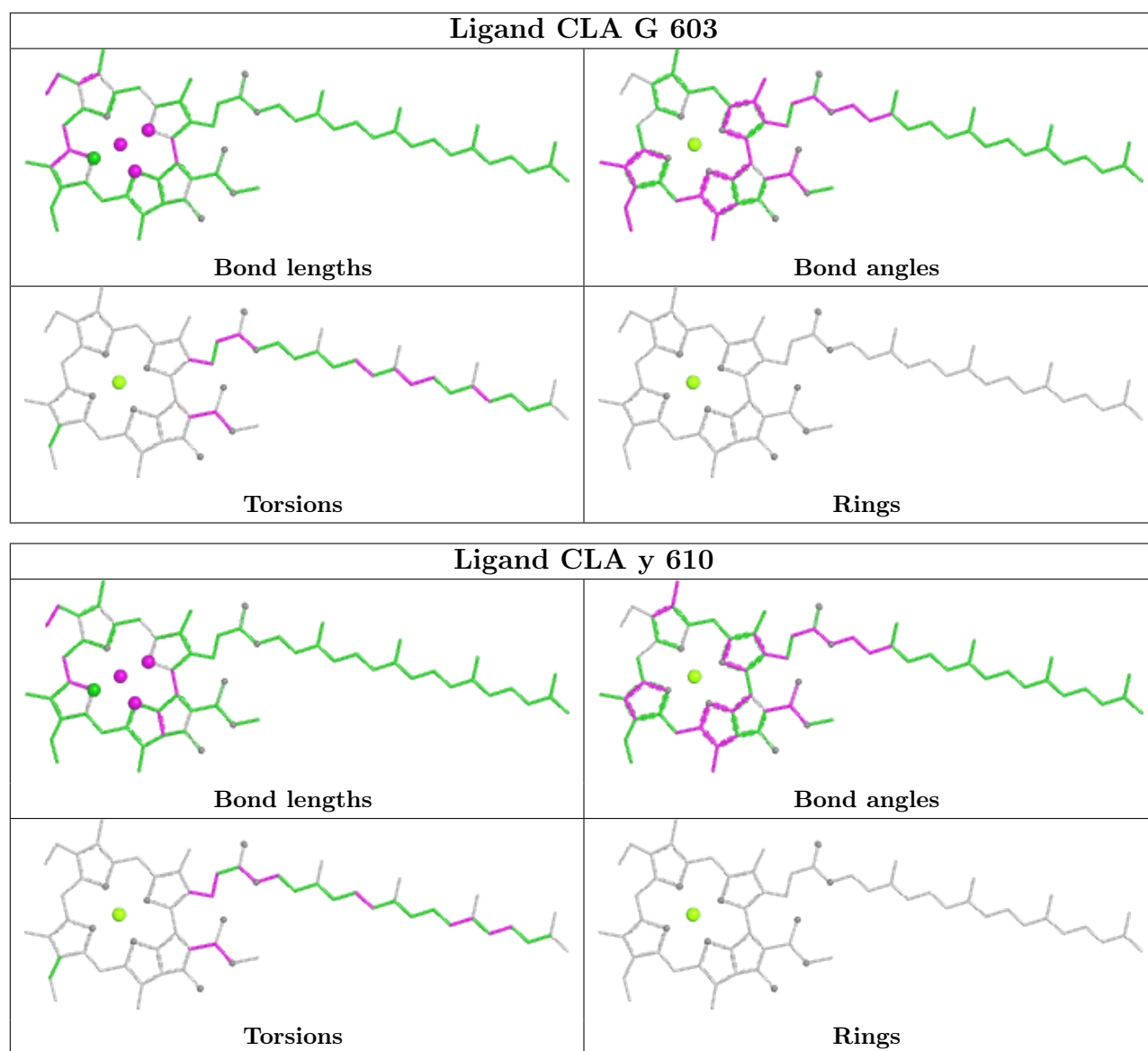


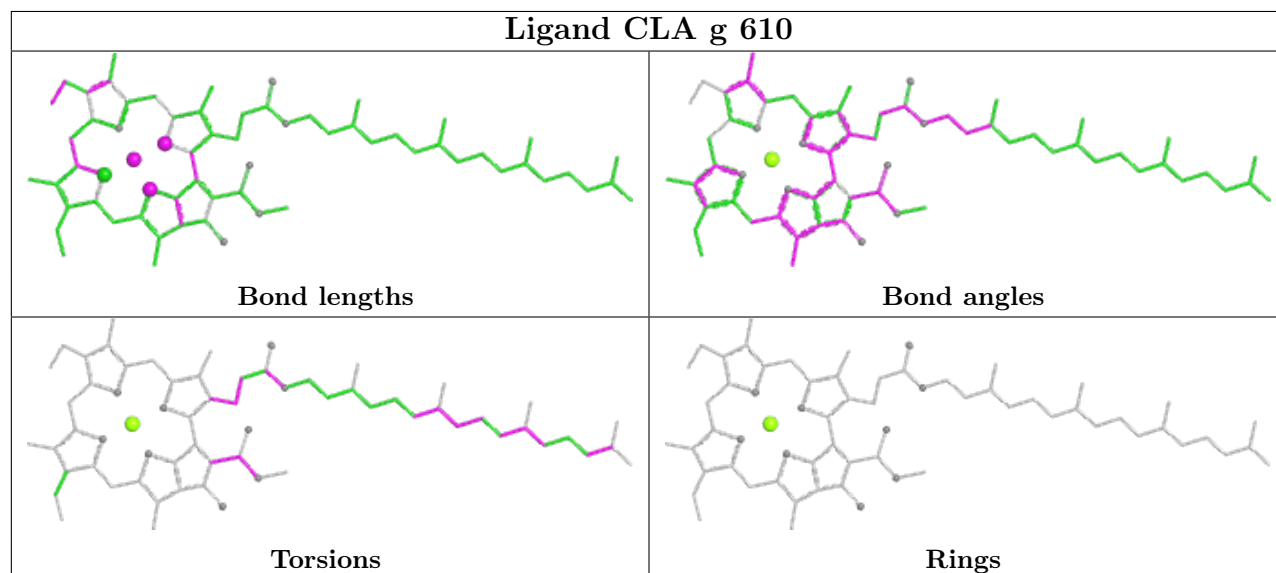
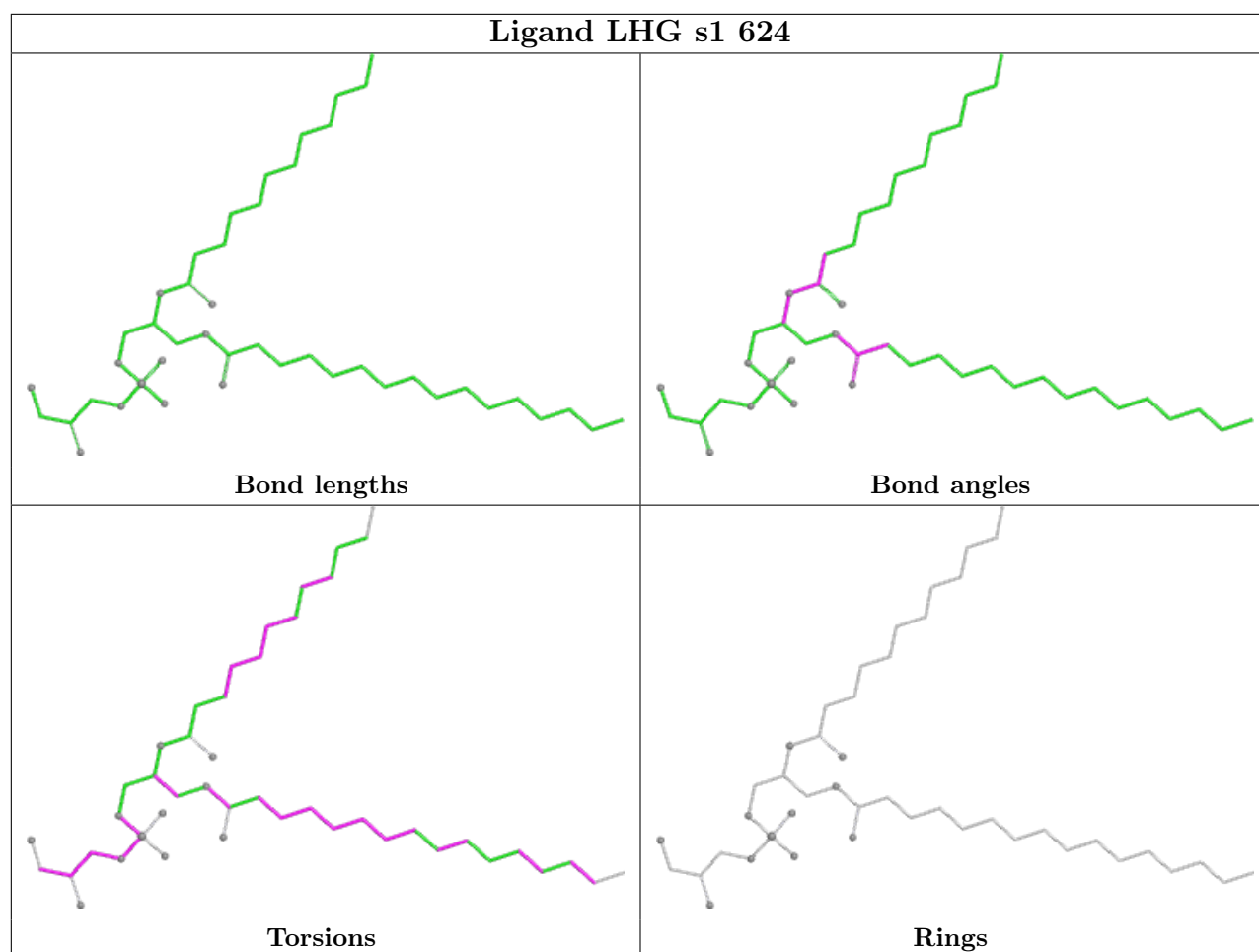
## Ligand LUT Y1 621

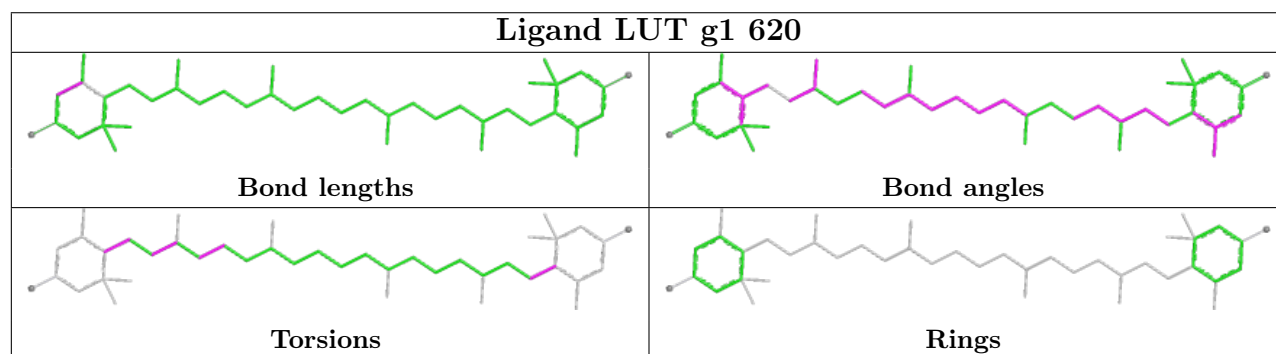
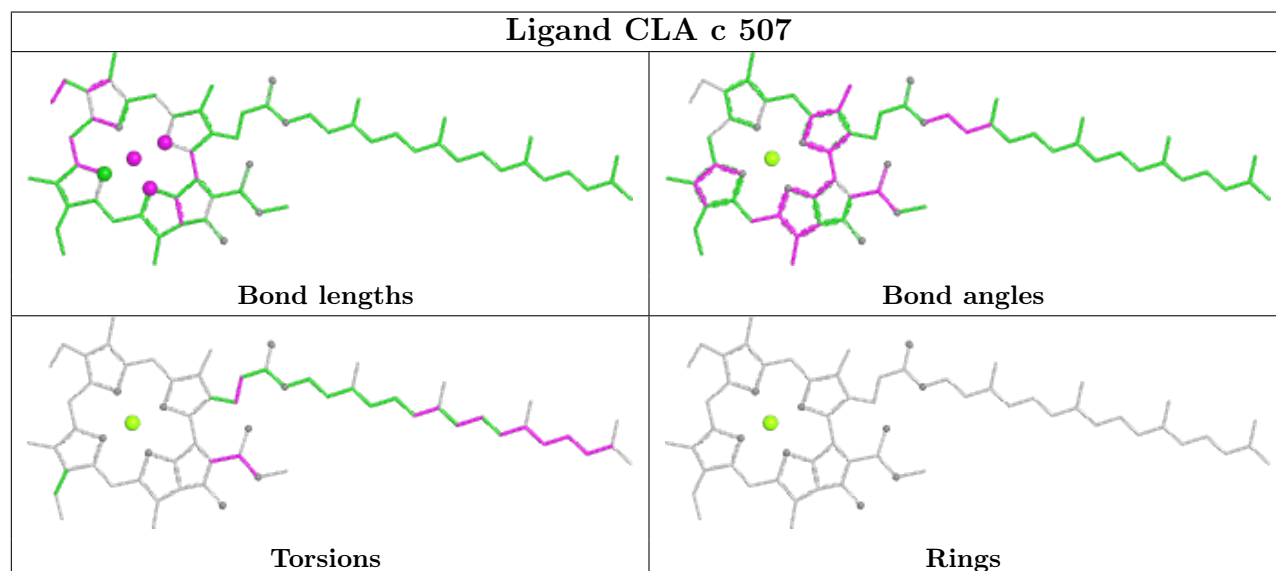
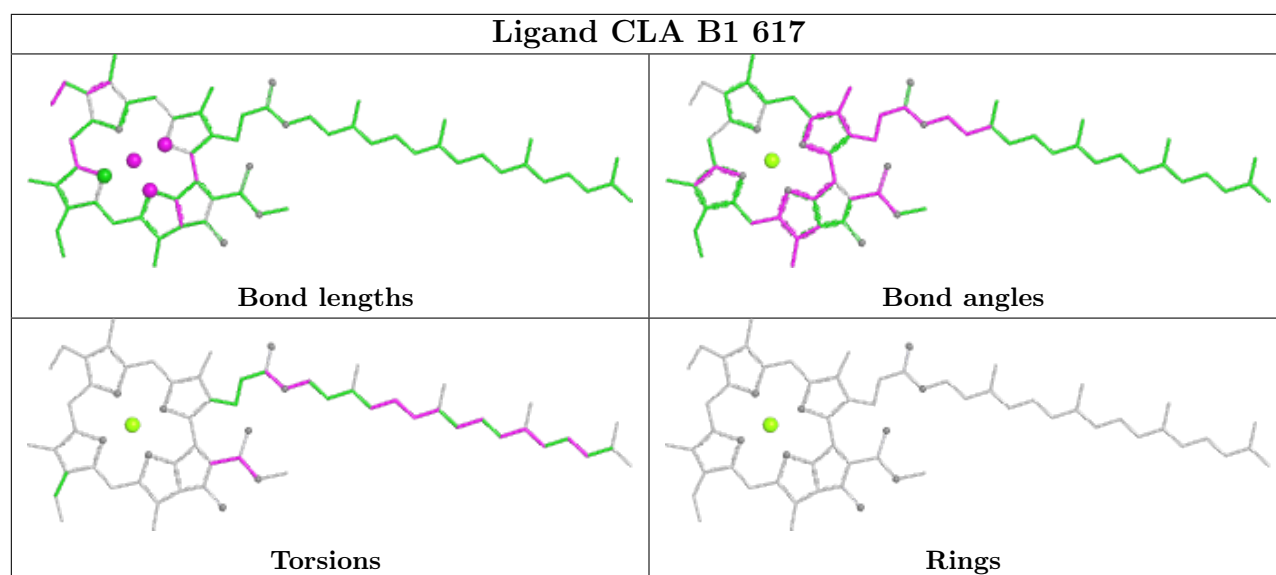


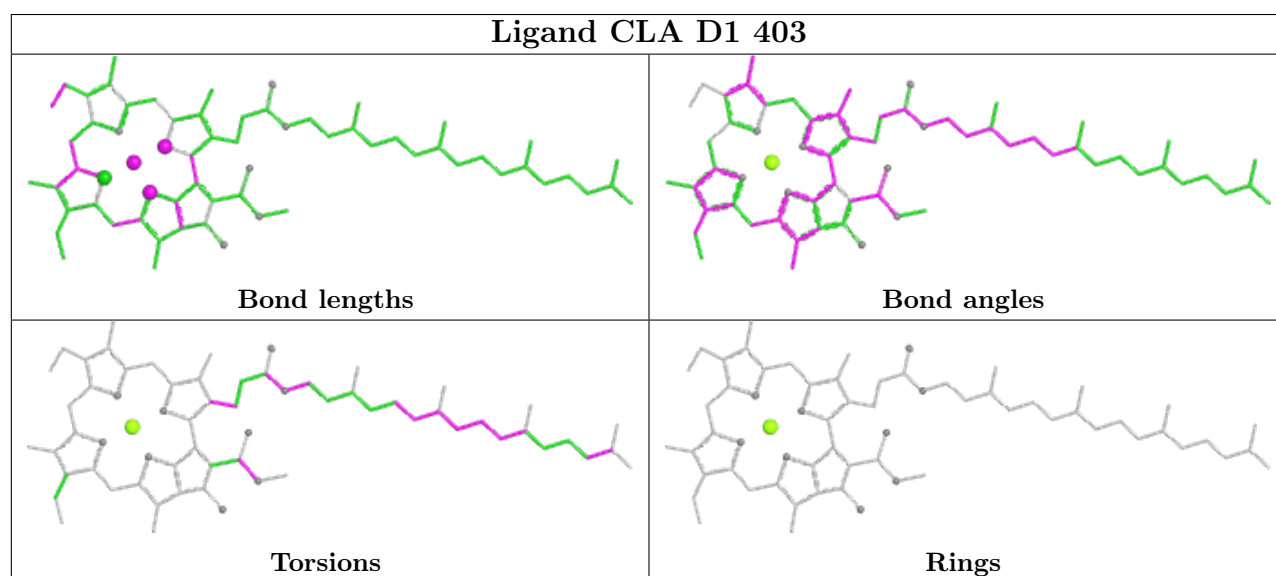
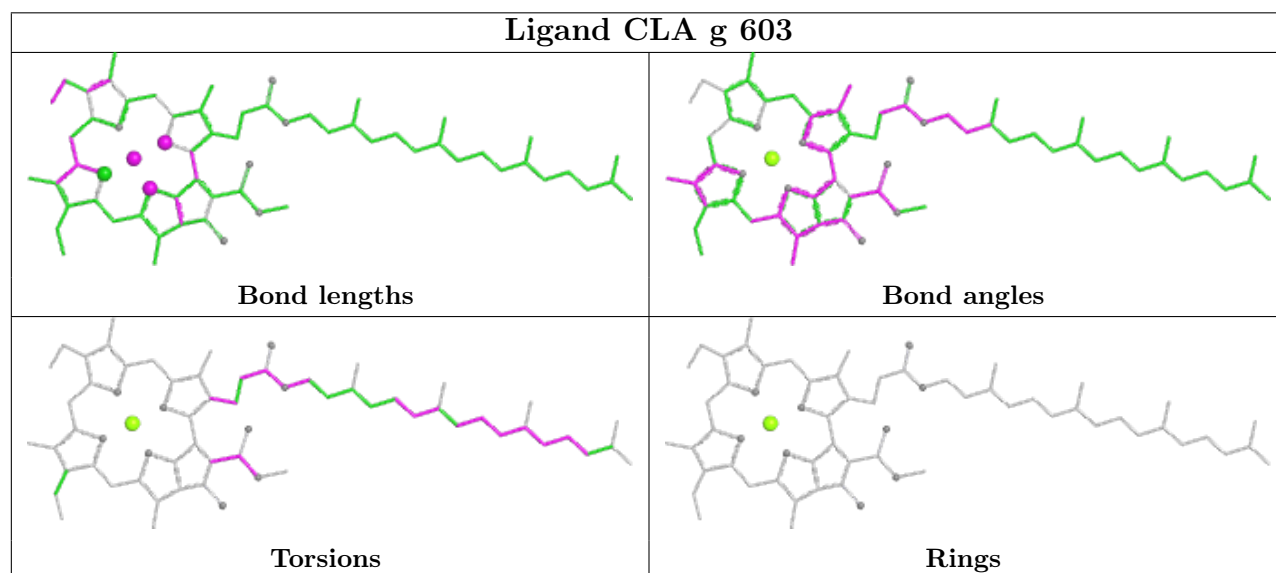
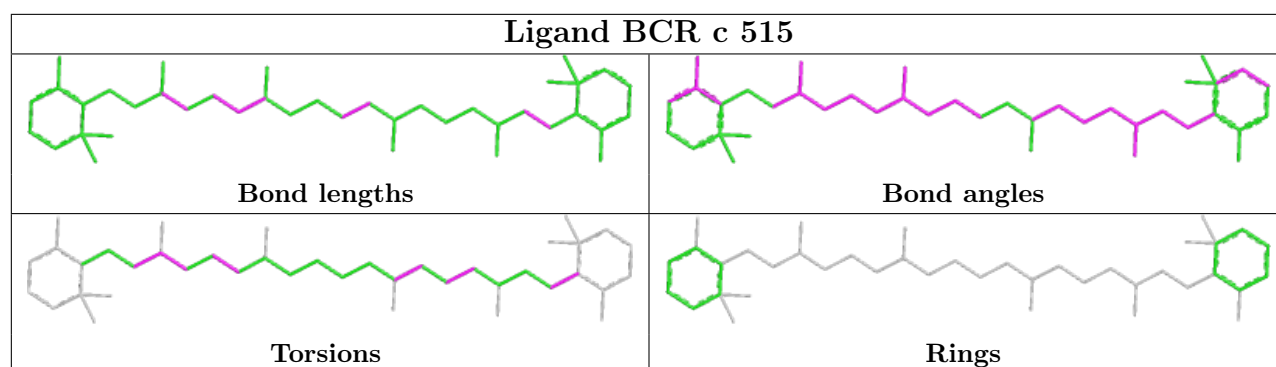


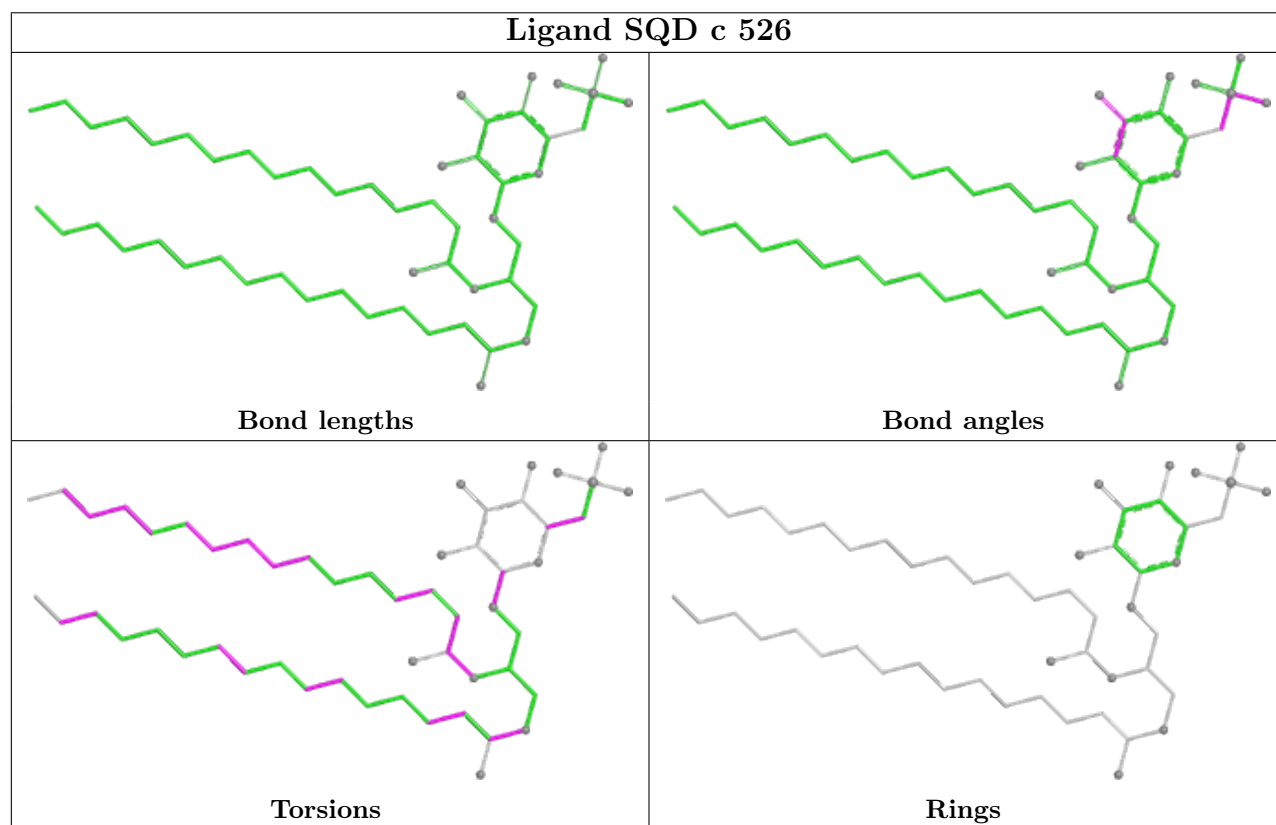
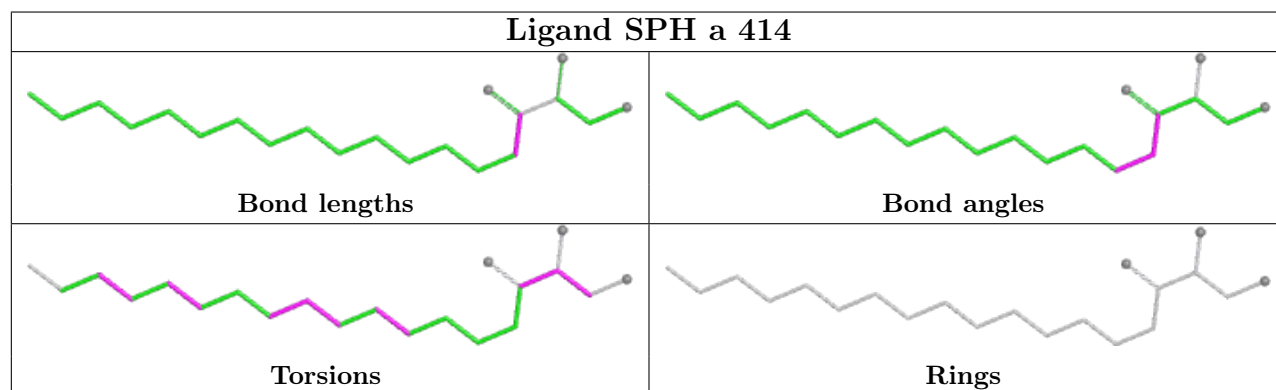
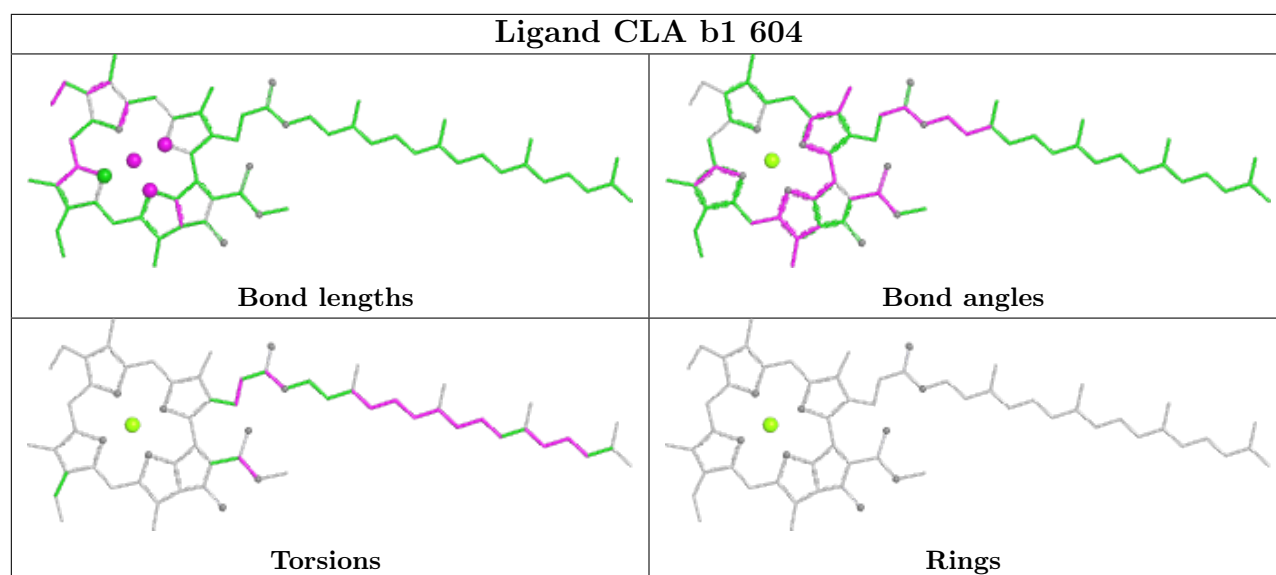


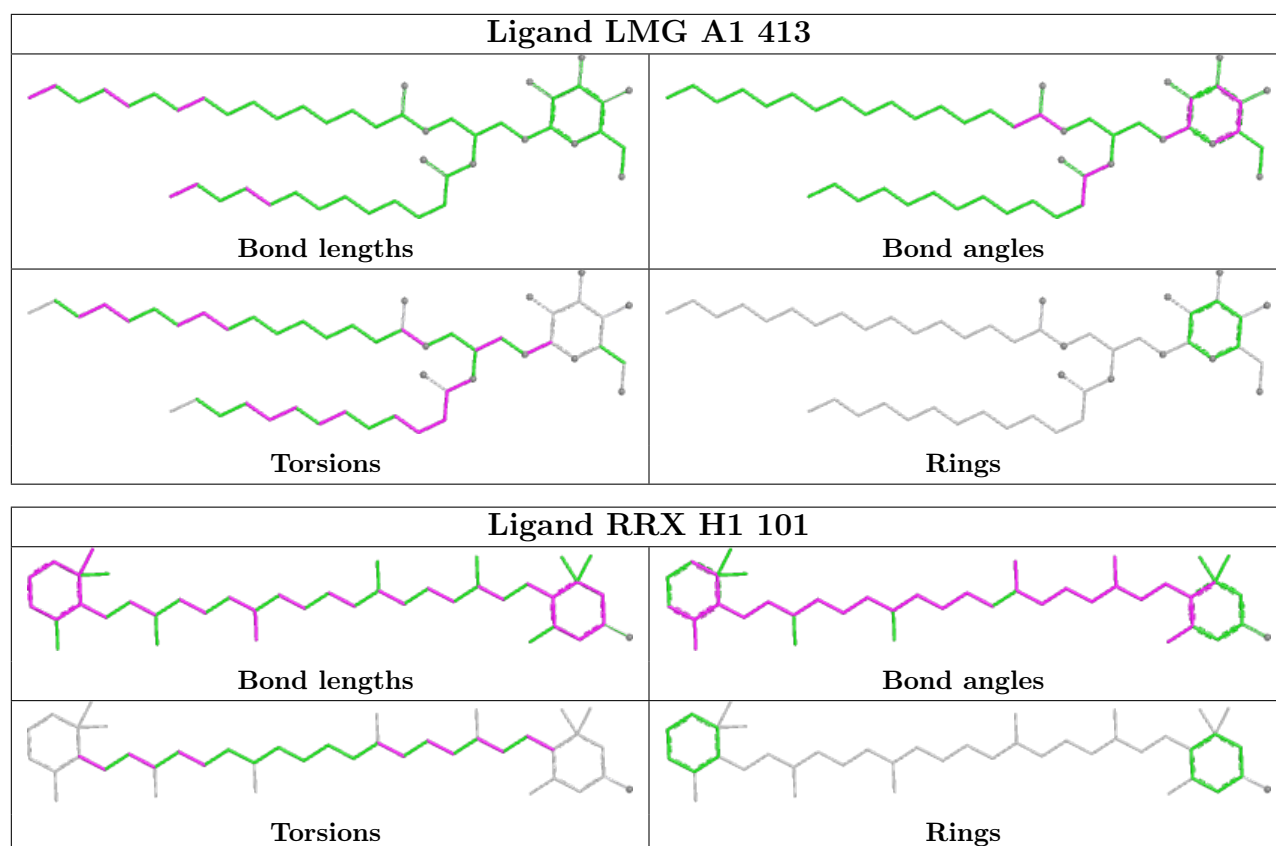




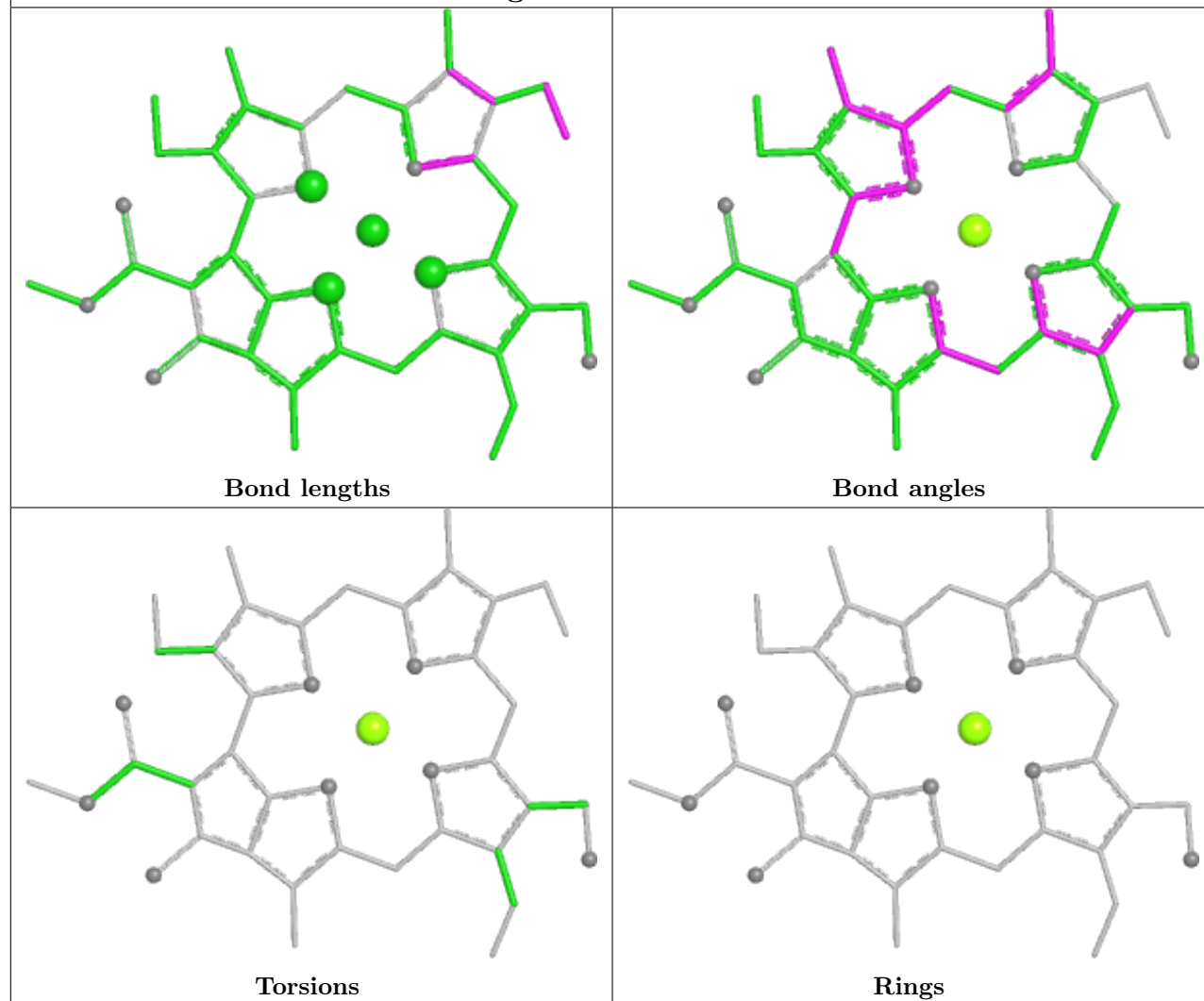




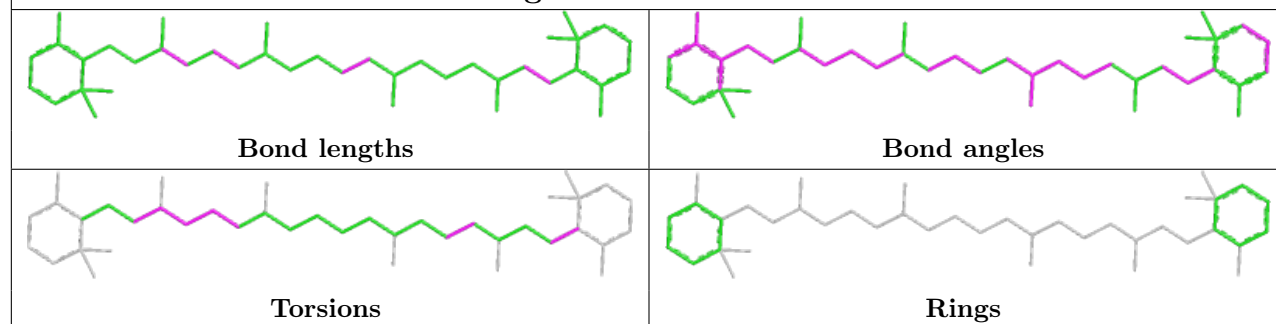


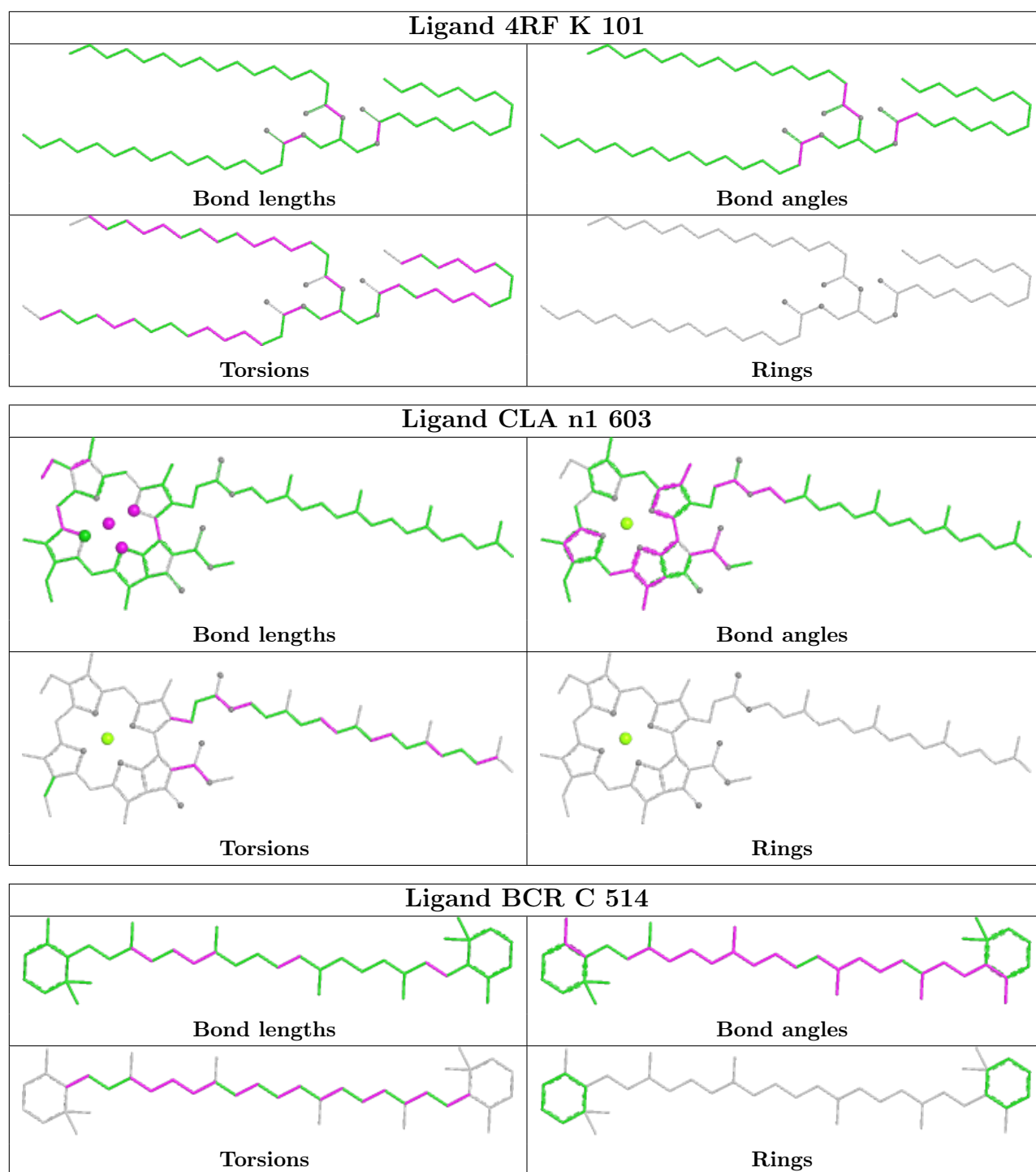


## Ligand CHL s 607

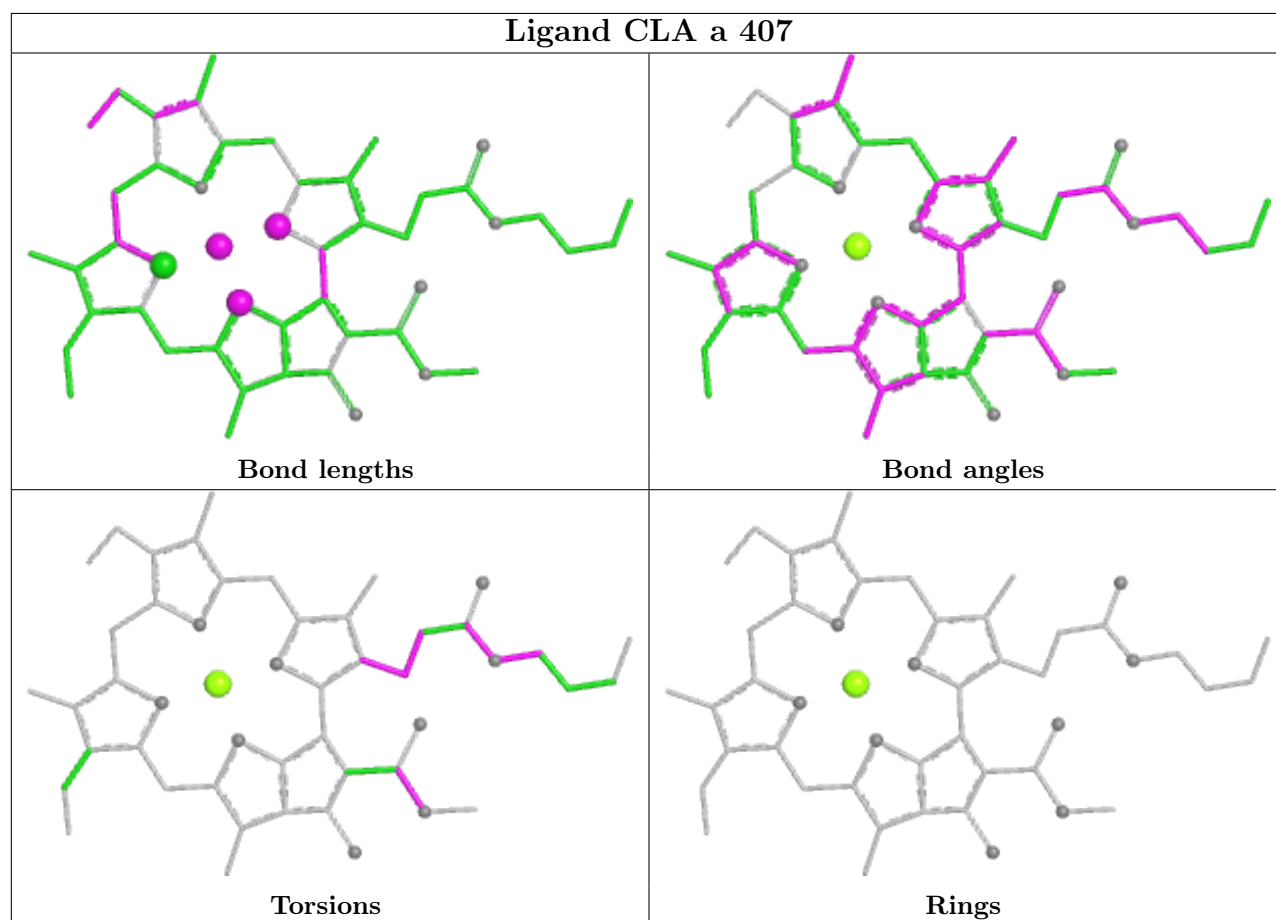
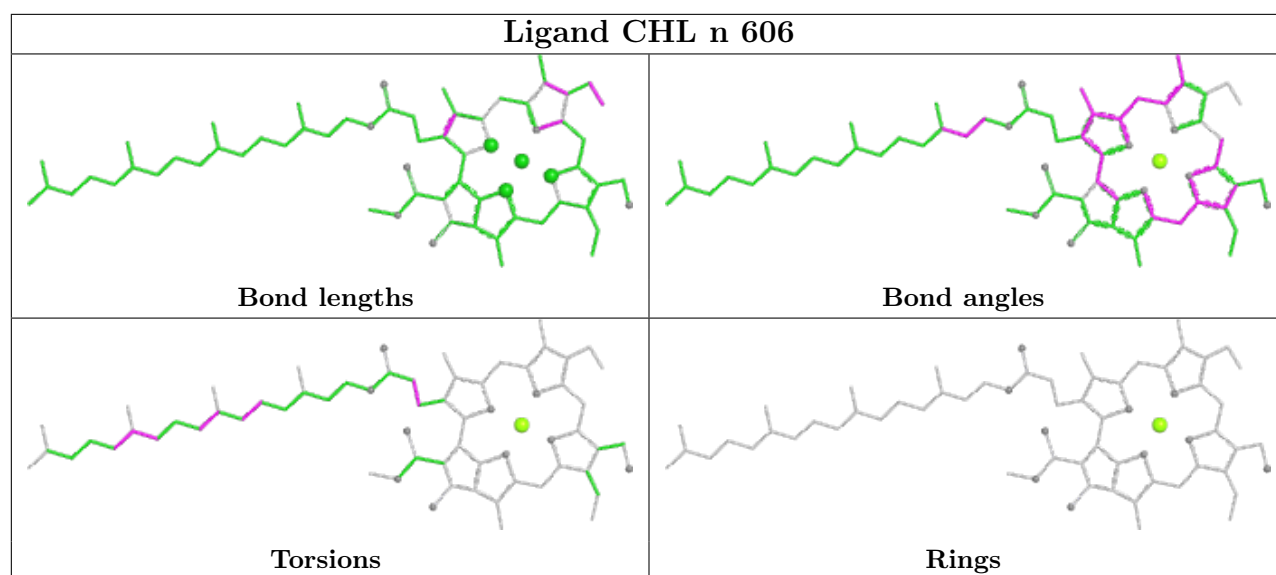


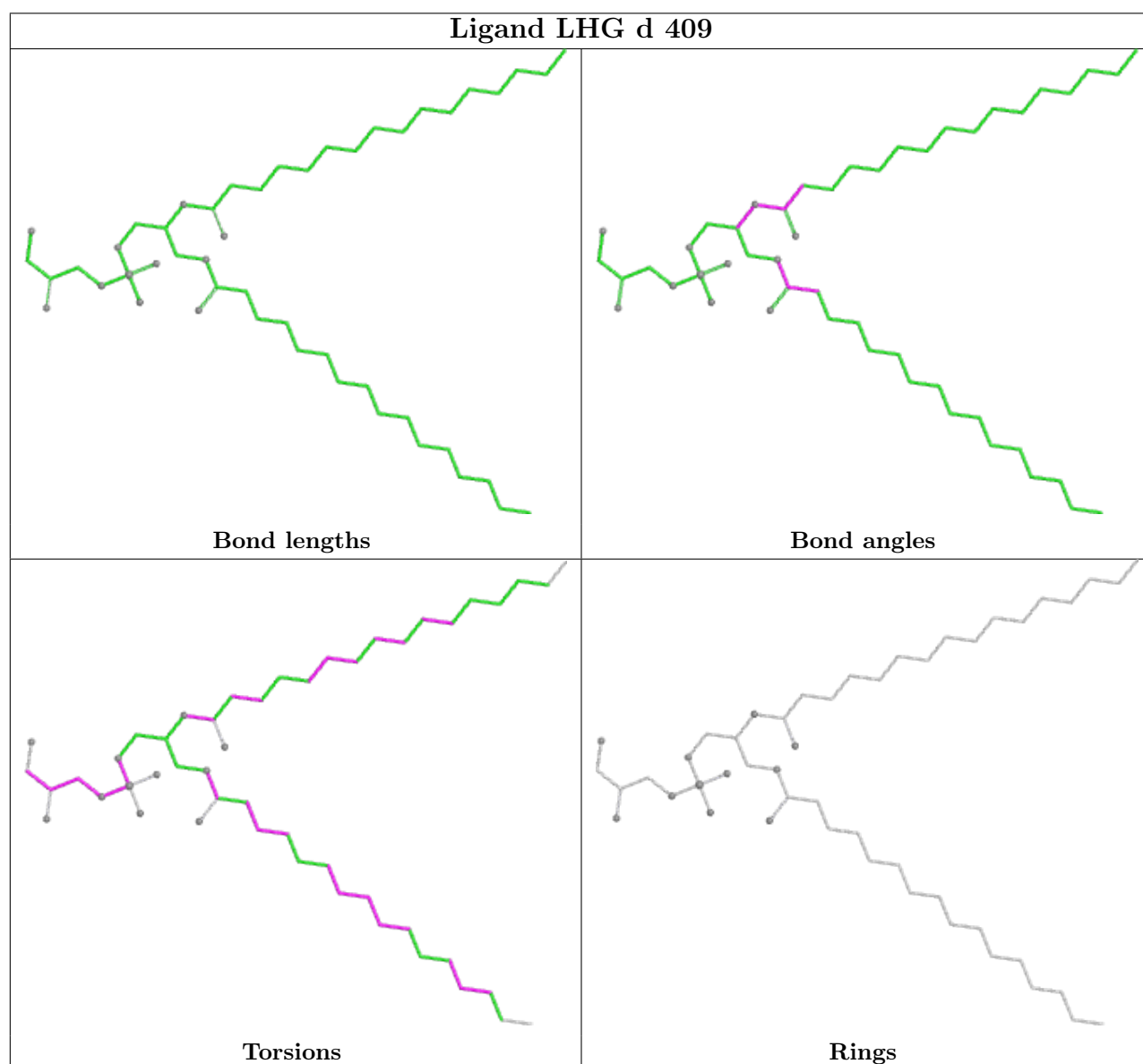
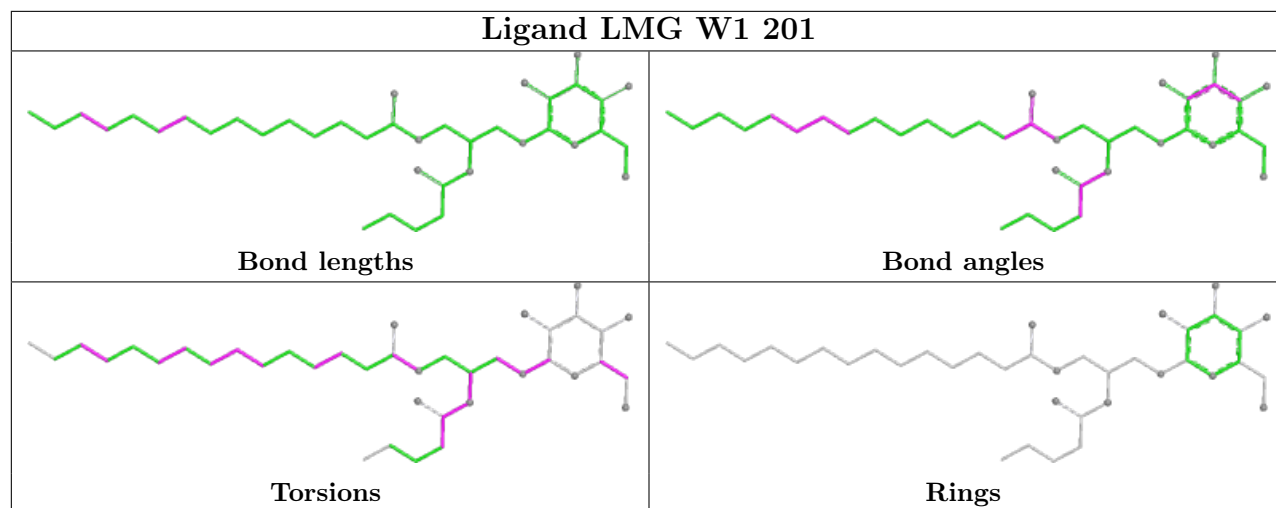
## Ligand BCR b1 619

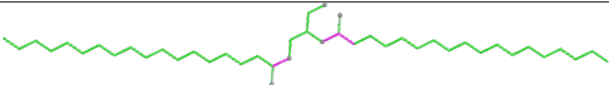
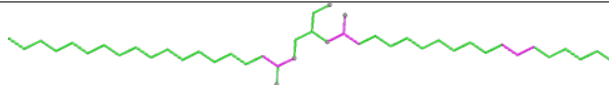
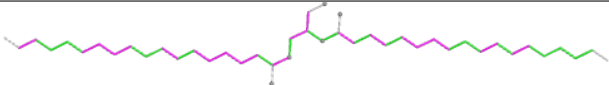
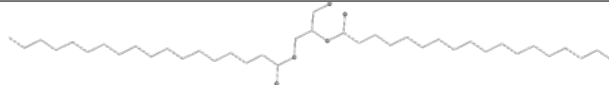


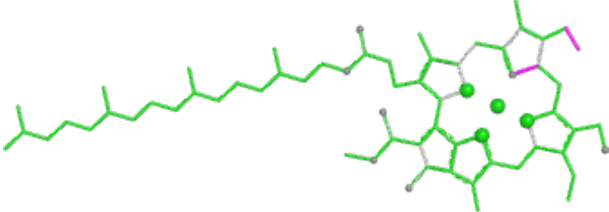
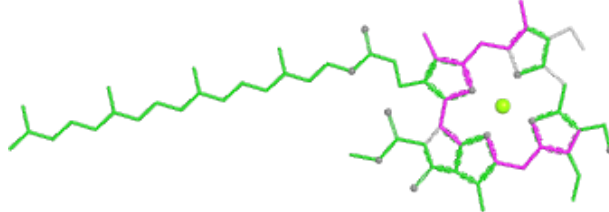
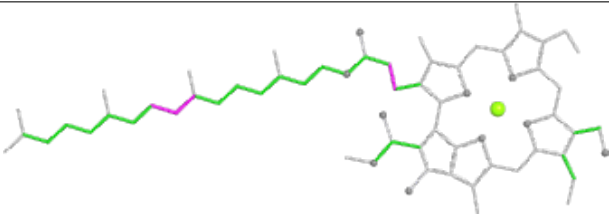
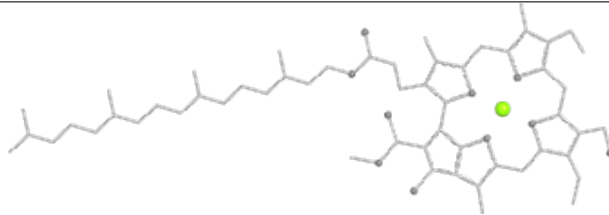


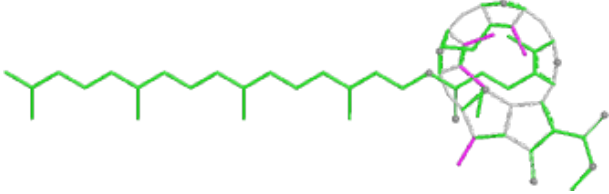
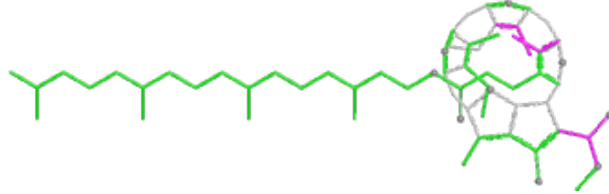
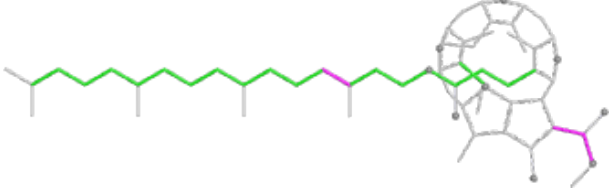
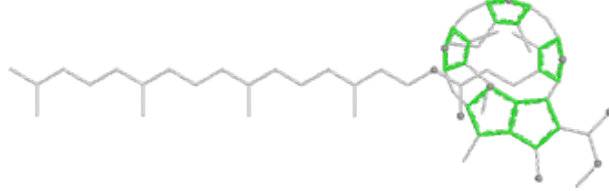




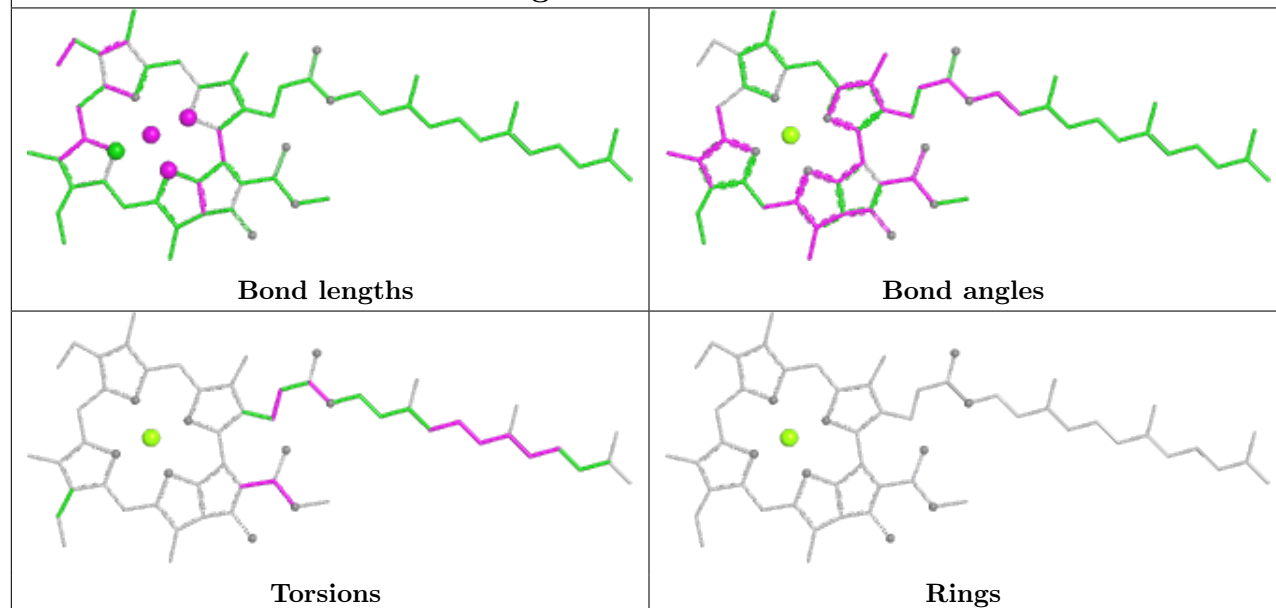


Ligand DGA C1 524	
	
Bond lengths	Bond angles
	
Torsions	Rings

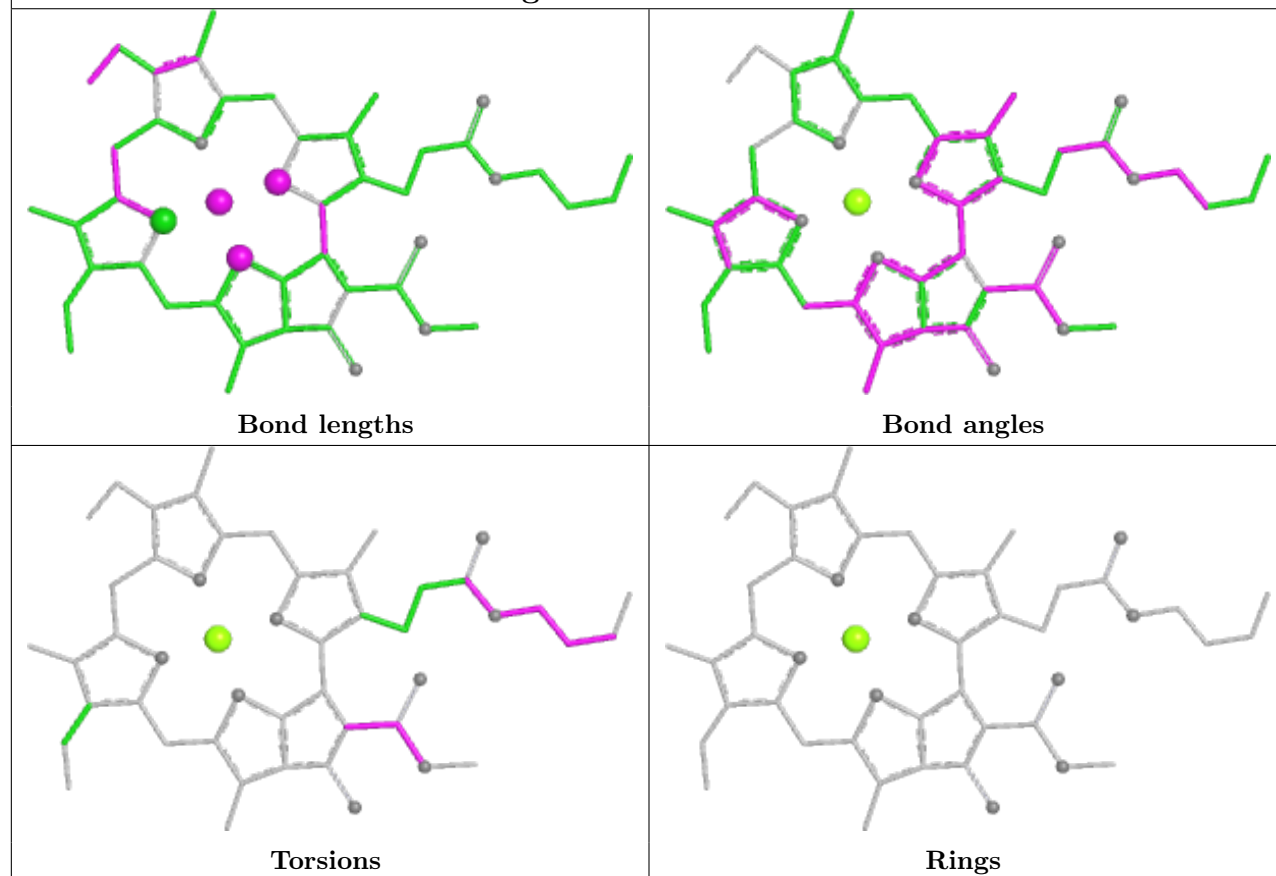
Ligand CHL y1 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

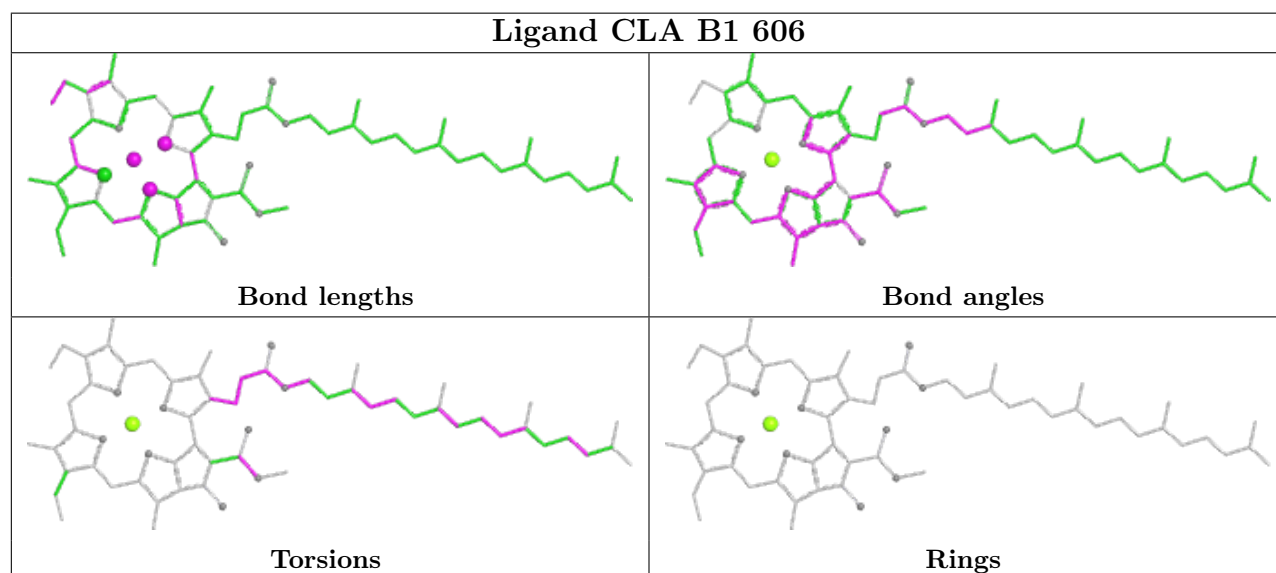
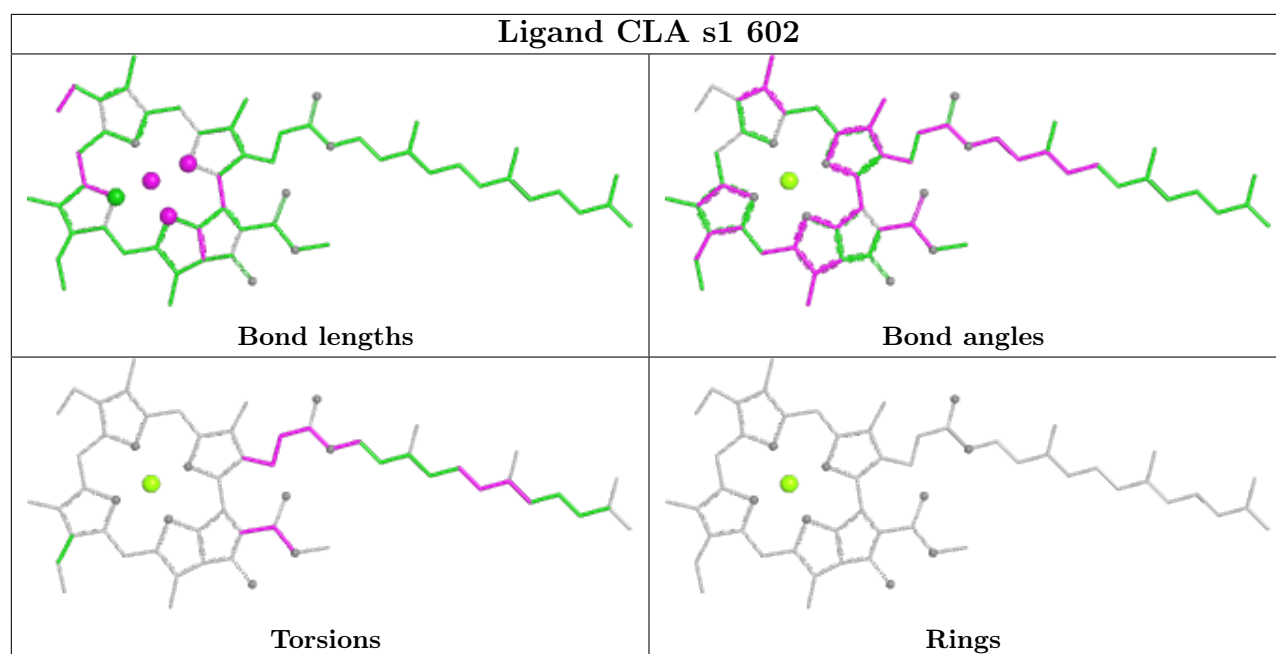
Ligand PHO A1 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

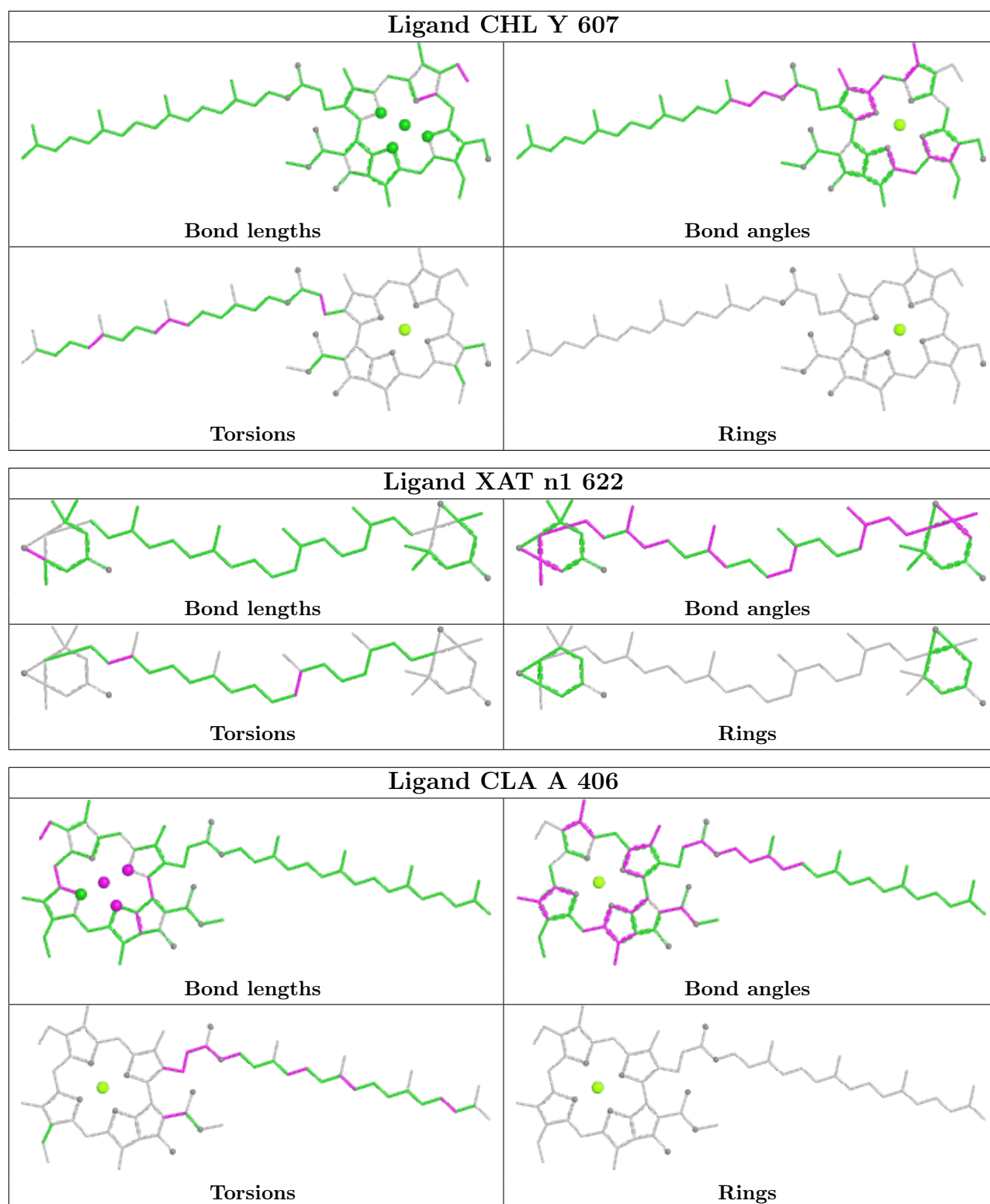
## Ligand CLA R 610

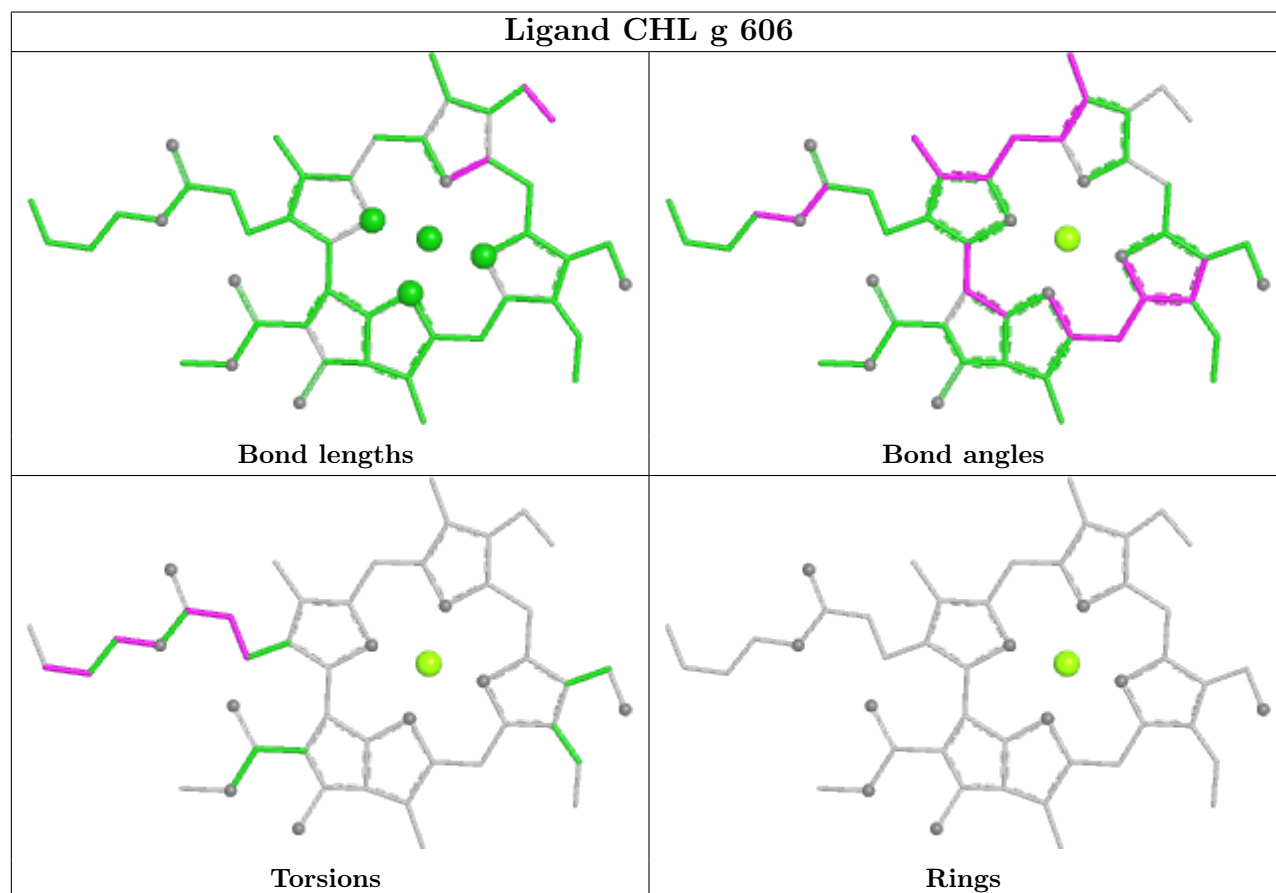
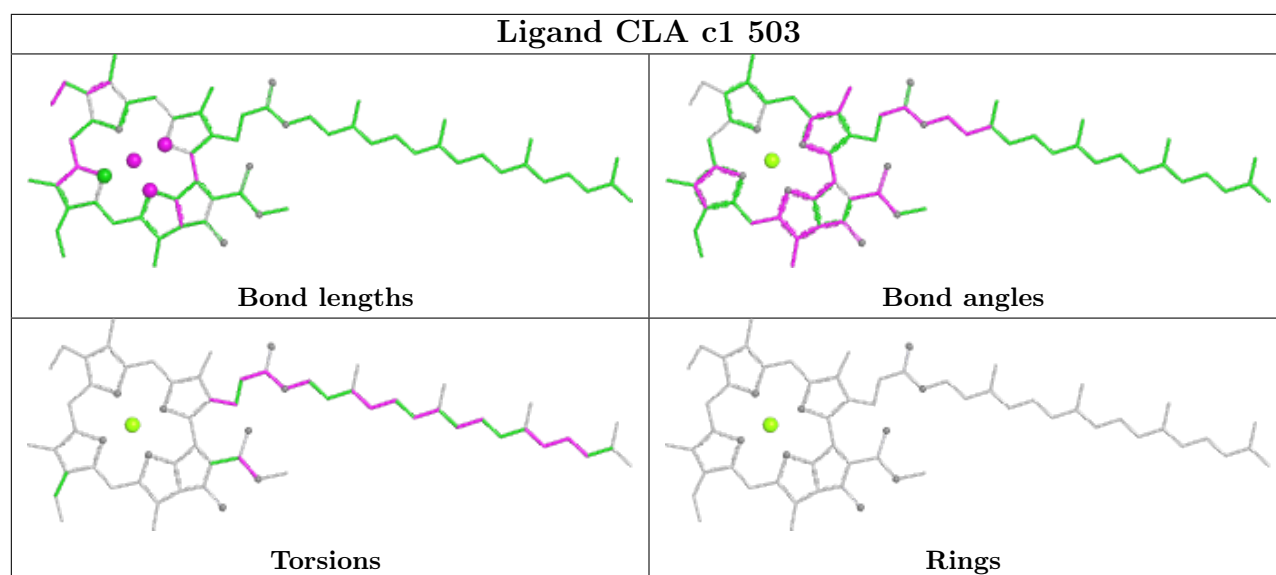


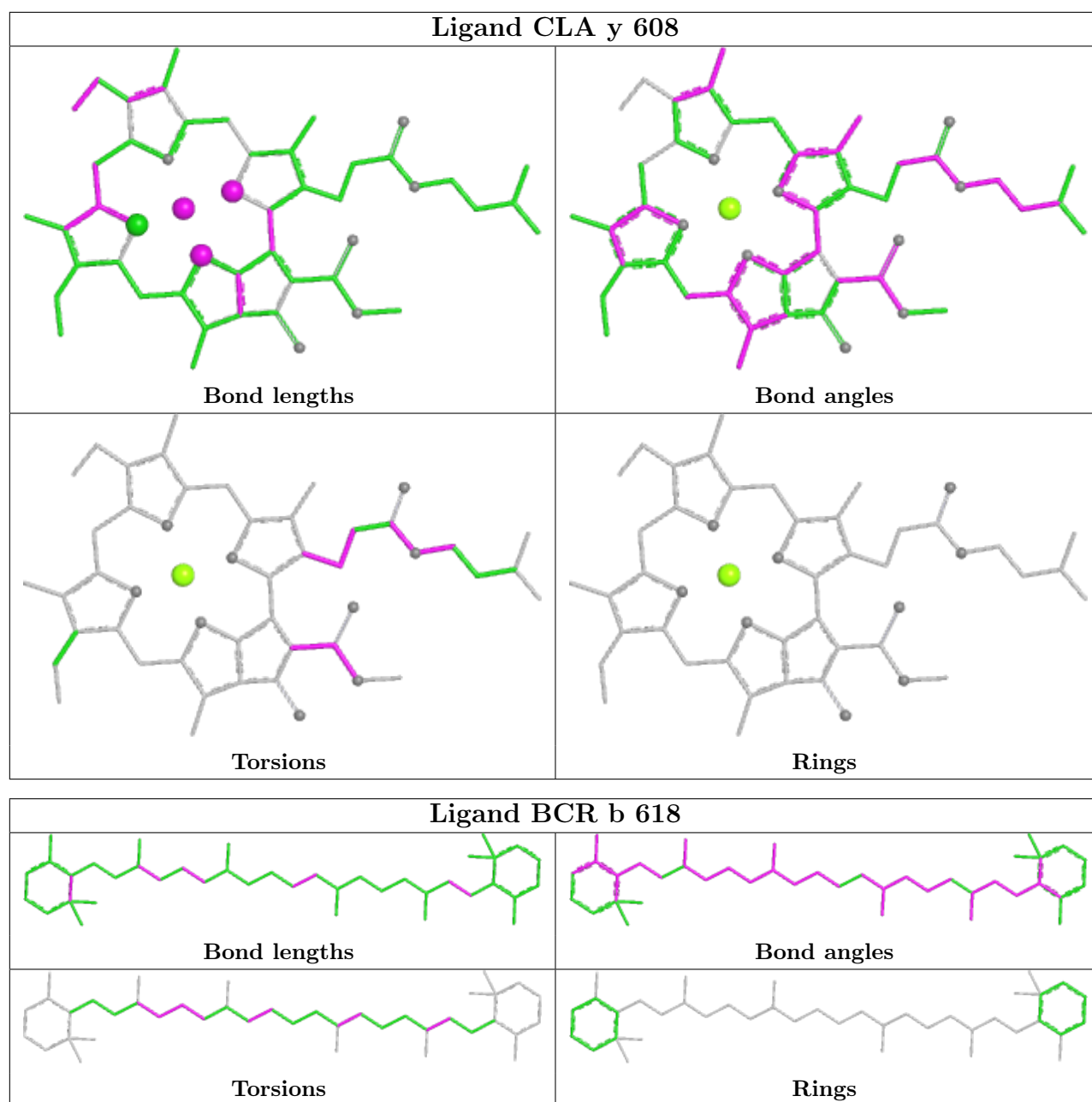
## Ligand CLA G1 604



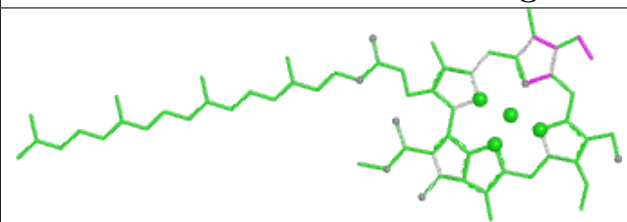
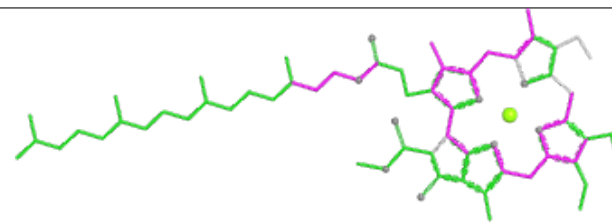
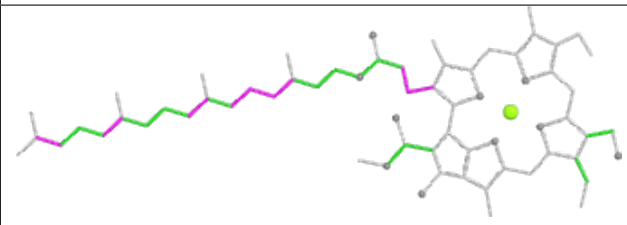
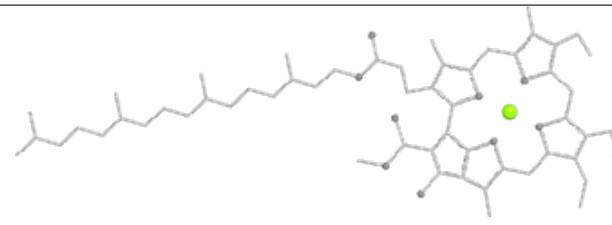


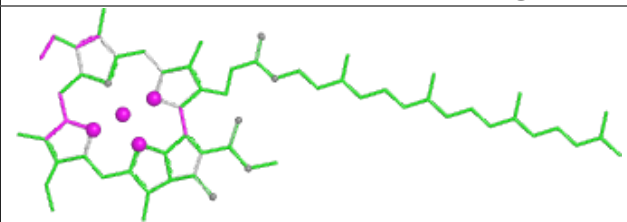
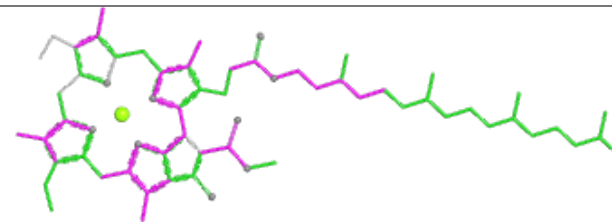
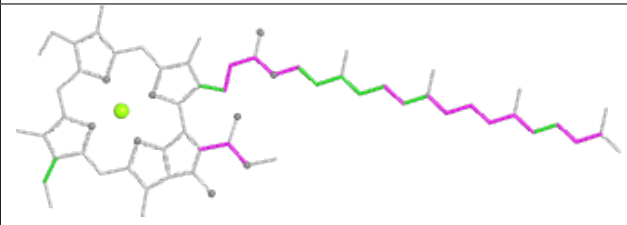
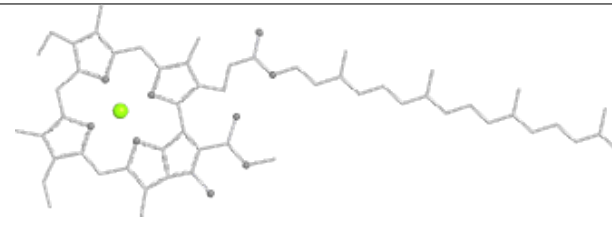


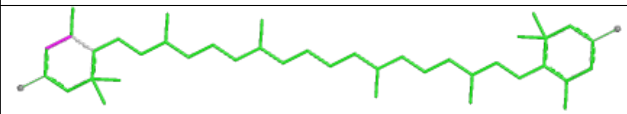
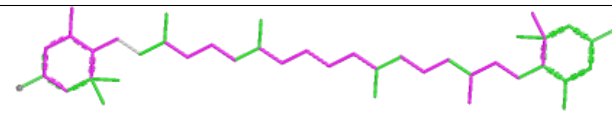
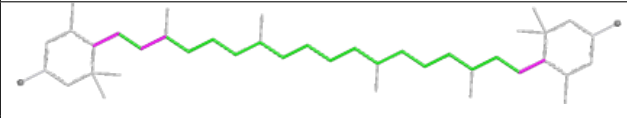
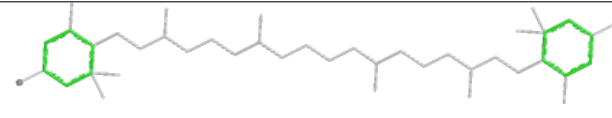


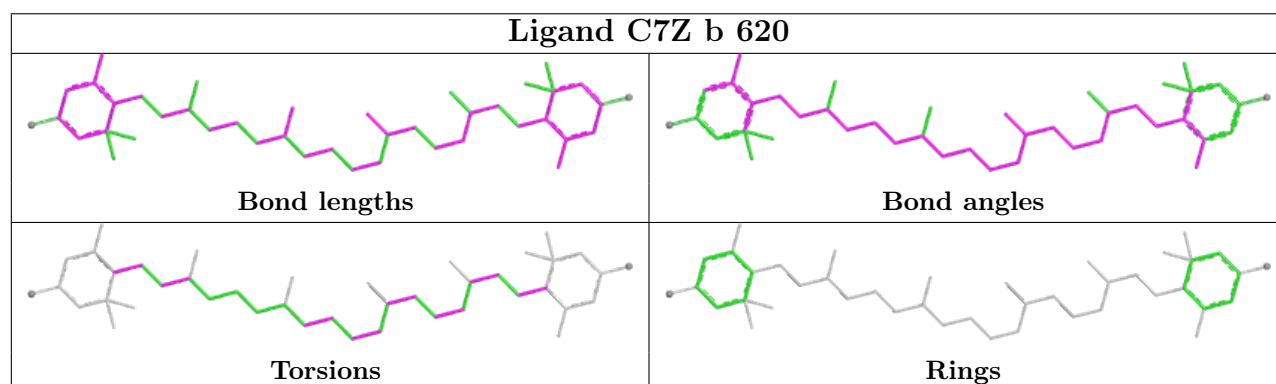
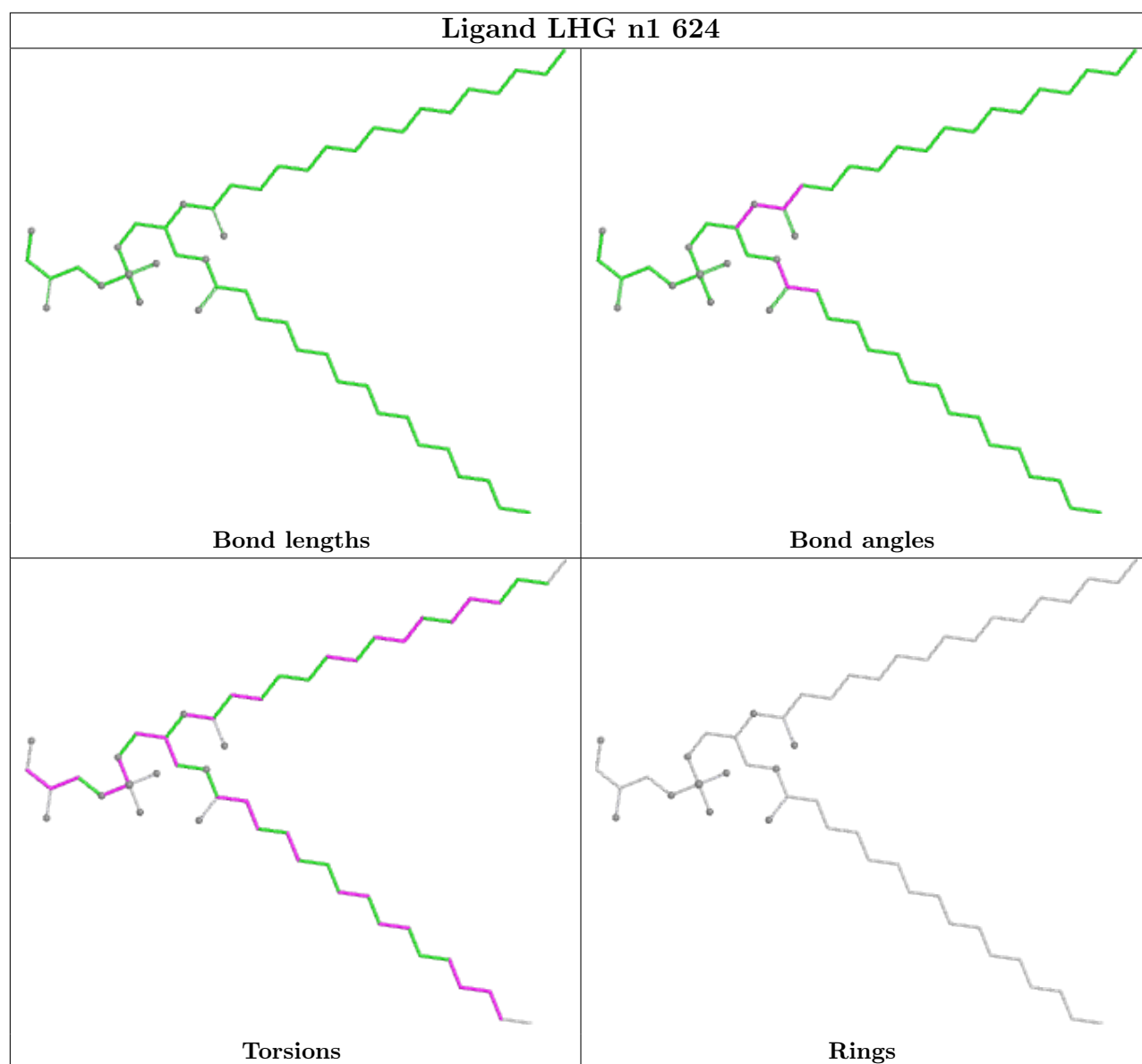


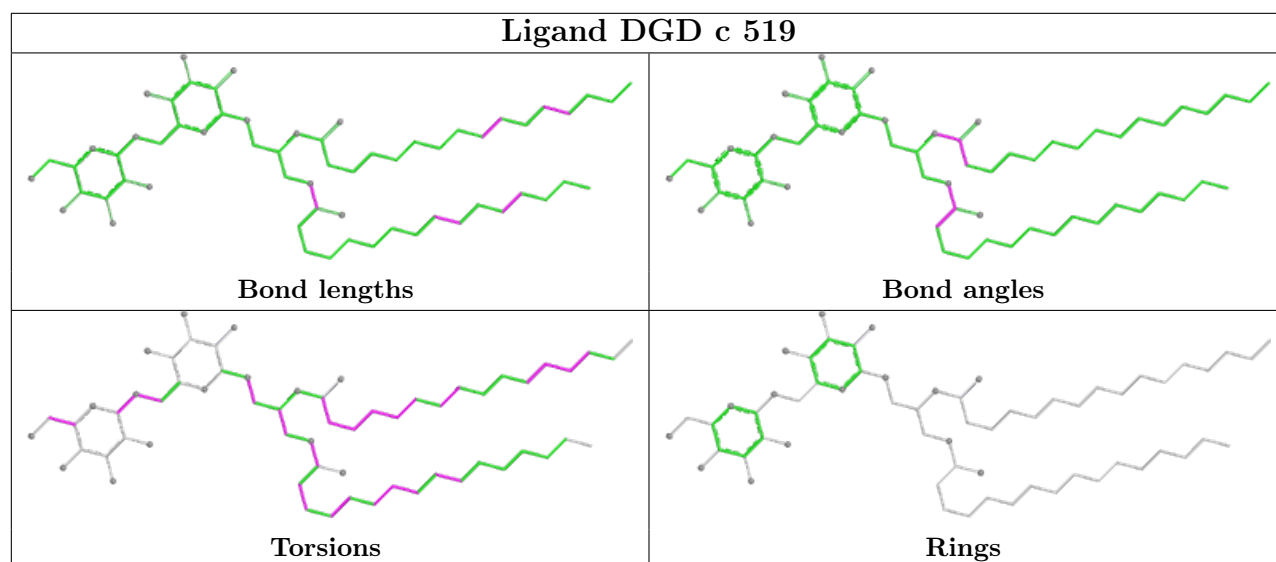
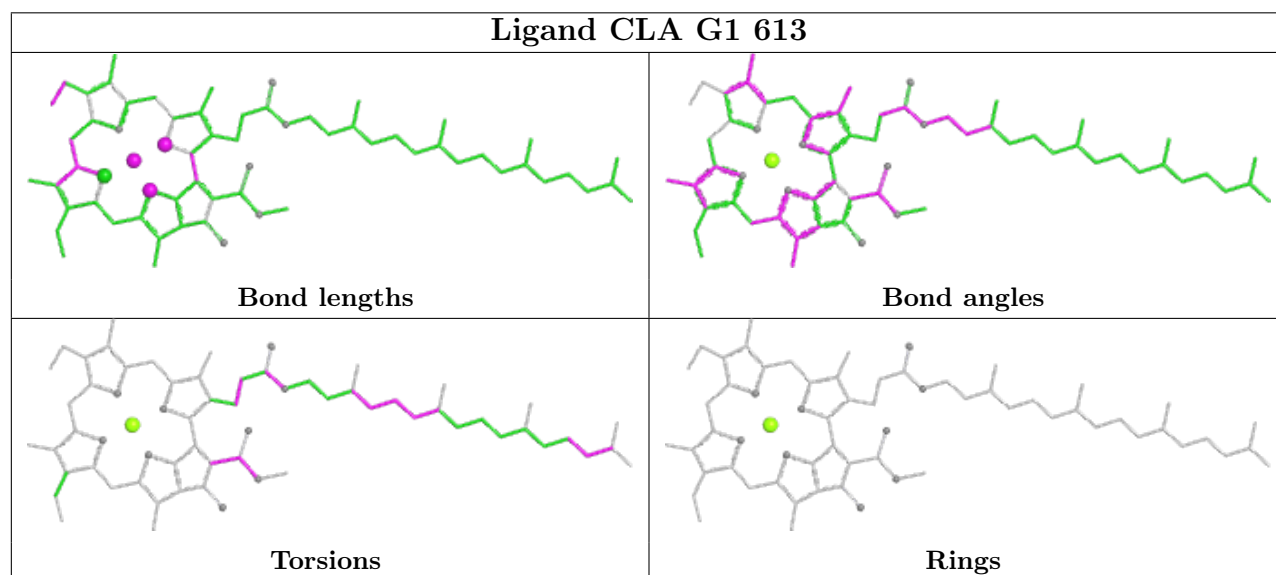
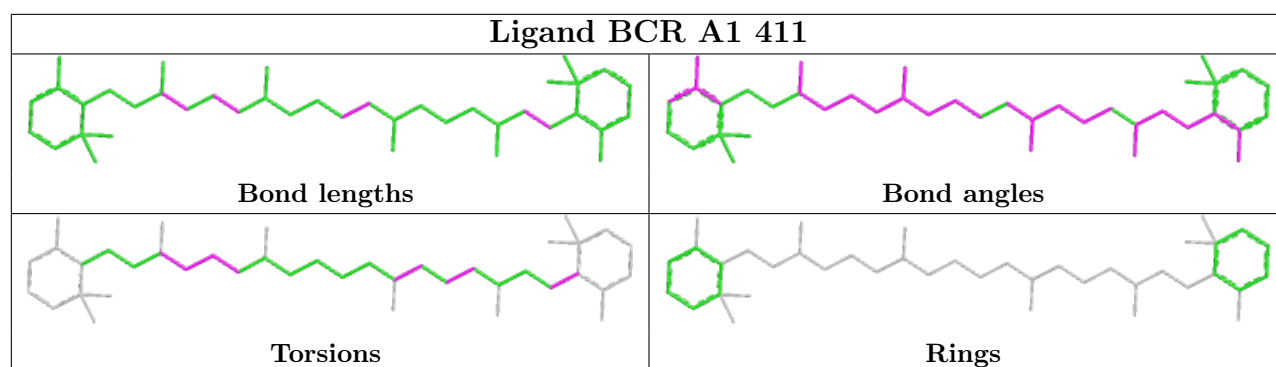


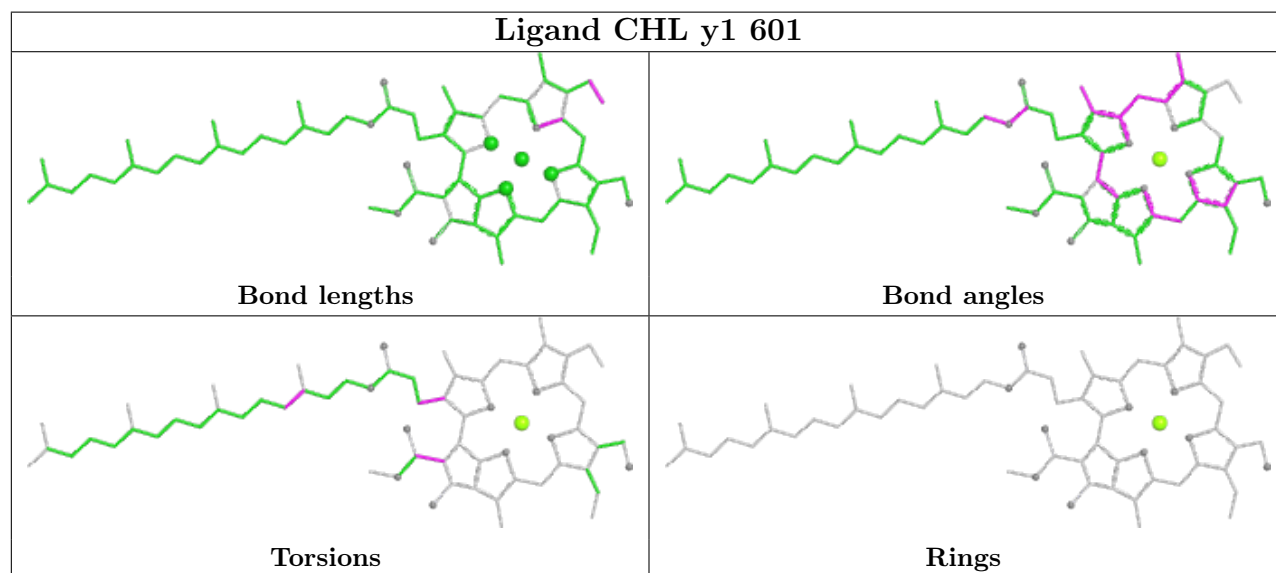
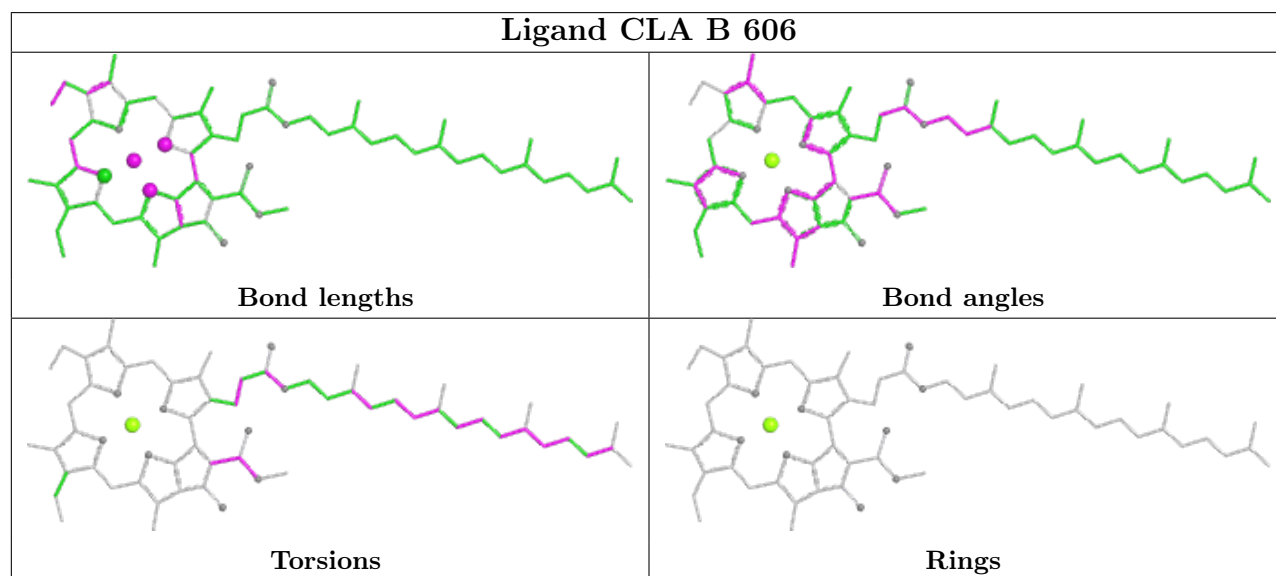
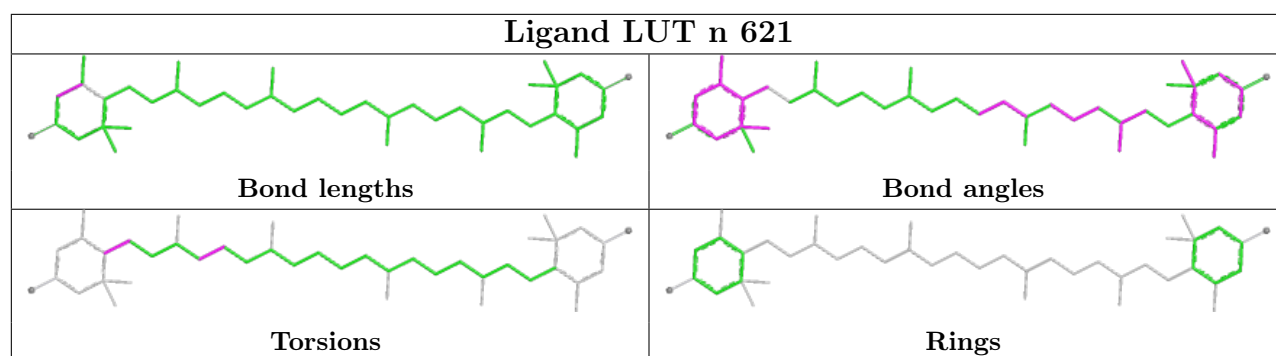
Ligand CHL N 606	
	
Bond lengths	Bond angles
	
Torsions	Rings

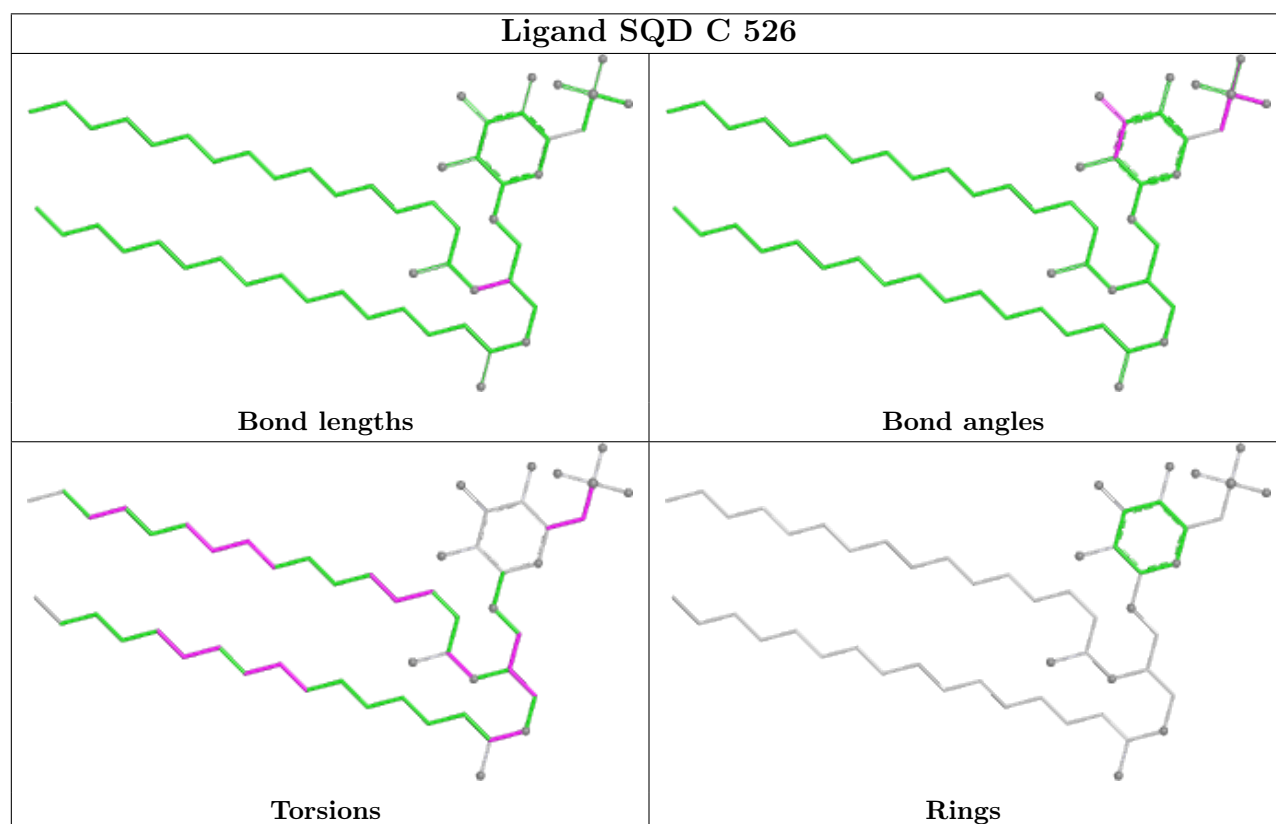
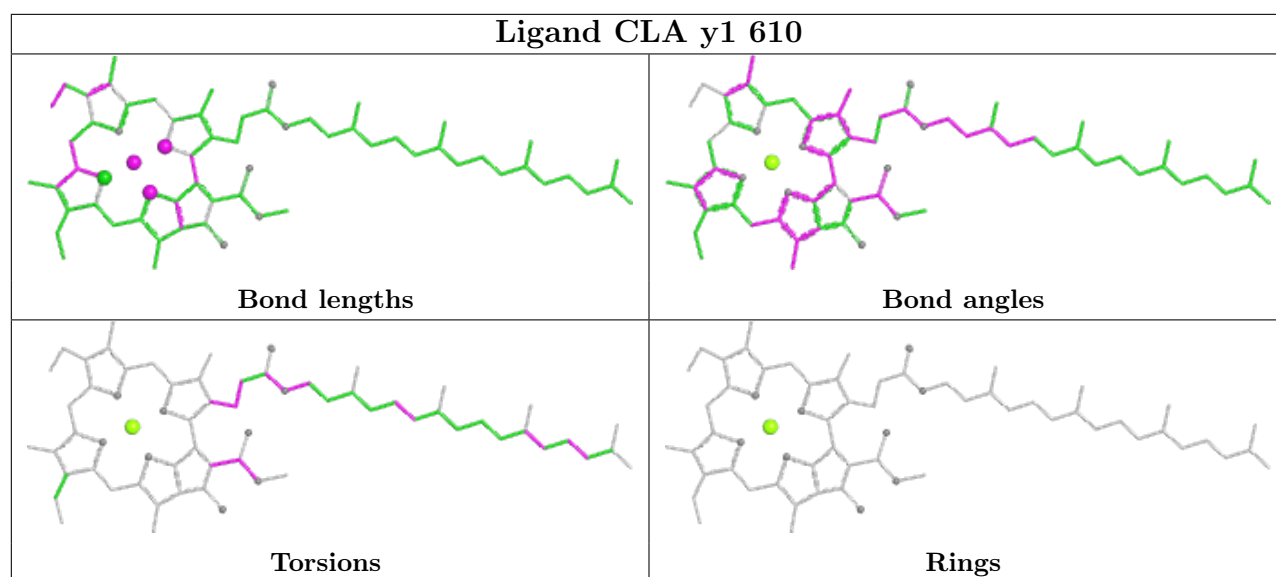
Ligand CLA B1 603	
	
Bond lengths	Bond angles
	
Torsions	Rings

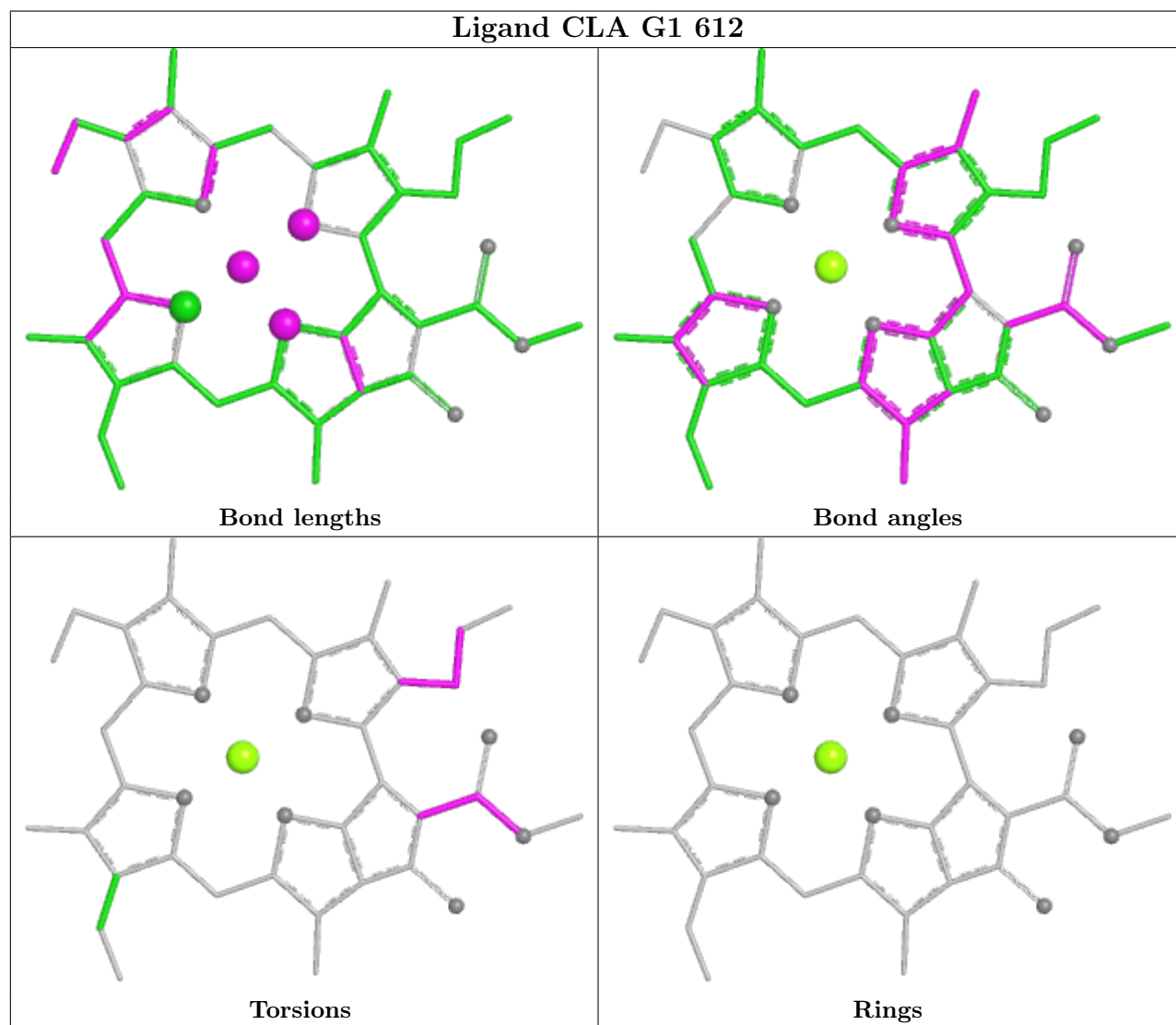
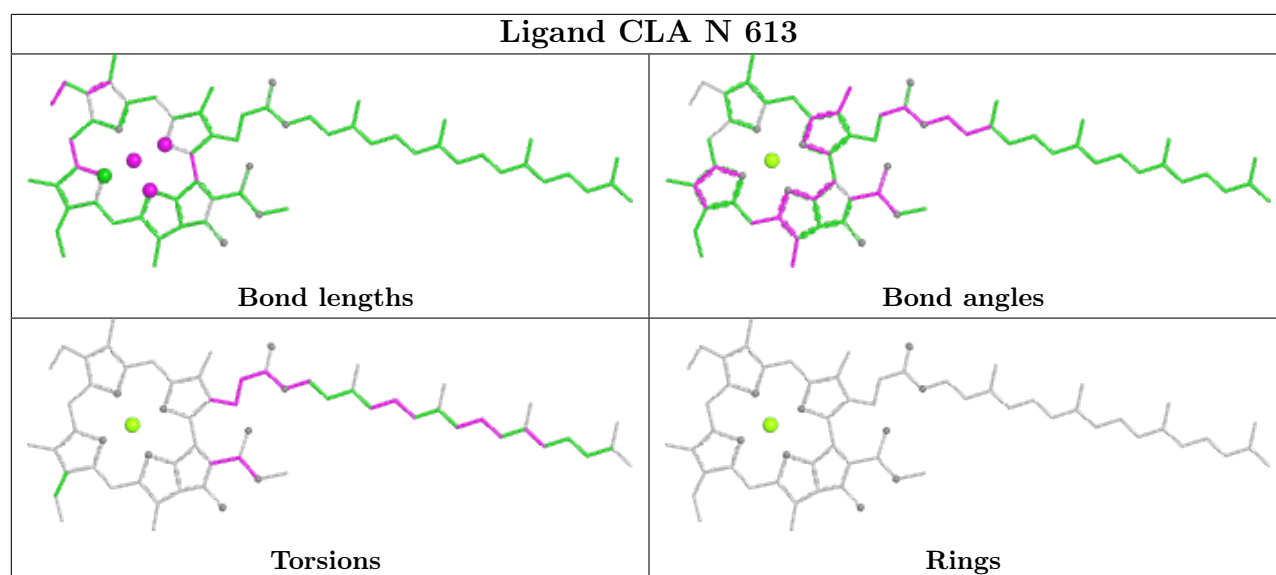
Ligand LUT Y 620	
	
Bond lengths	Bond angles
	
Torsions	Rings

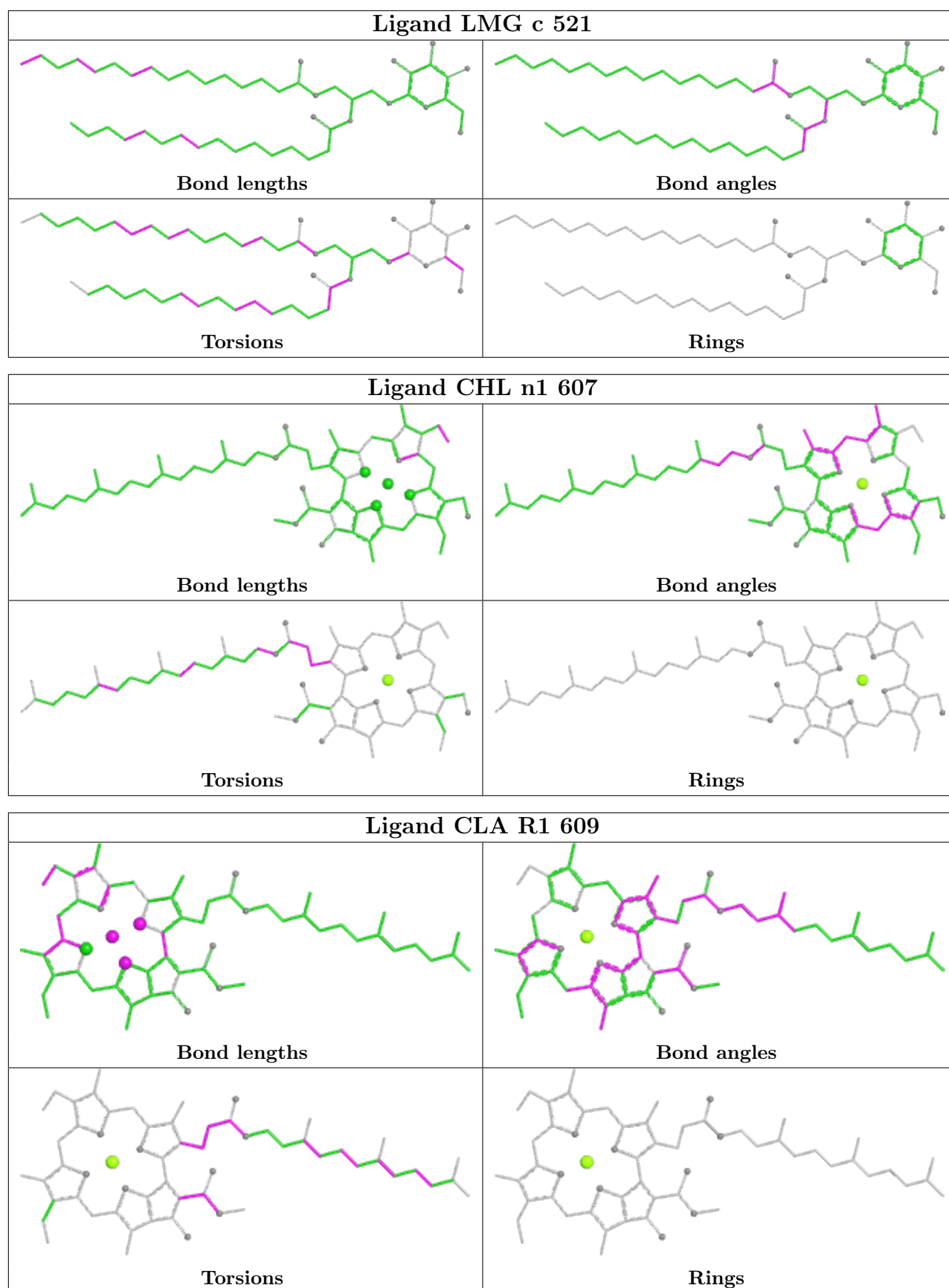


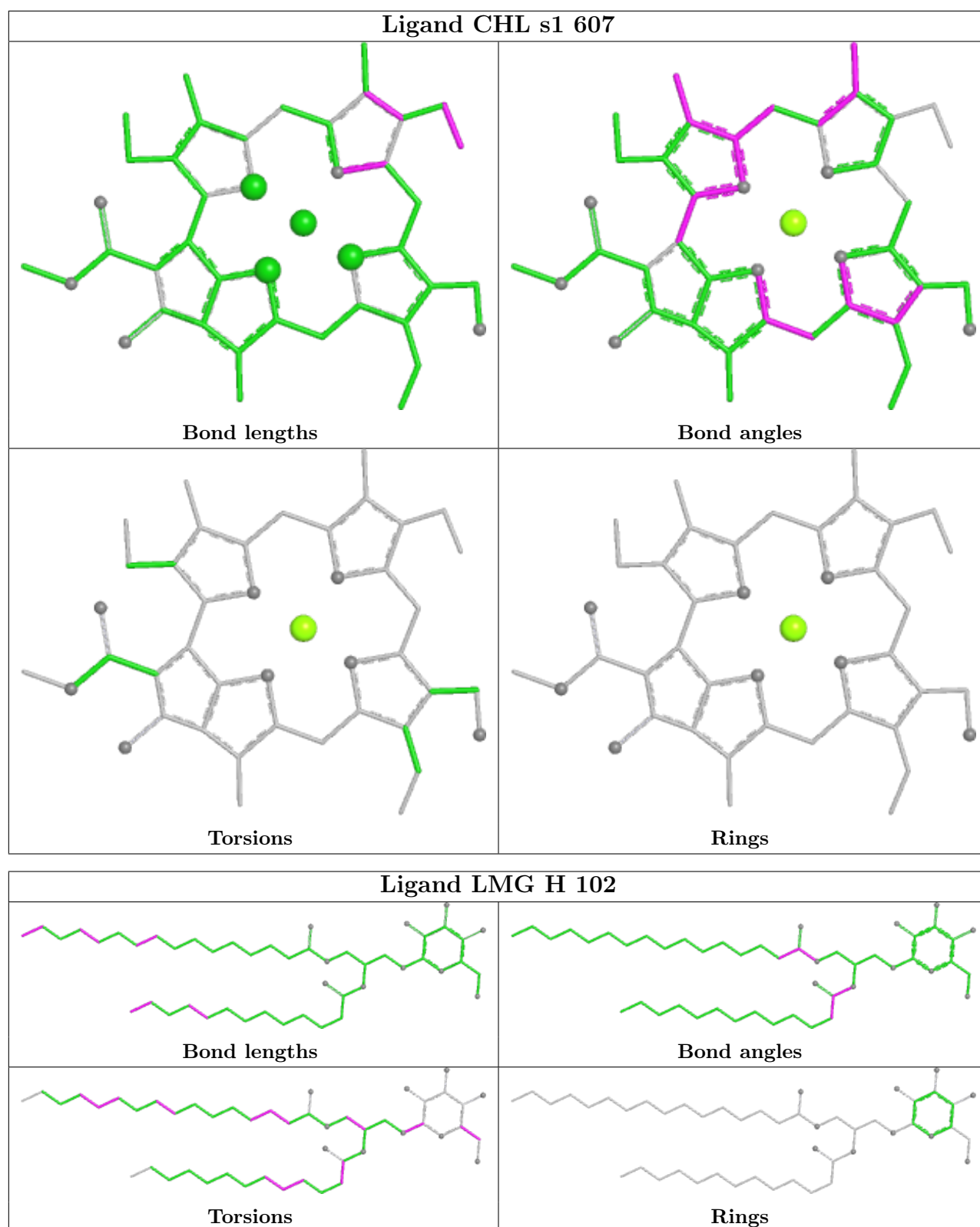






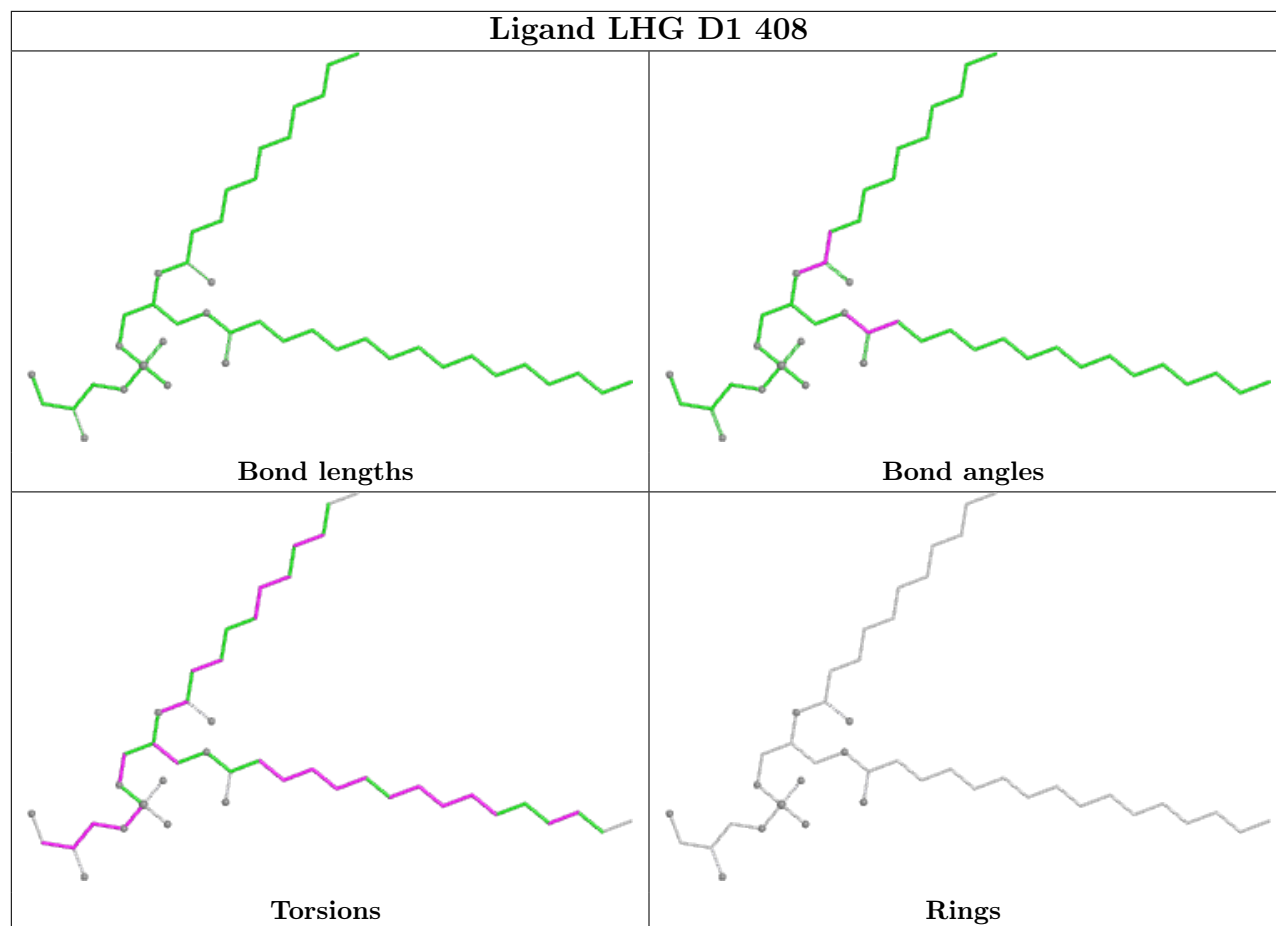




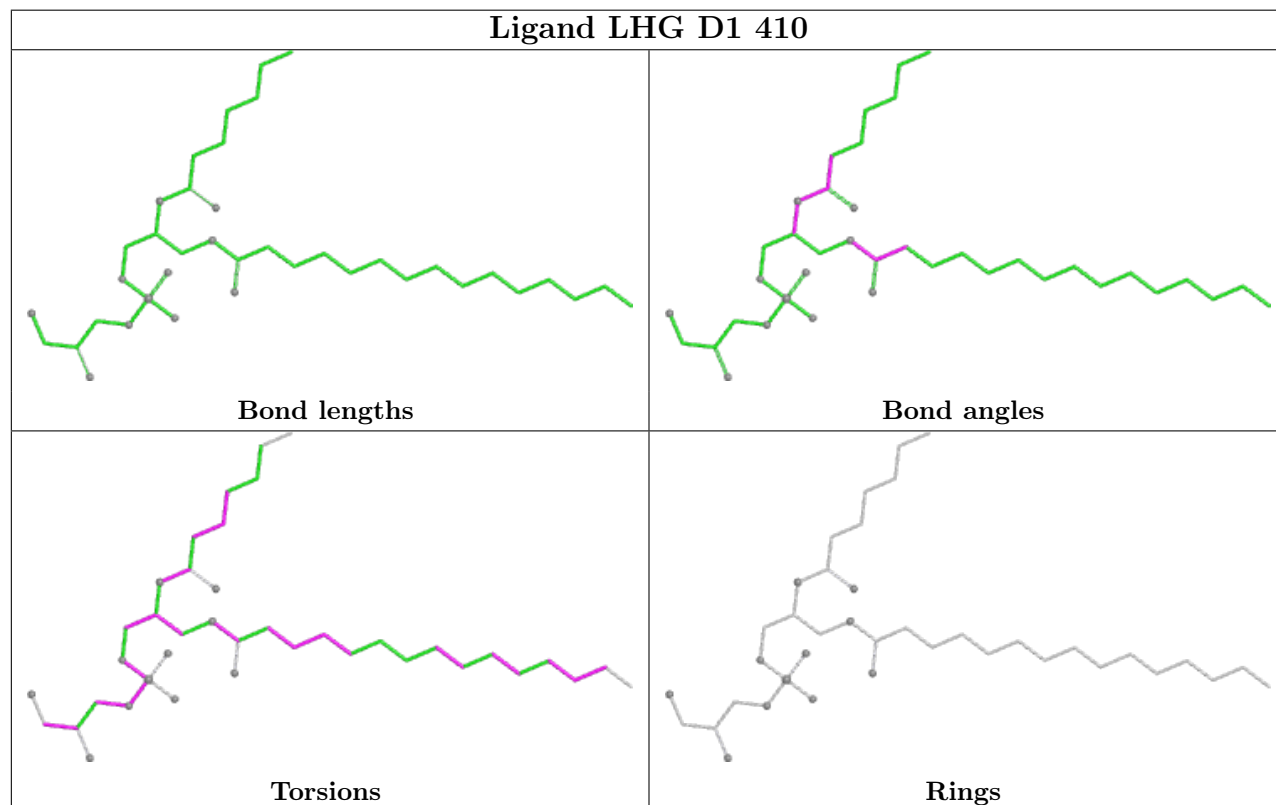


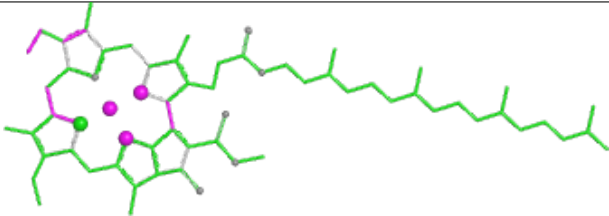
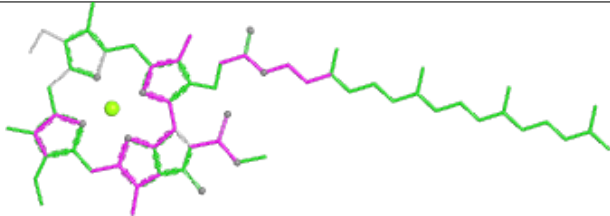
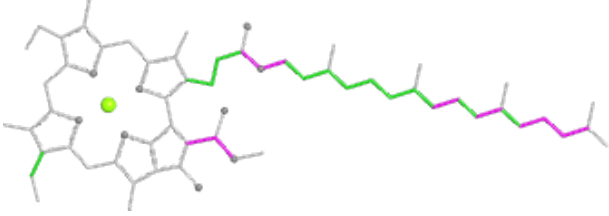
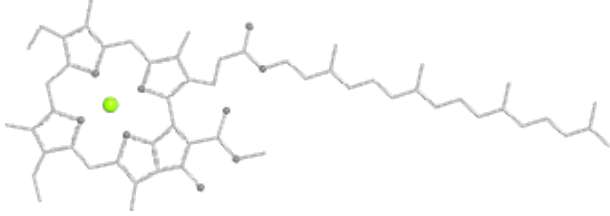


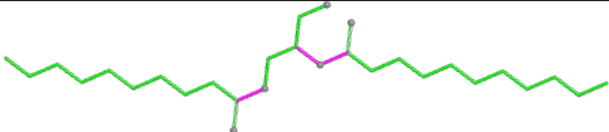
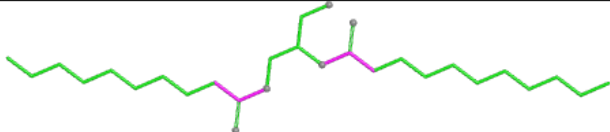
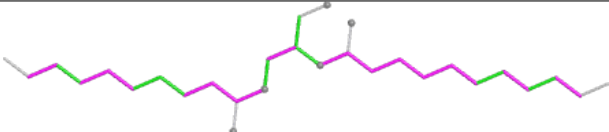
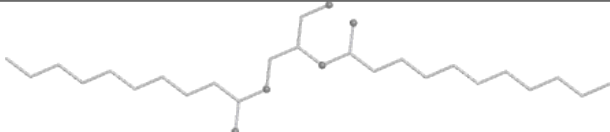
## Ligand LHG D1 408

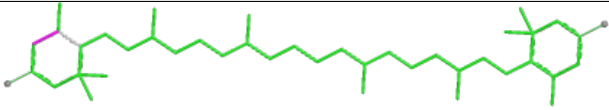
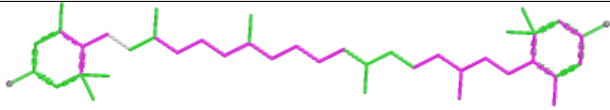
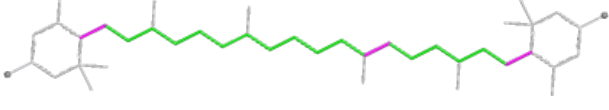
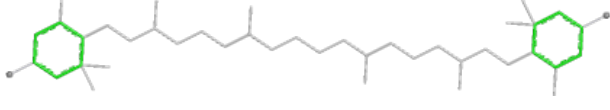


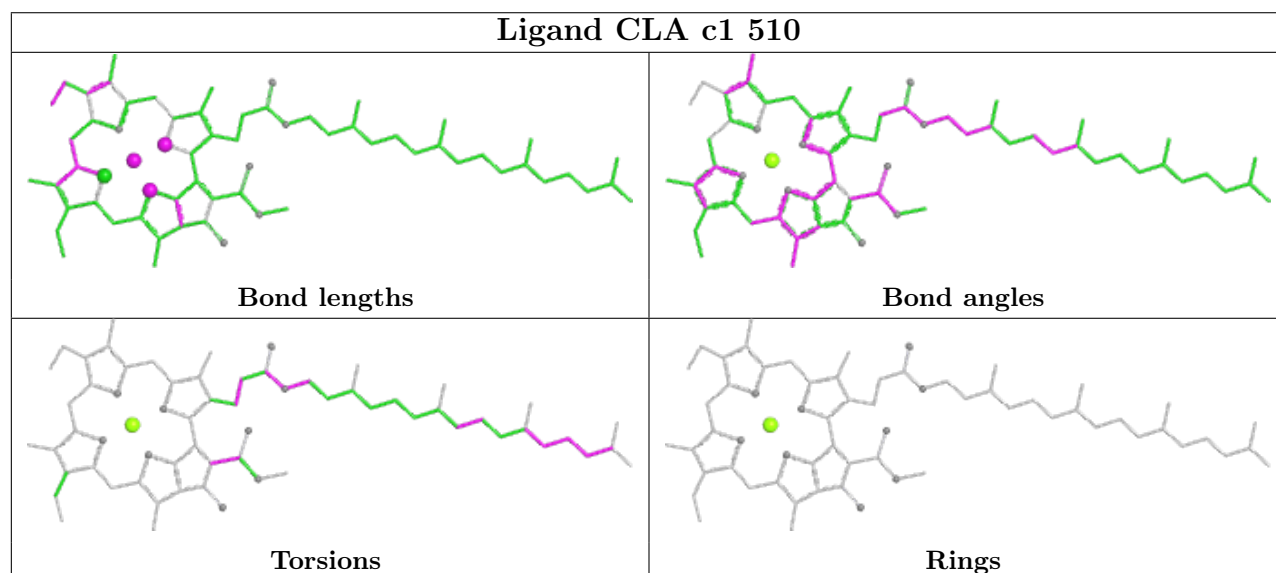
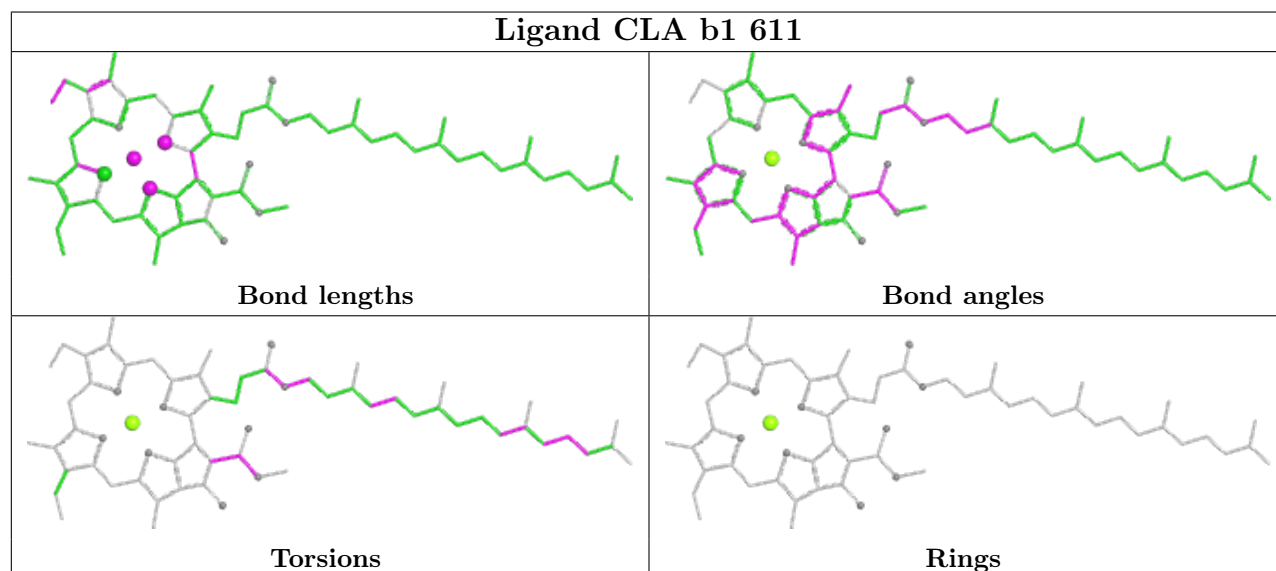
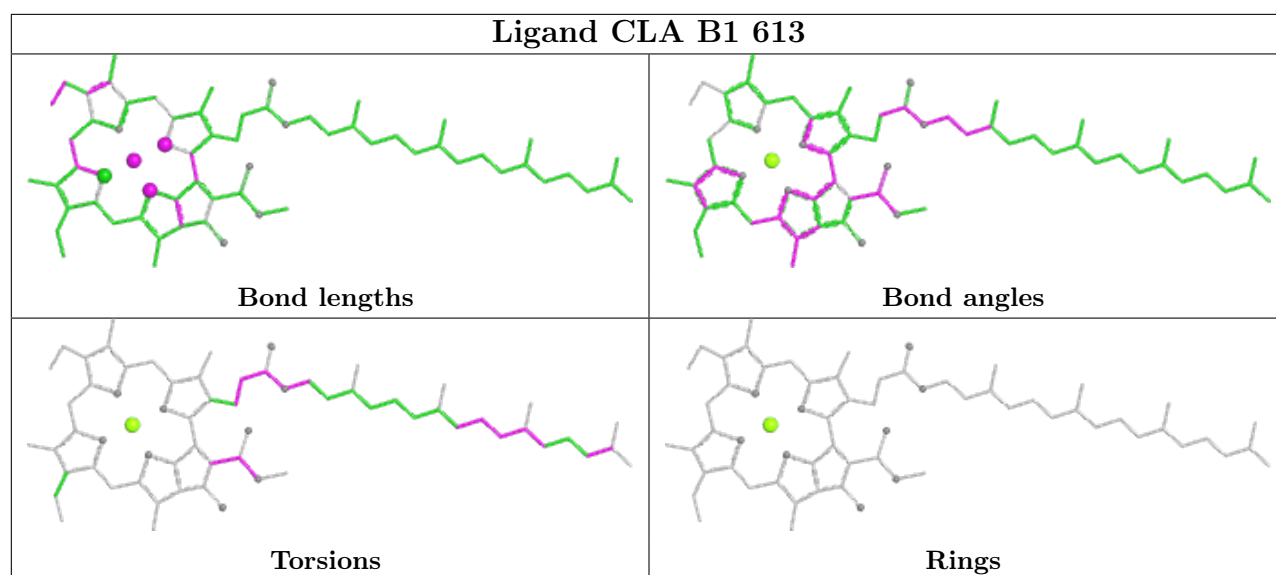
## Ligand LHG D1 410

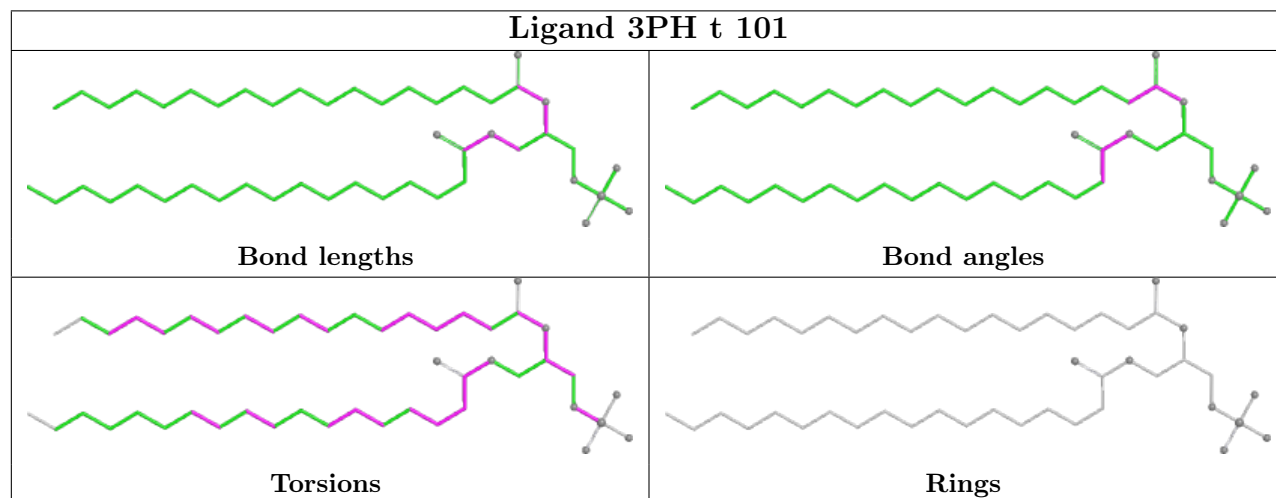
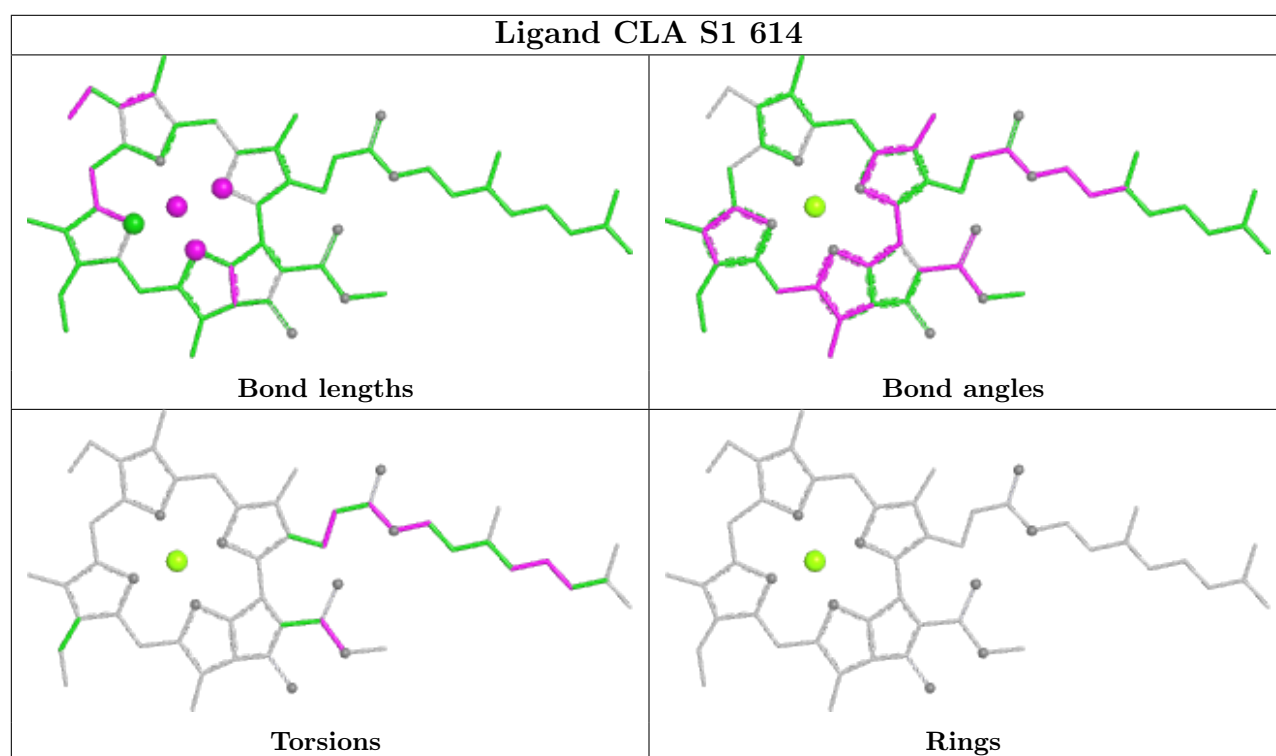
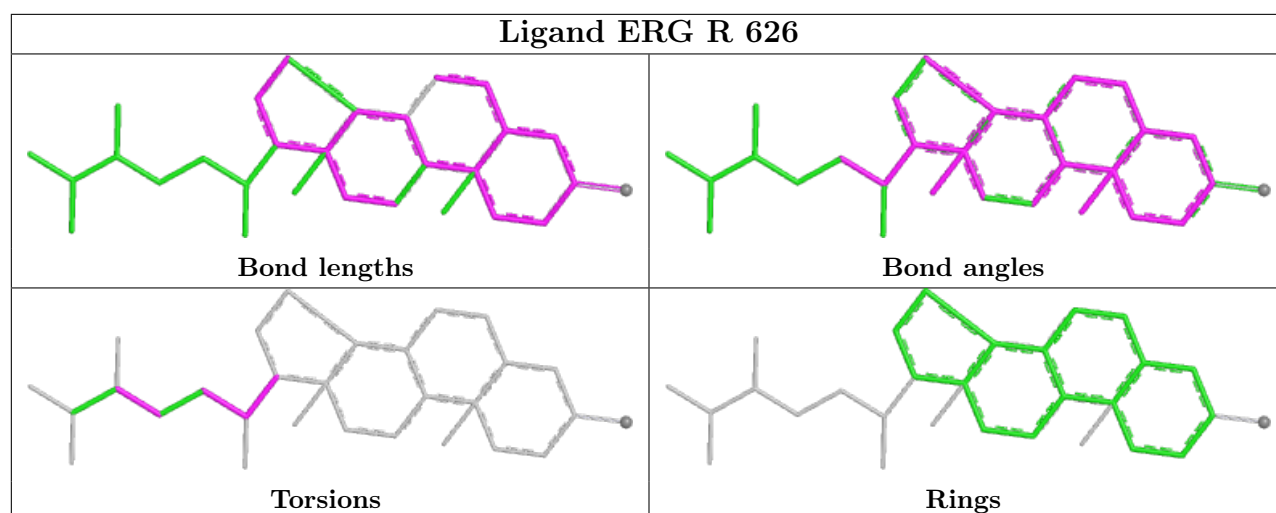


Ligand CLA B1 611	
	
Bond lengths	Bond angles
	
Torsions	Rings

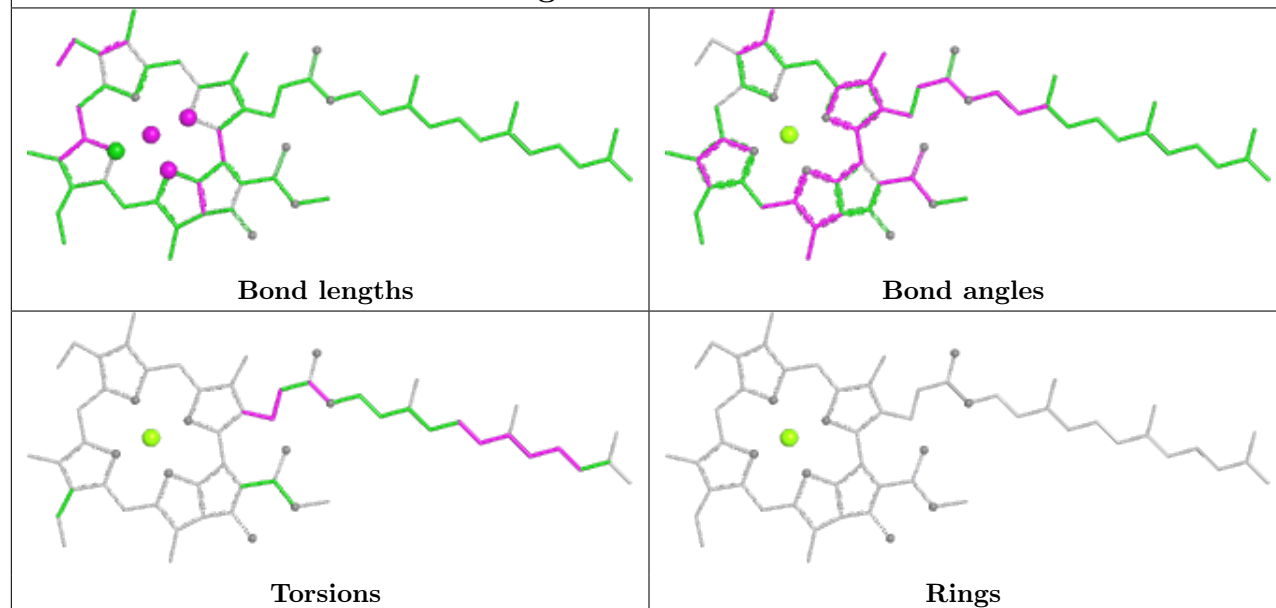
Ligand DGA j1 101	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand LUT s1 621	
	
Bond lengths	Bond angles
	
Torsions	Rings

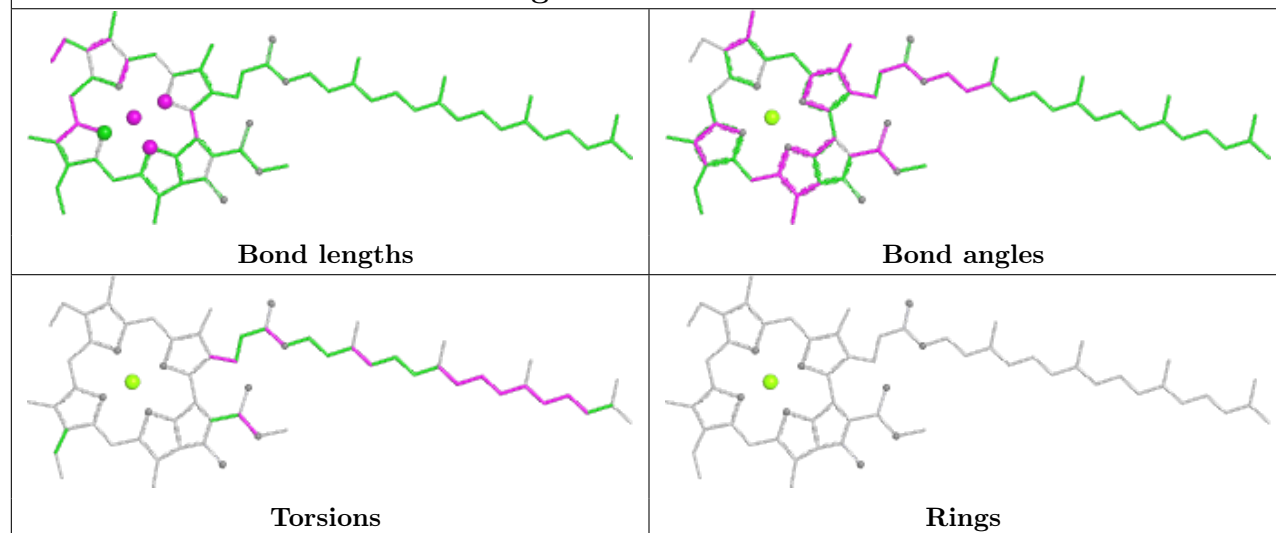


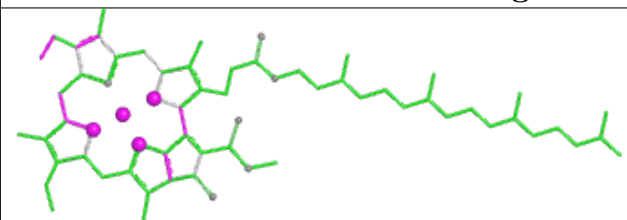
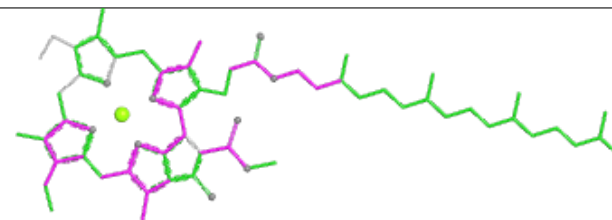
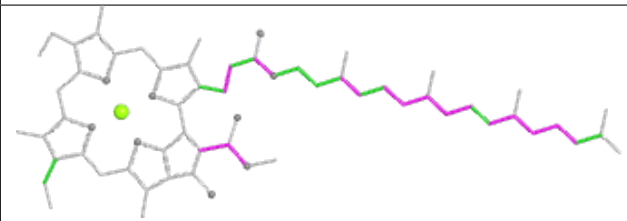
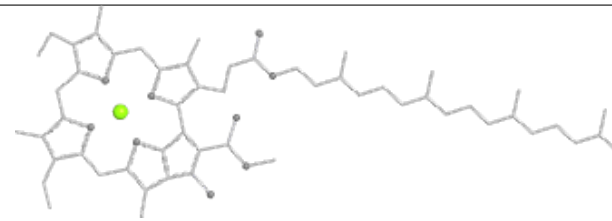


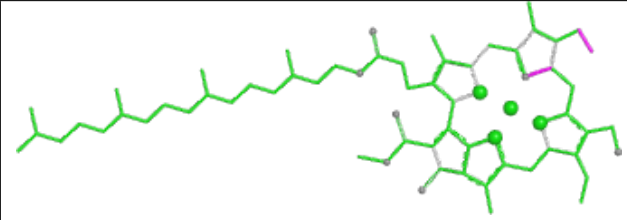
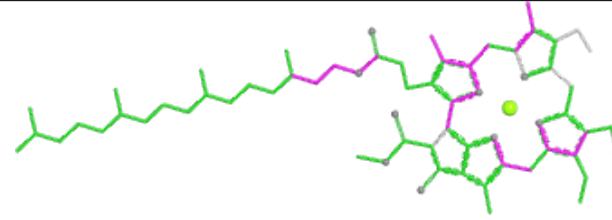
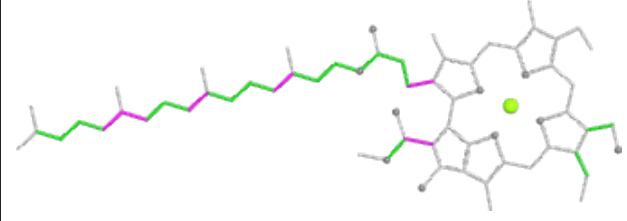
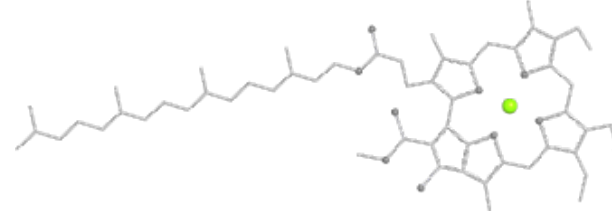
## Ligand CLA r 610

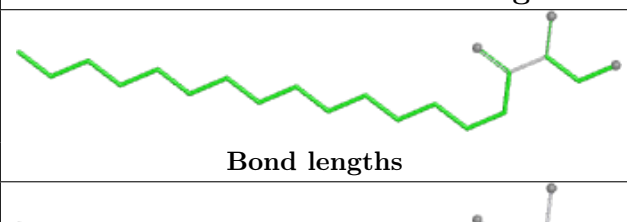
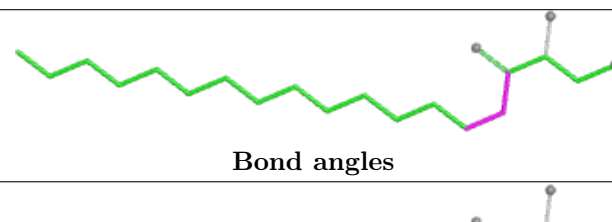




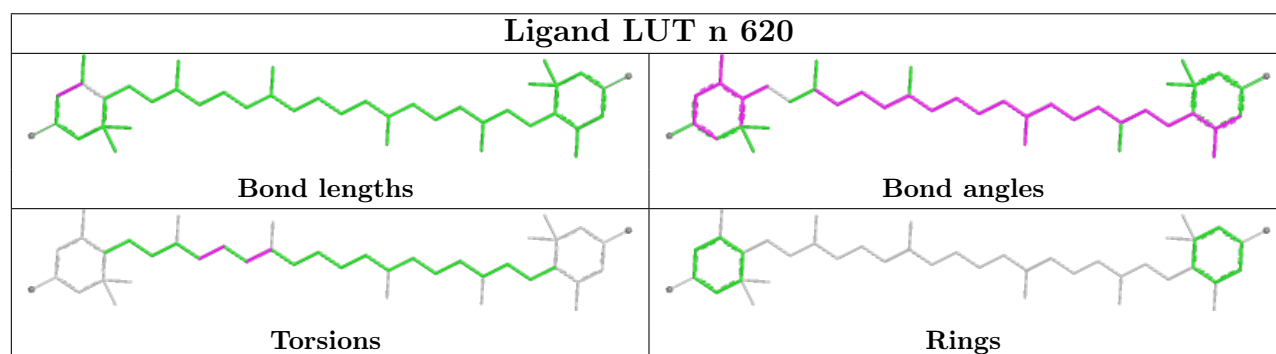
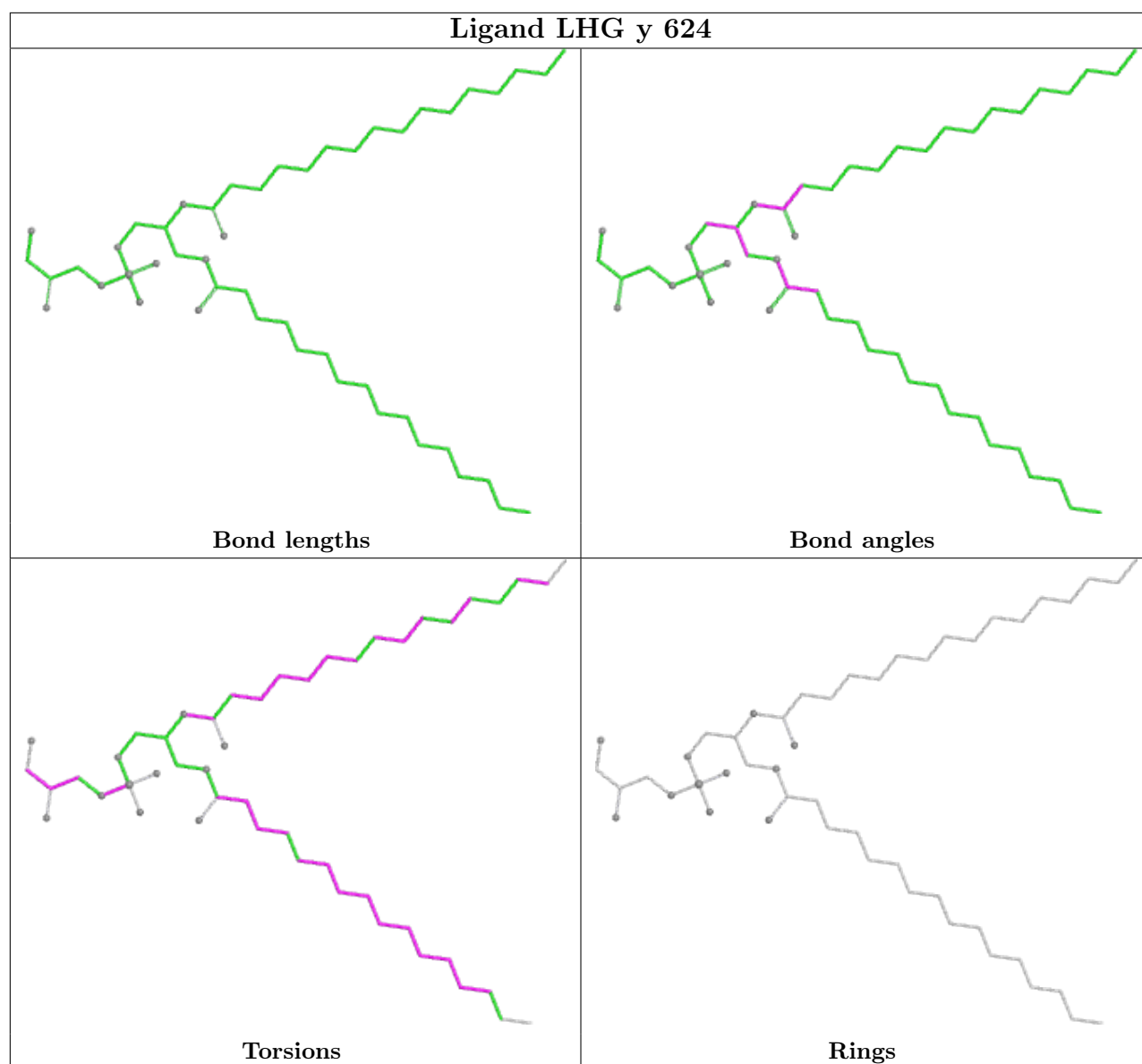
## Ligand CLA D 403

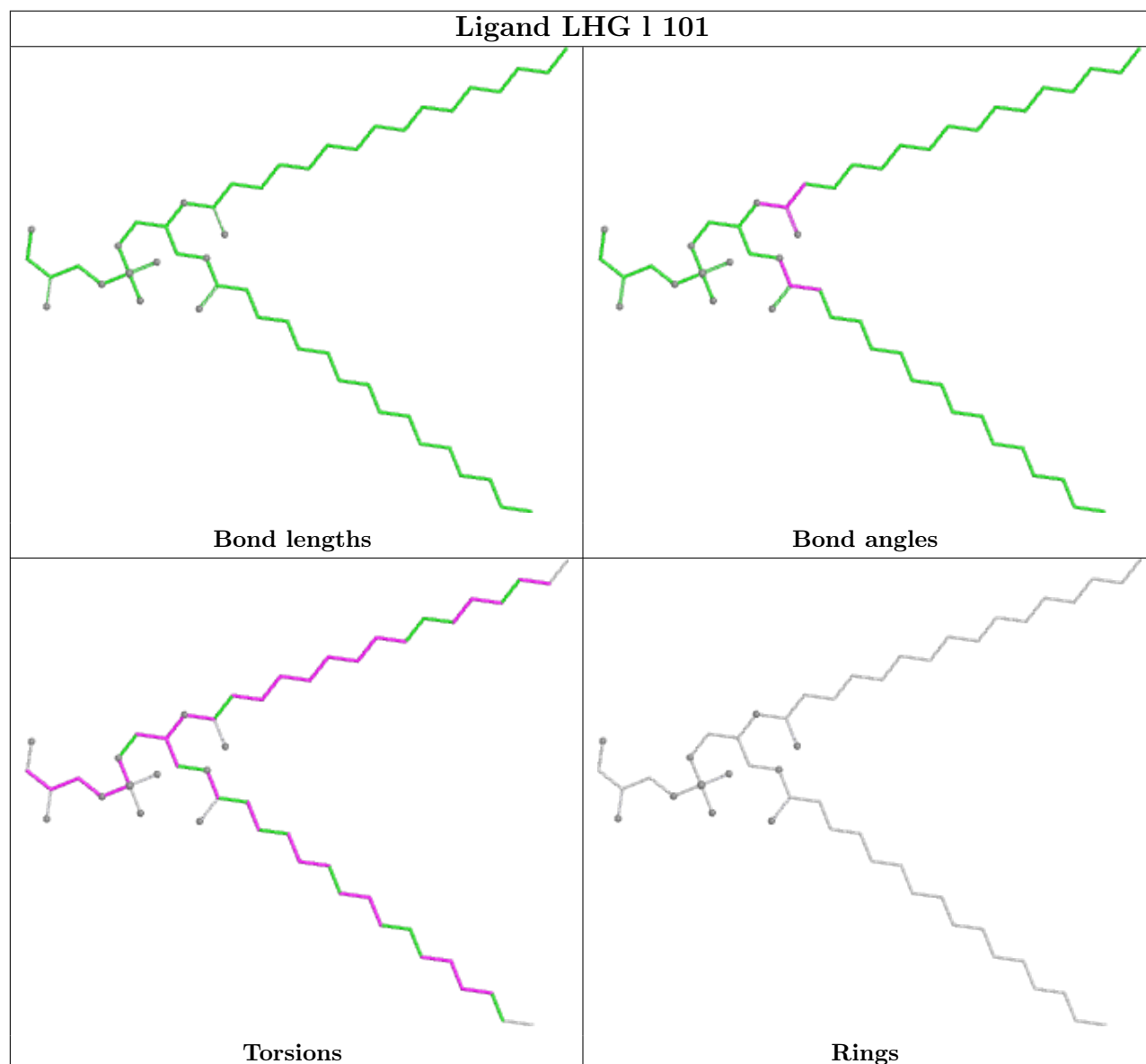
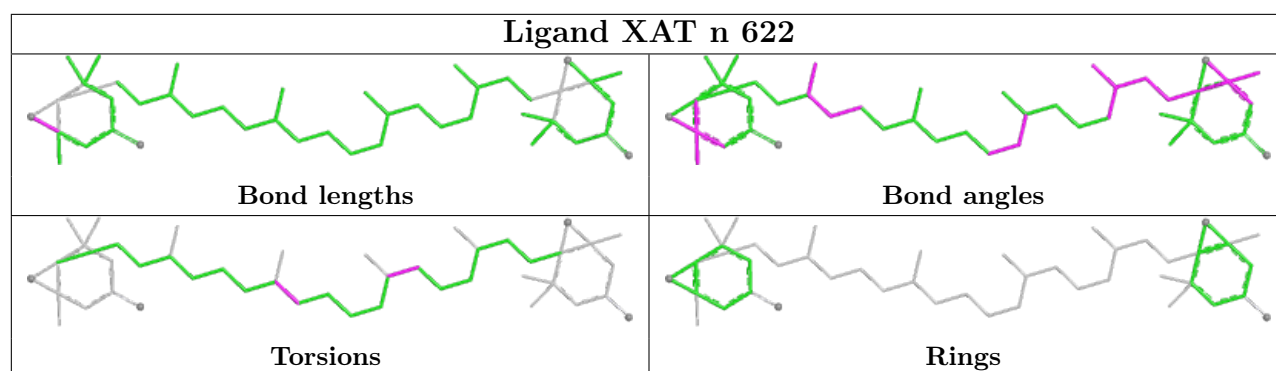


Ligand CLA Y1 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

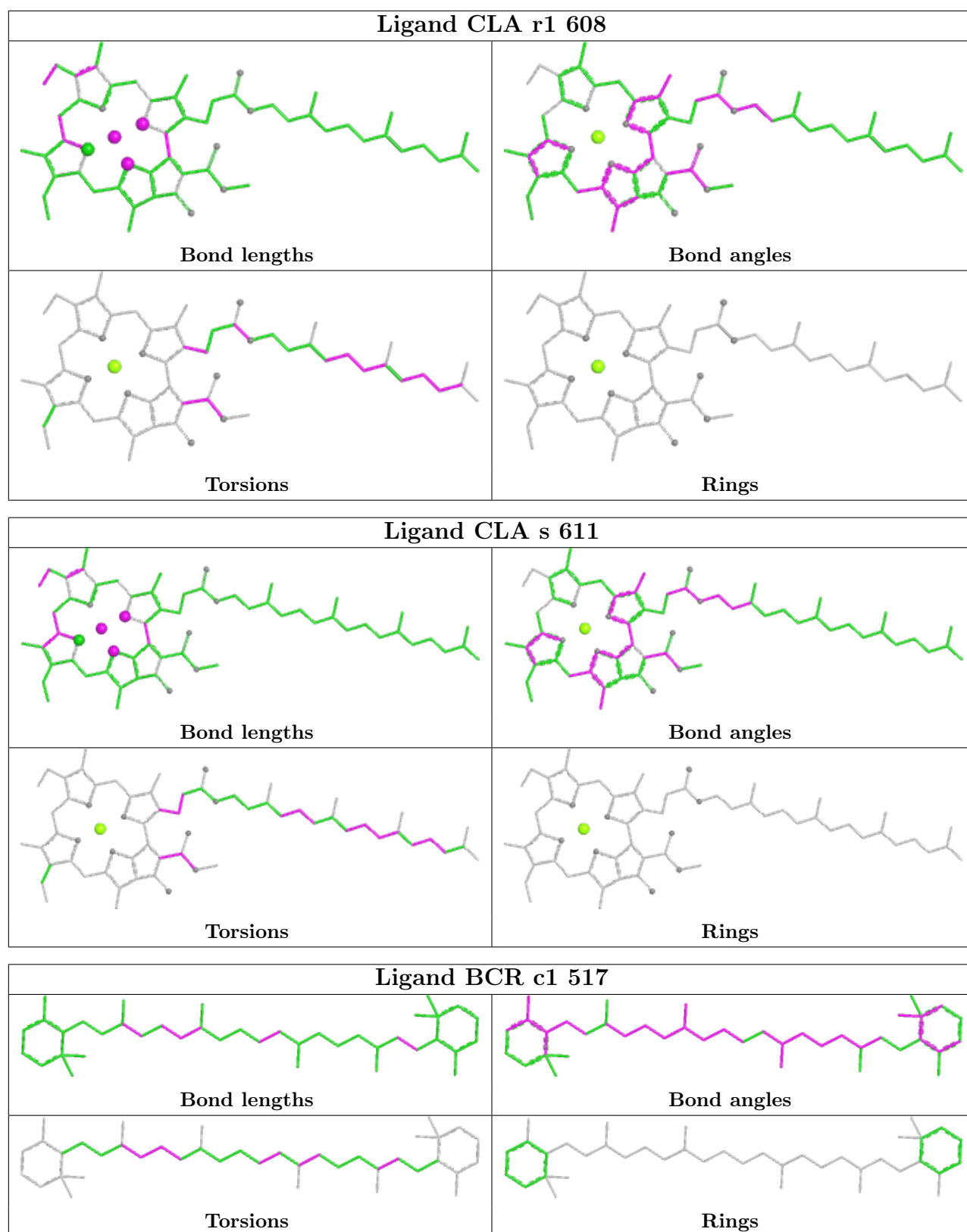
Ligand CHL n1 601	
	
Bond lengths	Bond angles
	
Torsions	Rings

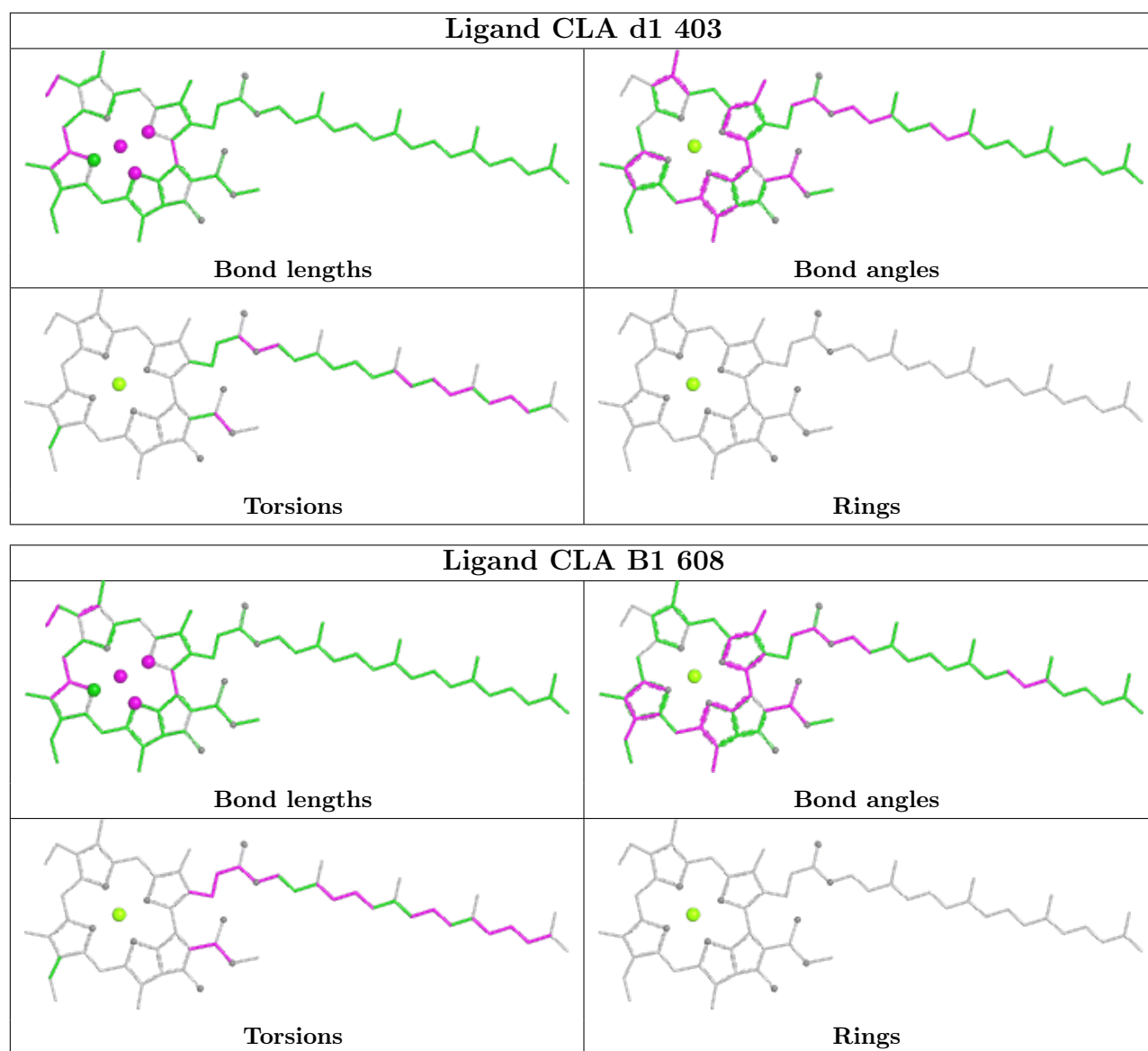
Ligand SPH Y1 625	
	
Bond lengths	Bond angles
	
Torsions	Rings

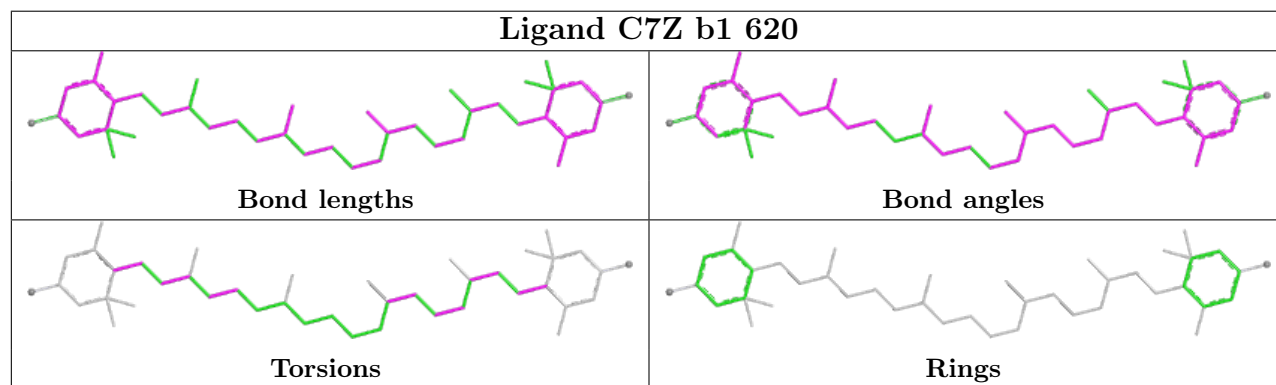
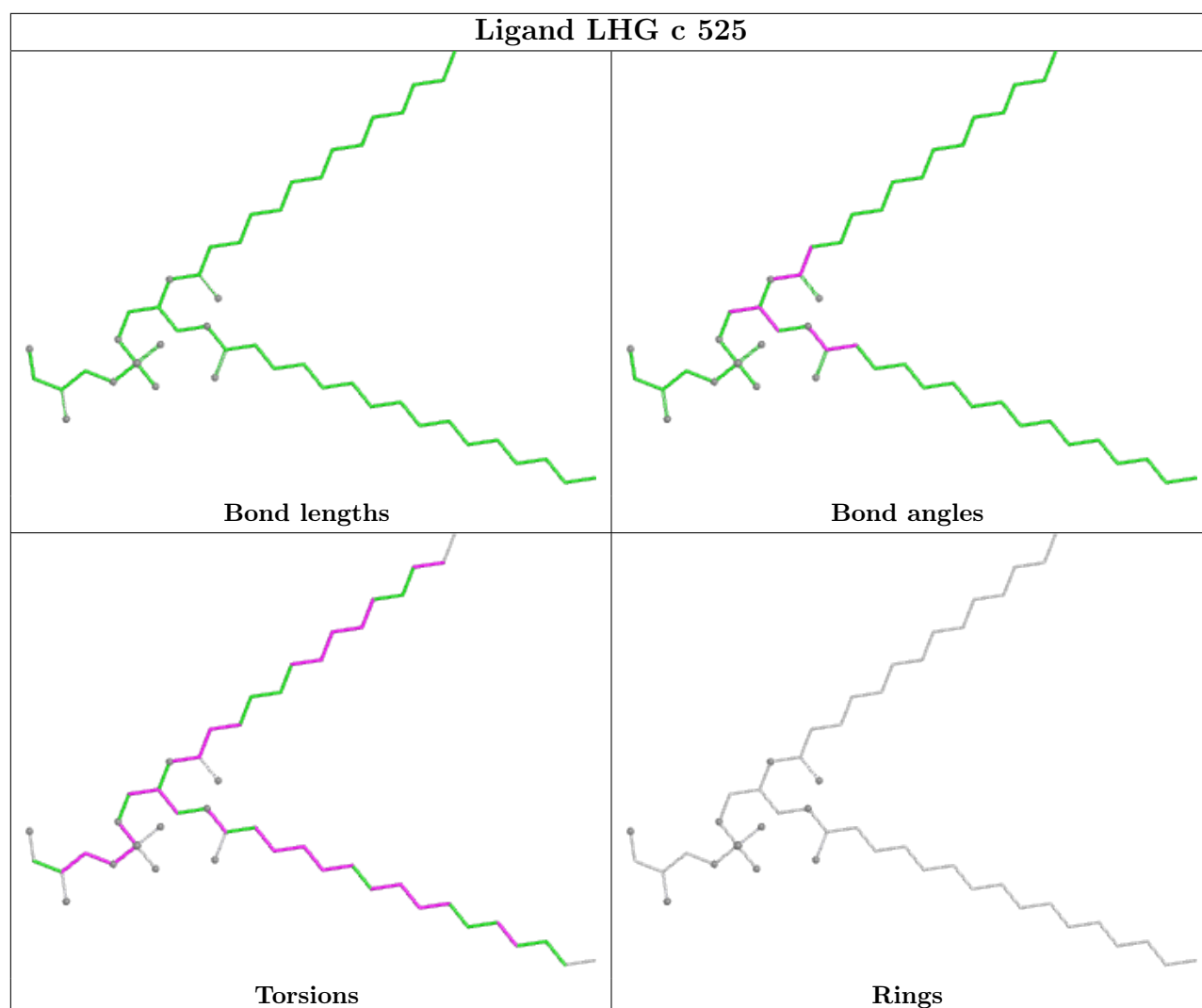


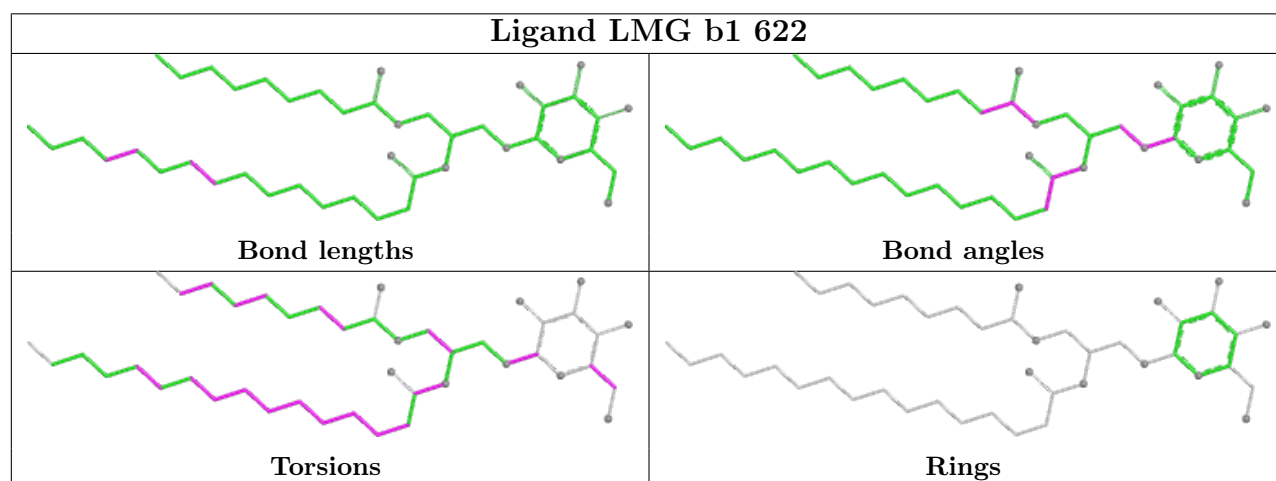
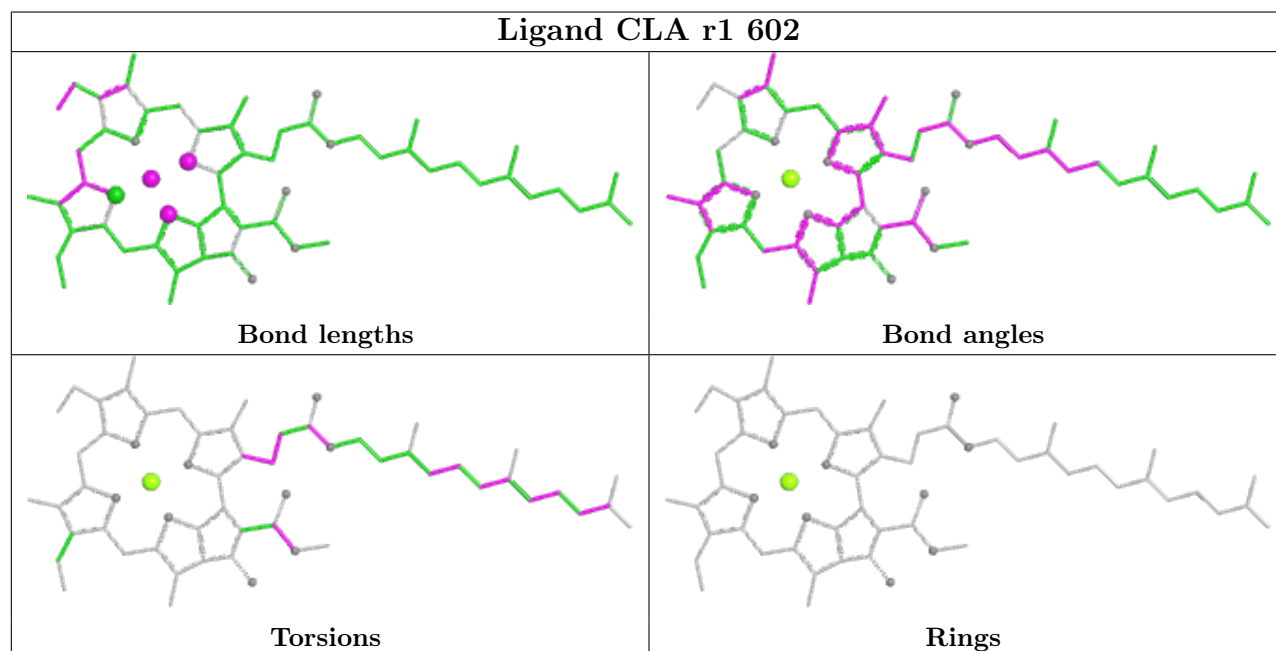
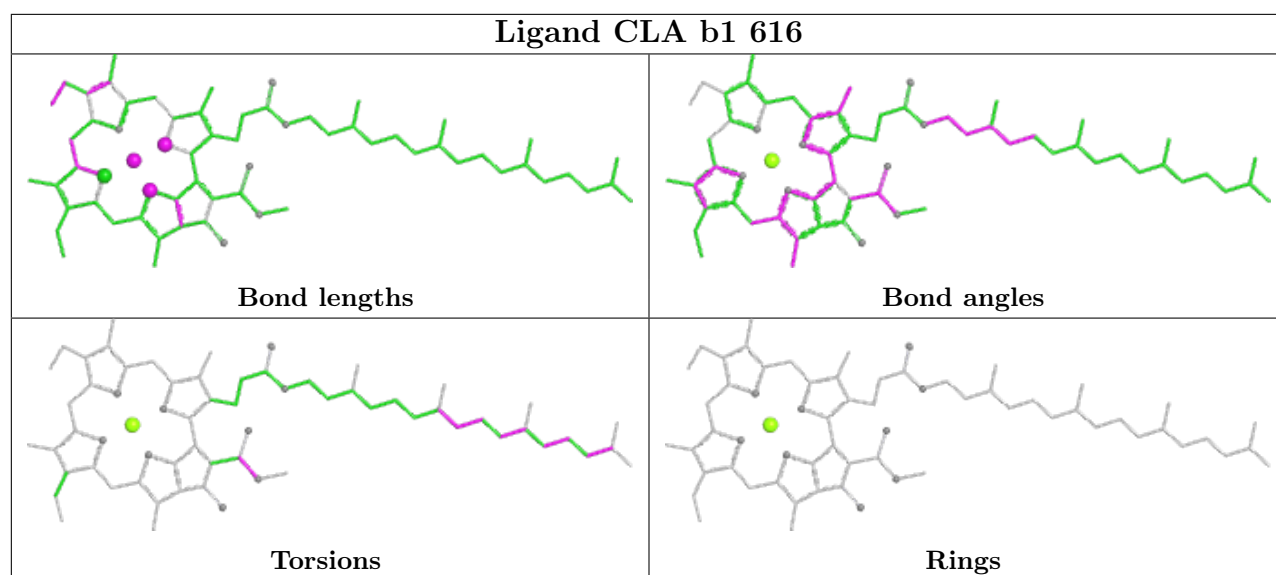


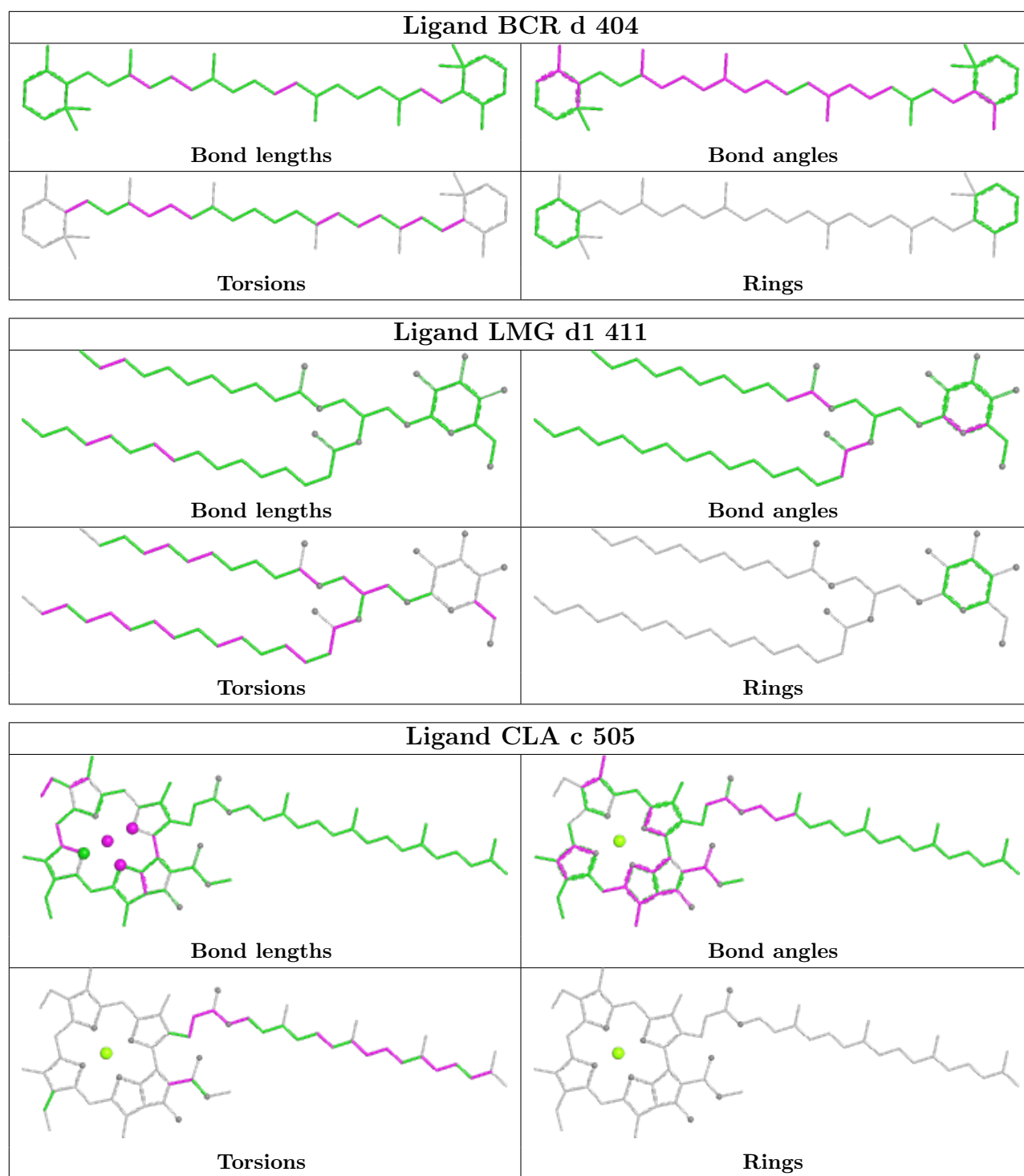


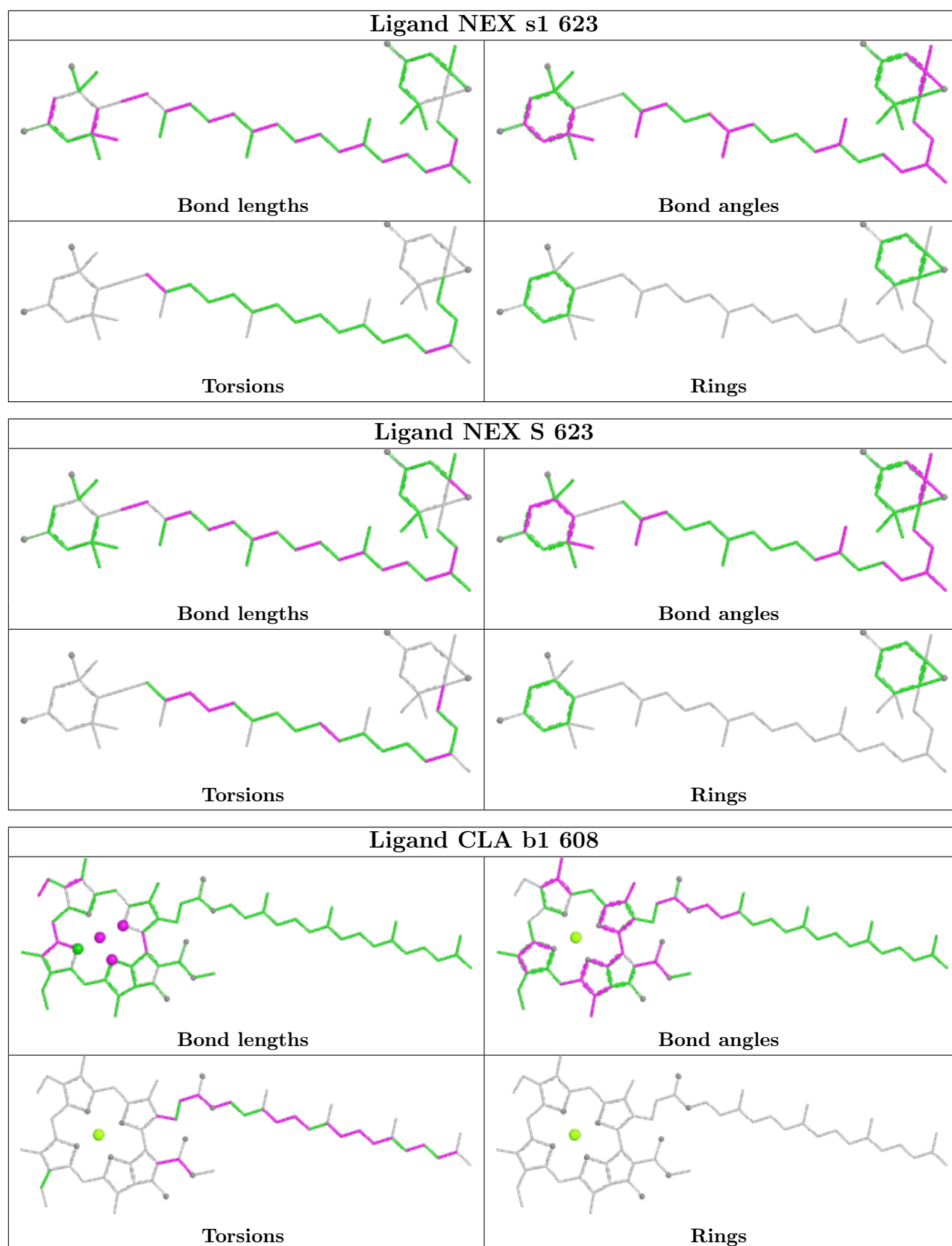


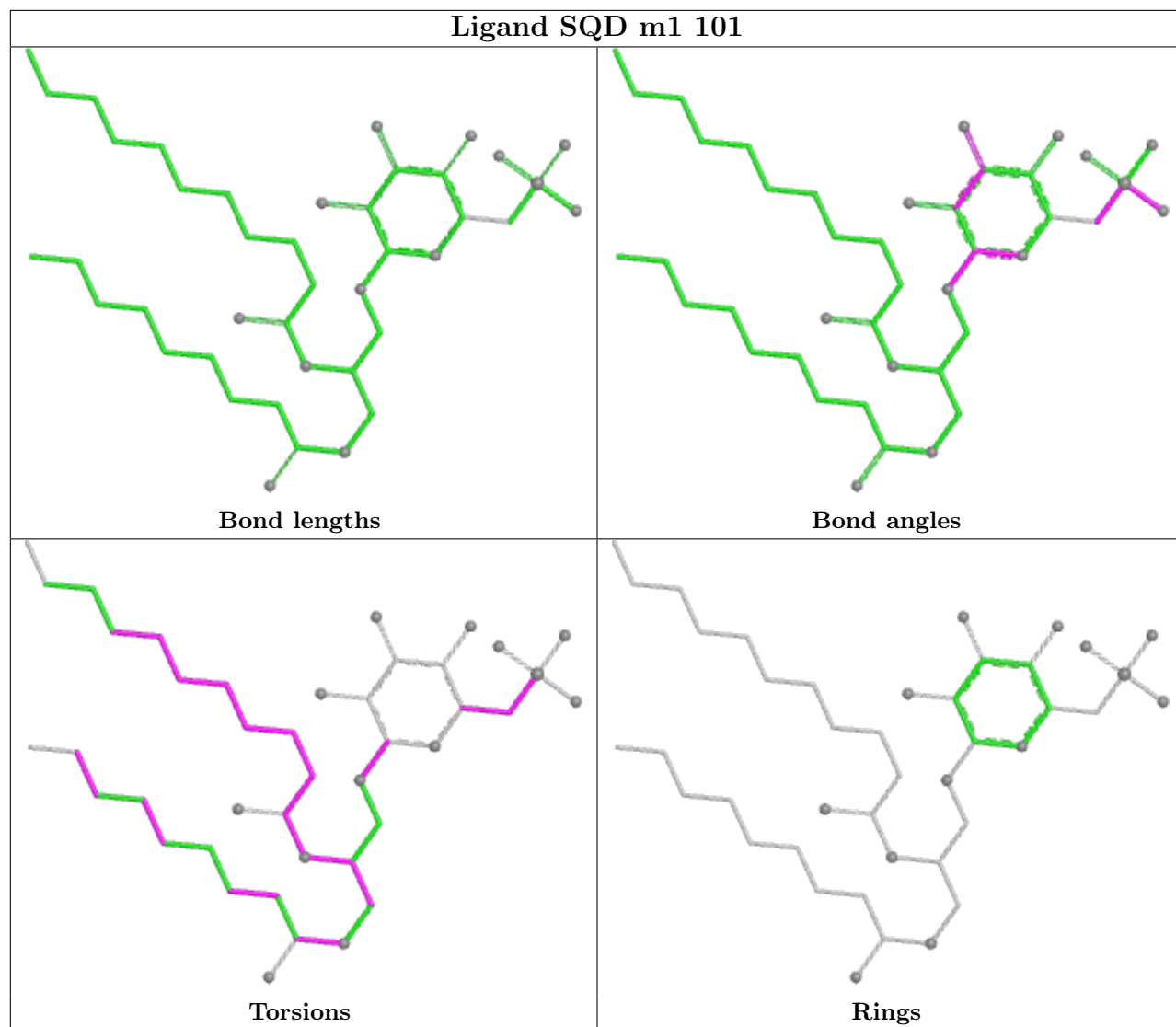


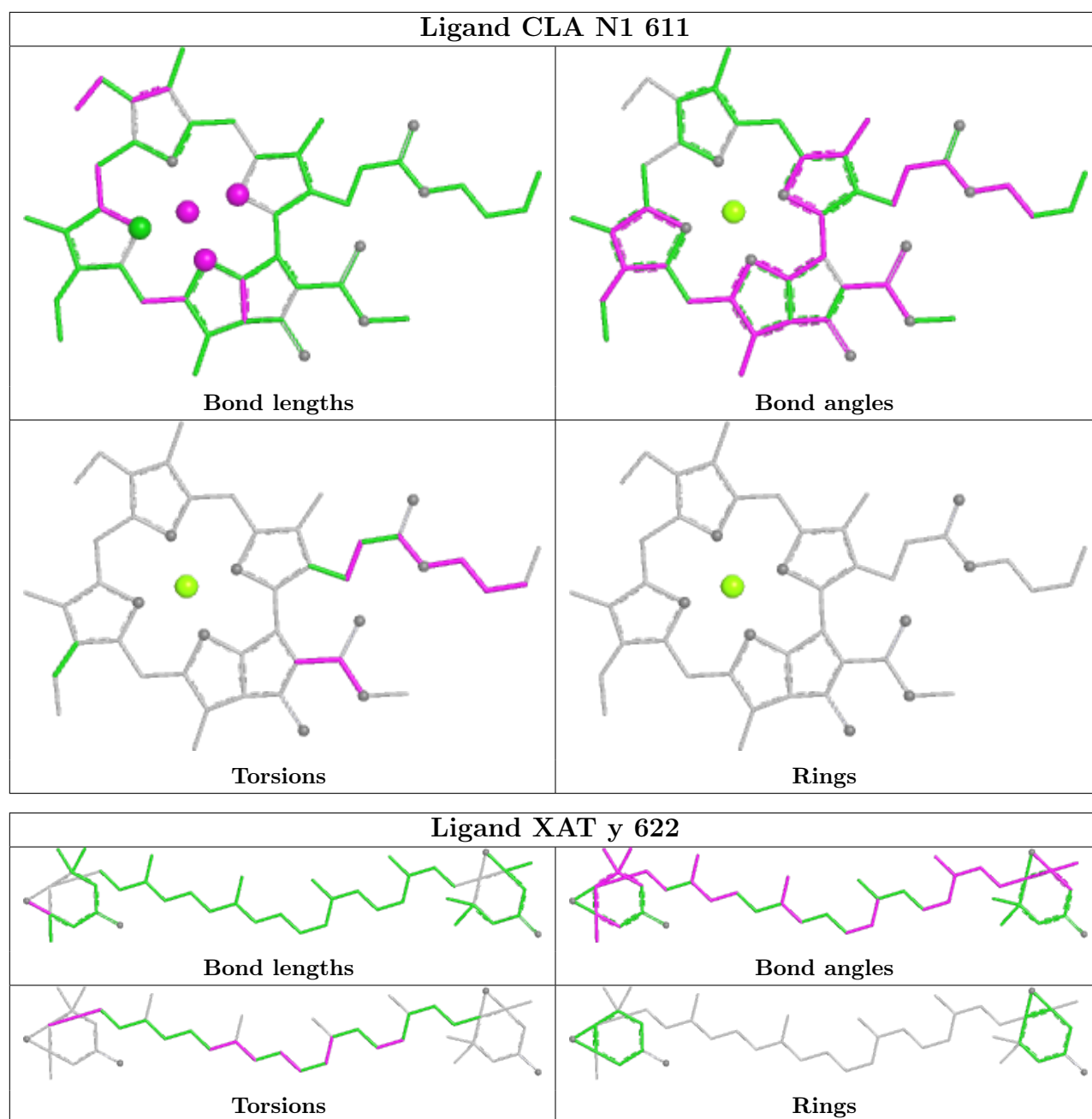




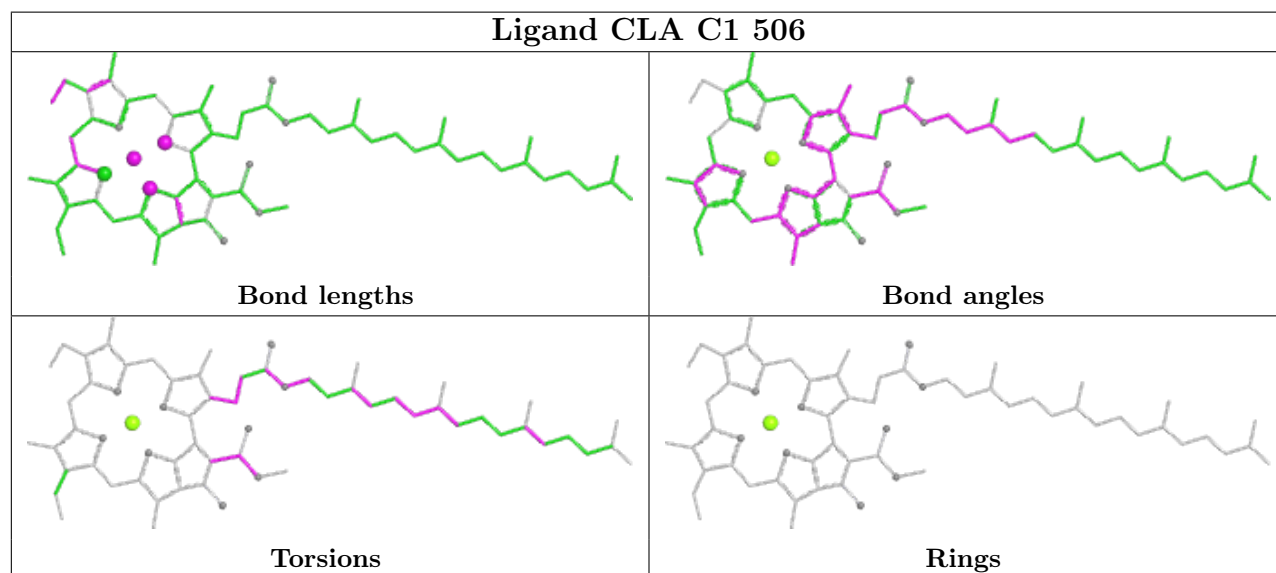
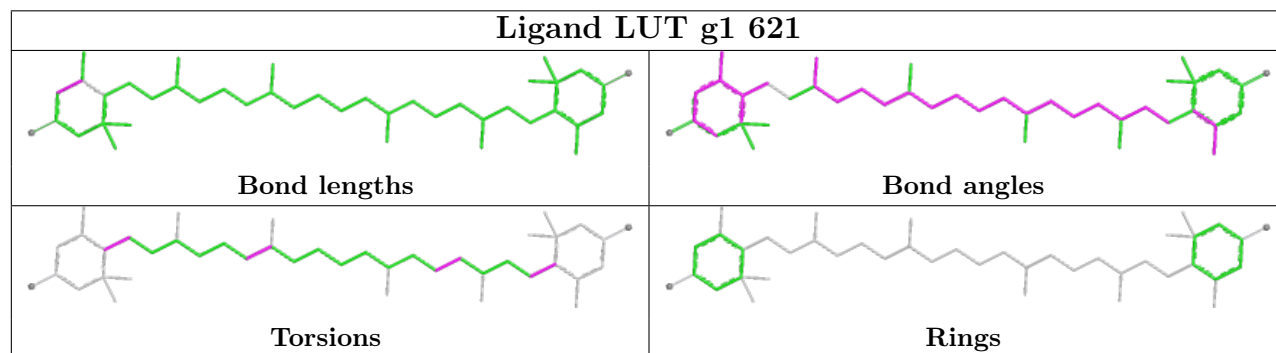
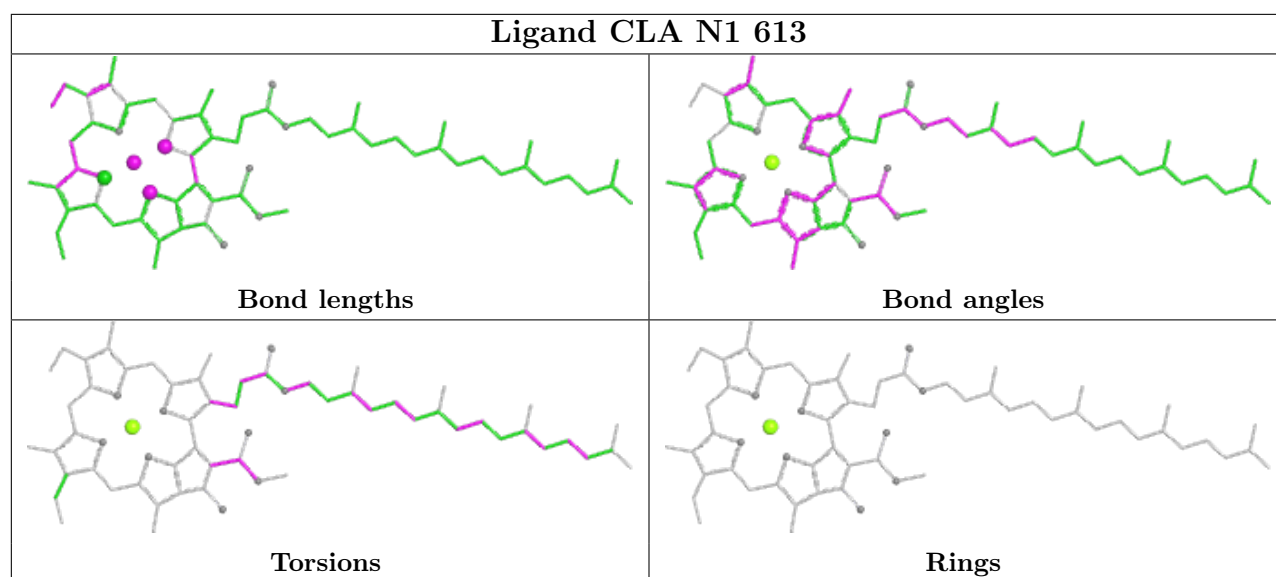


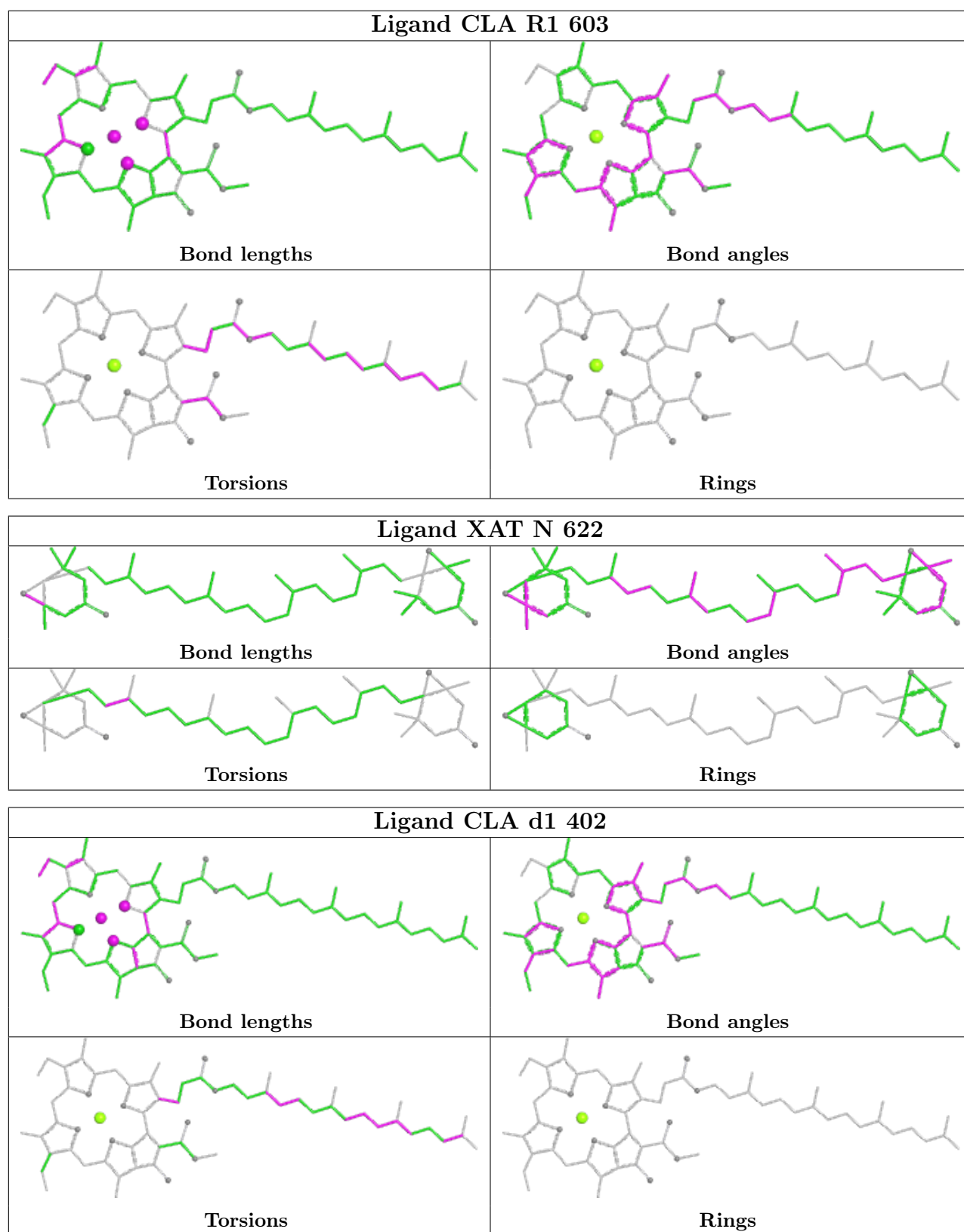


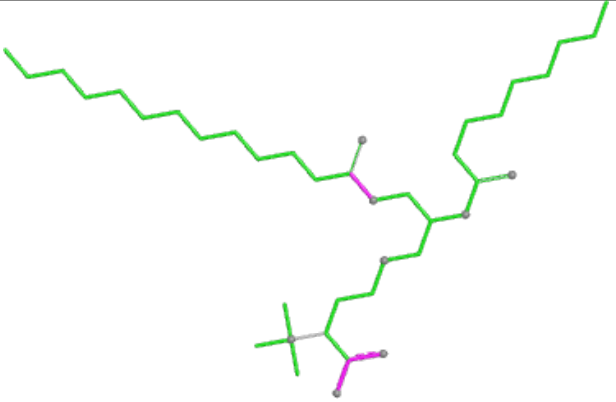
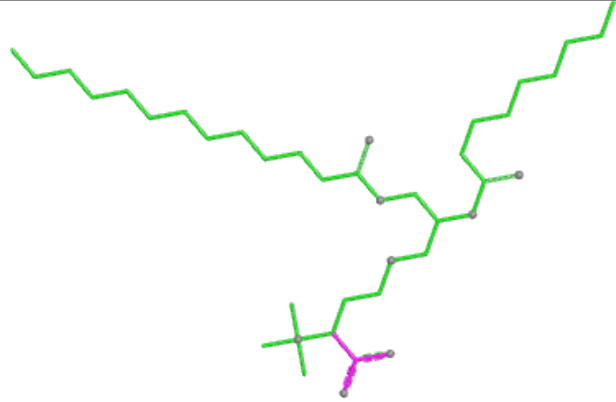
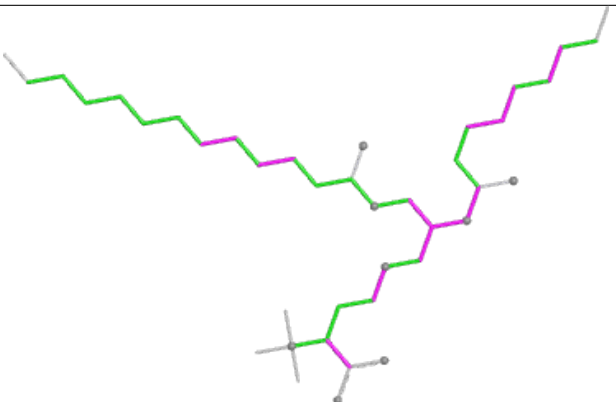
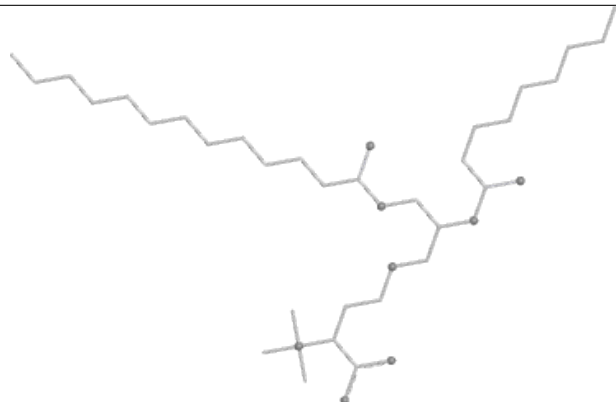


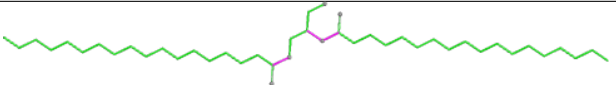
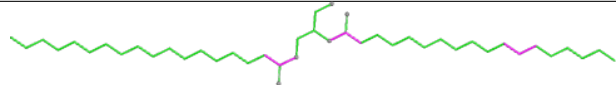
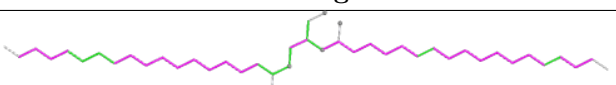
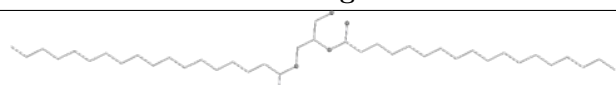




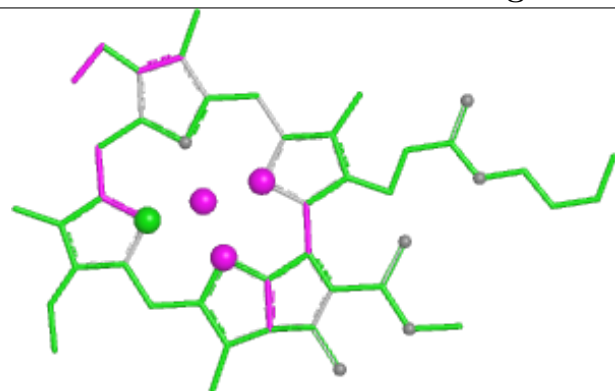




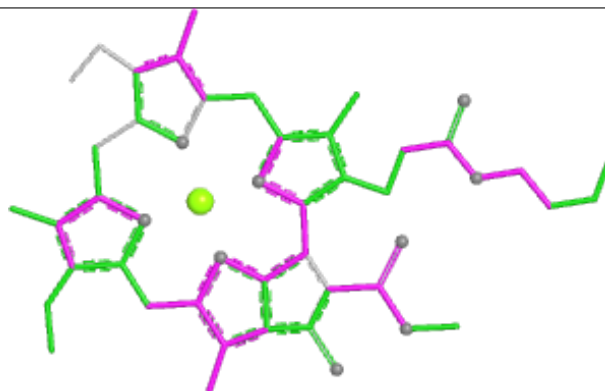
Ligand LMK c1 527	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand DGA c 524	
	
Bond lengths	Bond angles
	
Torsions	Rings

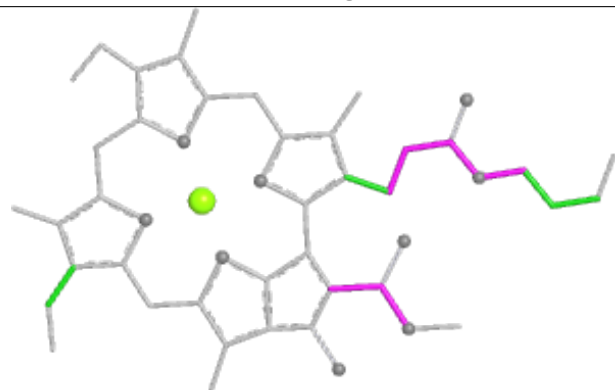
## Ligand CLA R1 604



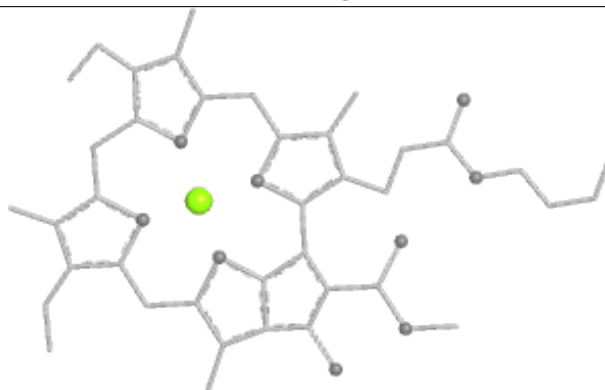
Bond lengths



Bond angles

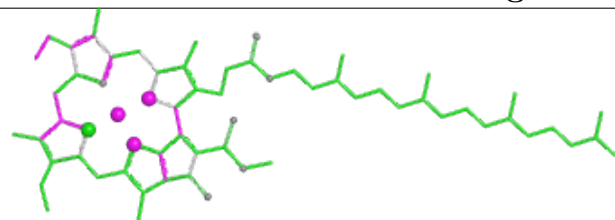


Torsions

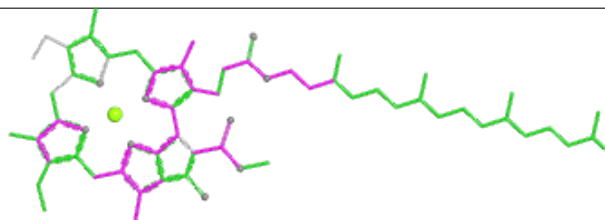


Rings

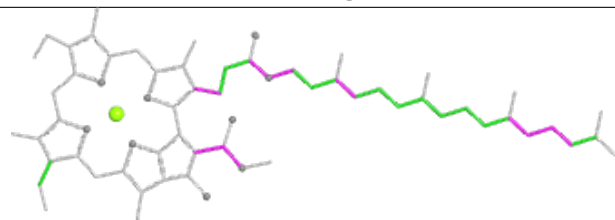
## Ligand CLA Y1 603



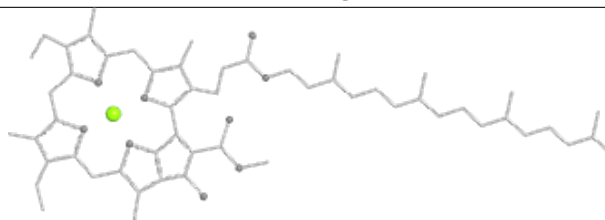
Bond lengths



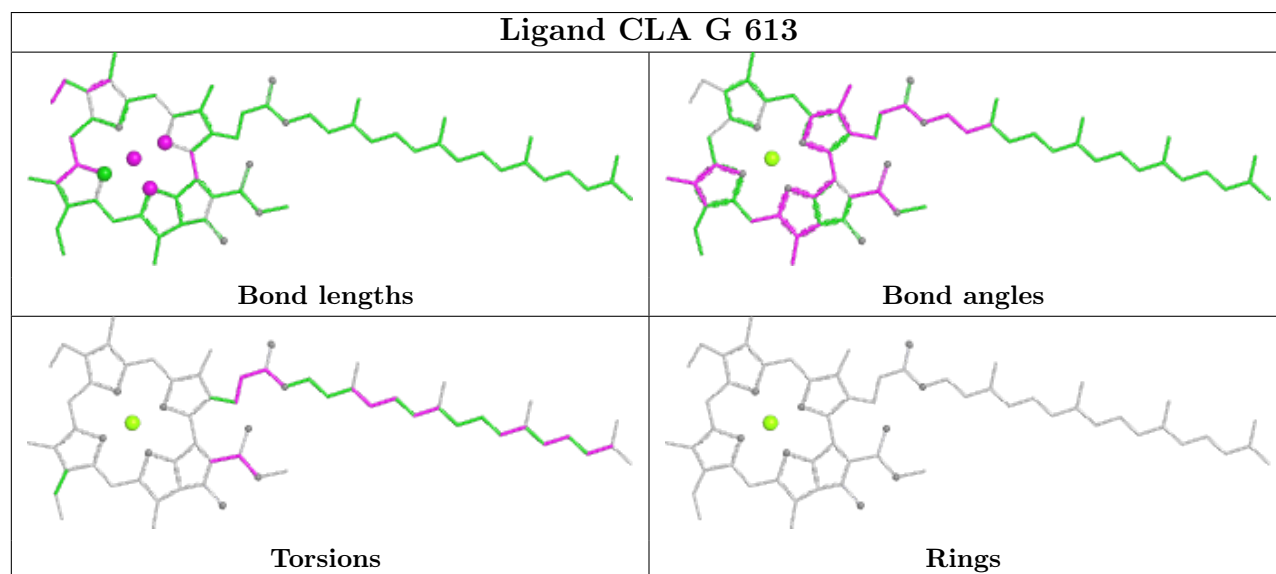
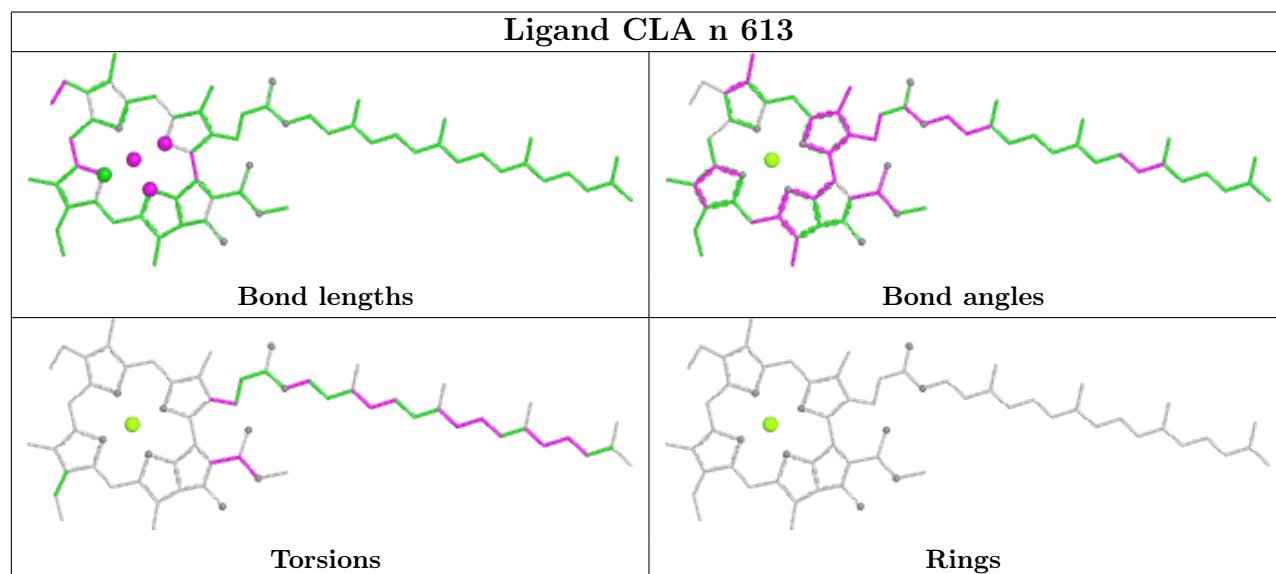
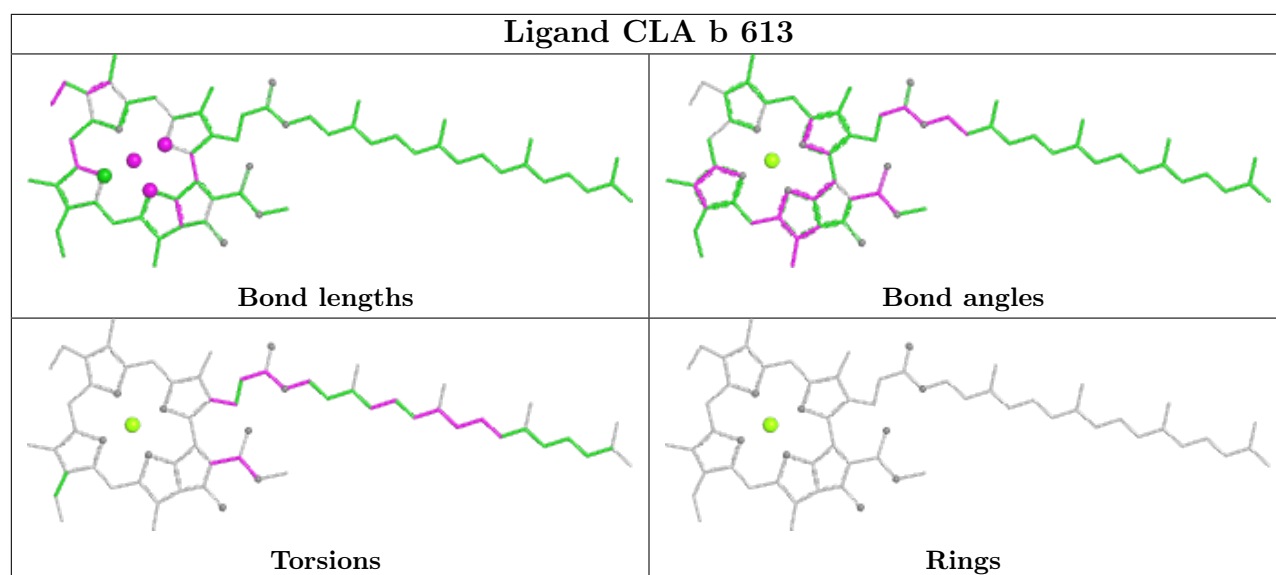
Bond angles

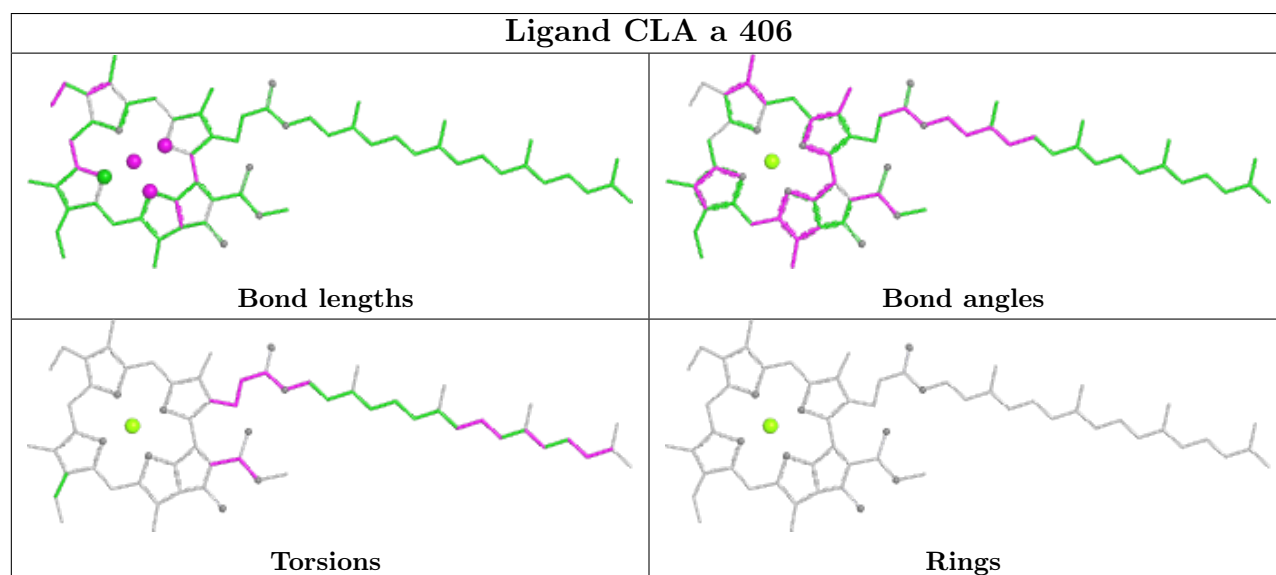
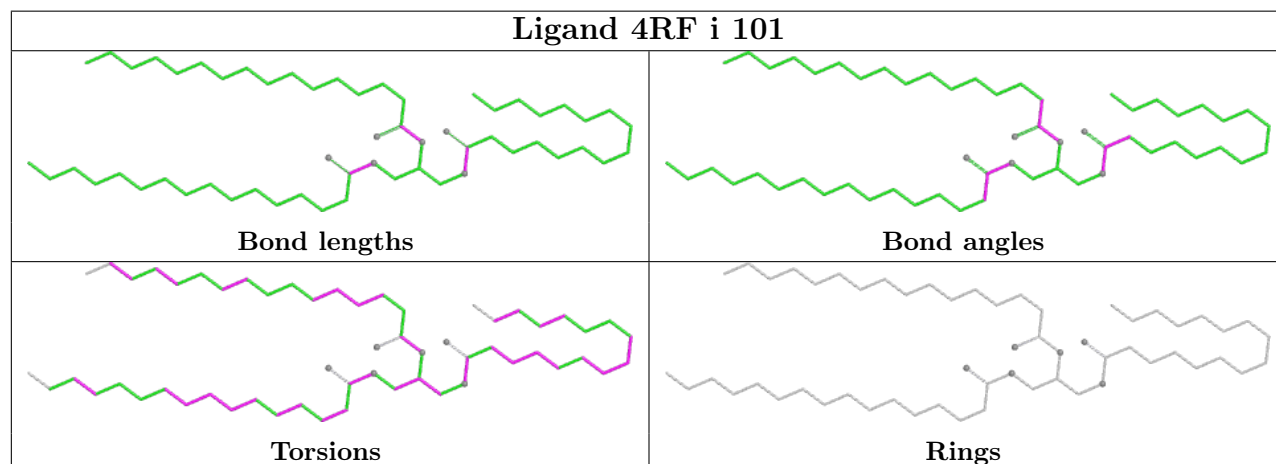
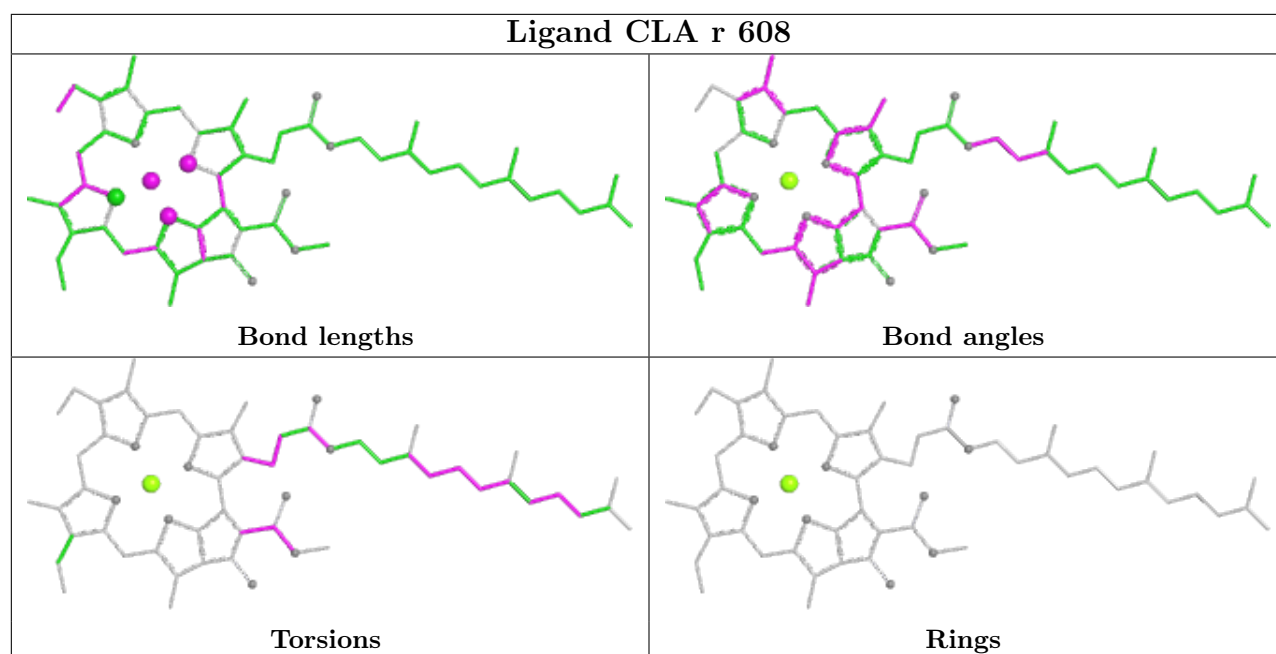


Torsions

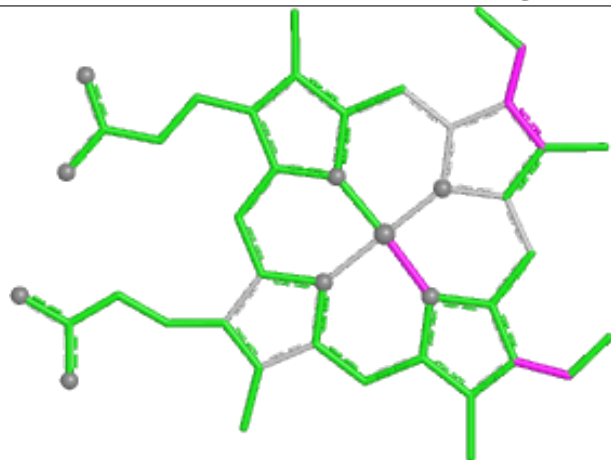


Rings

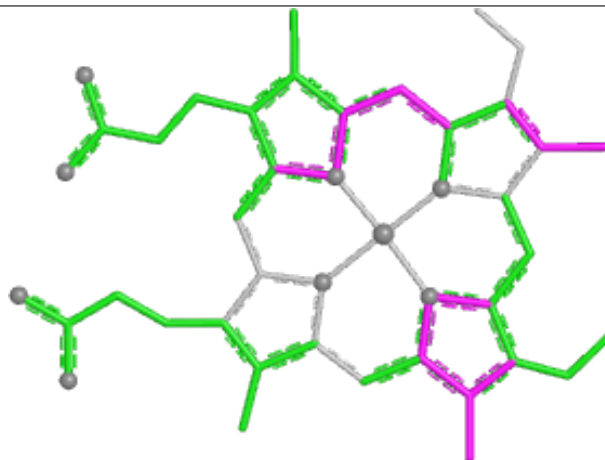




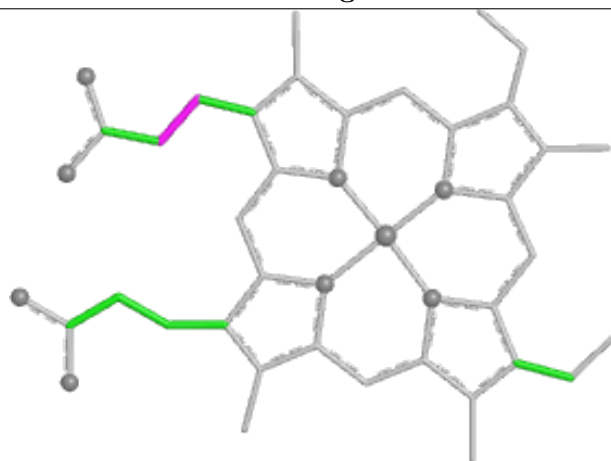
## Ligand HEM f 101



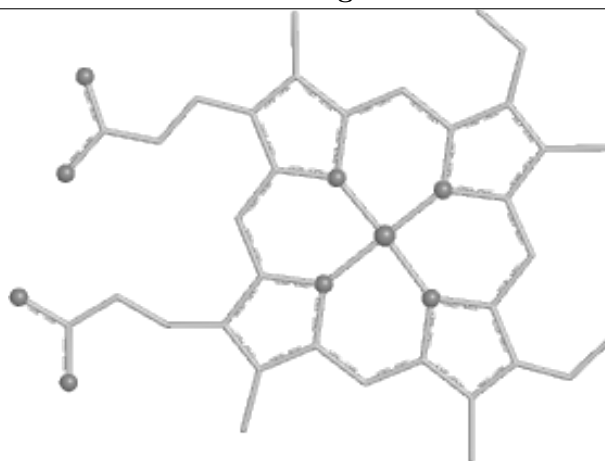
Bond lengths



Bond angles

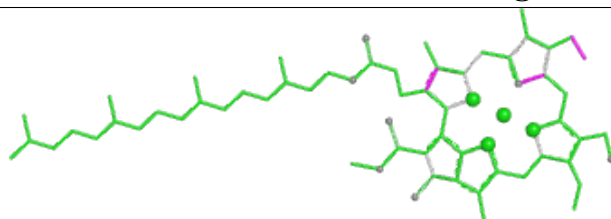


Torsions

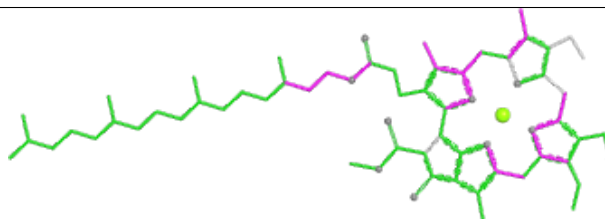


Rings

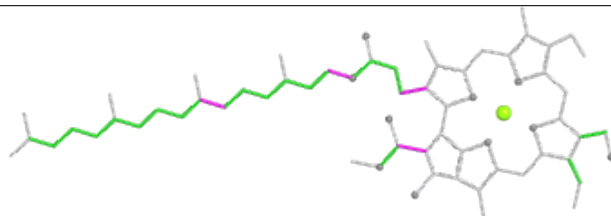
## Ligand CHL Y 601



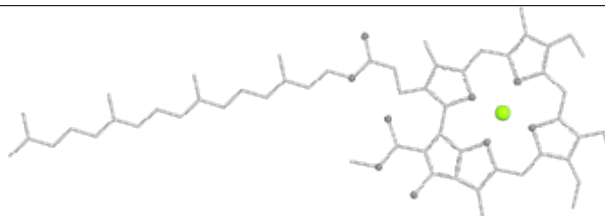
Bond lengths



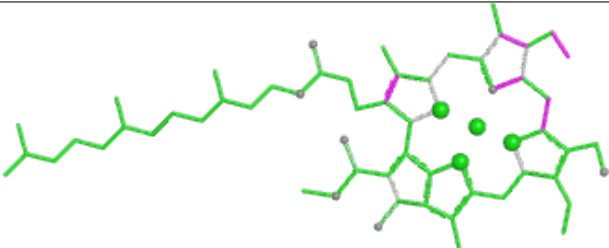
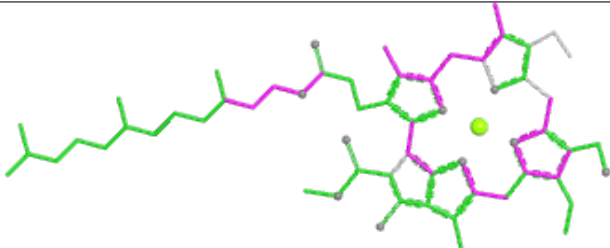
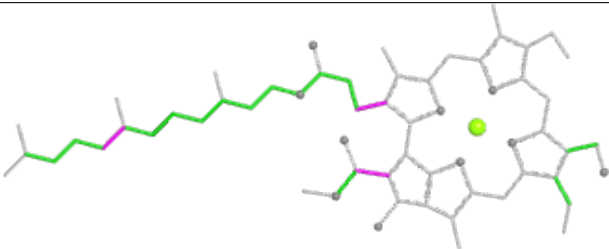
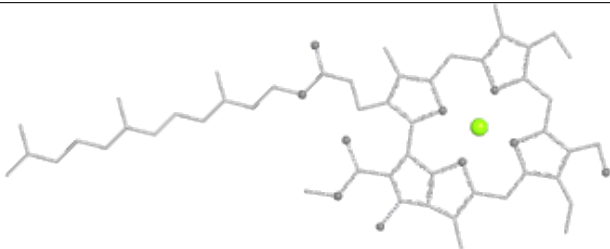
Bond angles

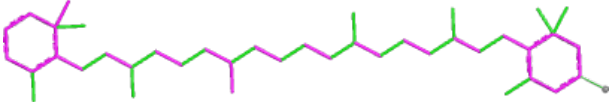

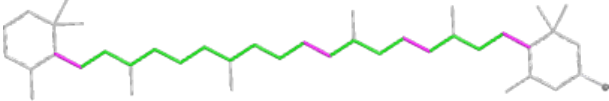



Torsions

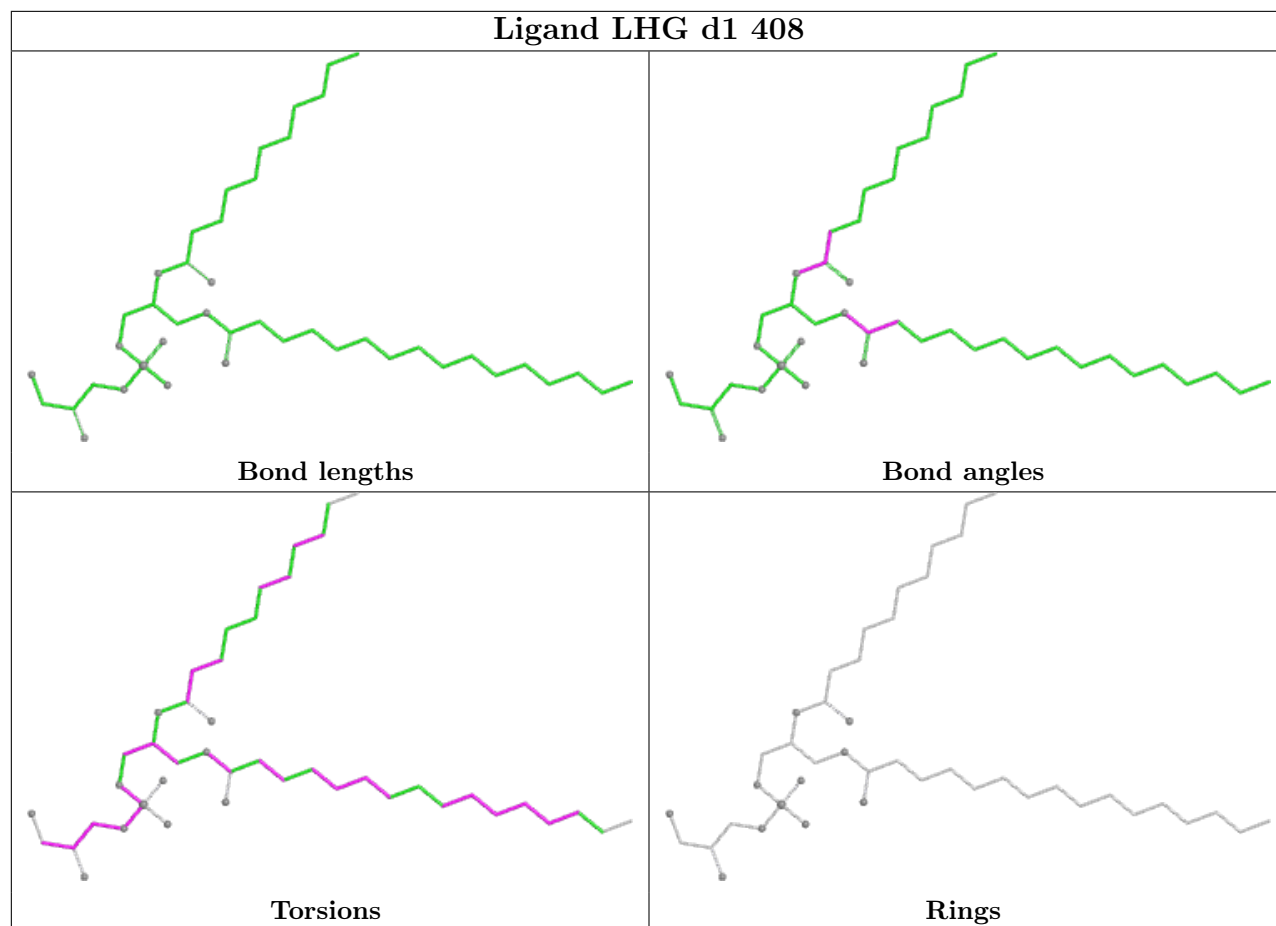


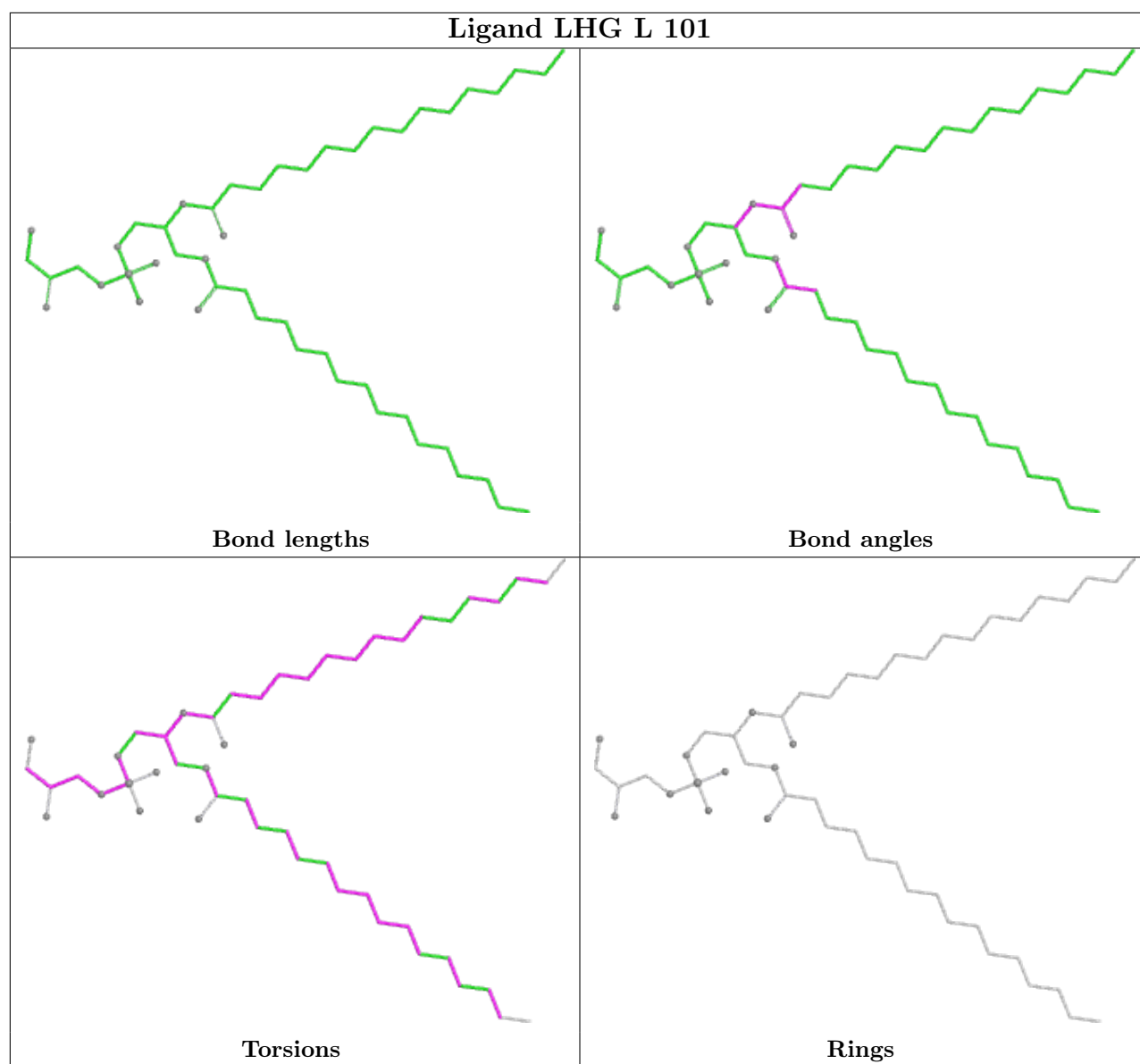
Rings

Ligand CHL s1 608	
	
Bond lengths	Bond angles
	
Torsions	Rings

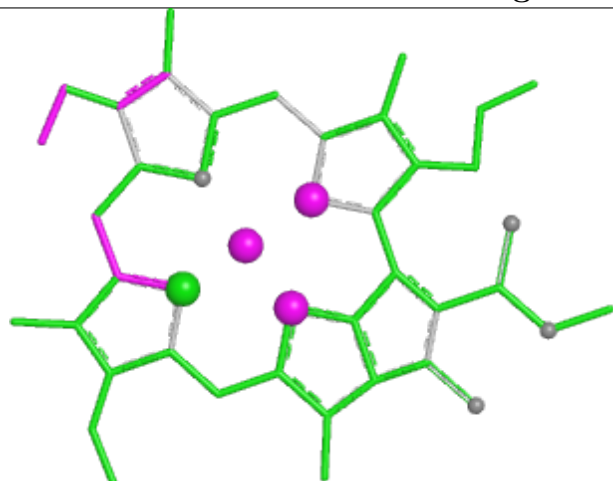
Ligand RRX h 101	
	
Bond lengths	Bond angles
	
Torsions	Rings



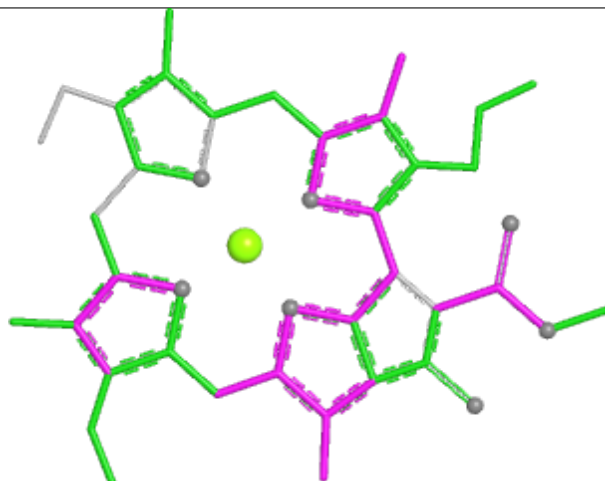




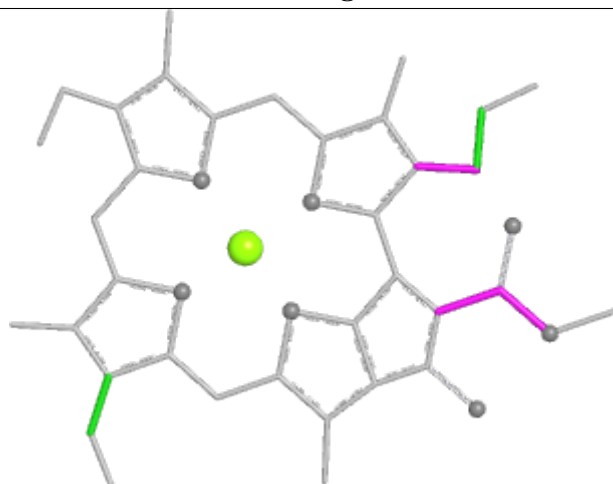
## Ligand CLA G 612



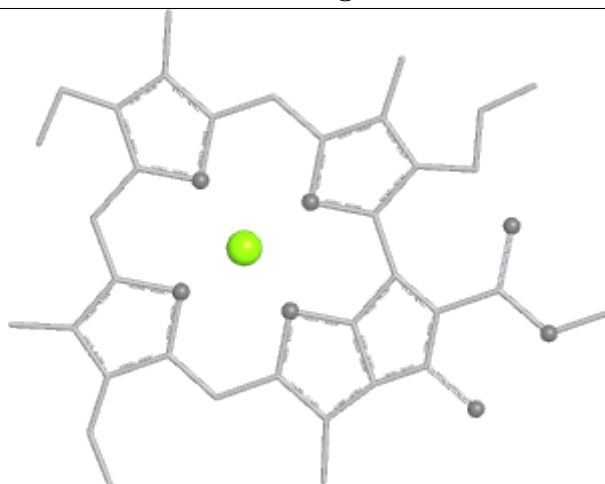
Bond lengths



Bond angles

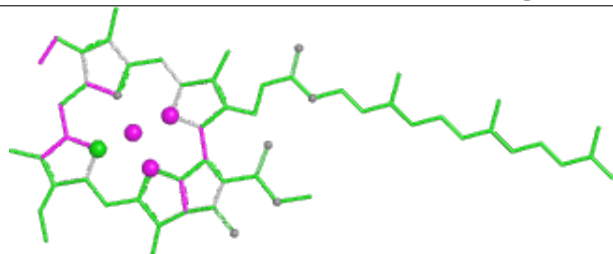


Torsions

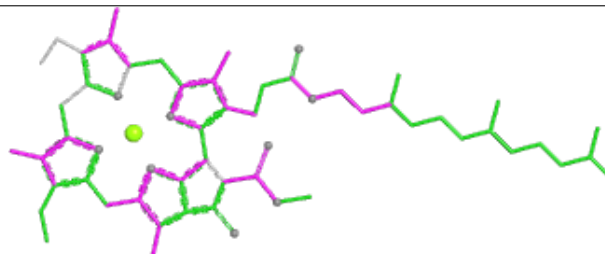


Rings

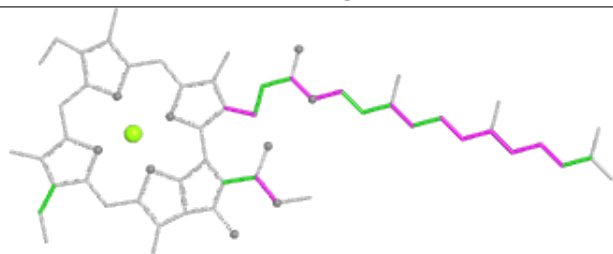
## Ligand CLA a 410



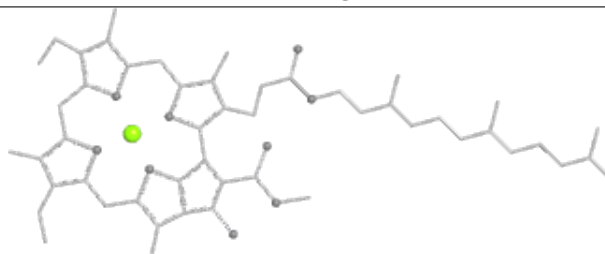
Bond lengths



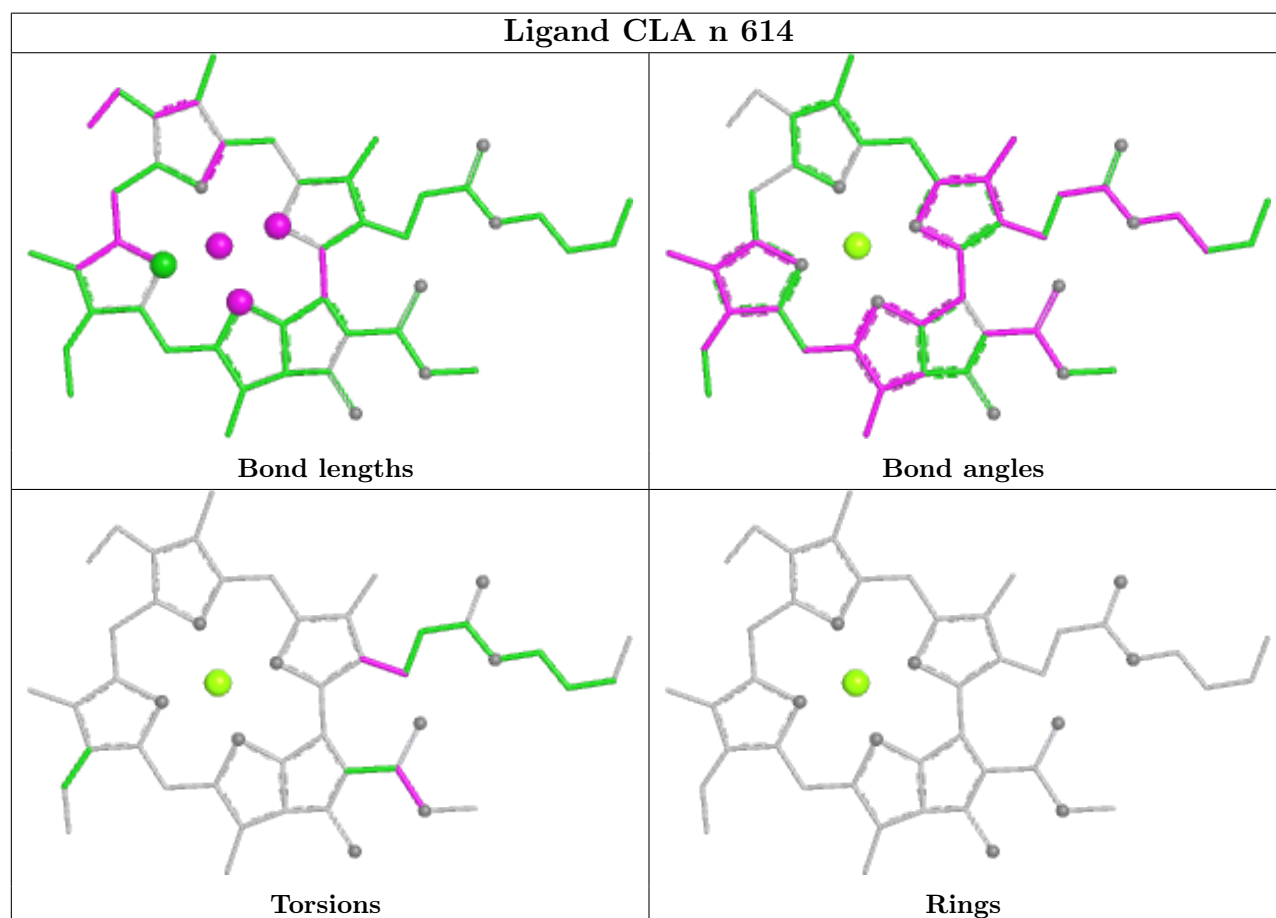
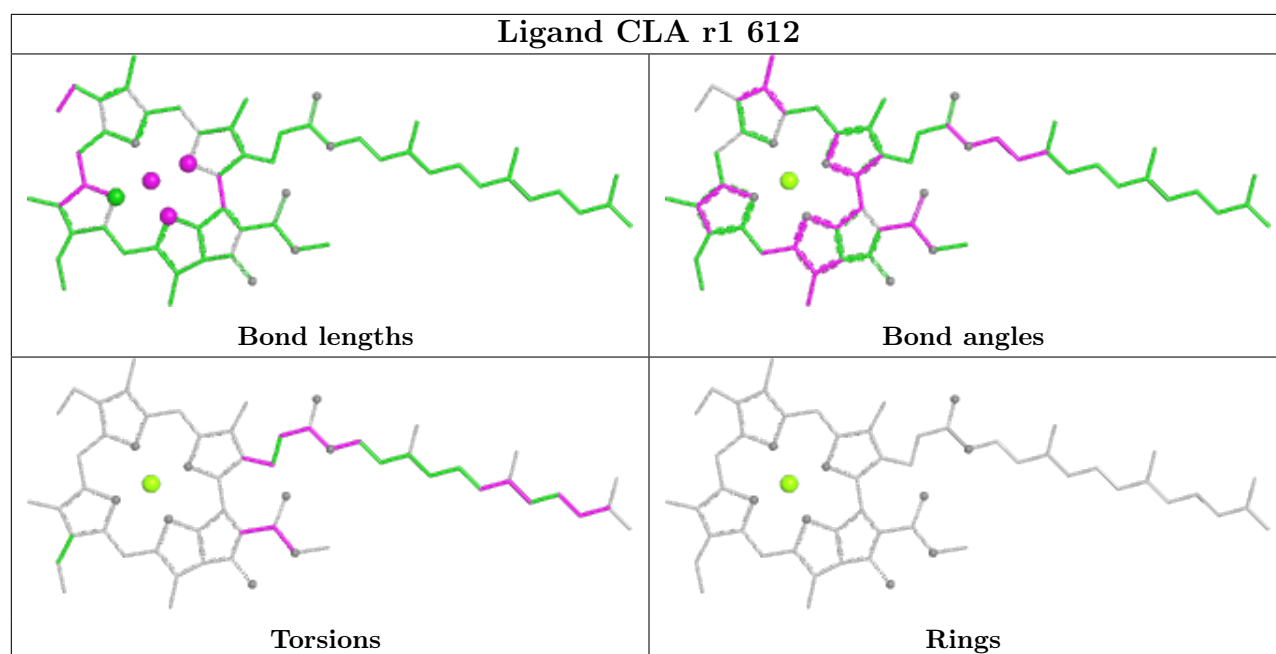
Bond angles

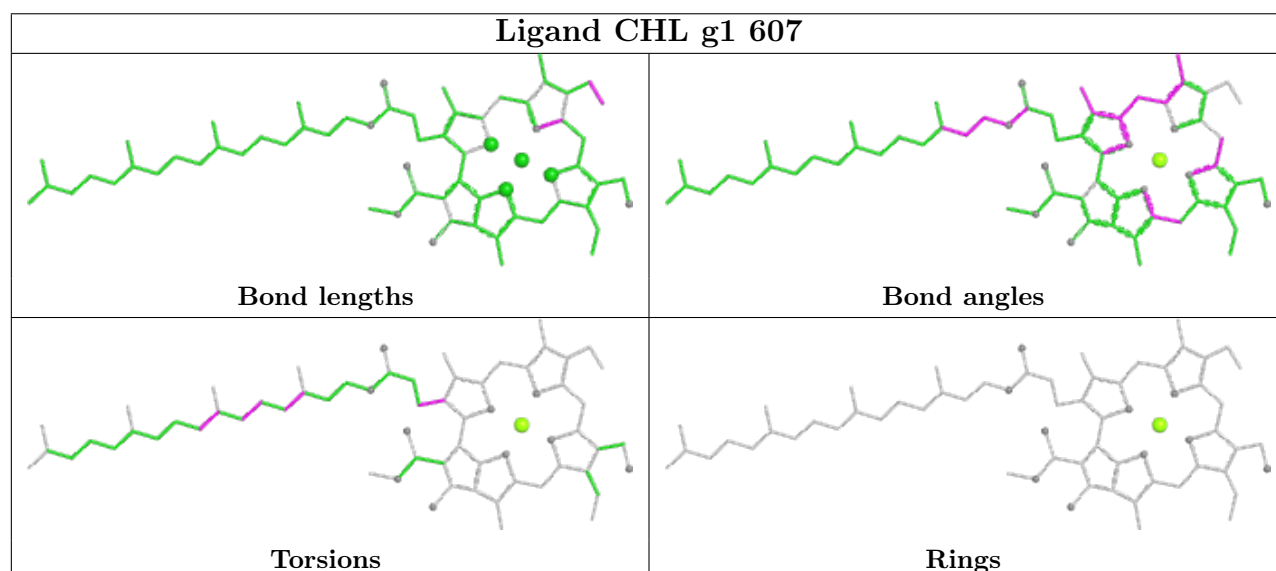
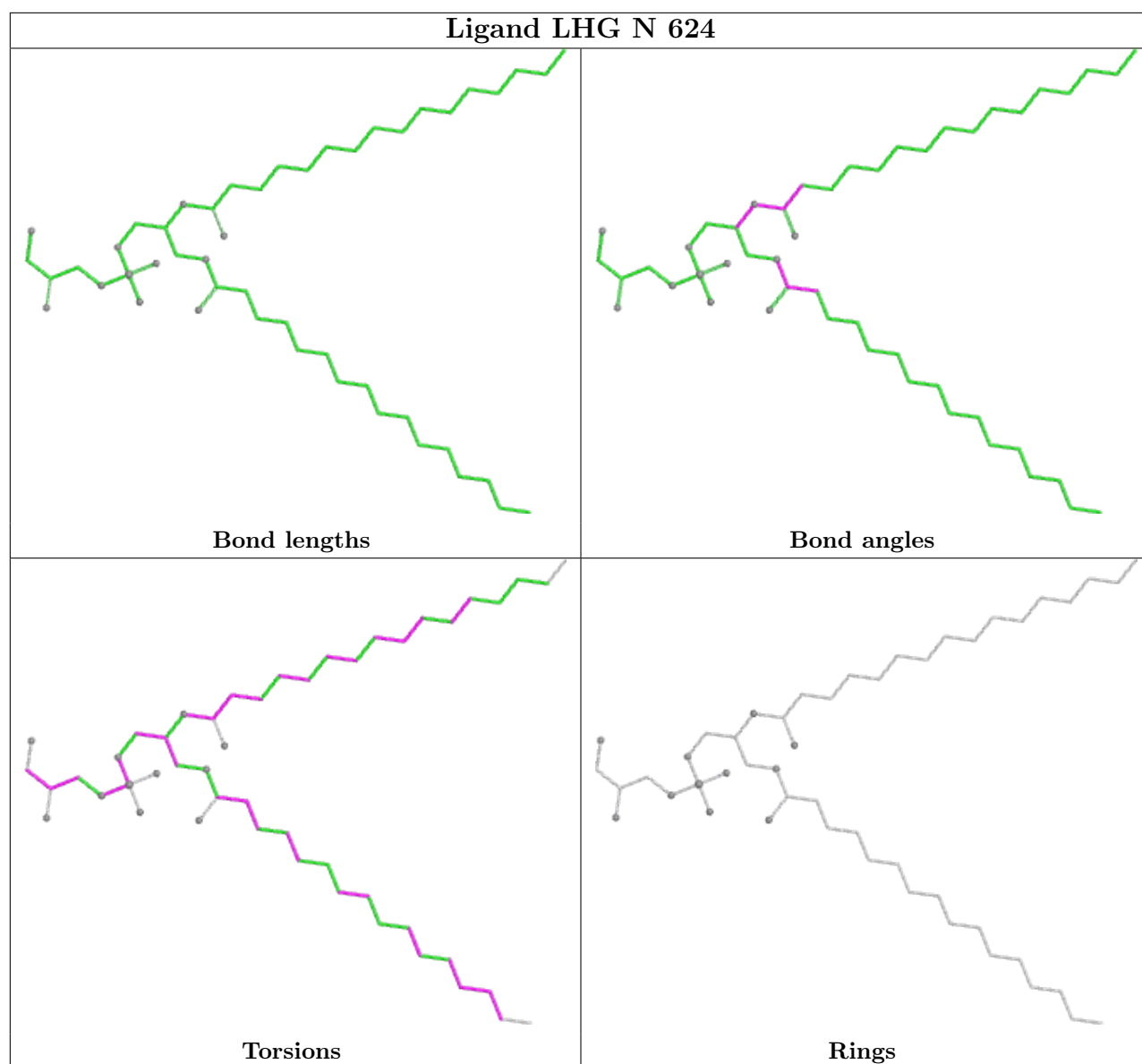


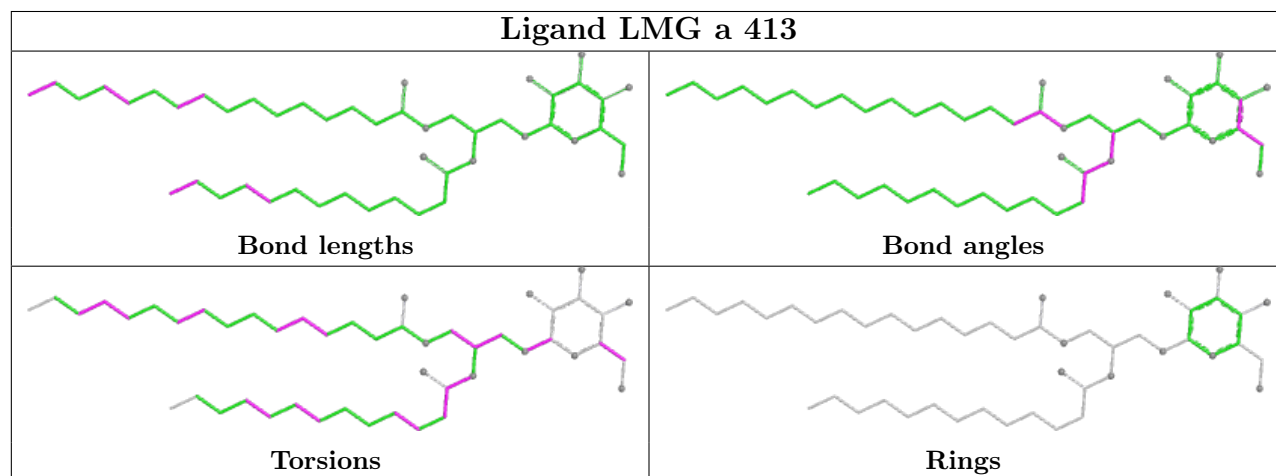
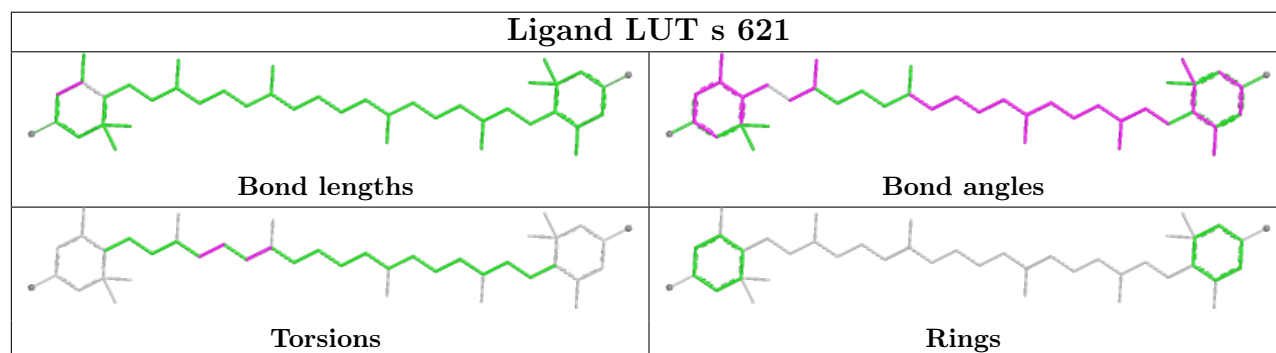
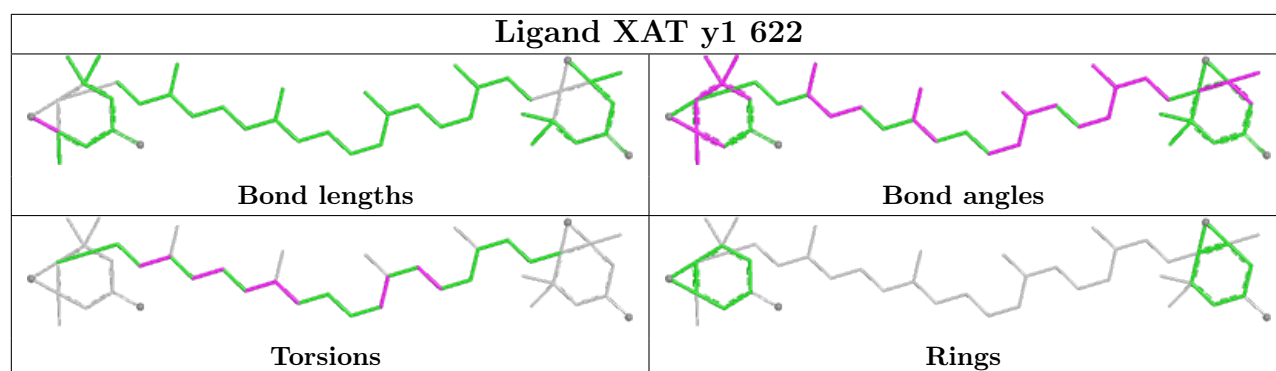
Torsions

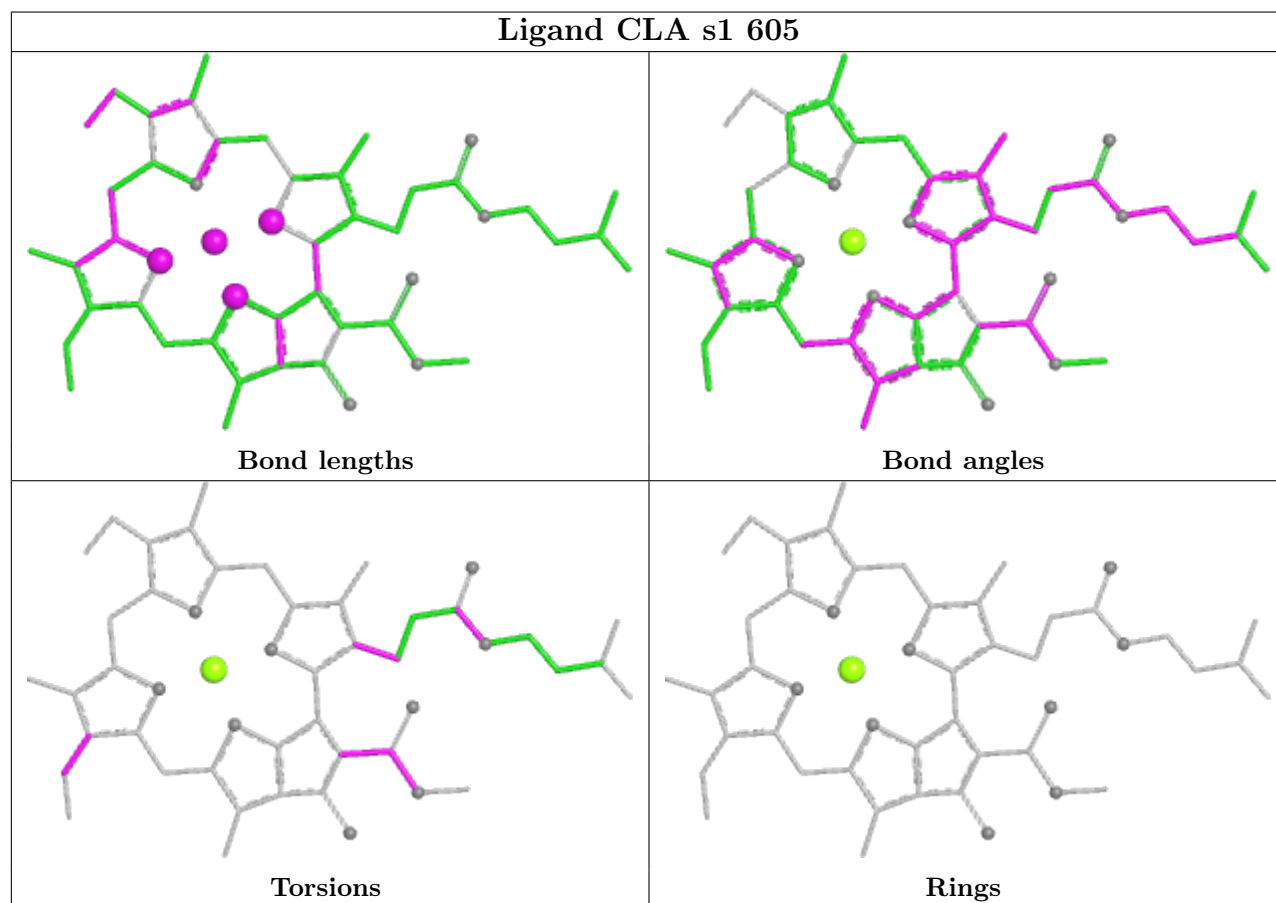
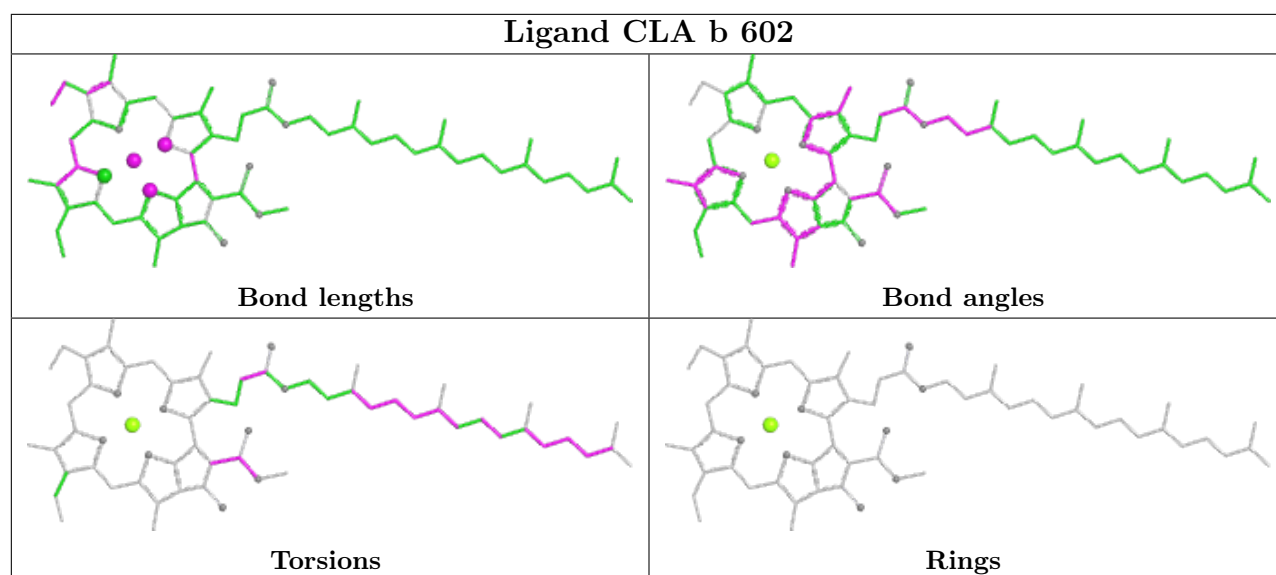


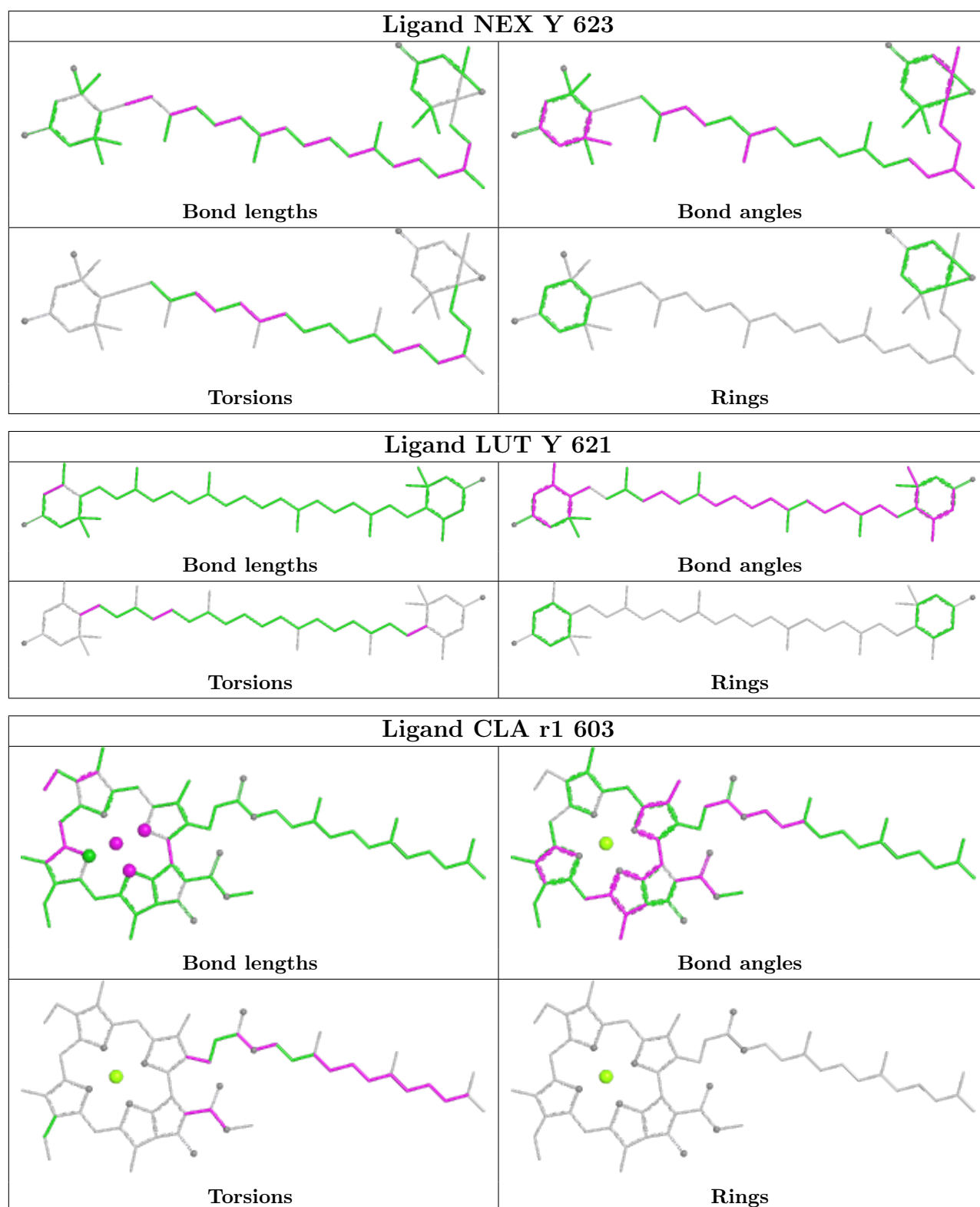
Rings



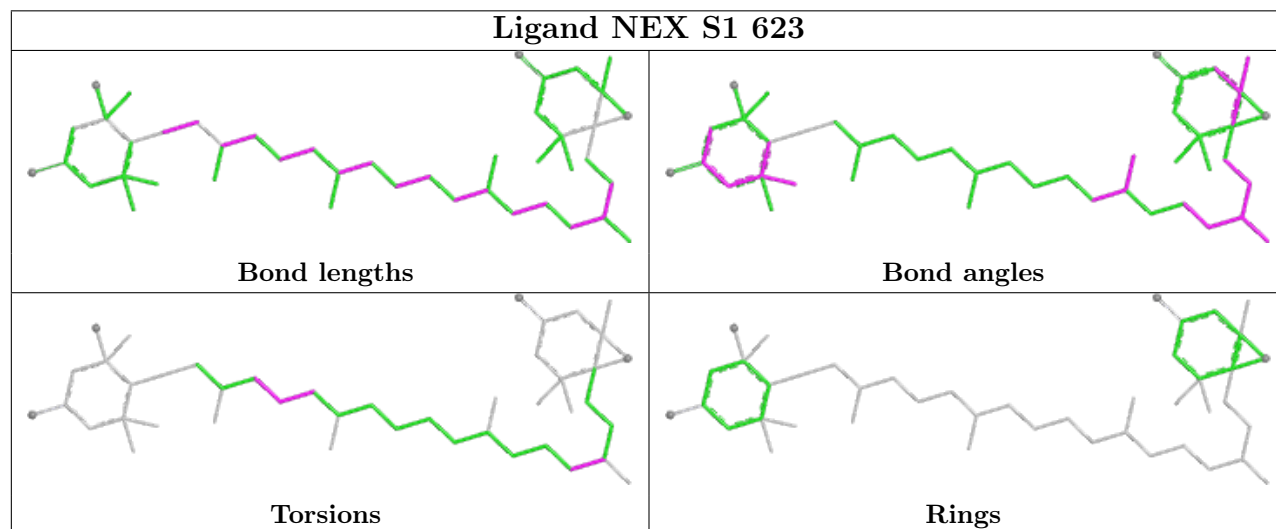
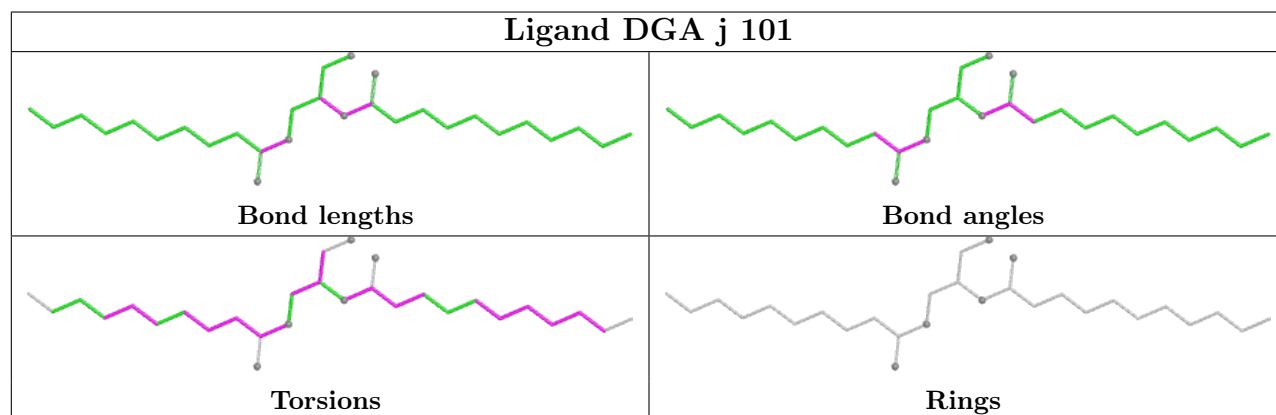
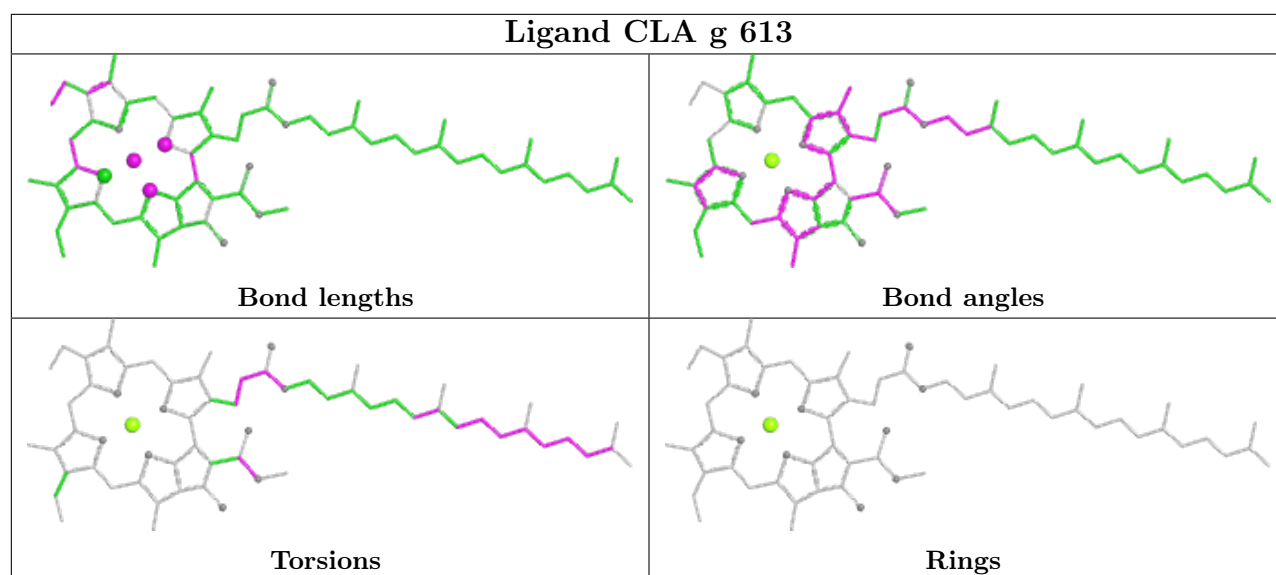


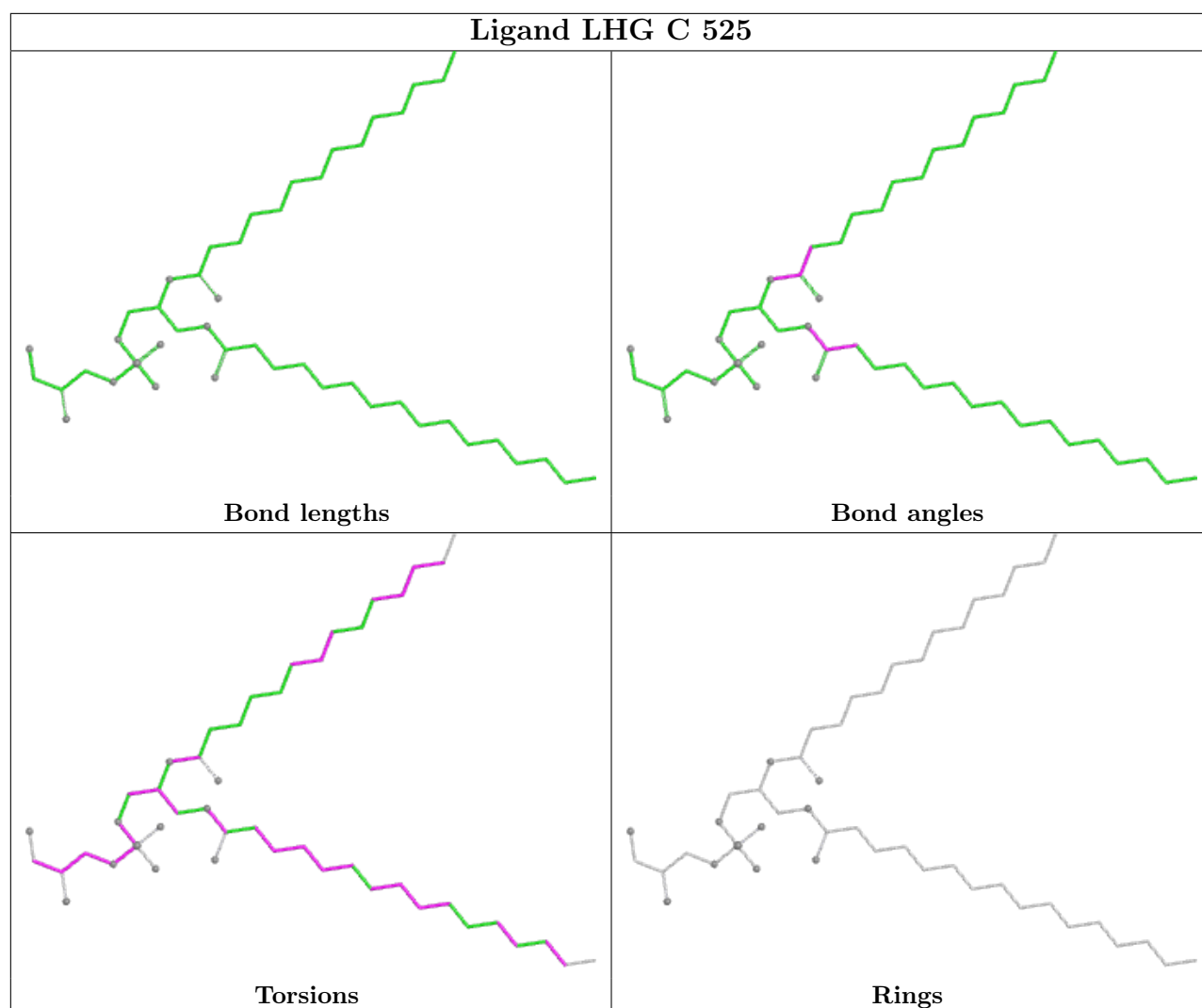


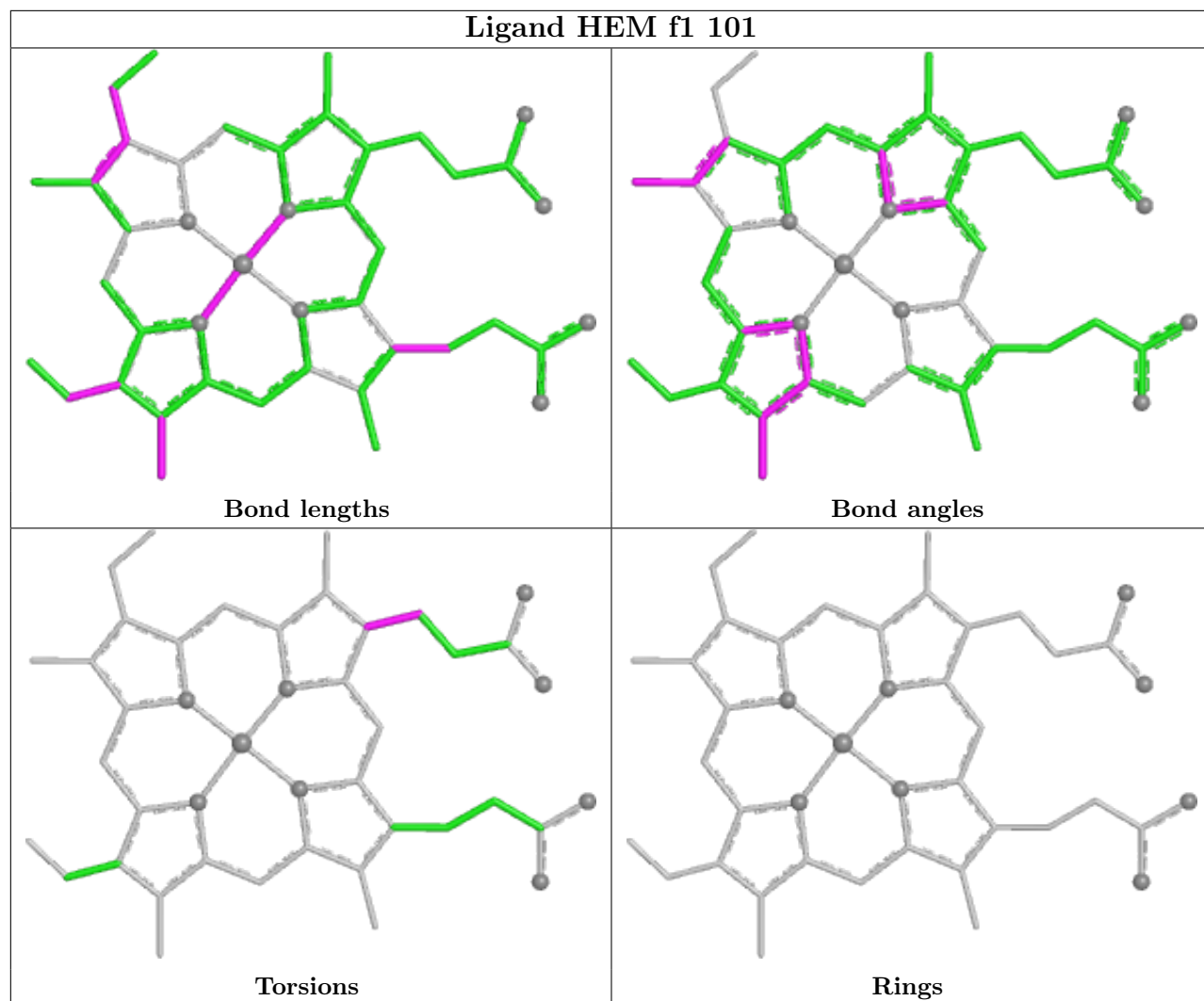


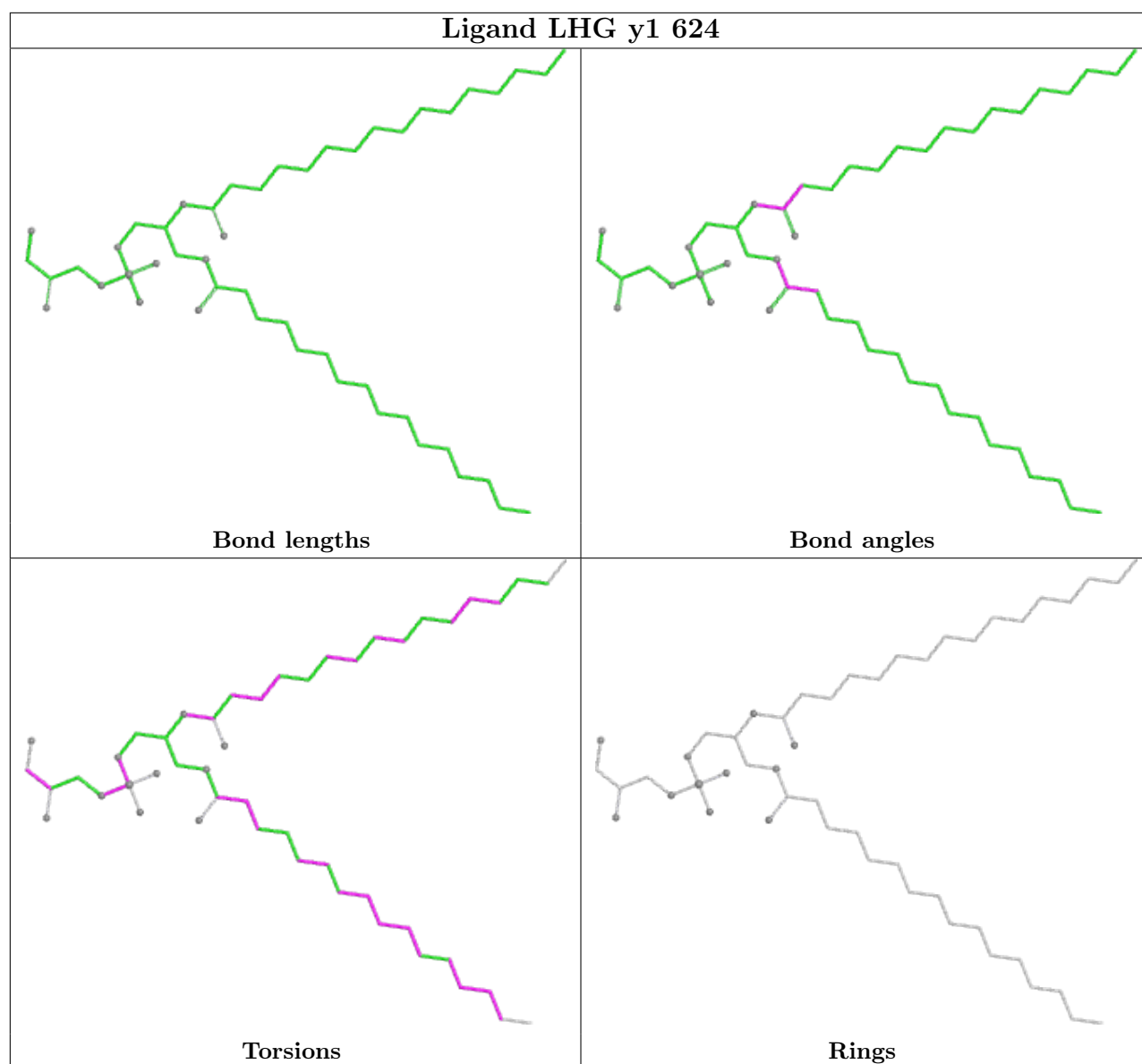


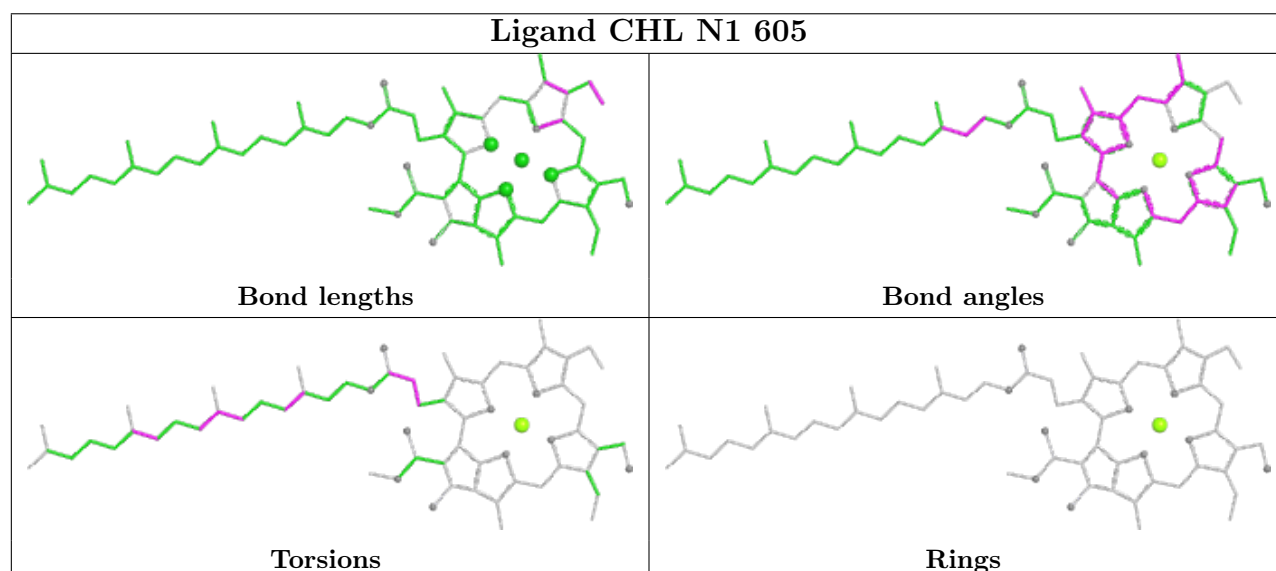
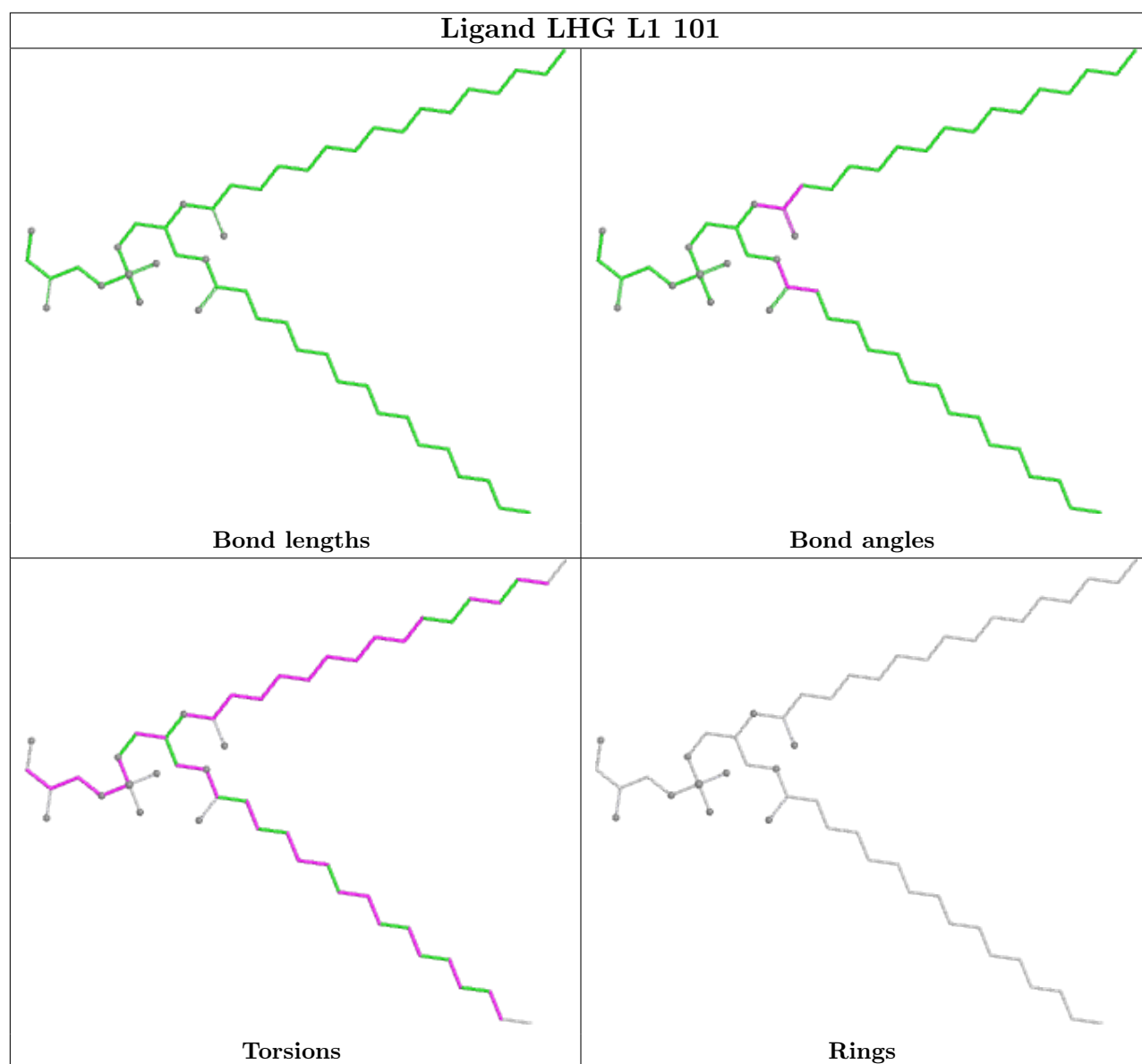


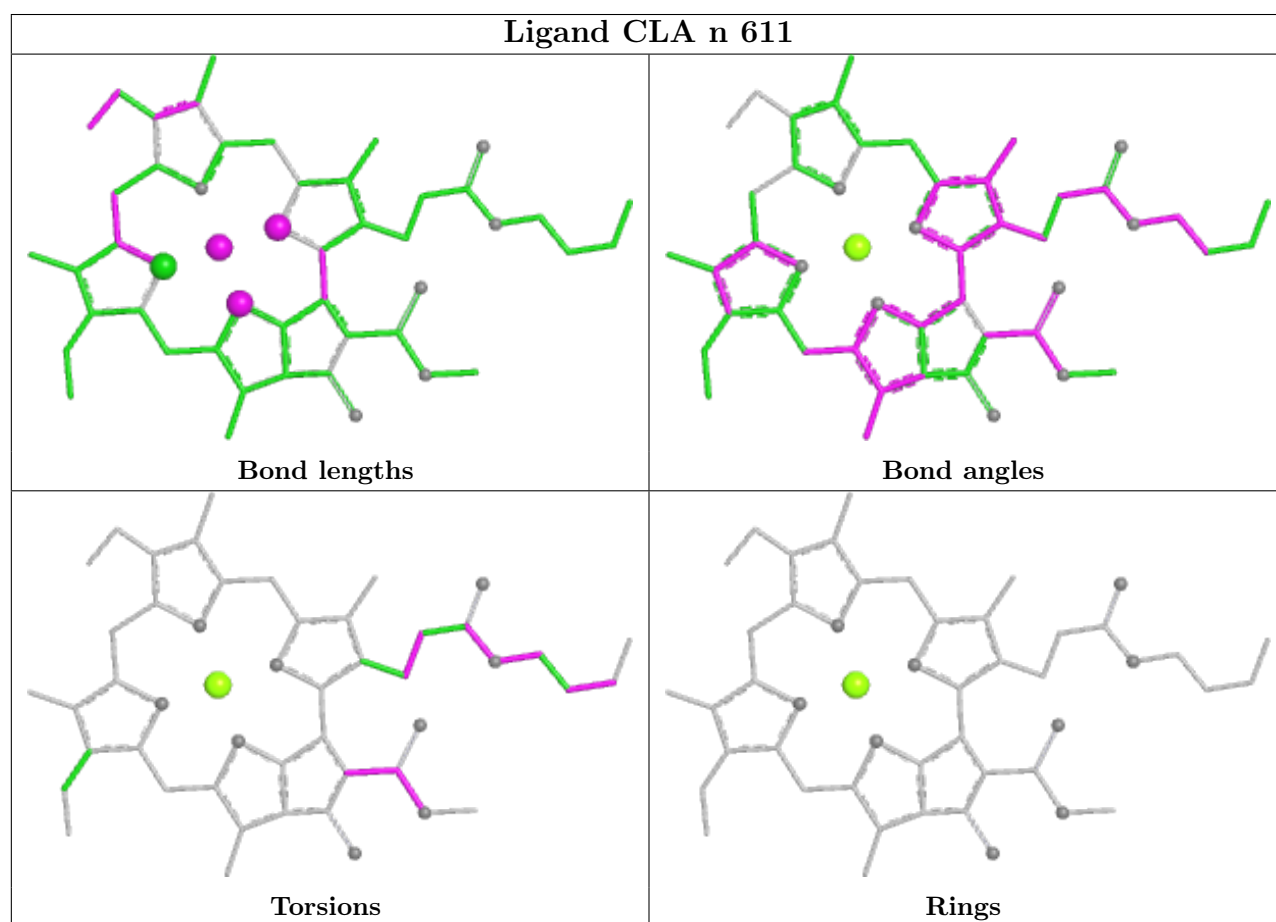
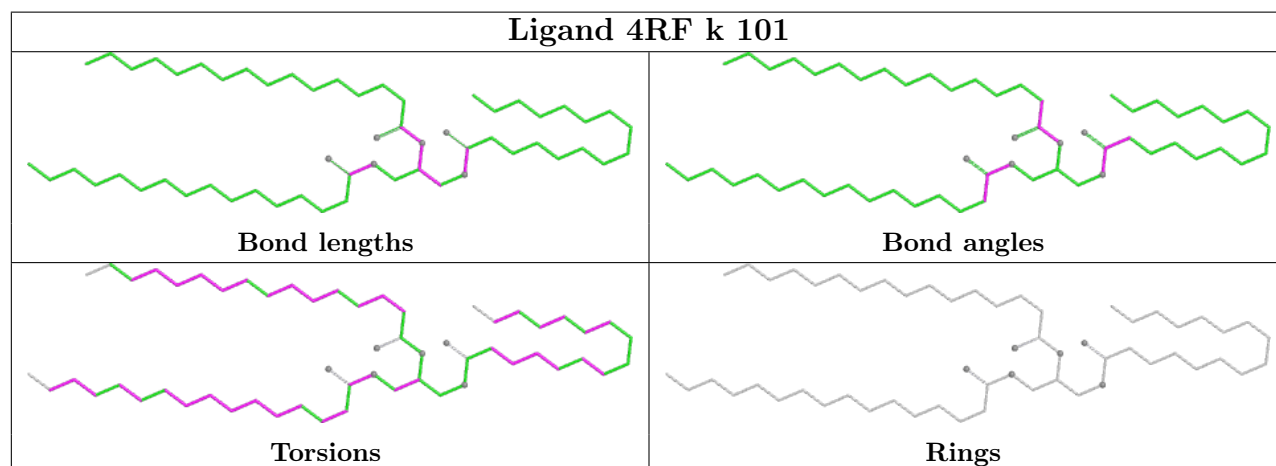
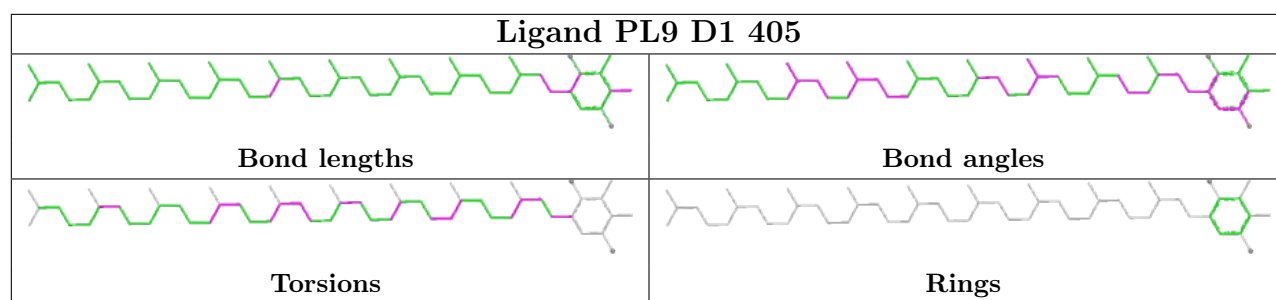


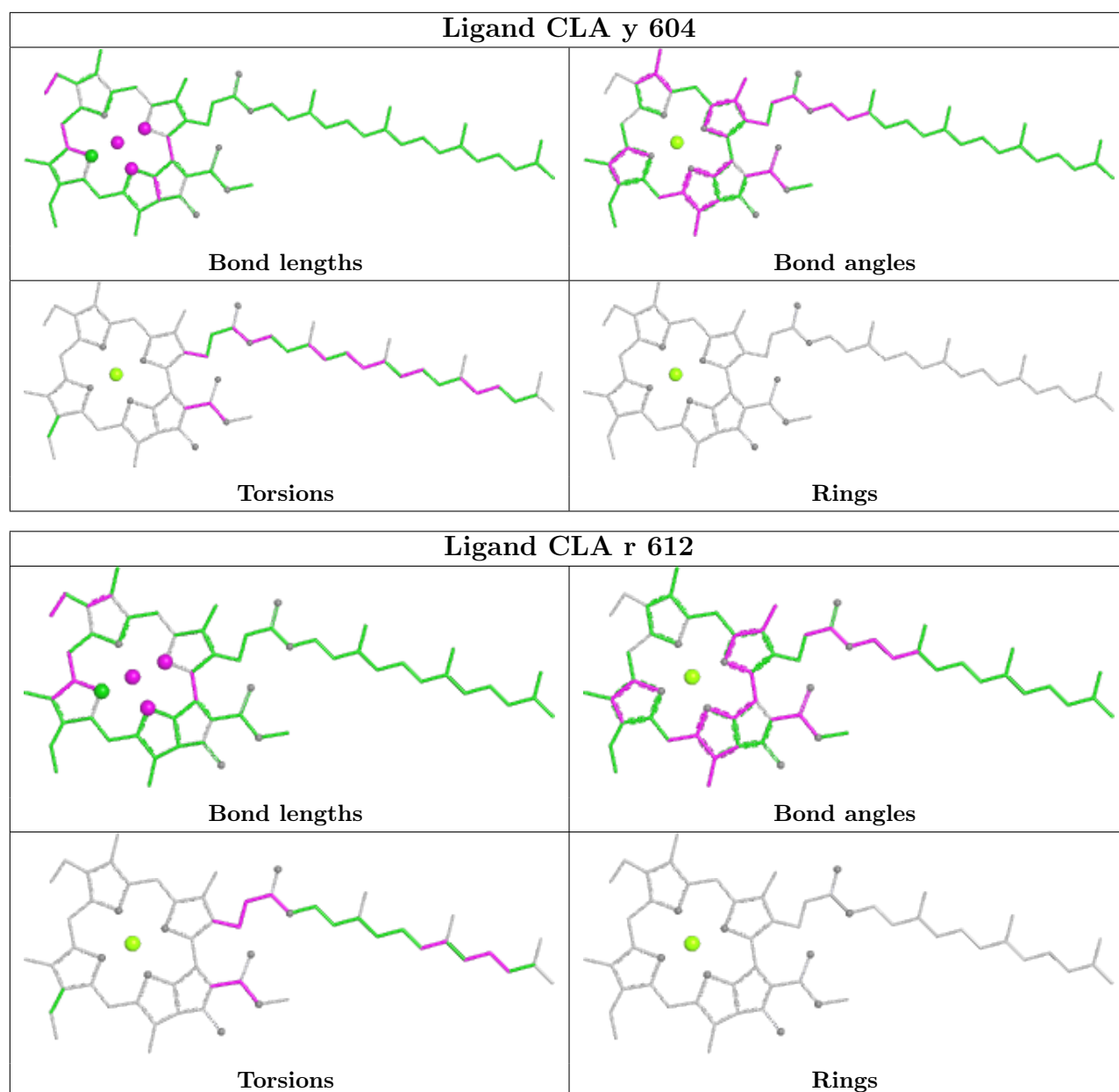


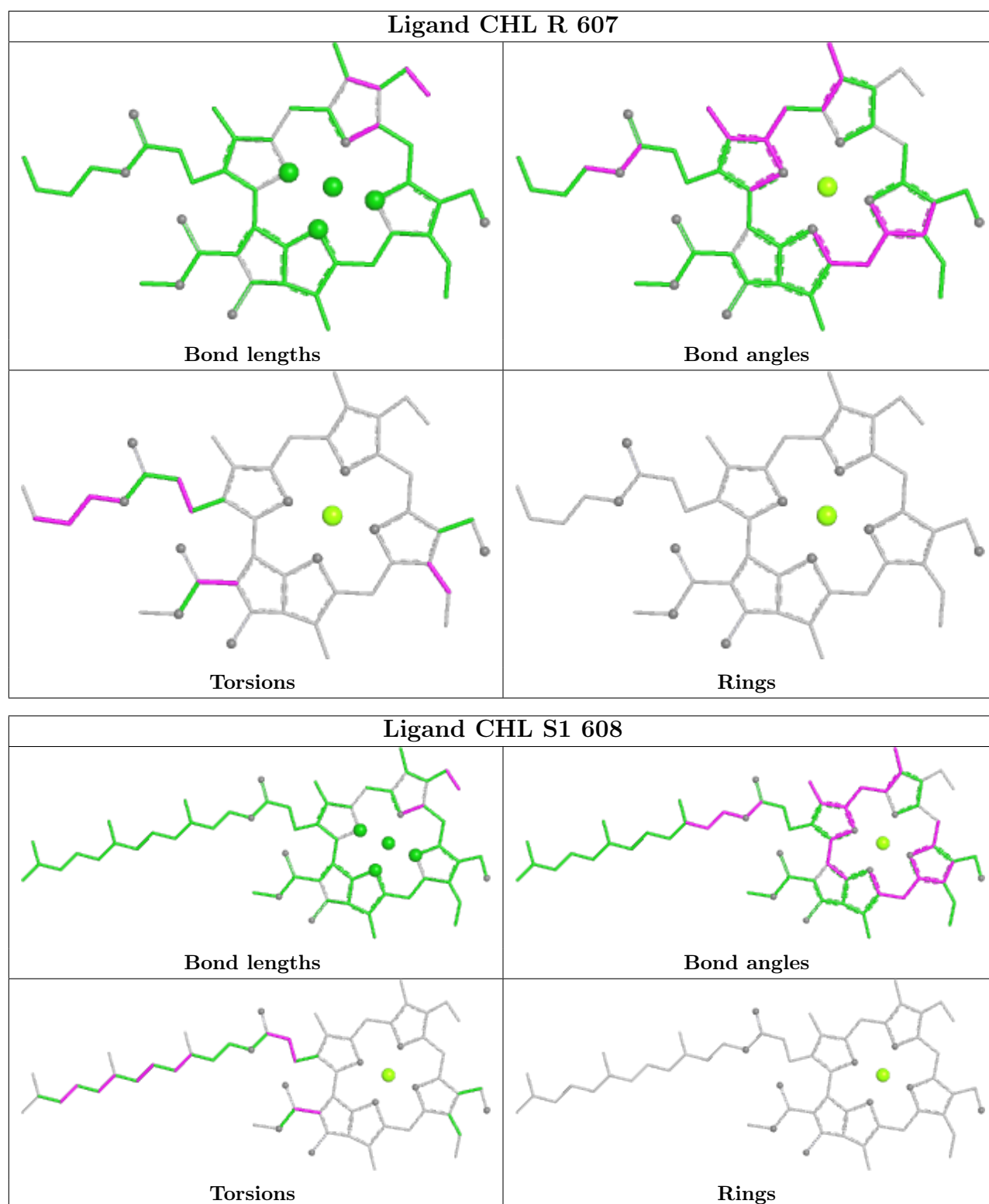




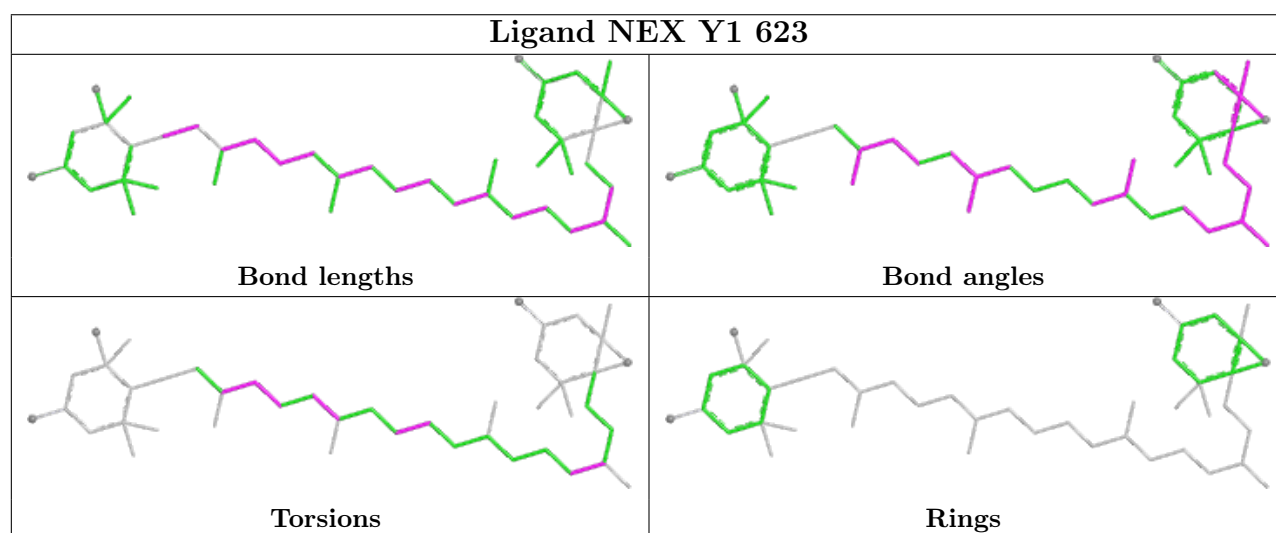
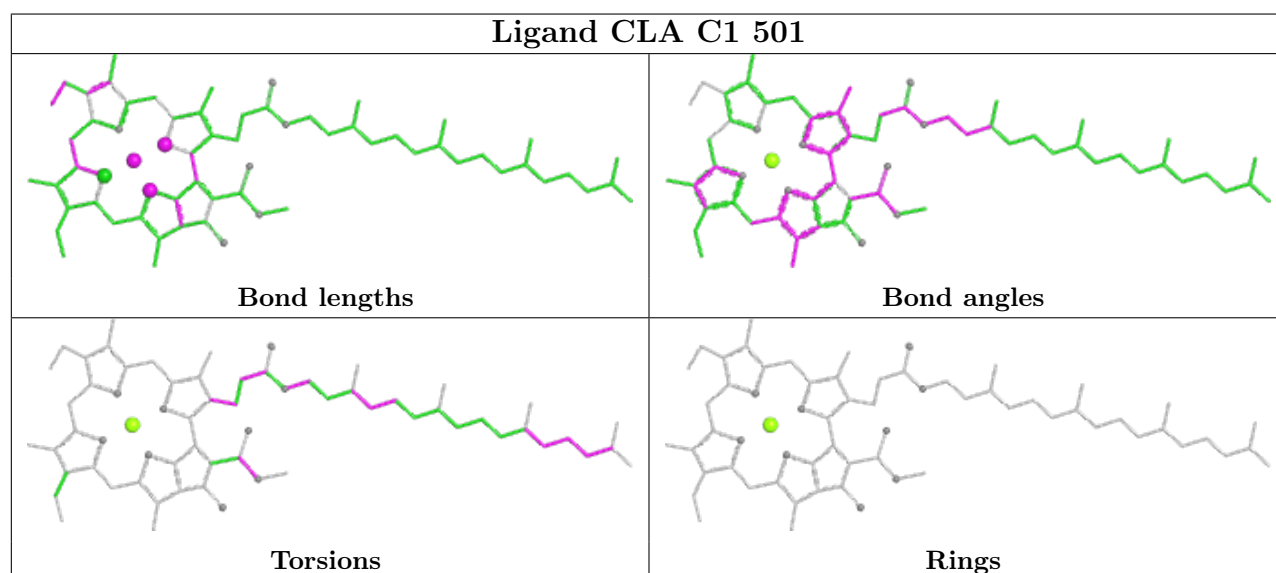
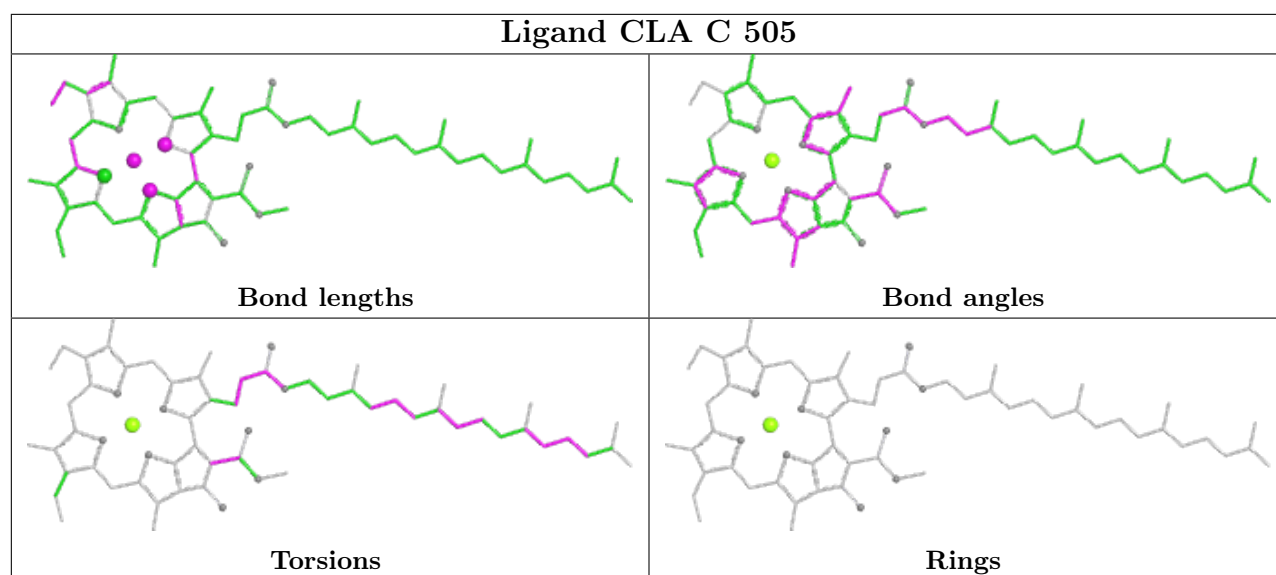


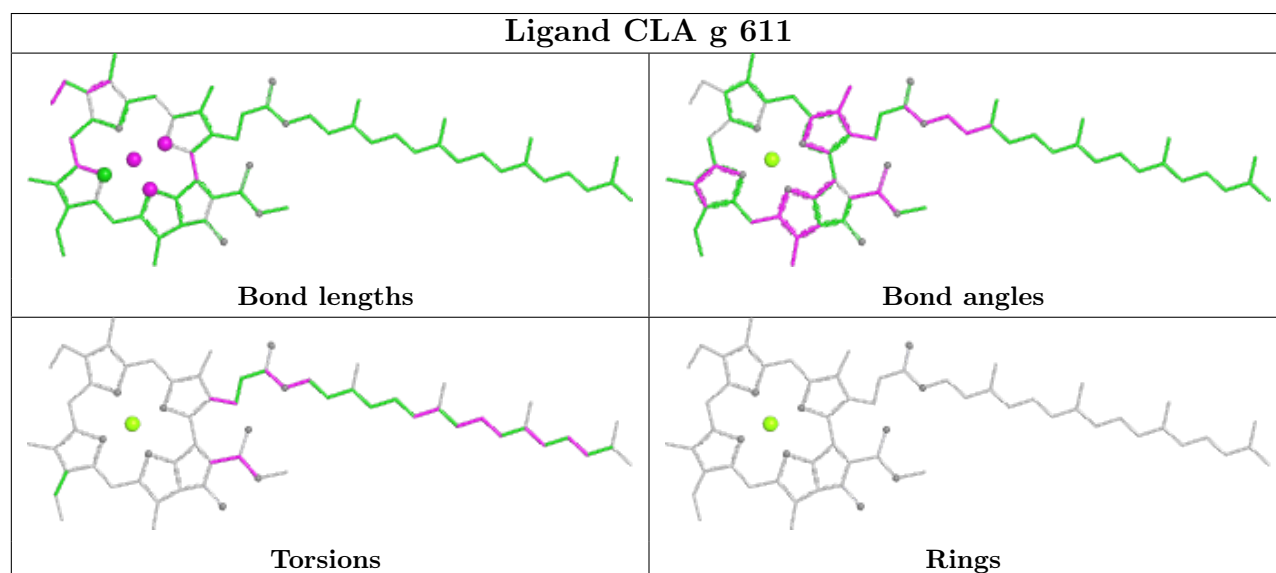
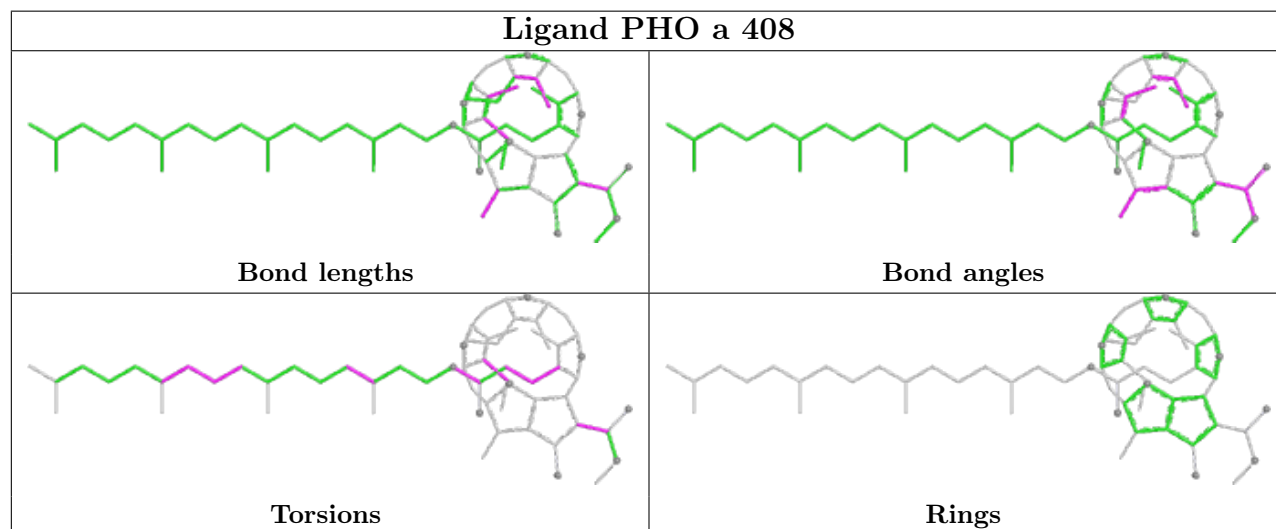
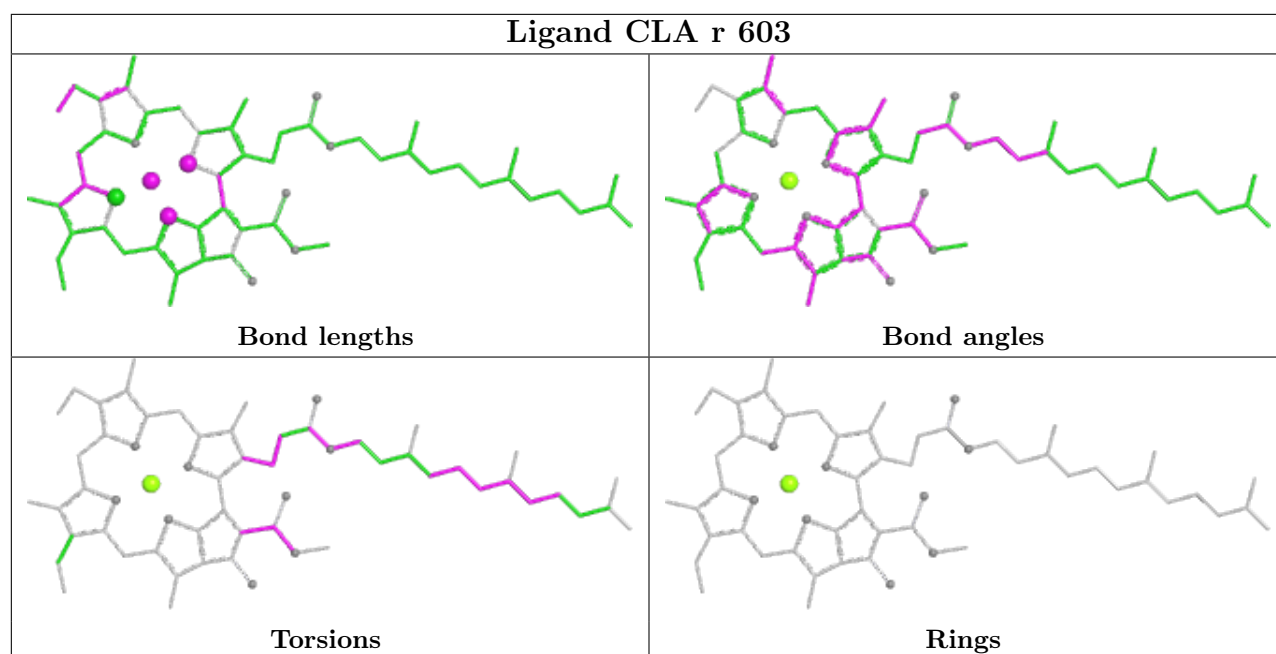


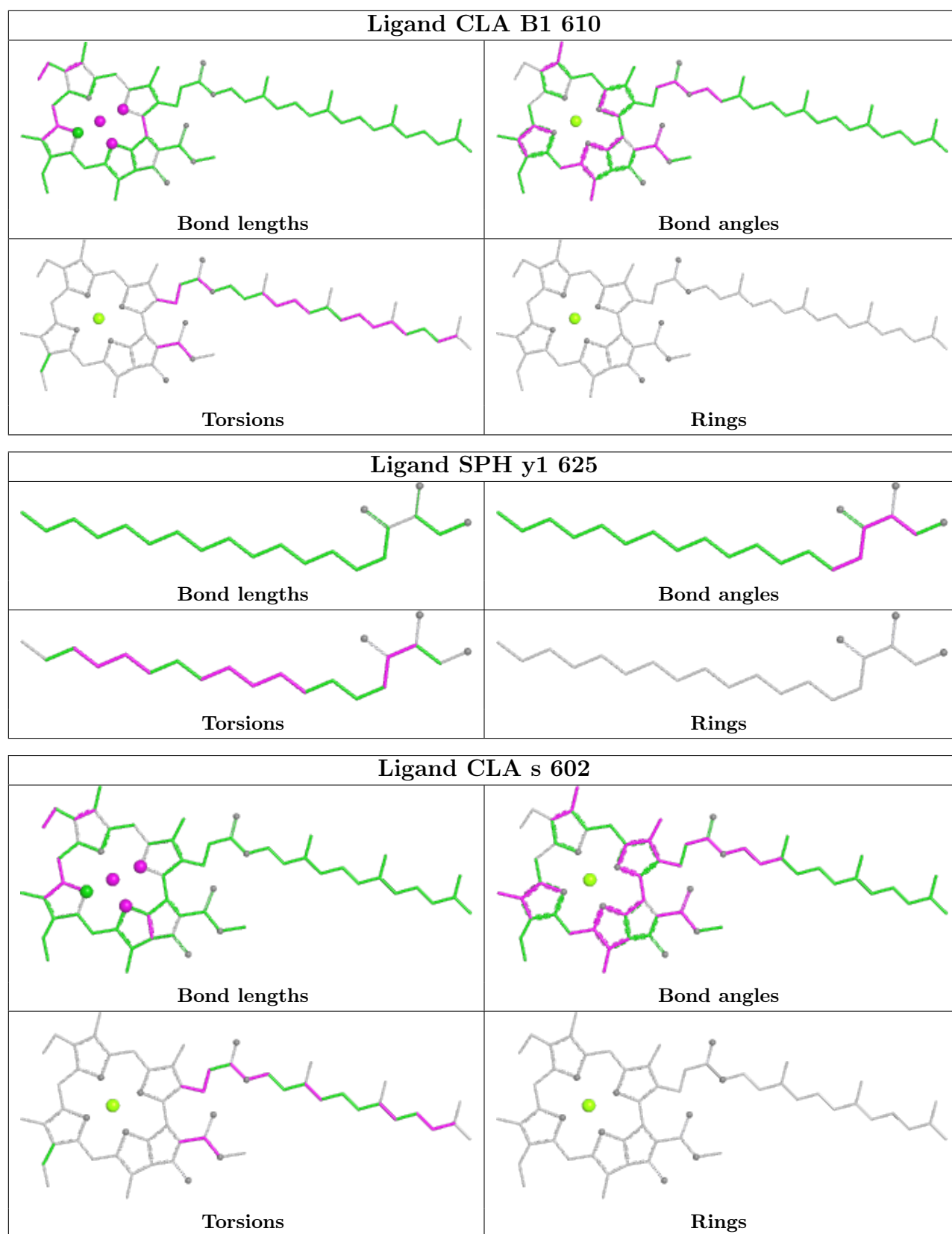


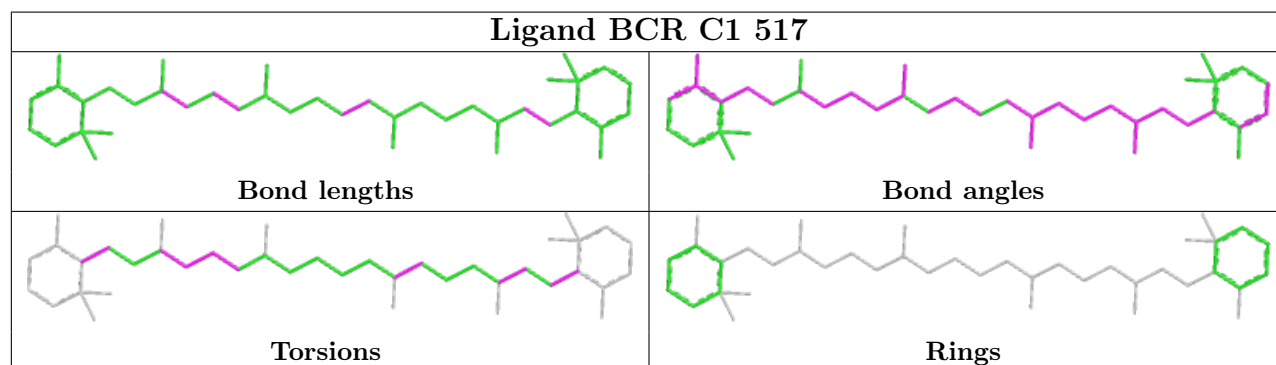
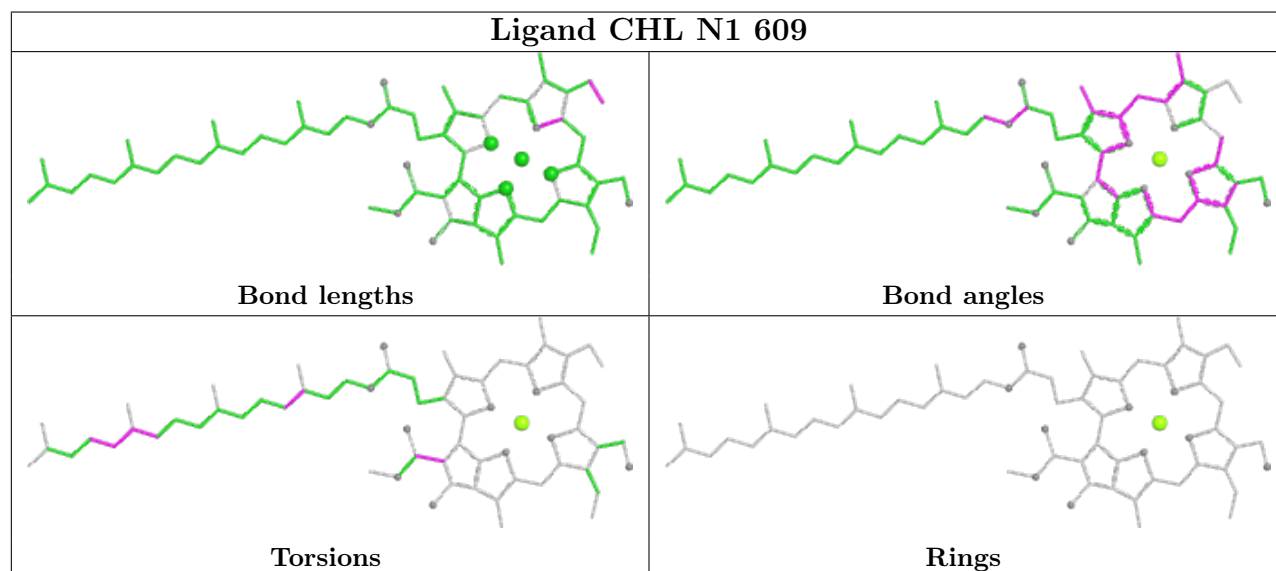
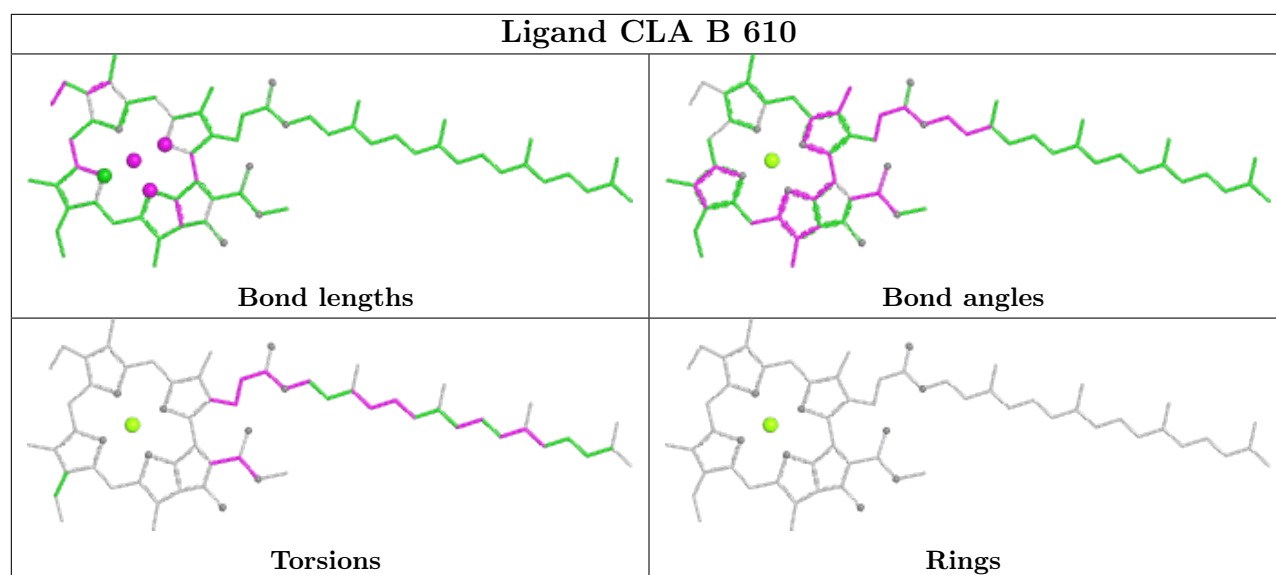


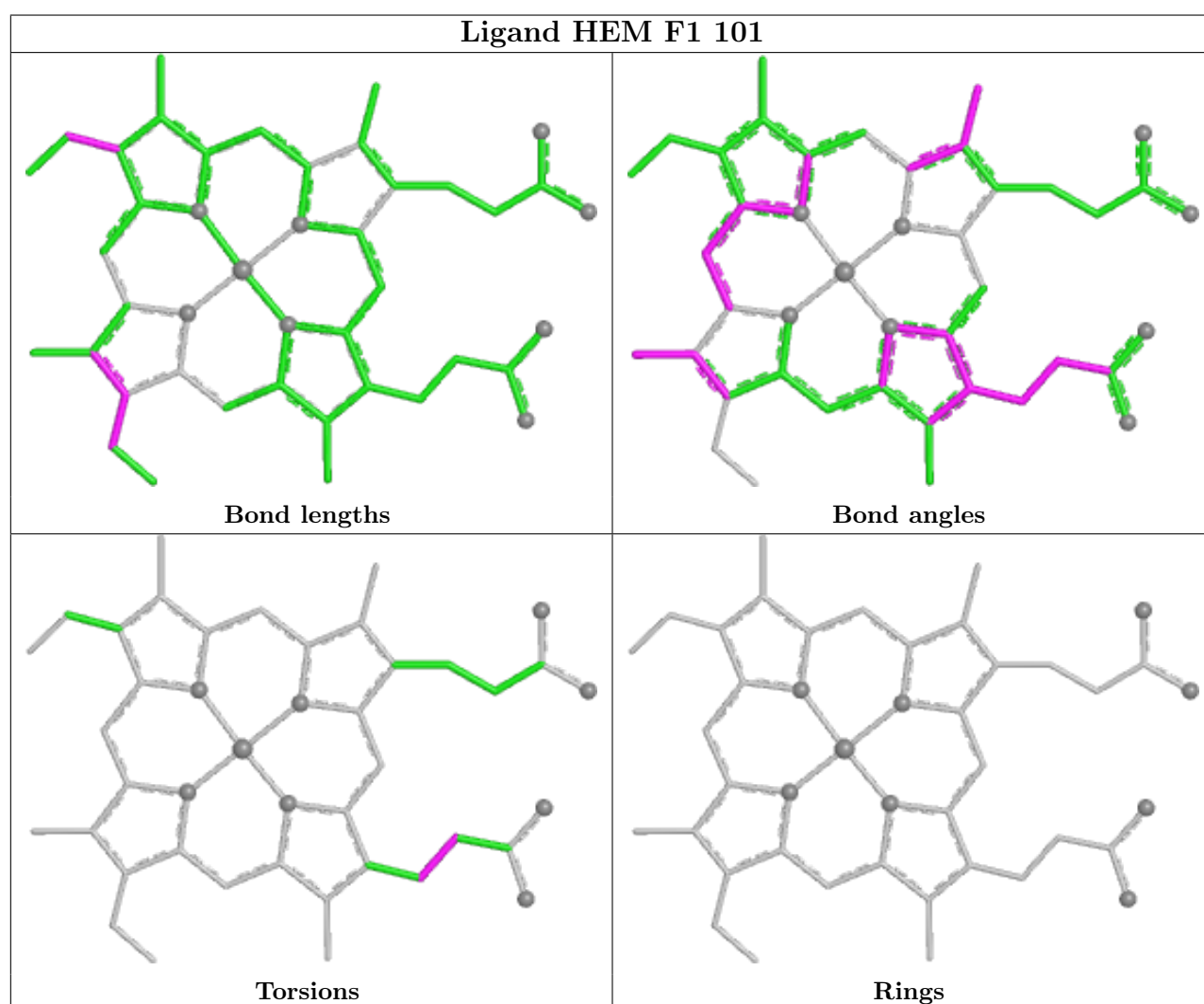
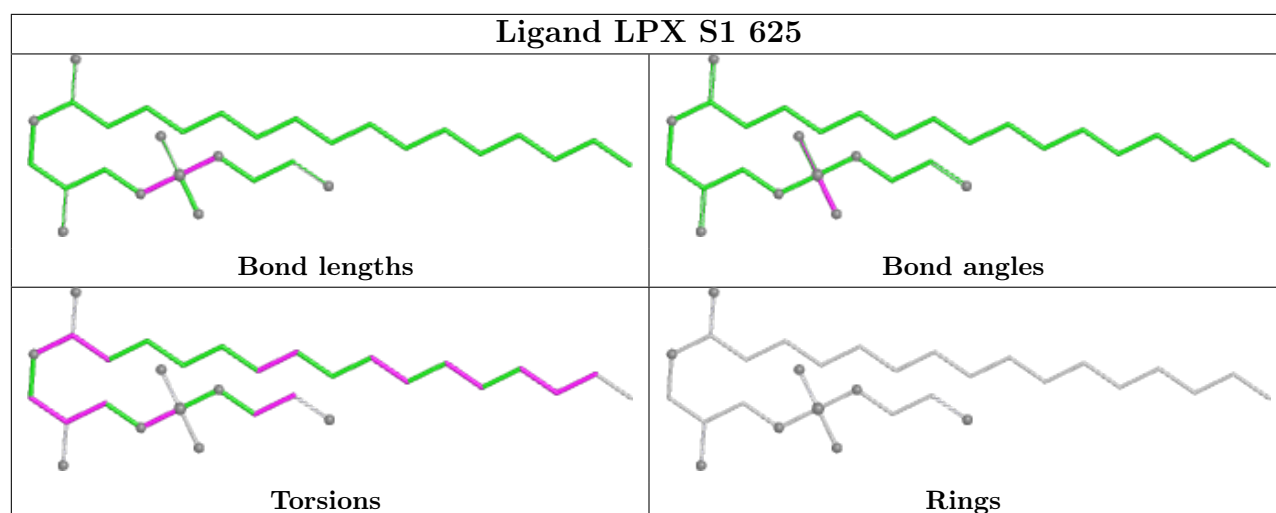


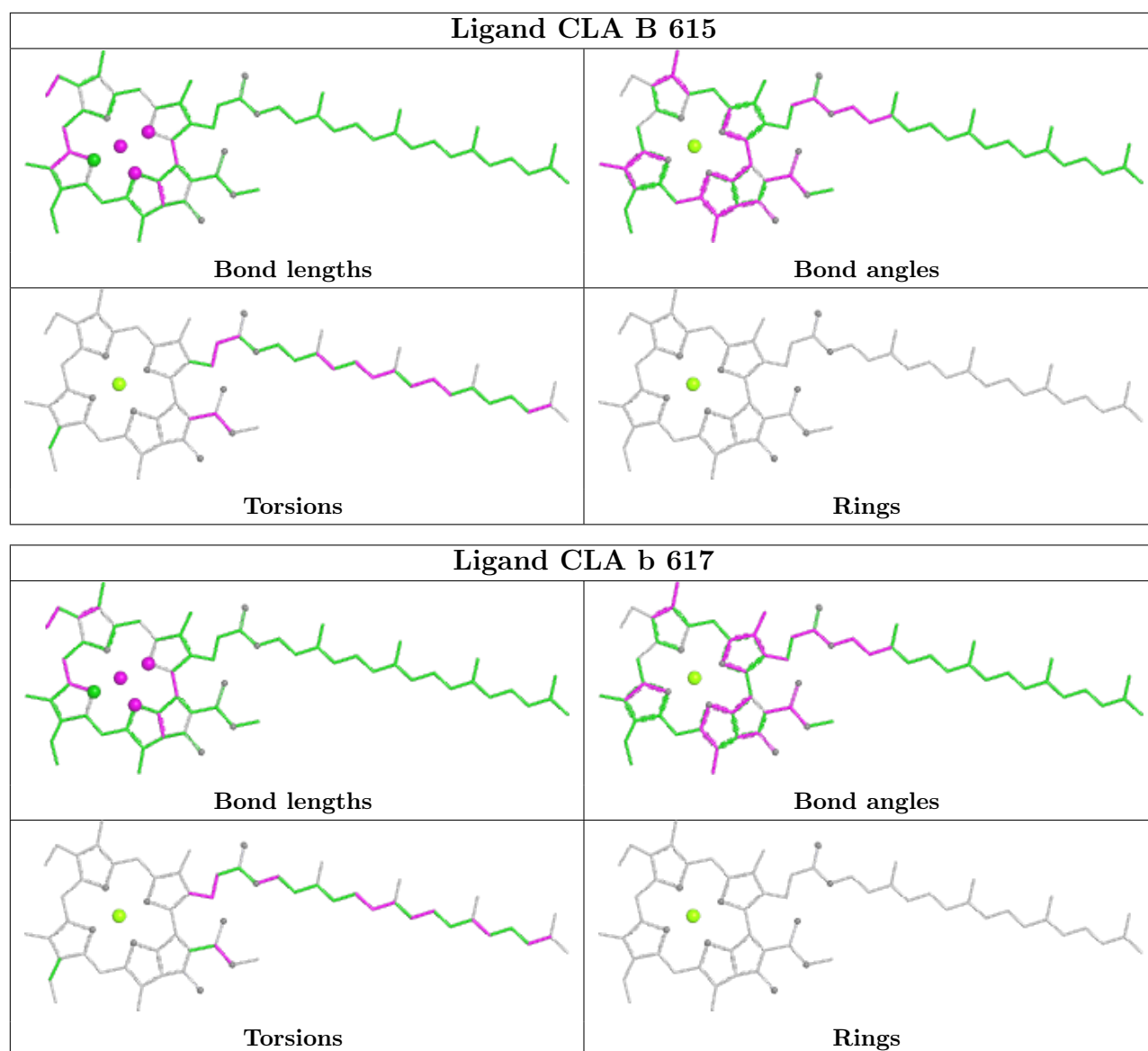


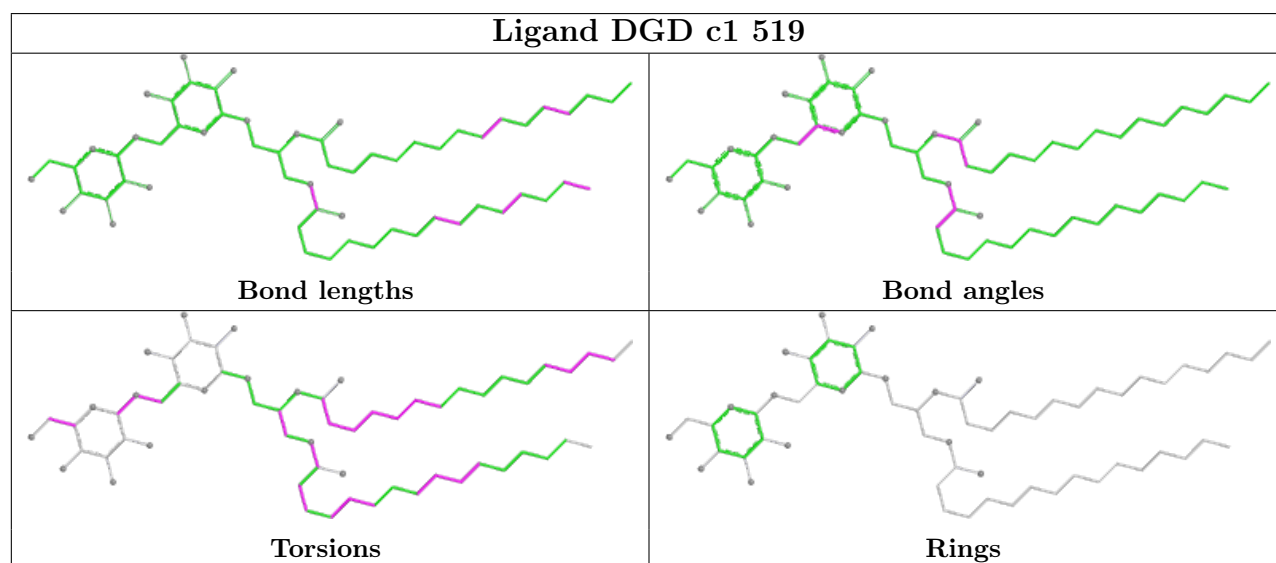
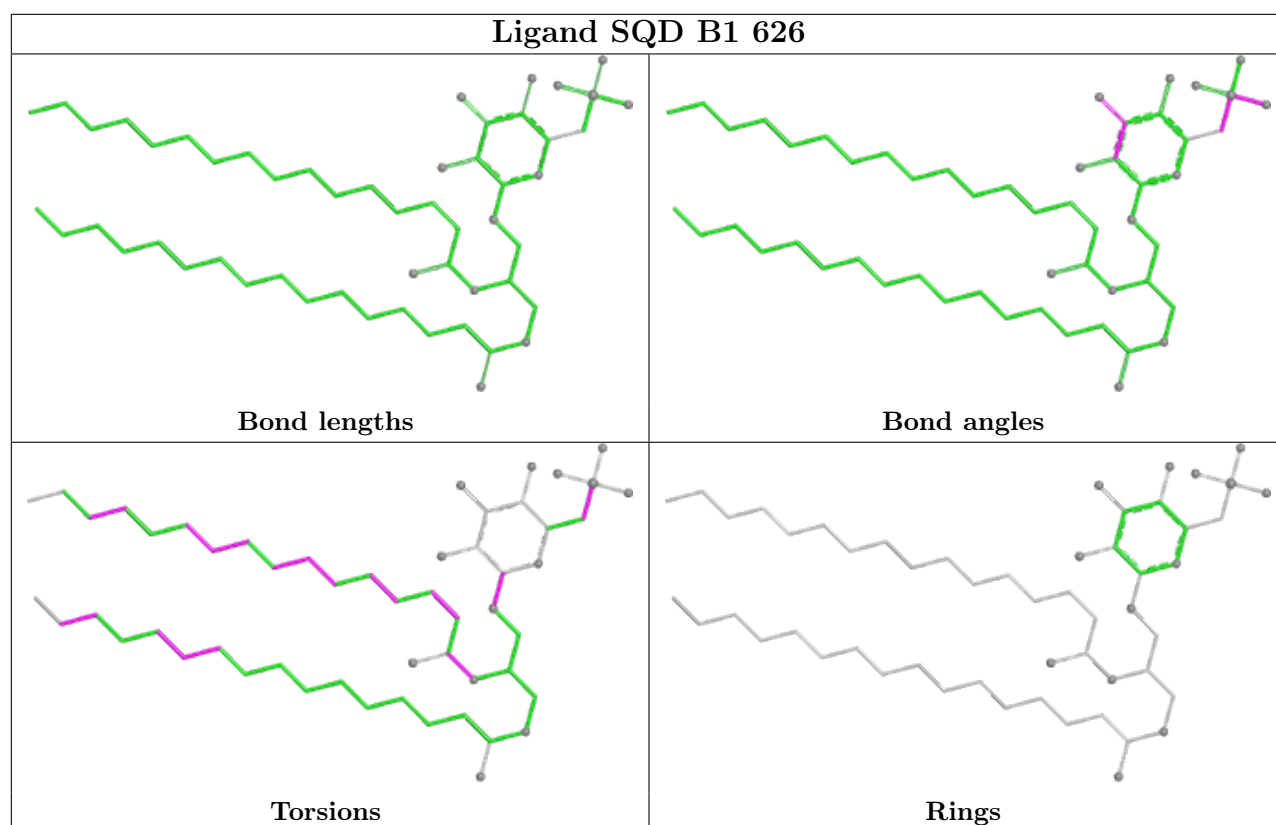


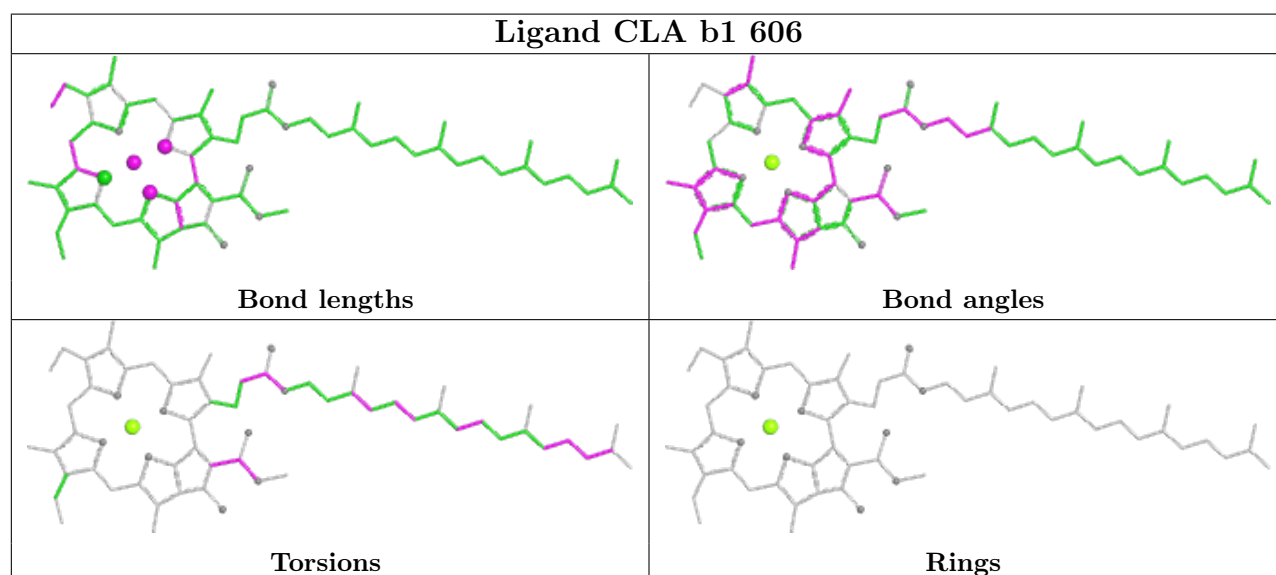
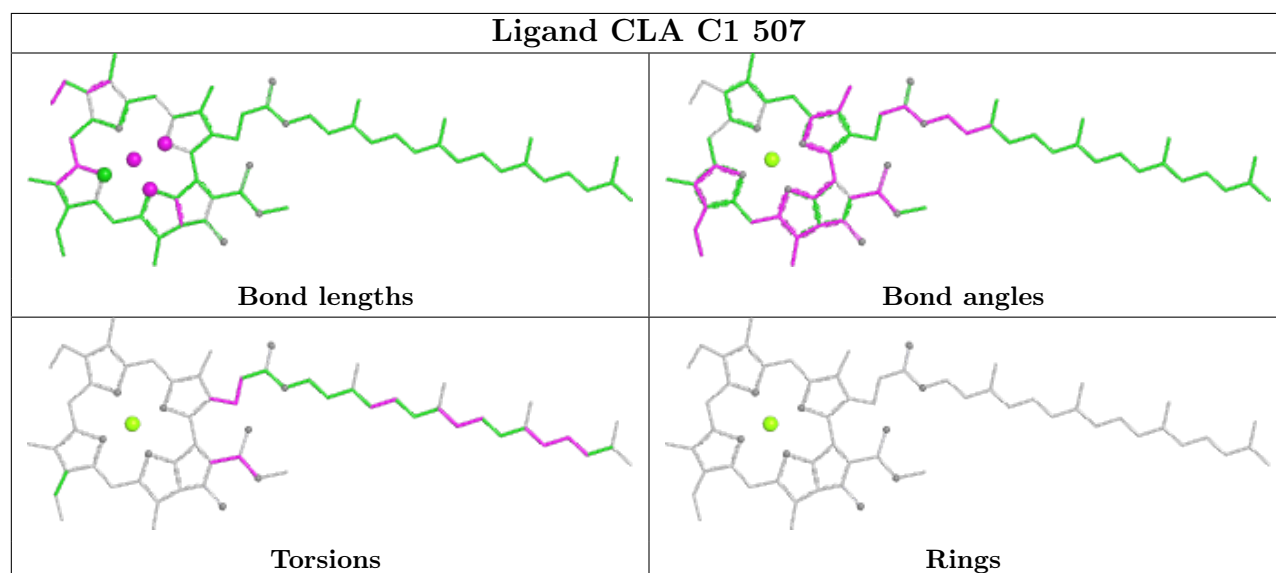
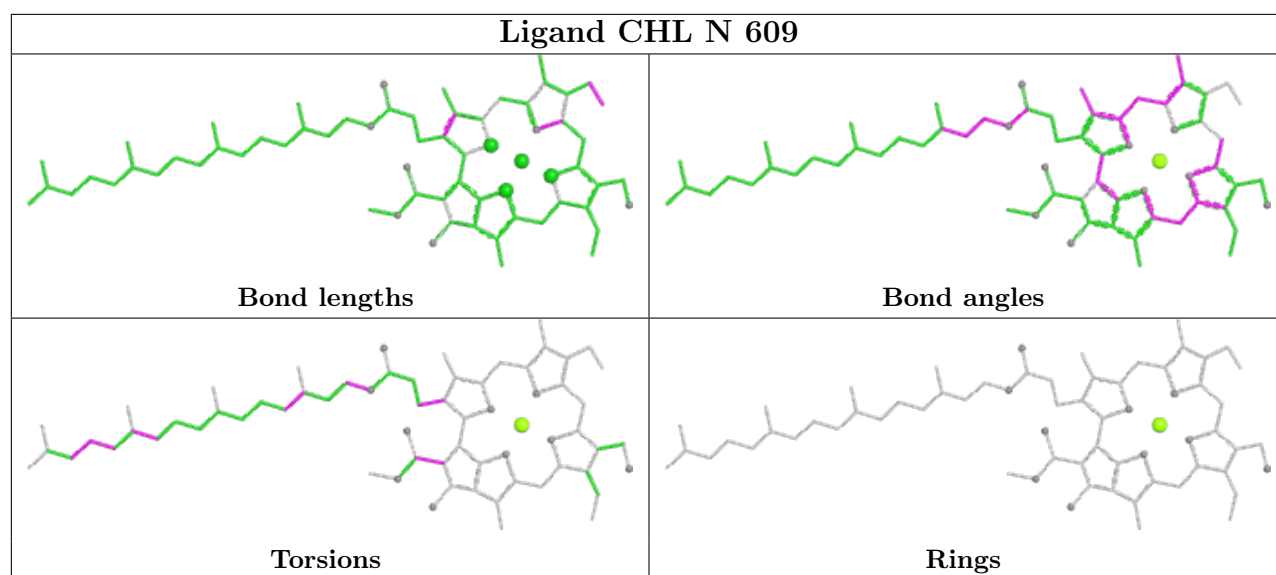




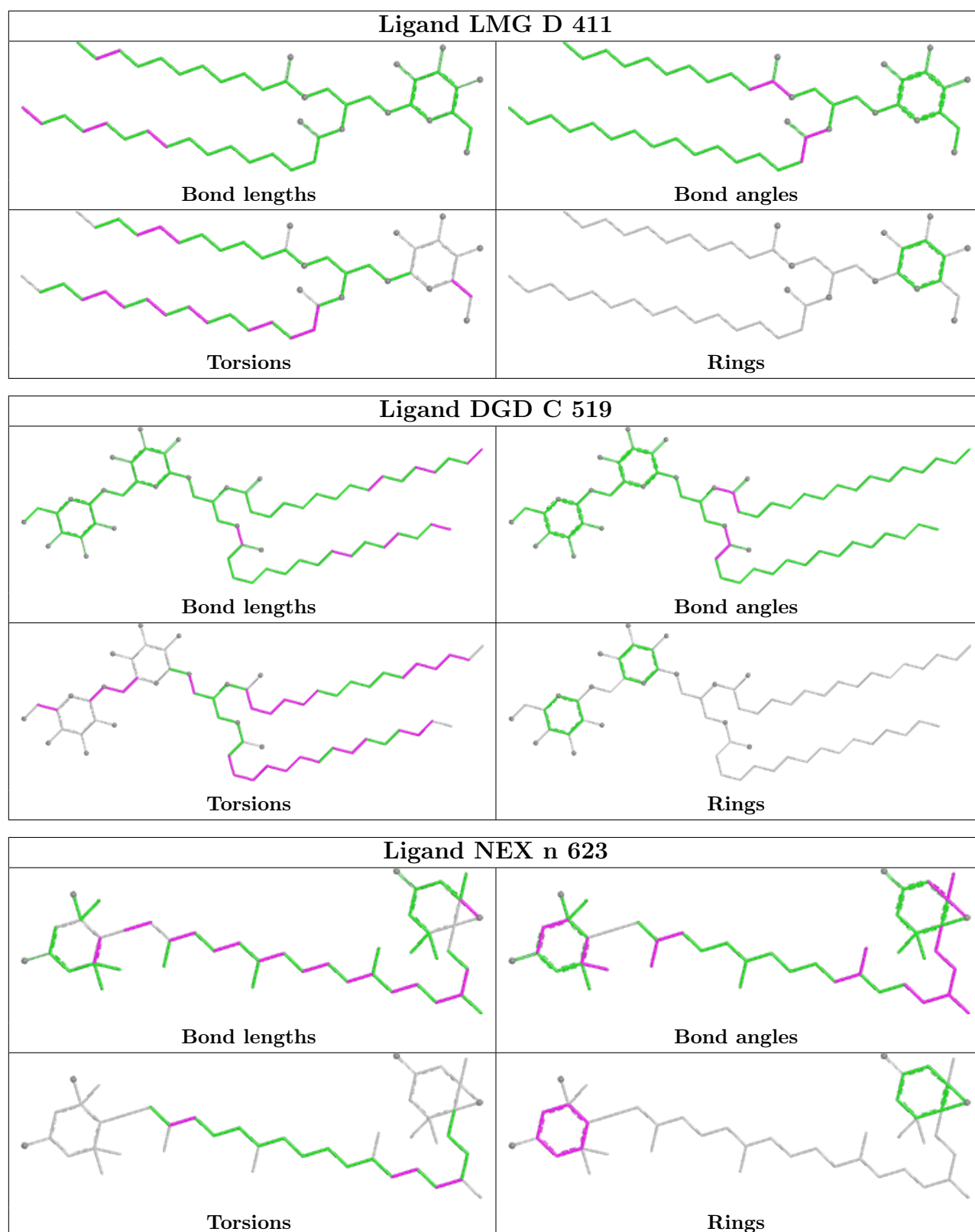


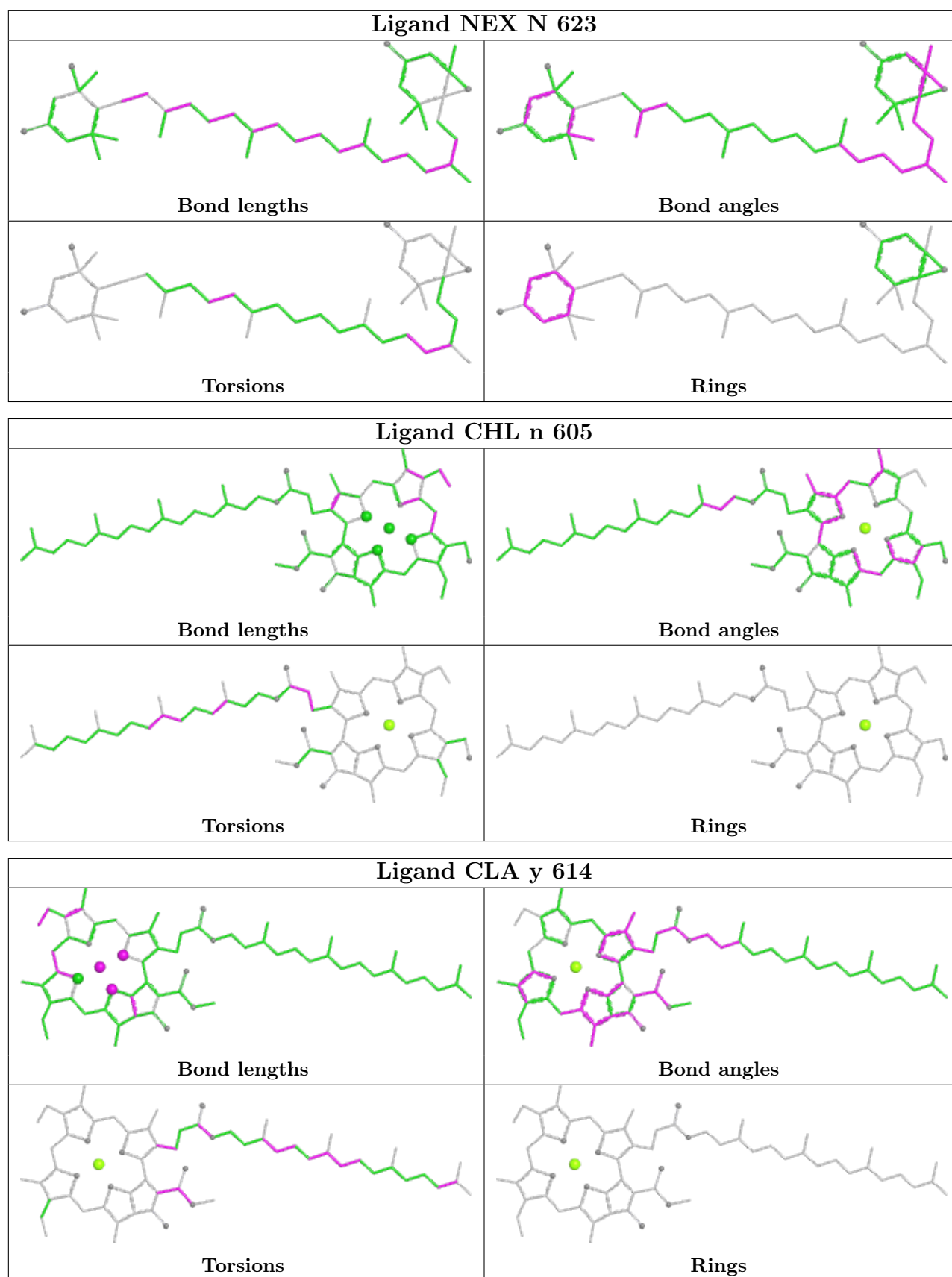


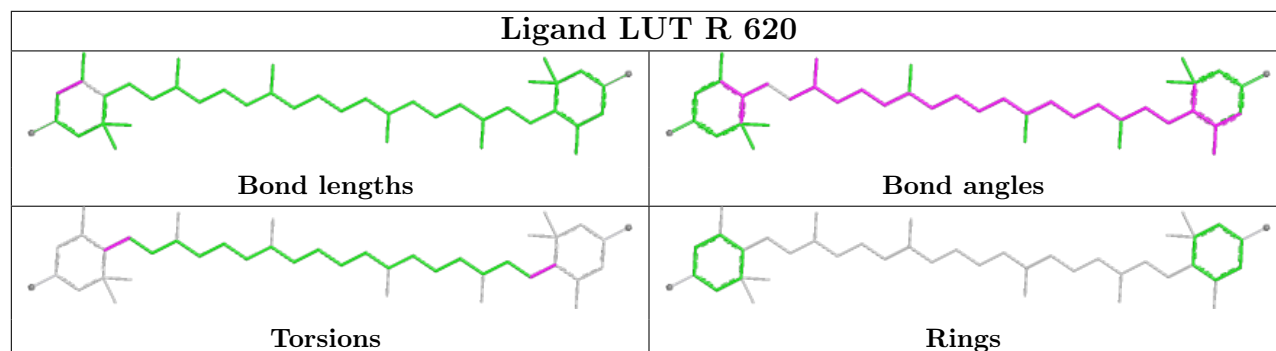
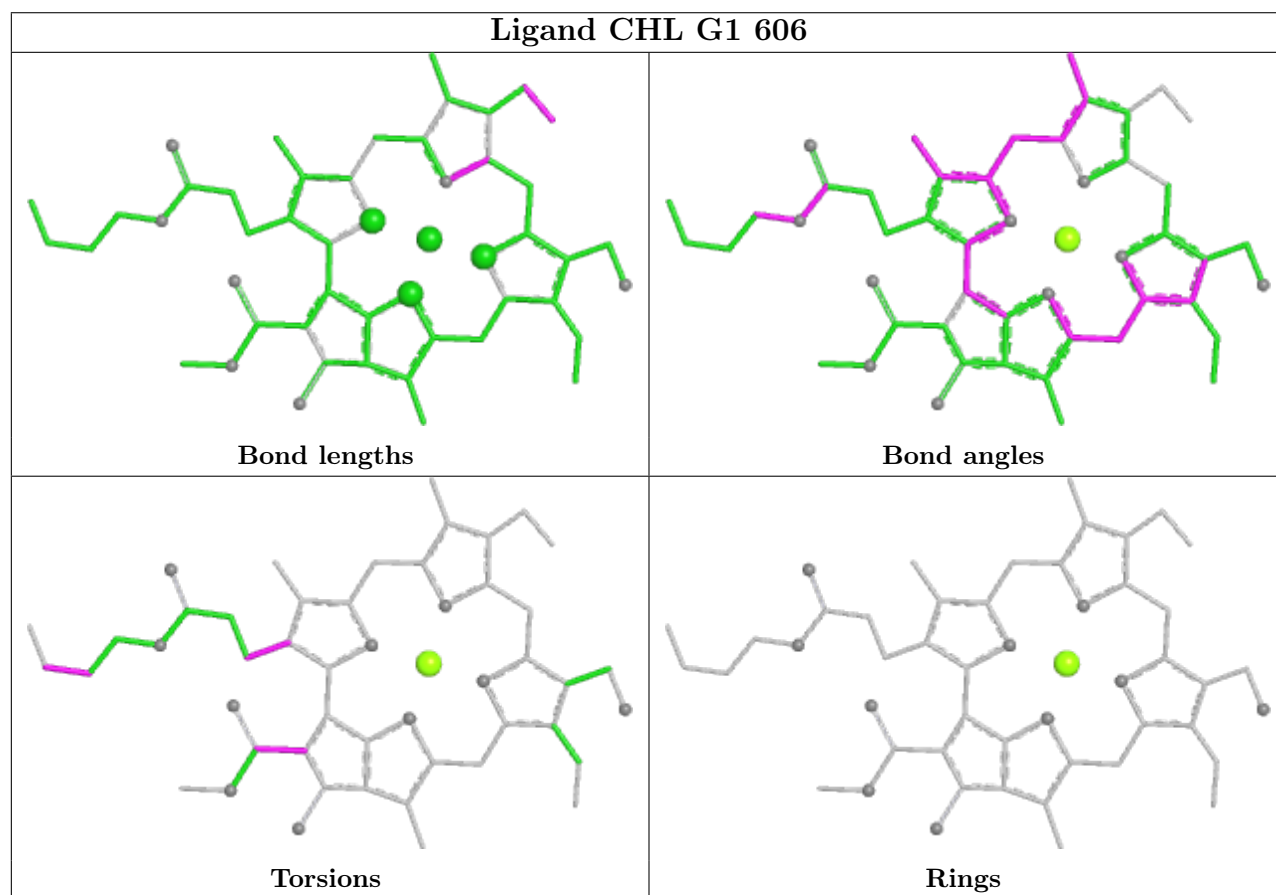
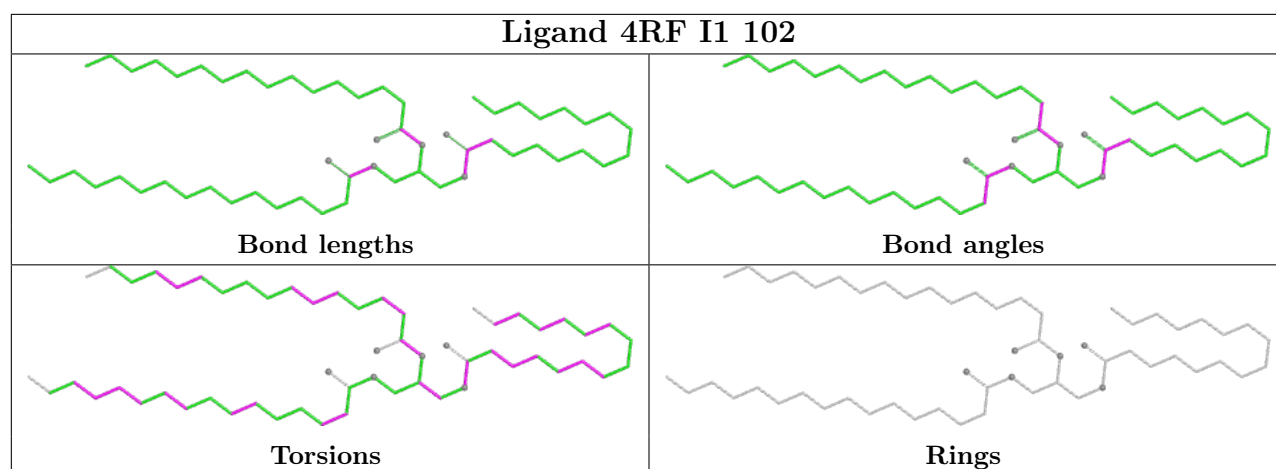


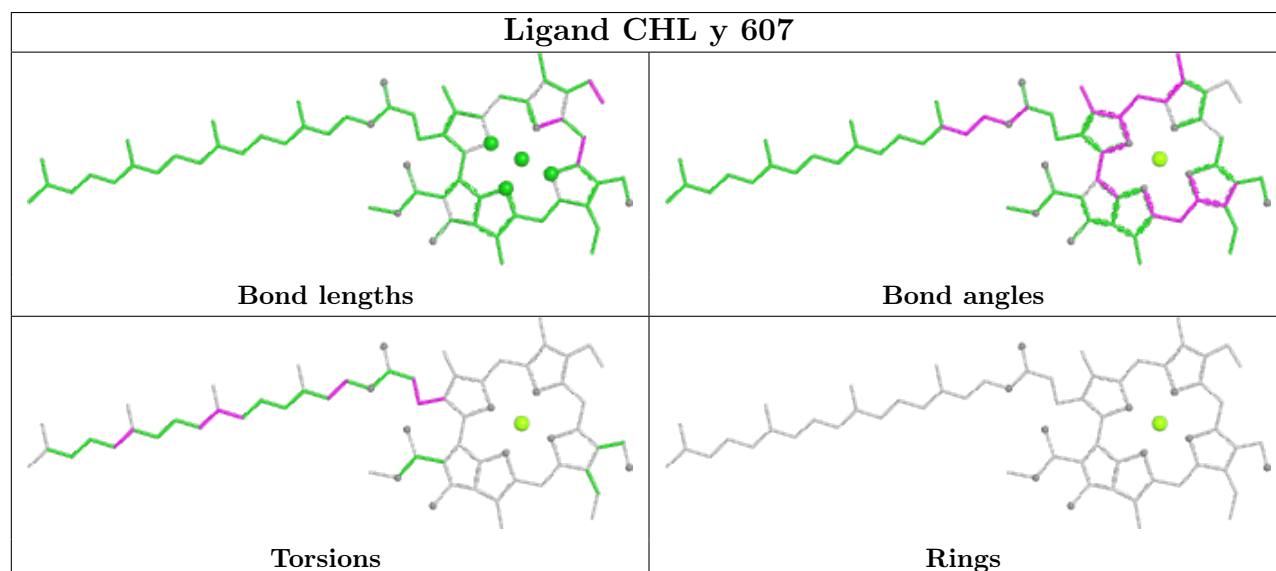
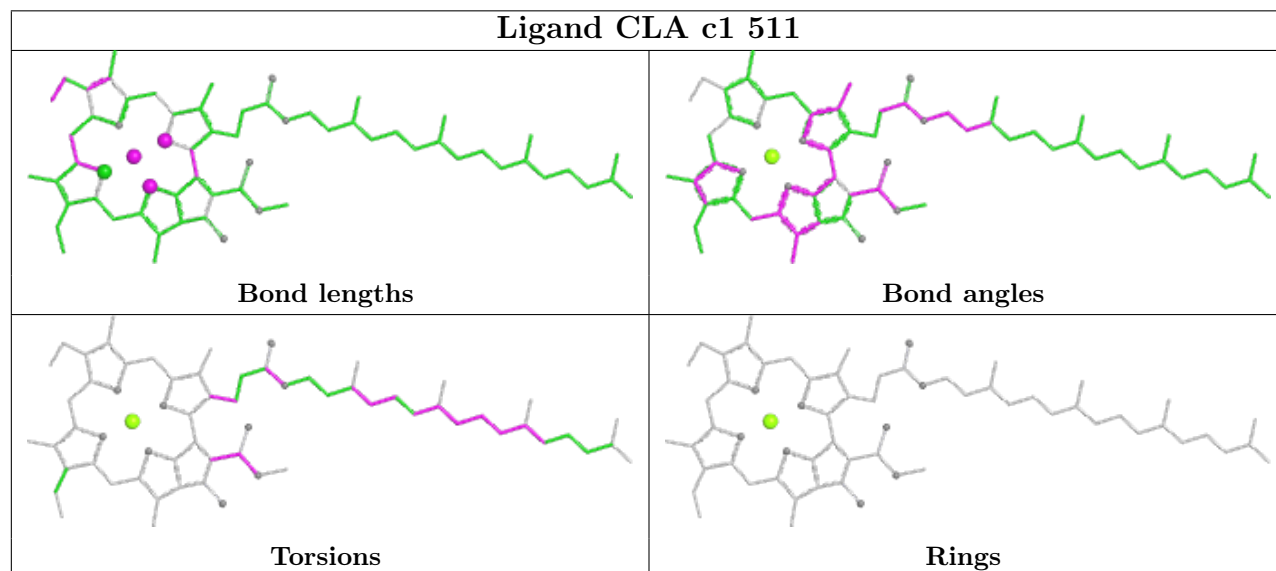
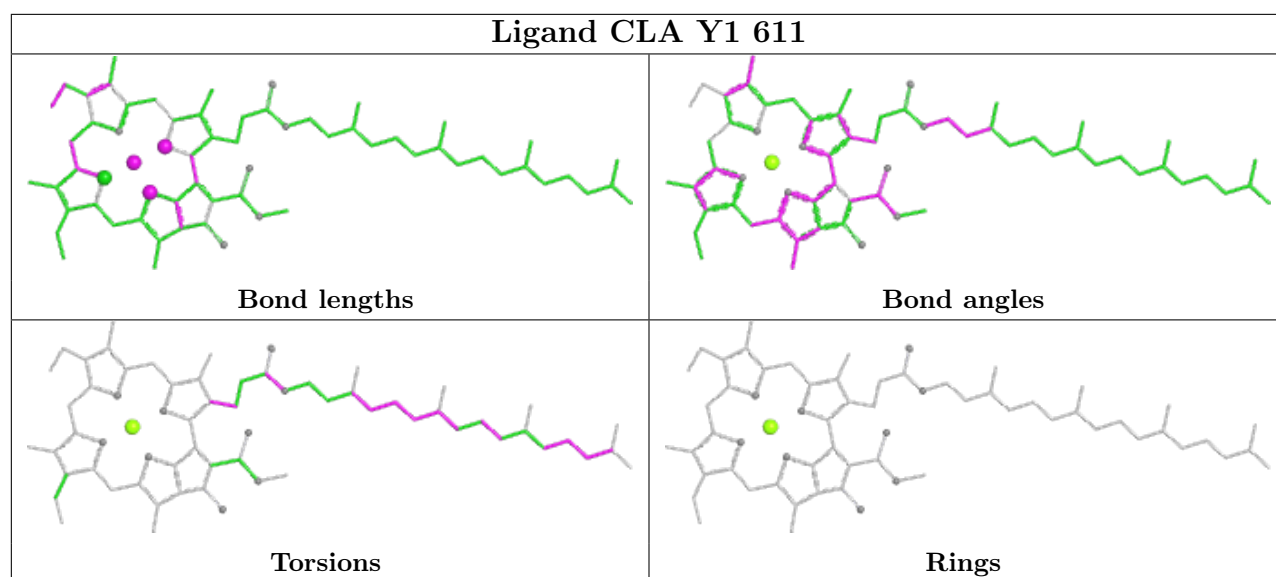


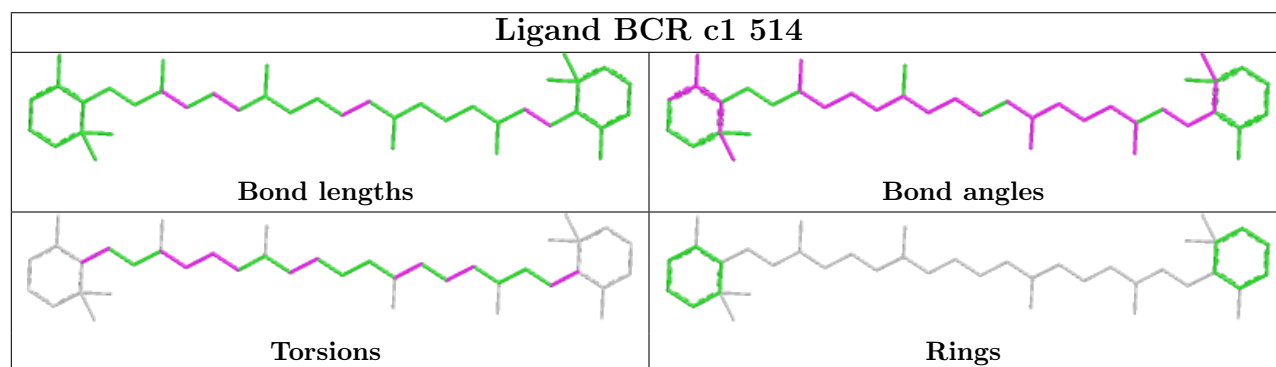
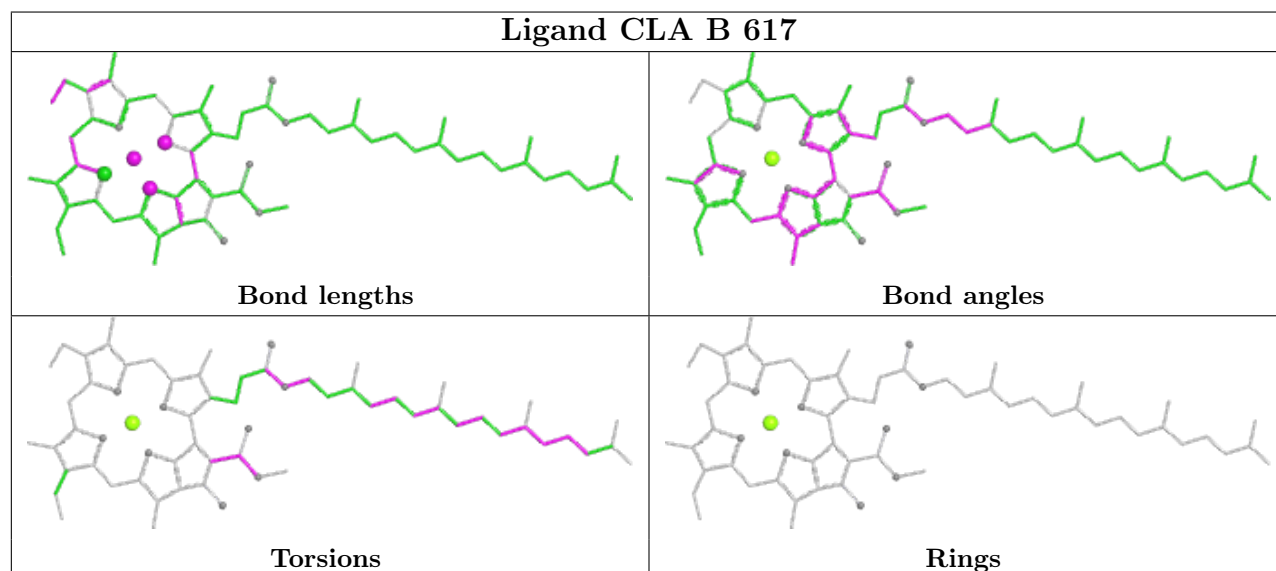
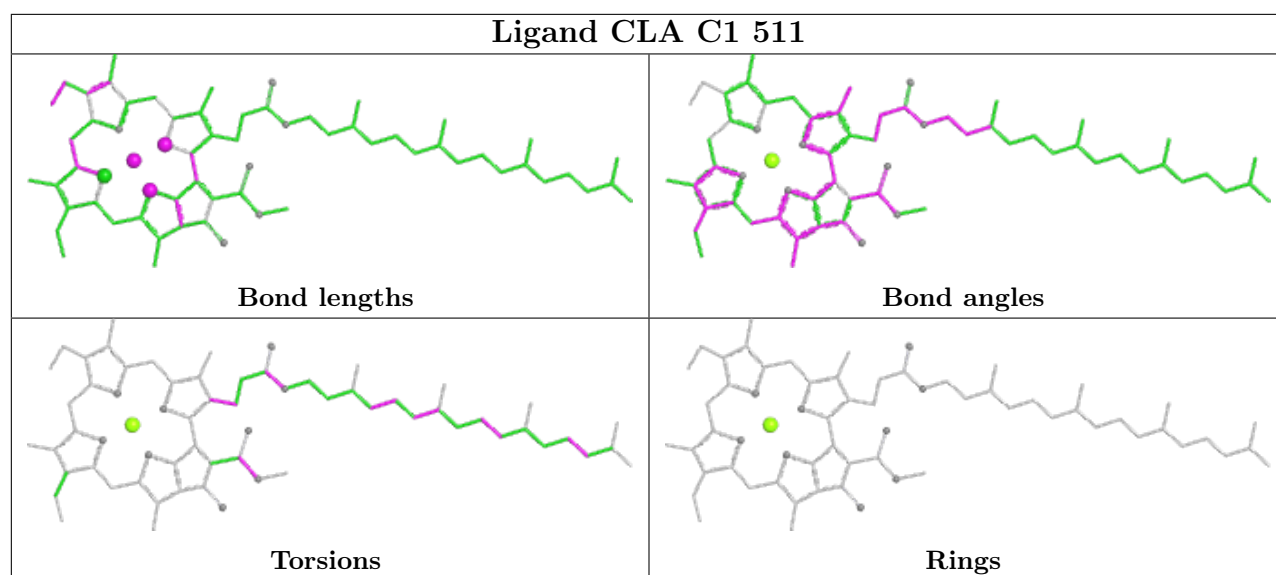


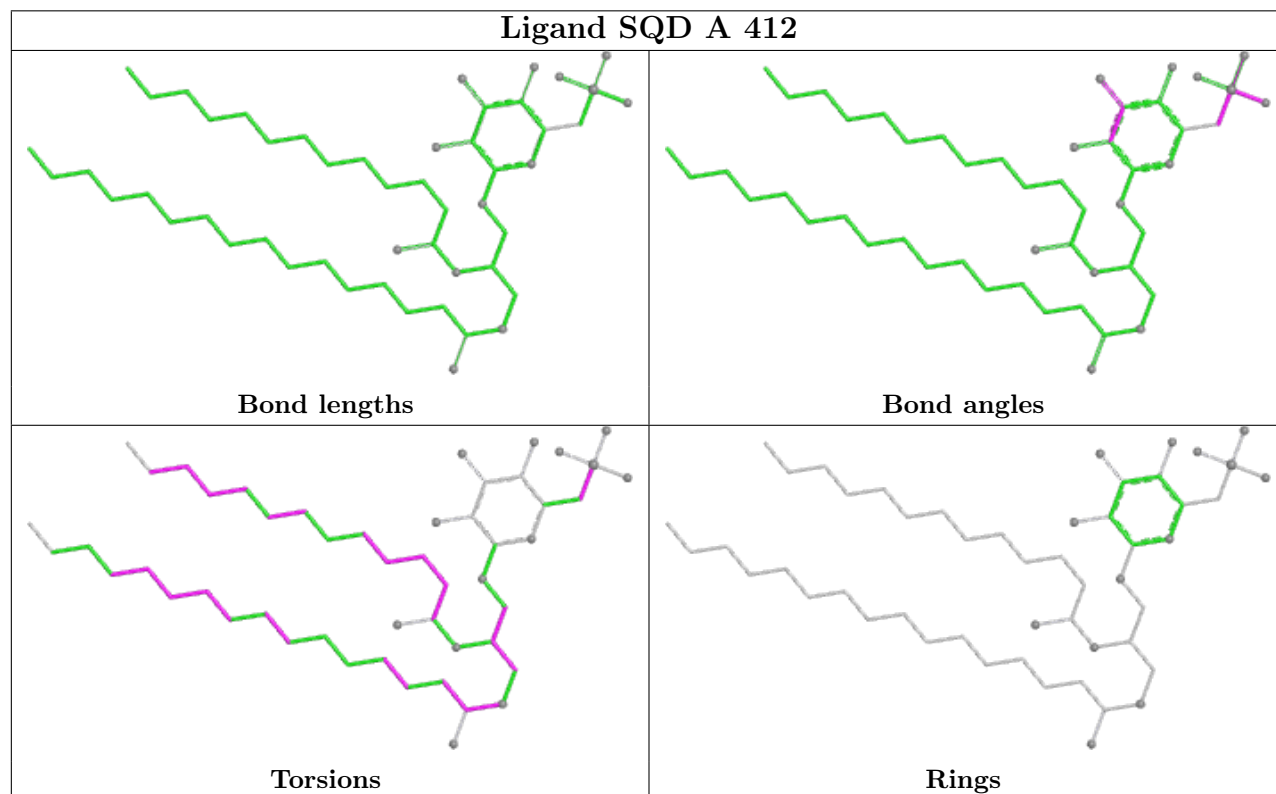
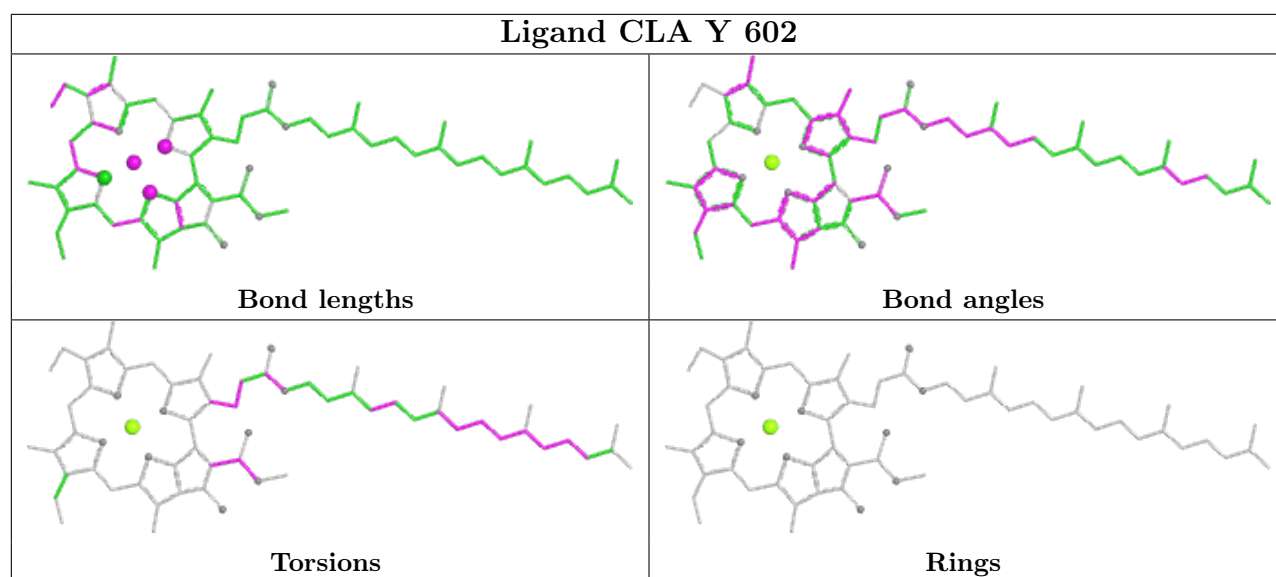


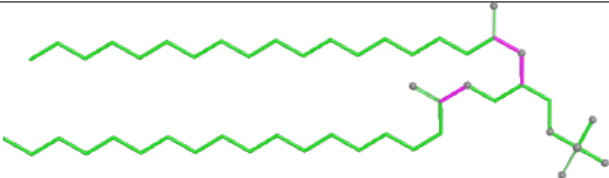
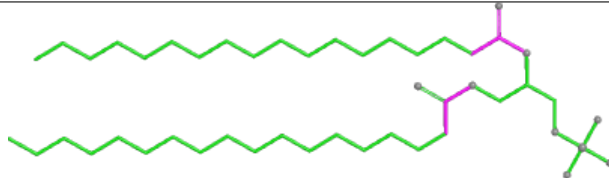
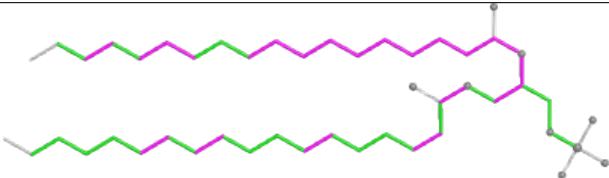
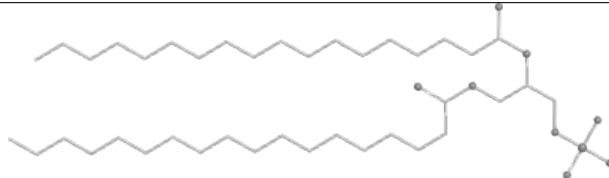


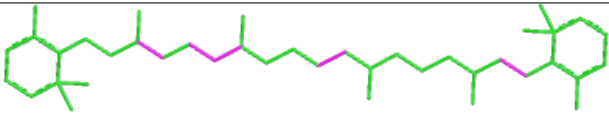
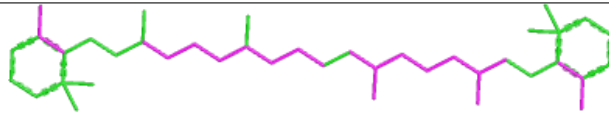
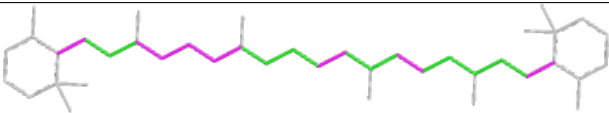
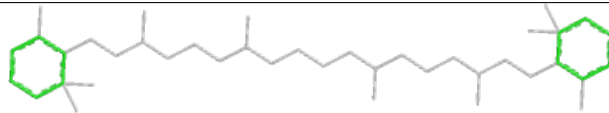


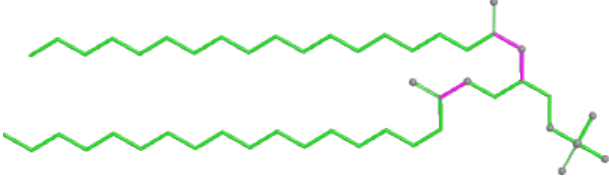
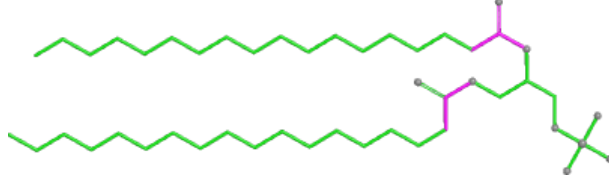
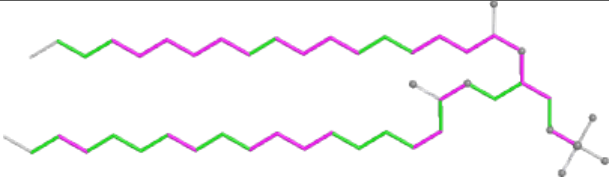
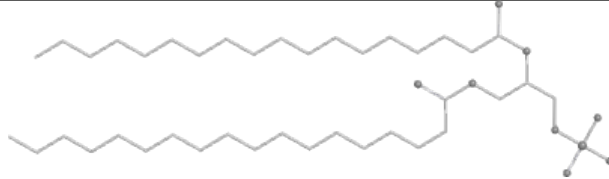


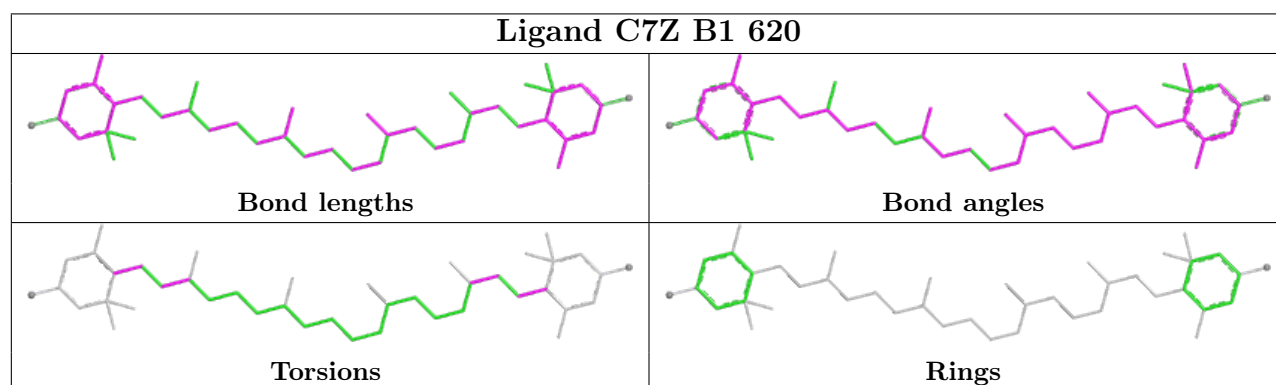
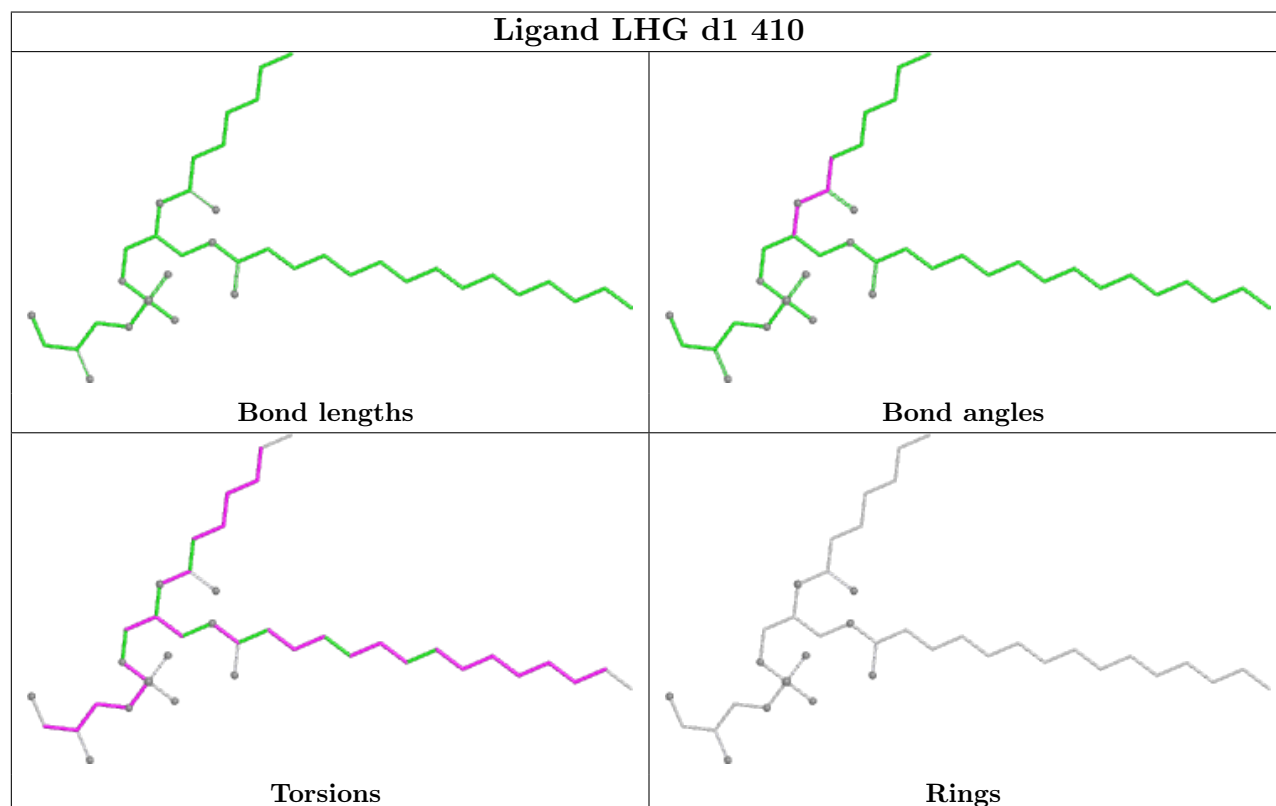
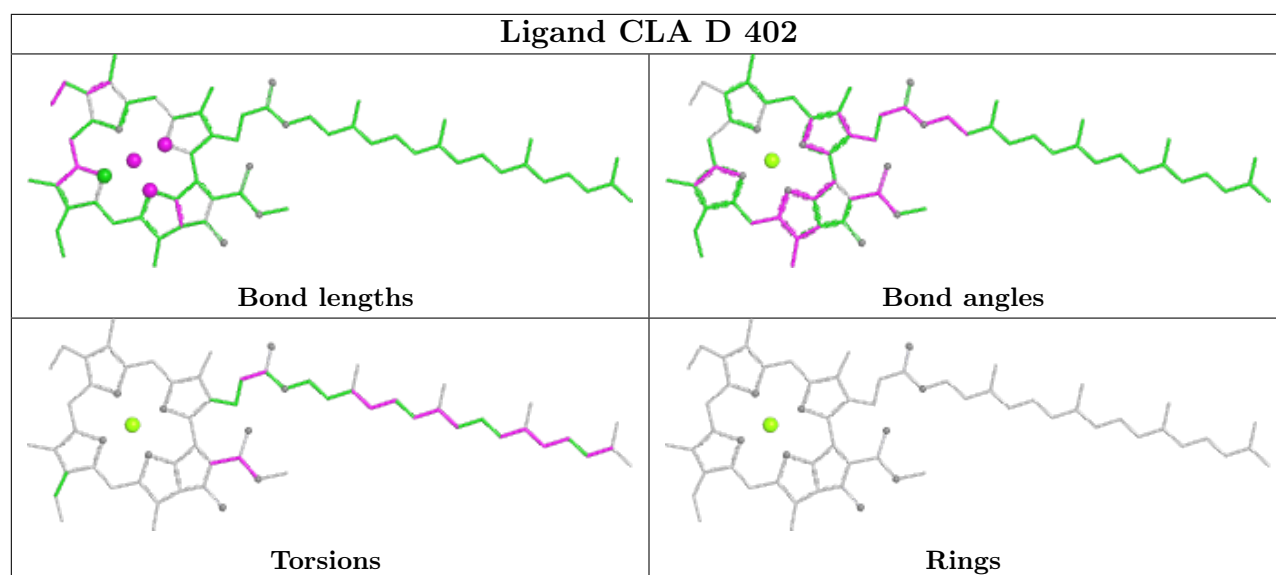




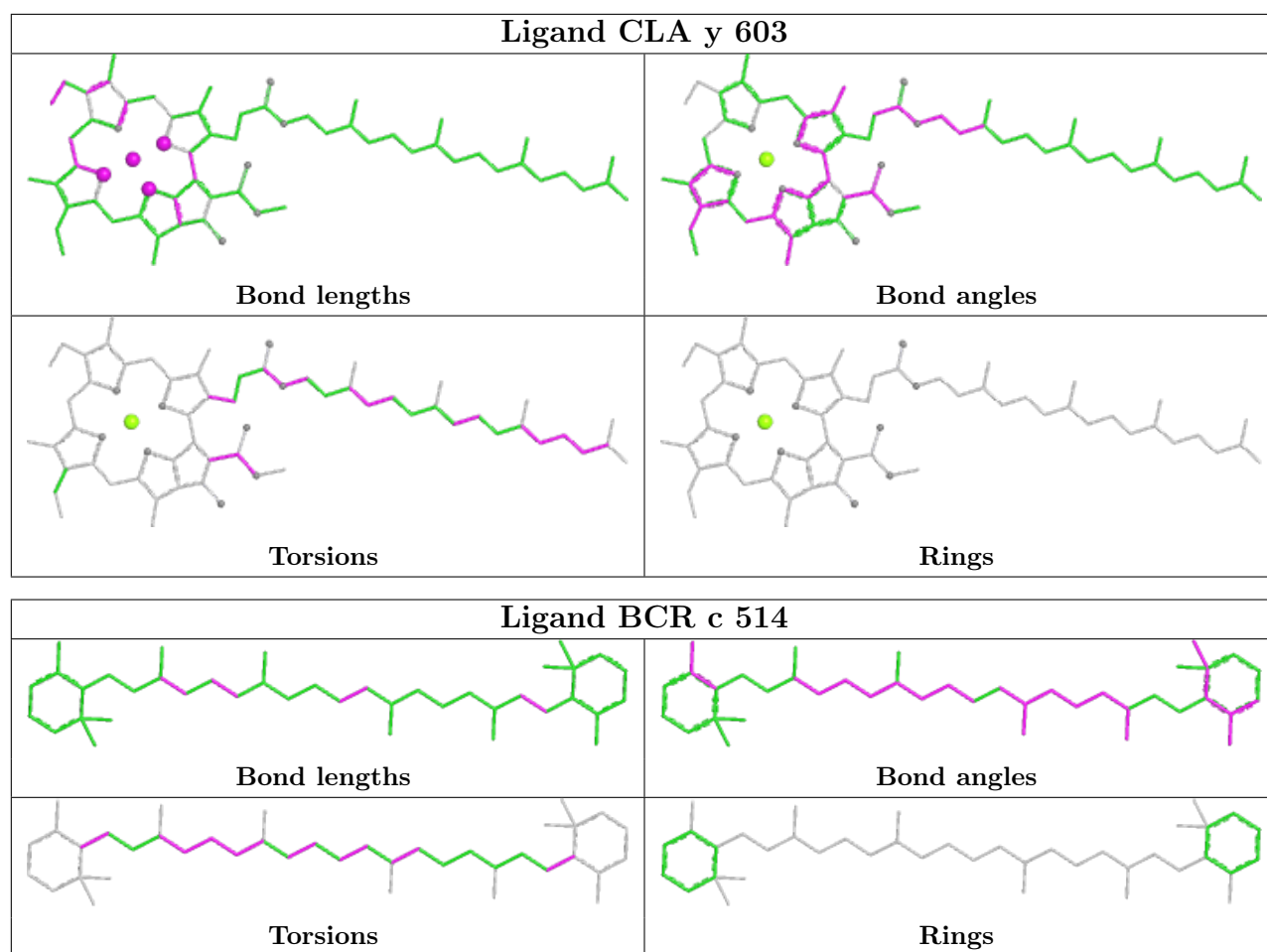
Ligand 3PH s 626			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

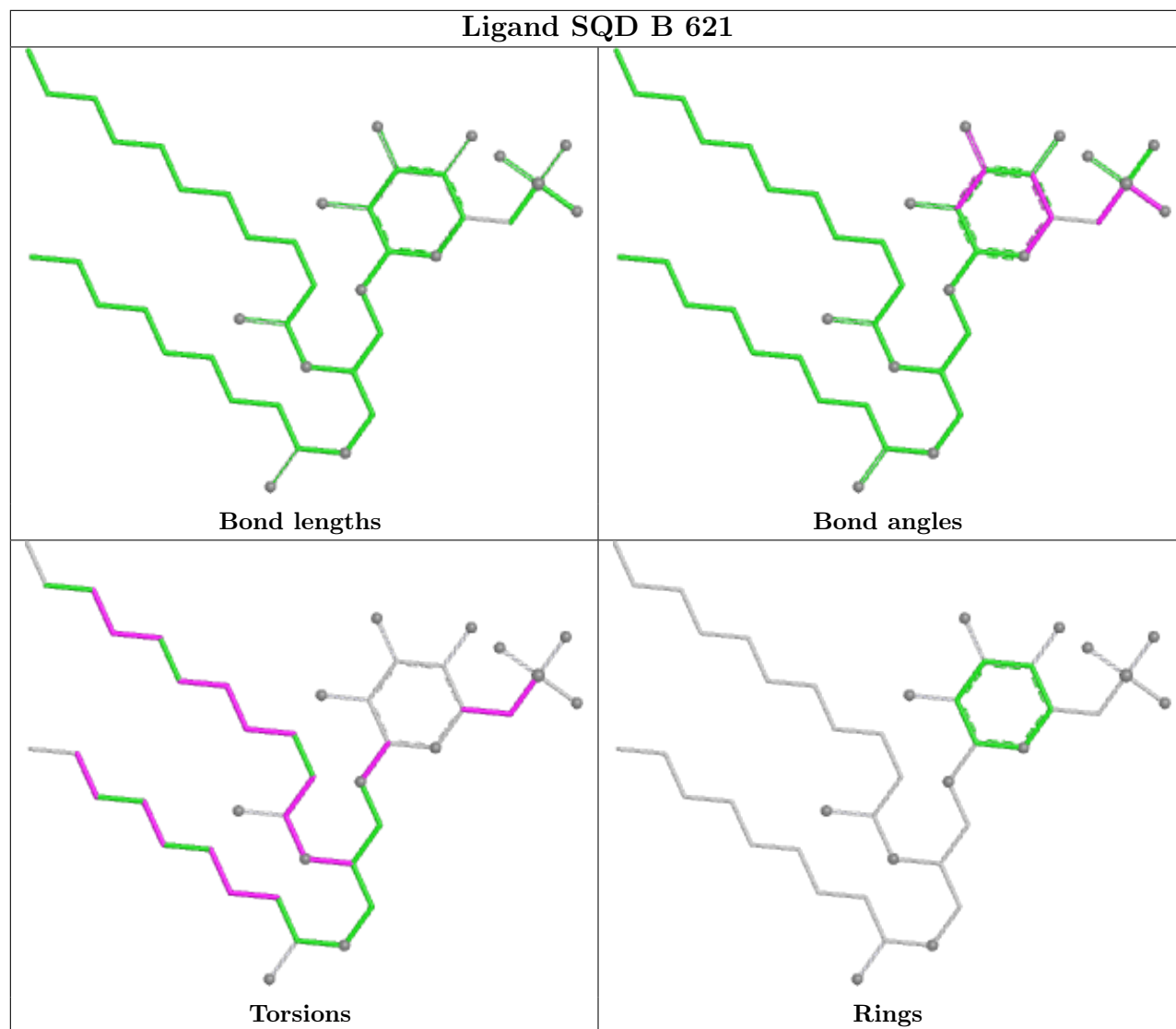
Ligand BCR C1 514			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

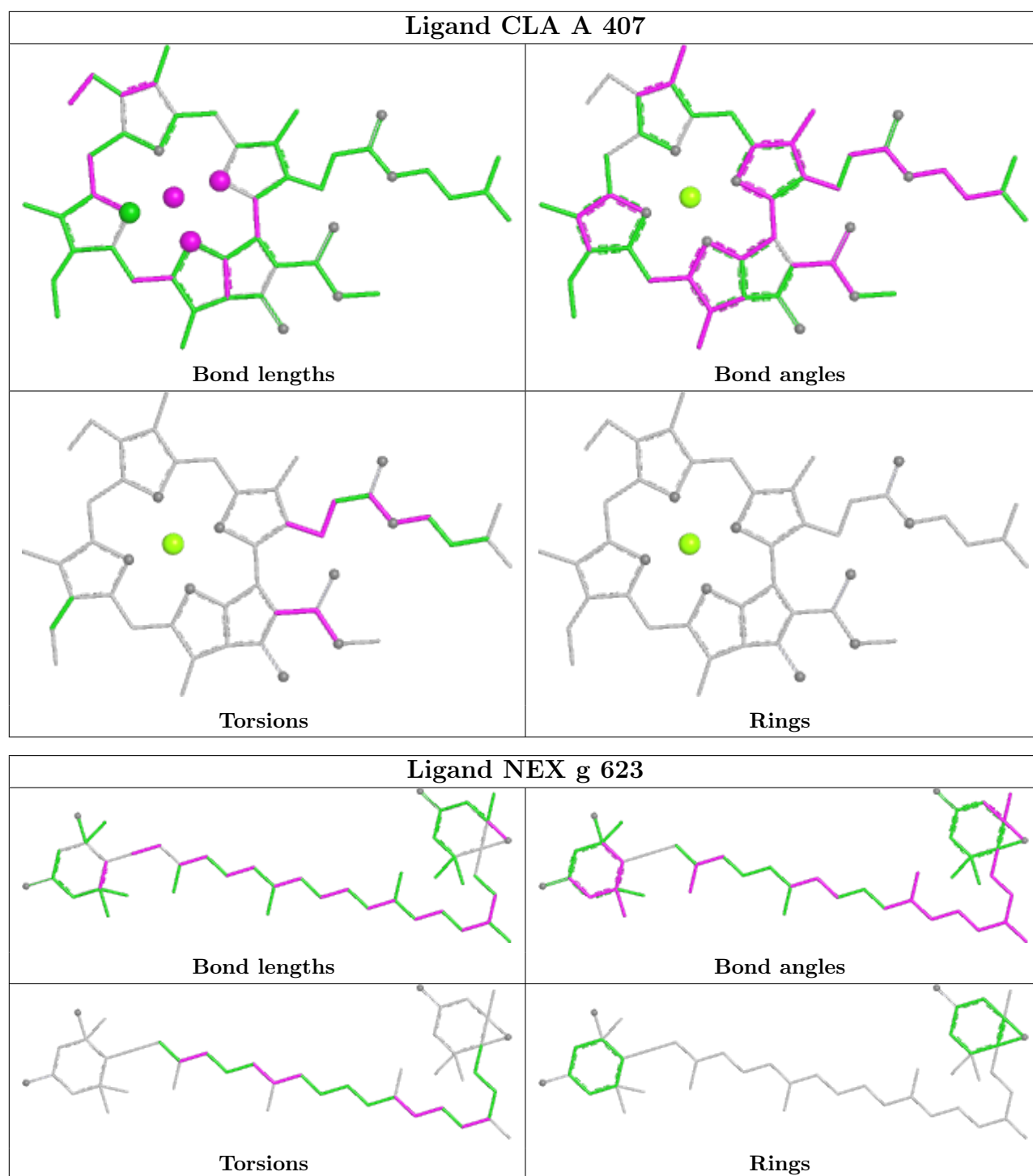
Ligand 3PH s1 626			
			
Bond lengths	Bond angles		
			
Torsions	Rings		

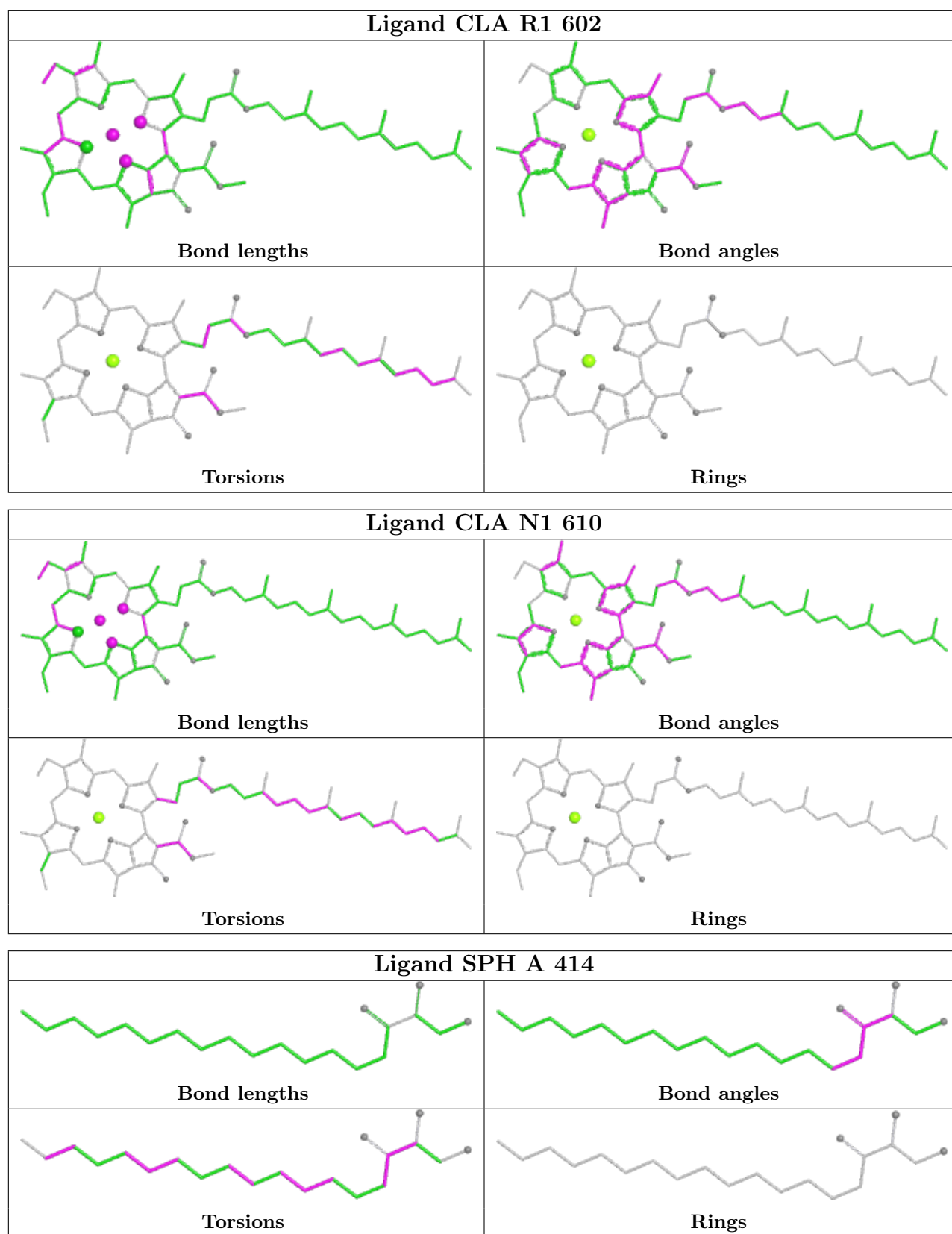


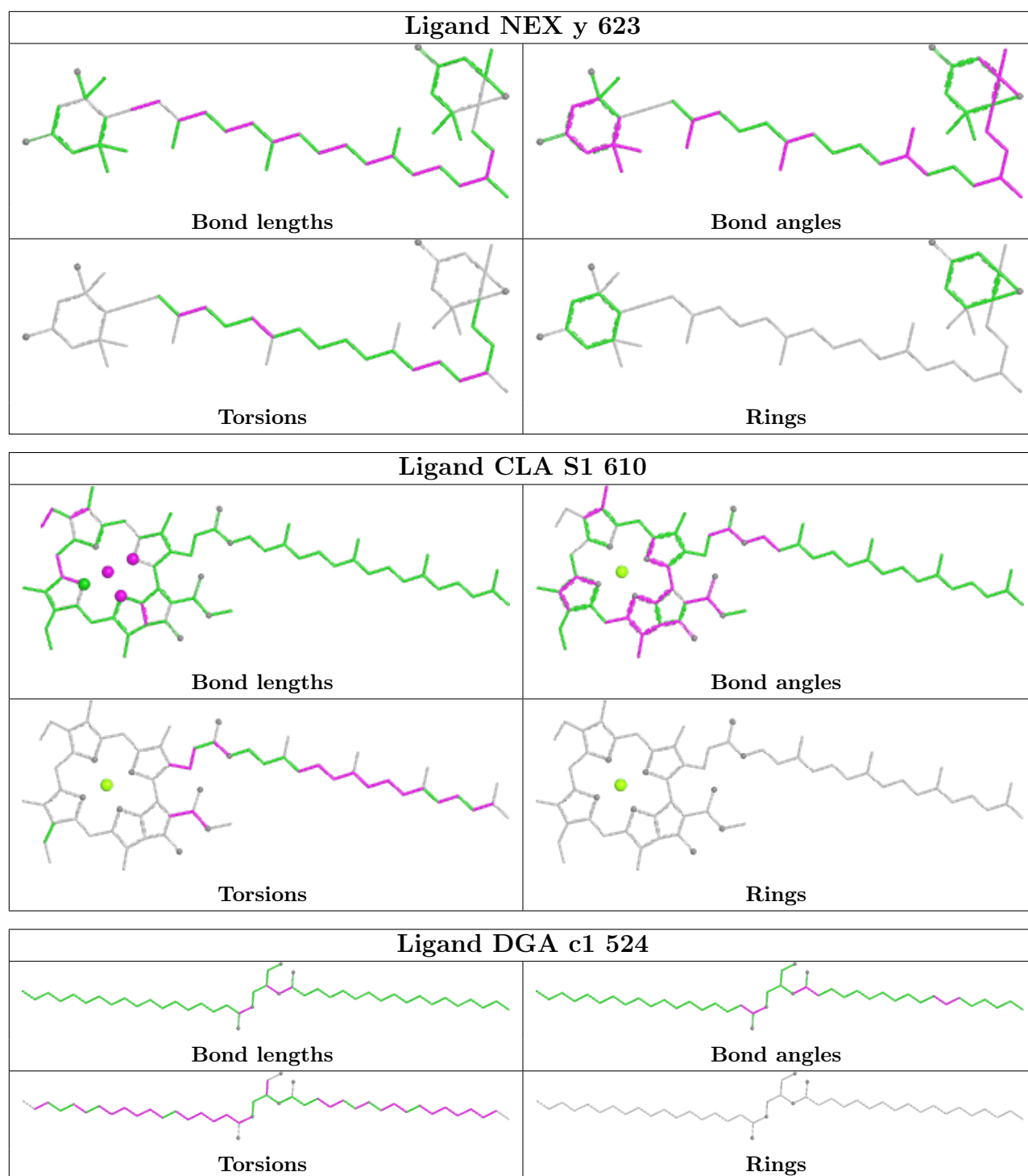


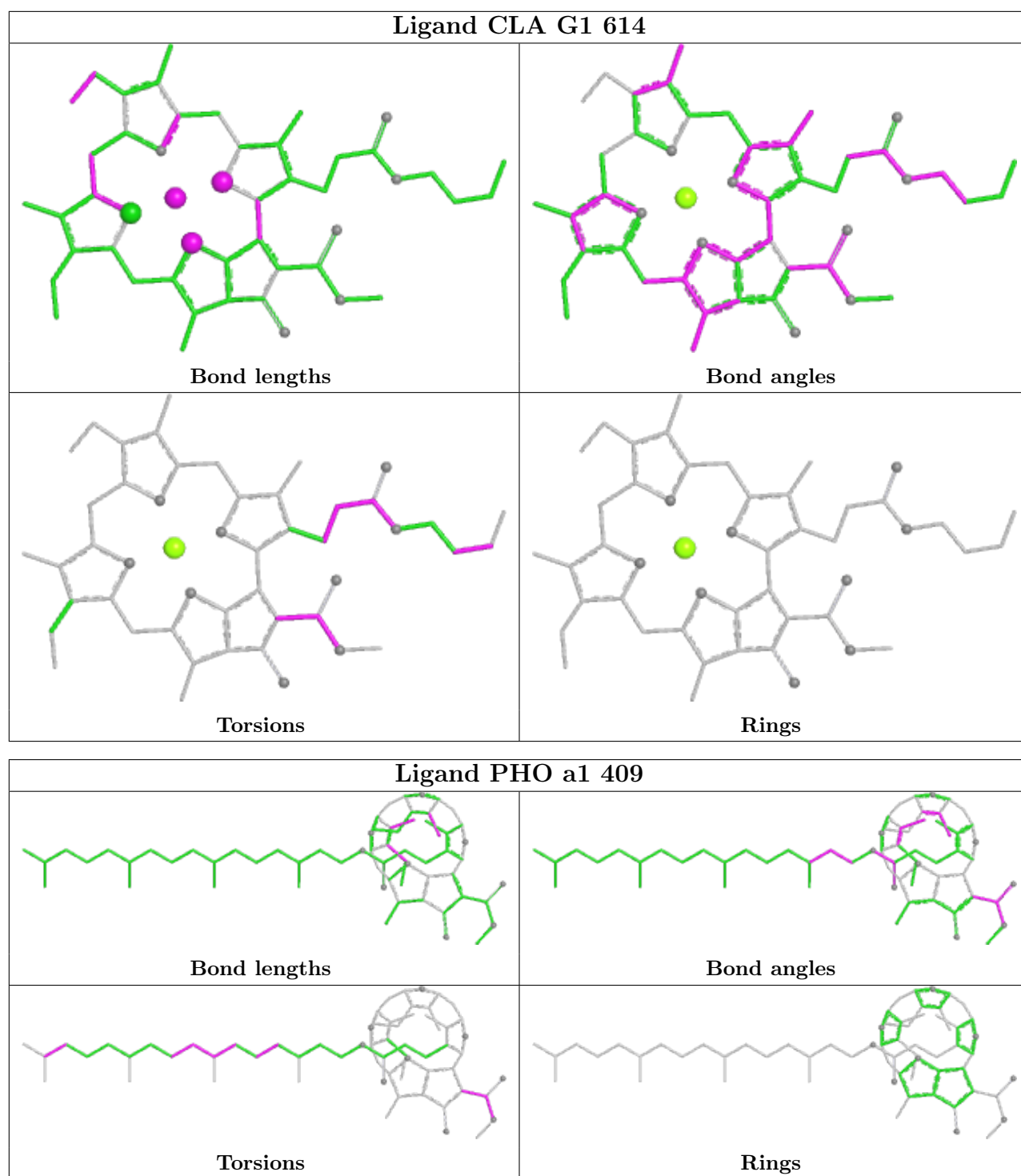


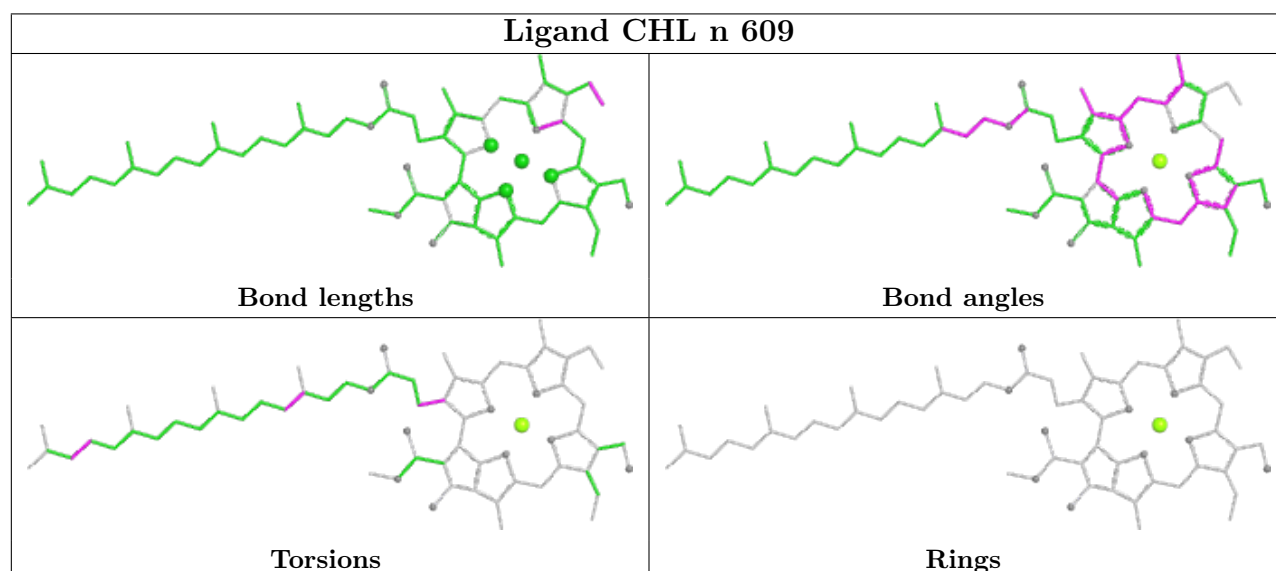
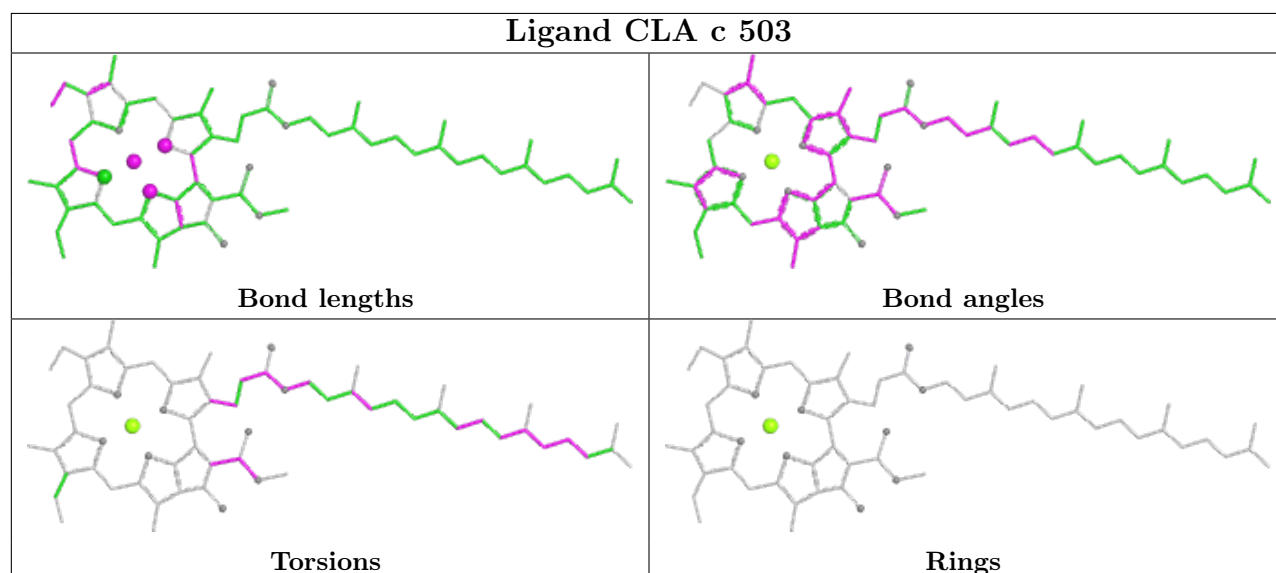
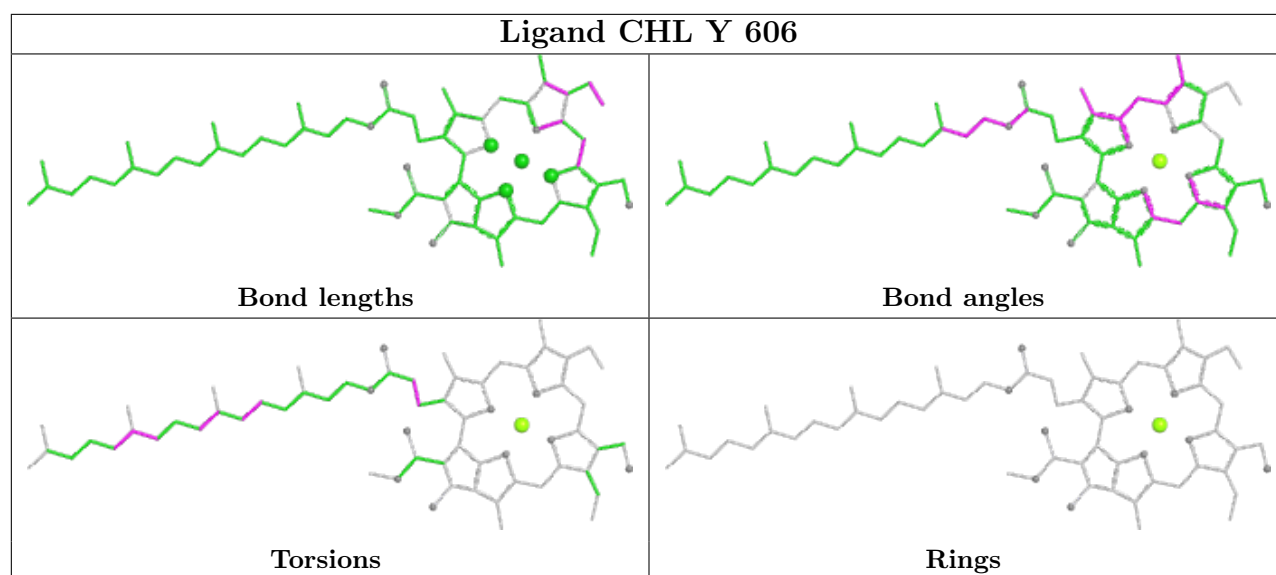


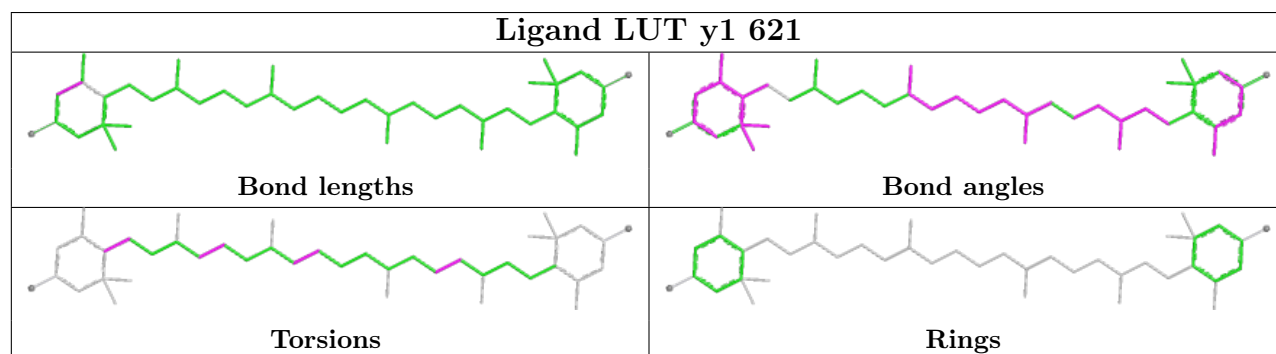
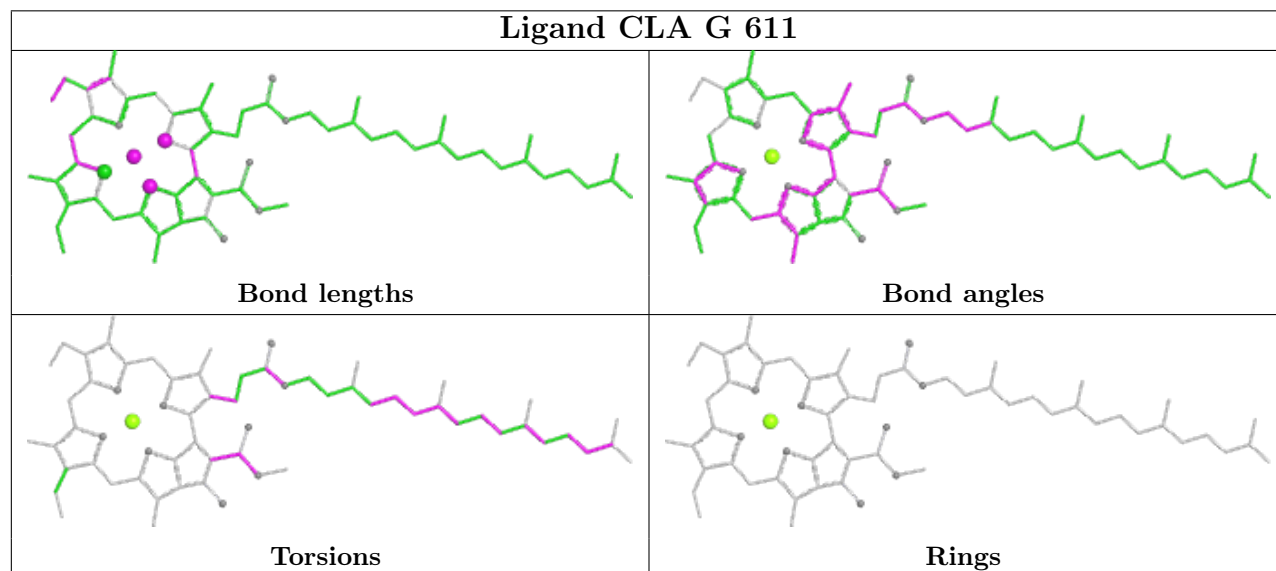
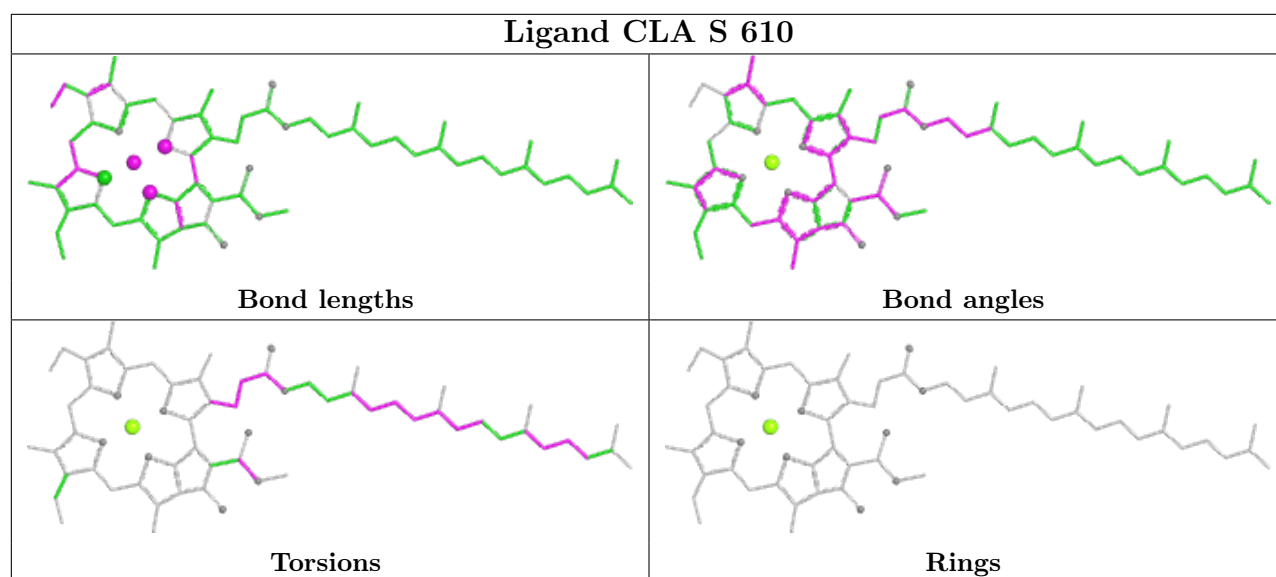




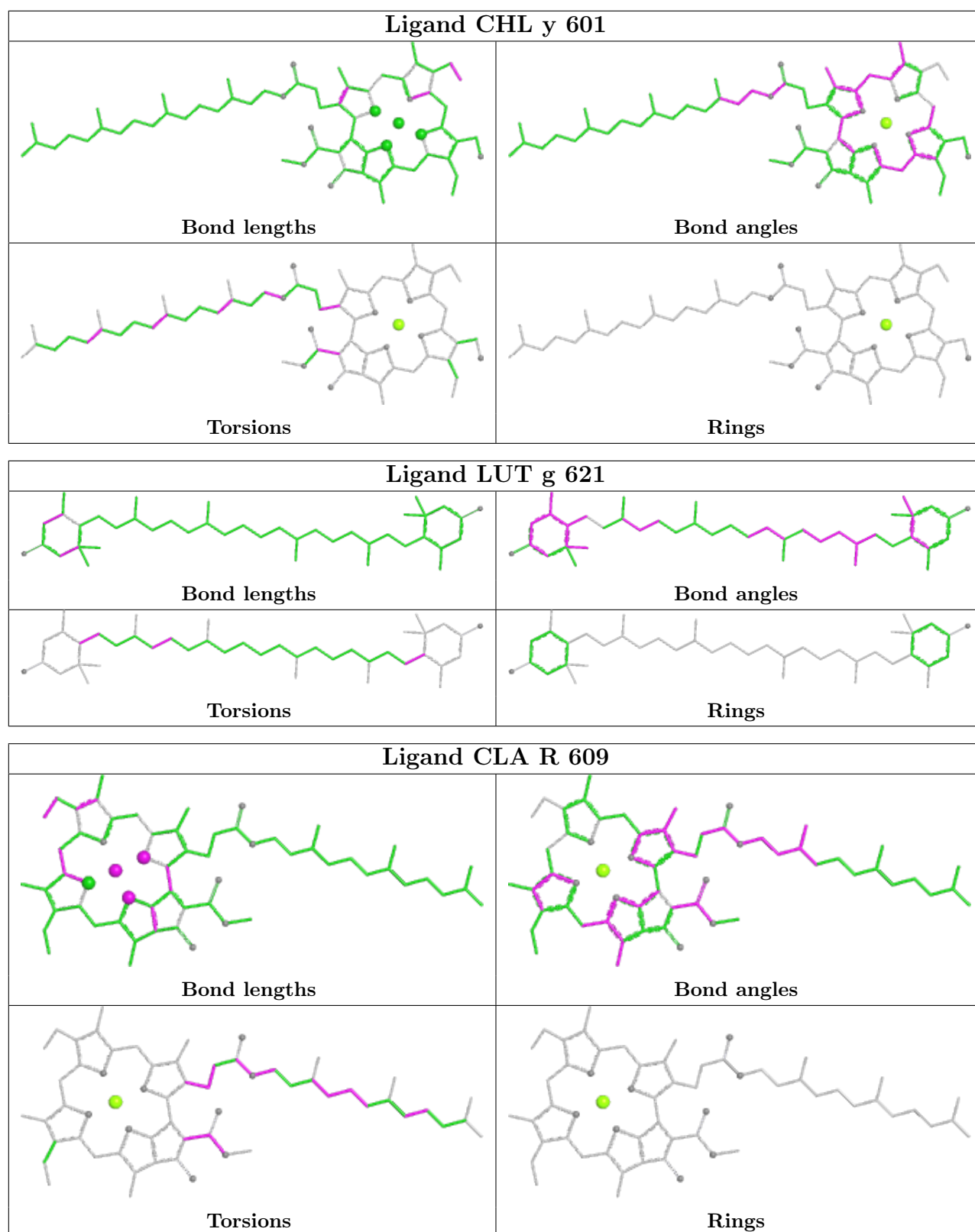


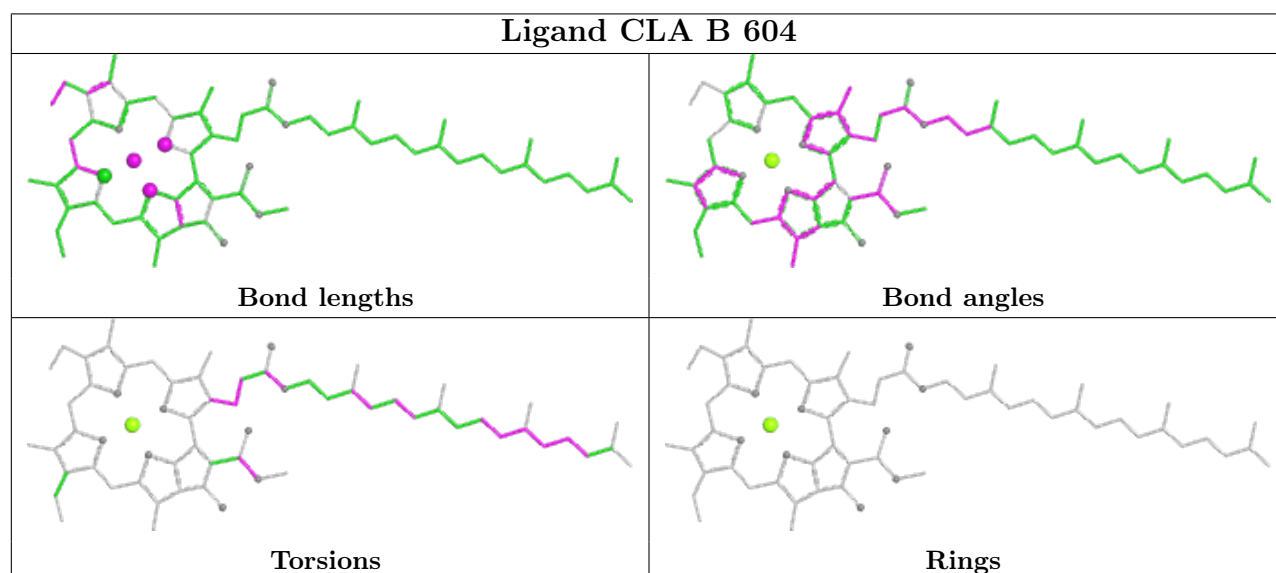
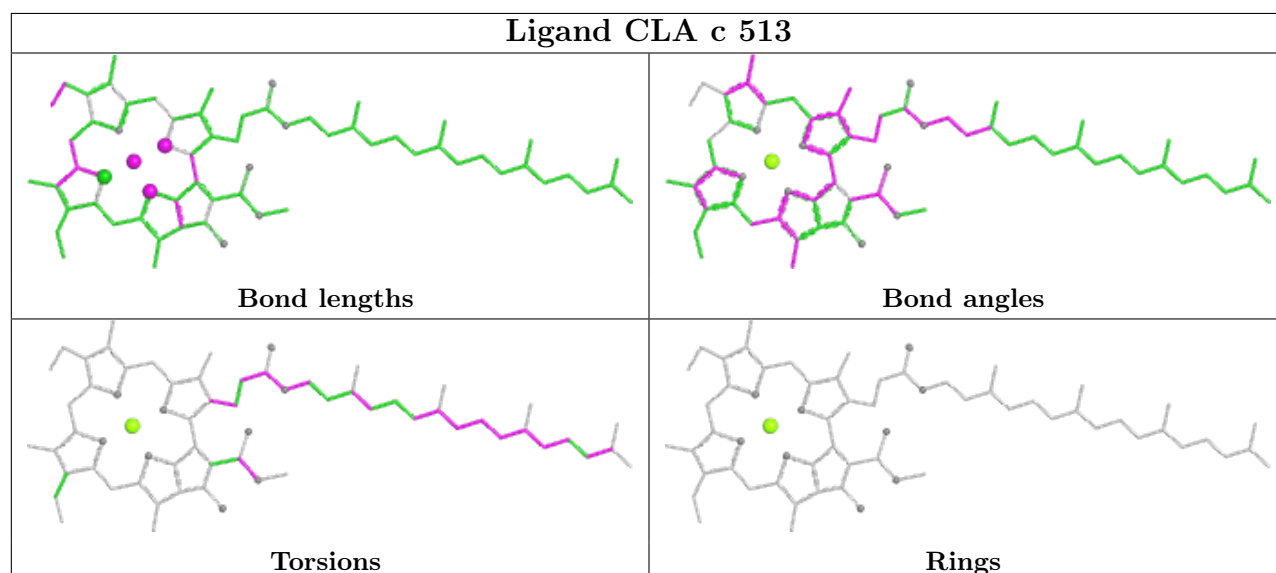
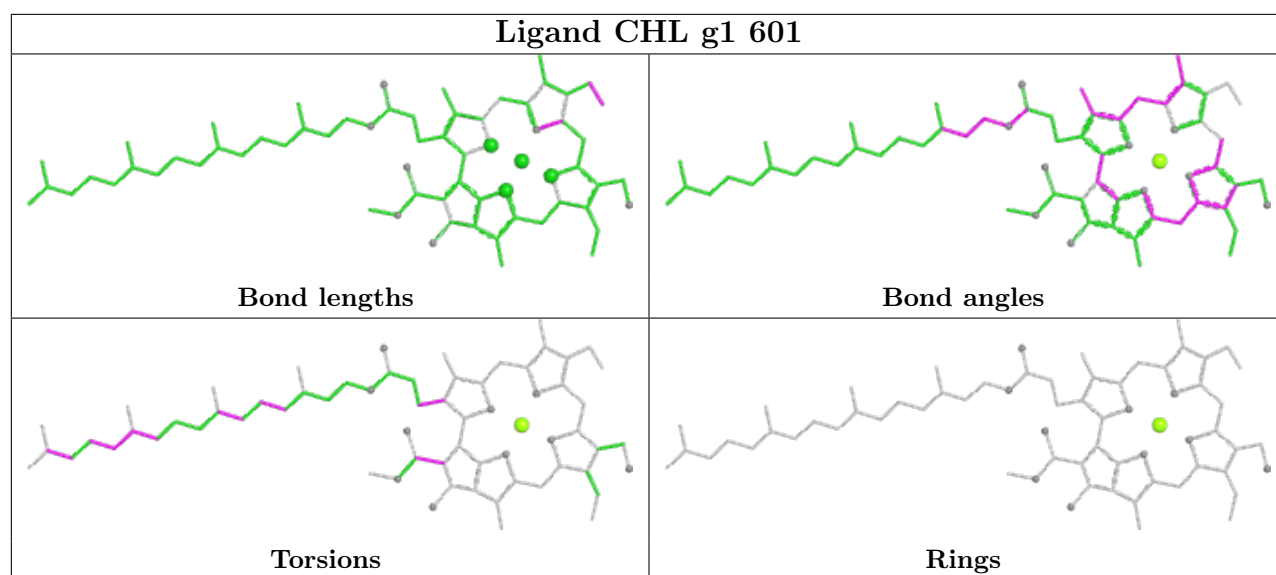


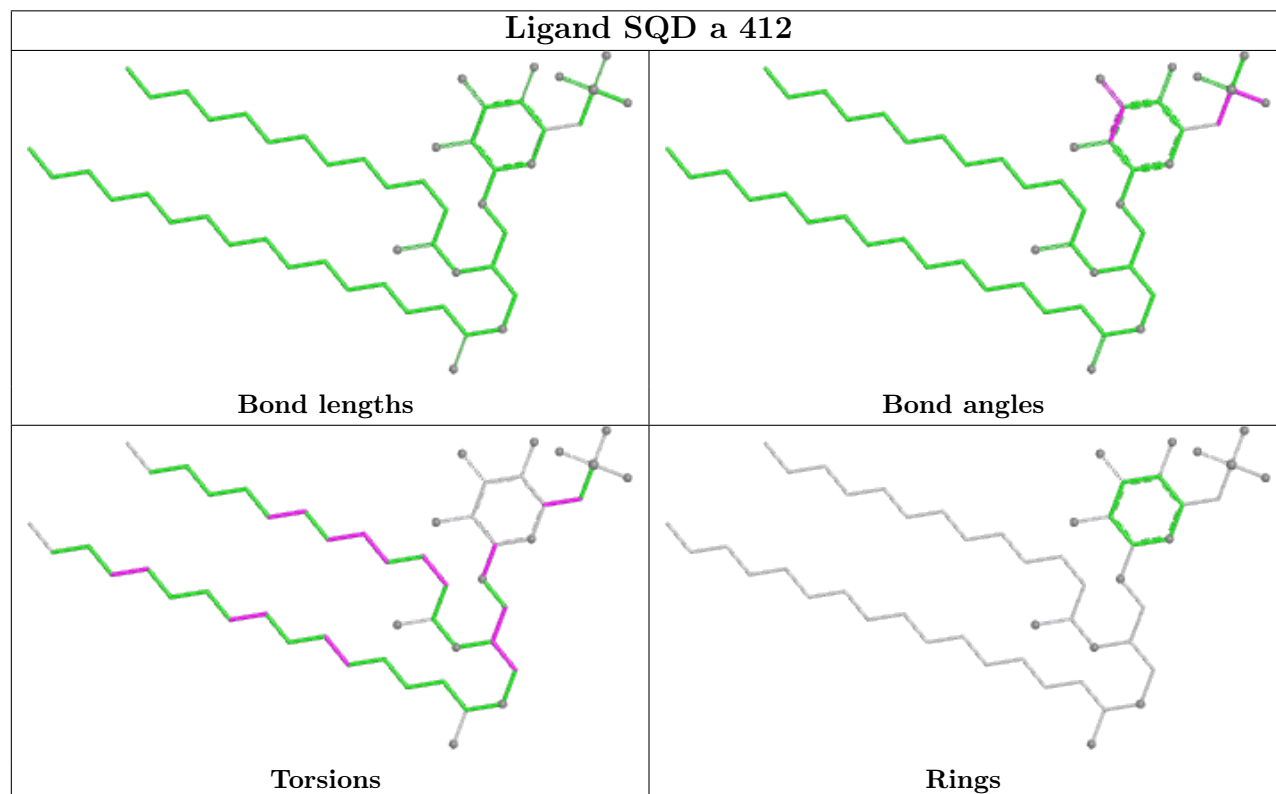
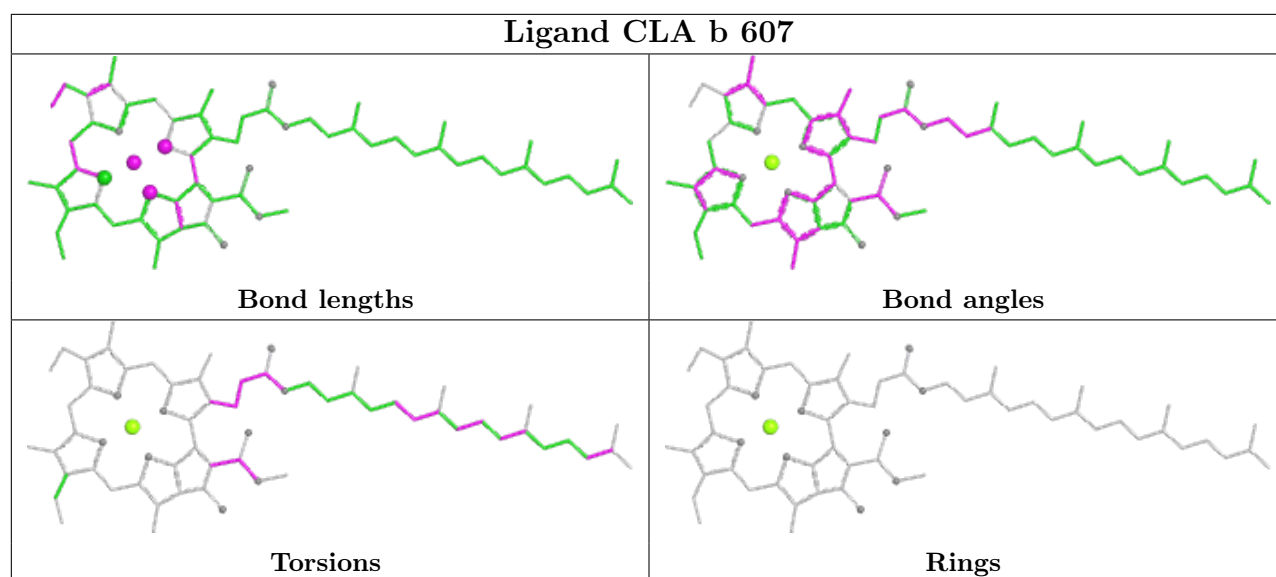


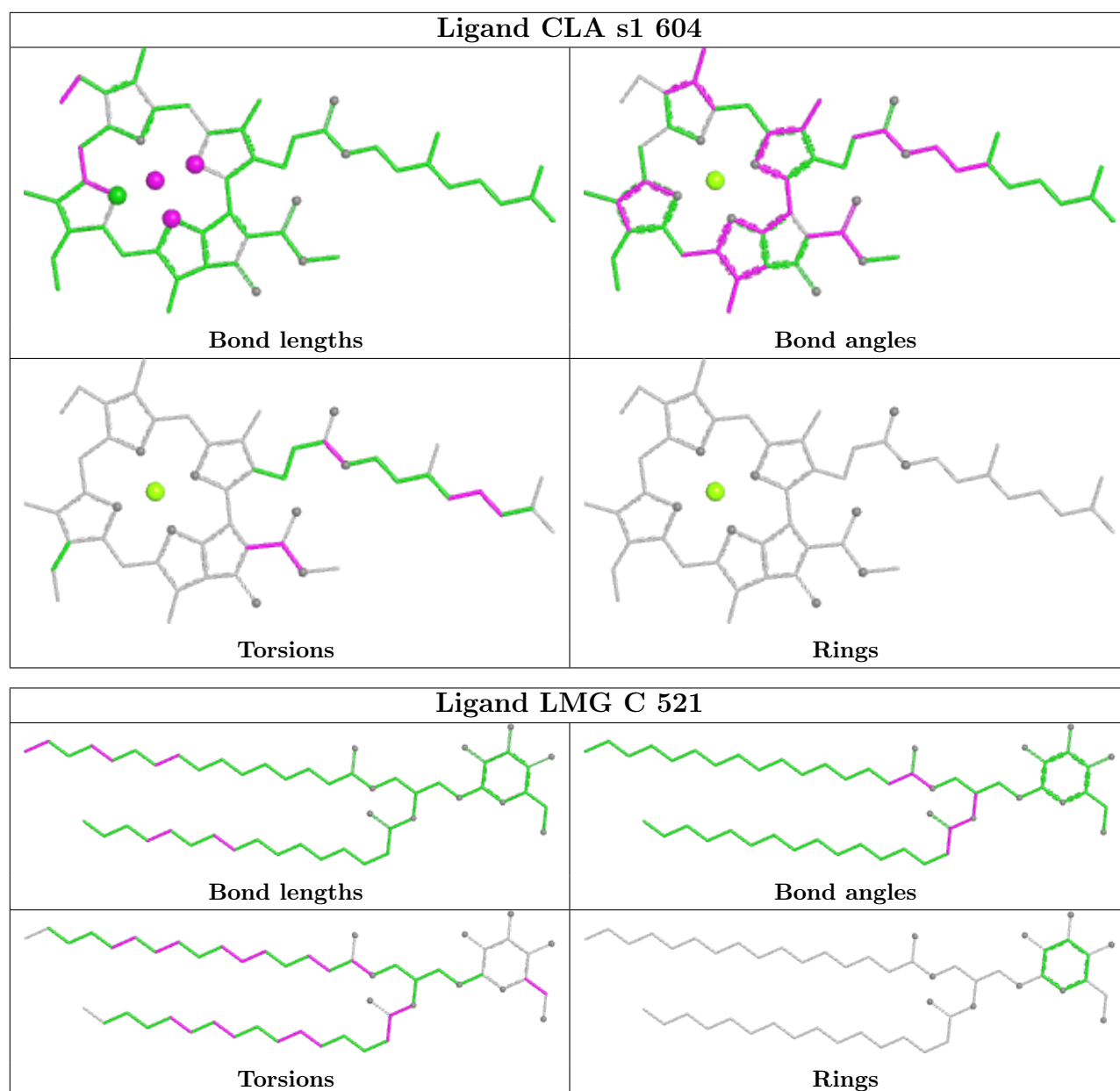


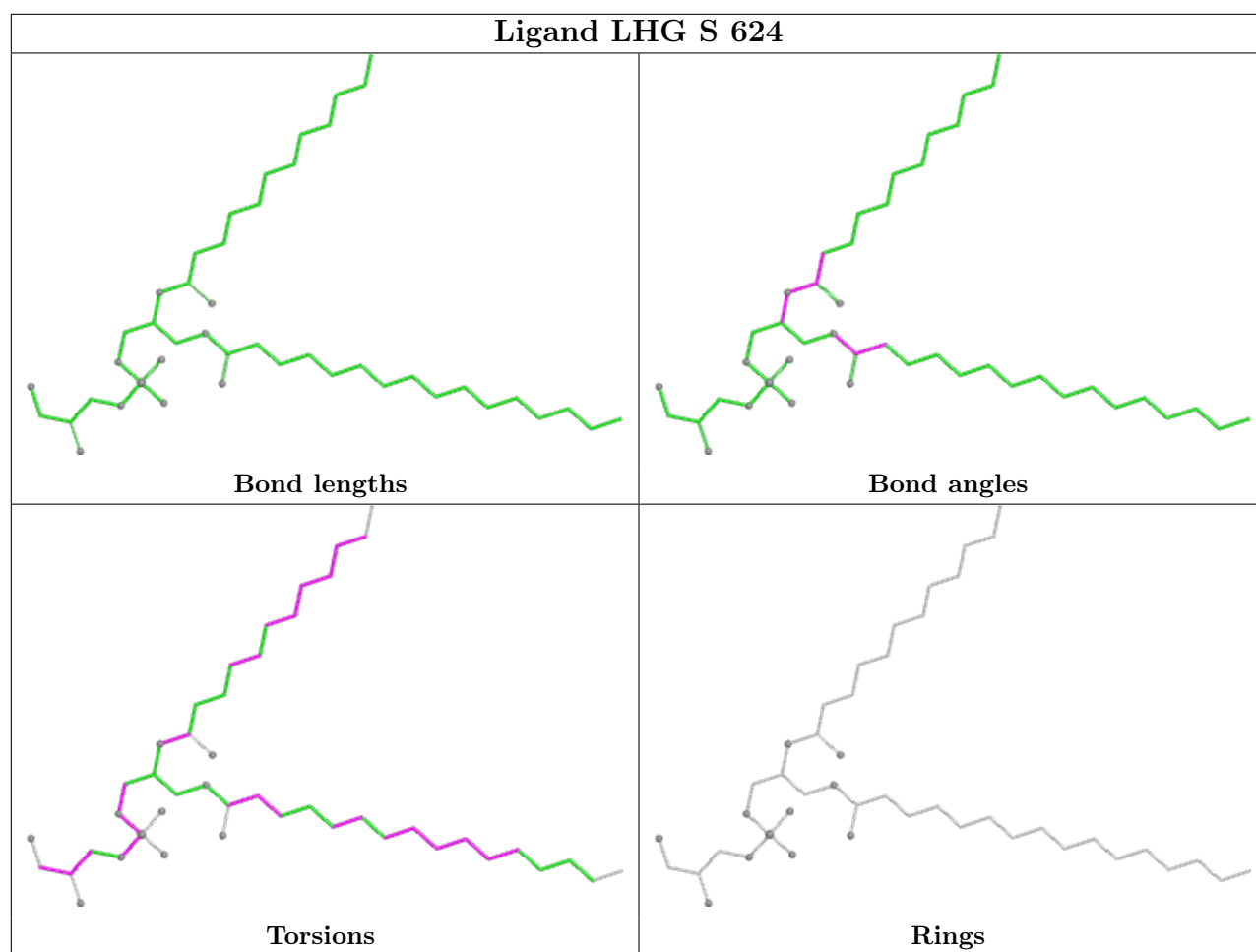


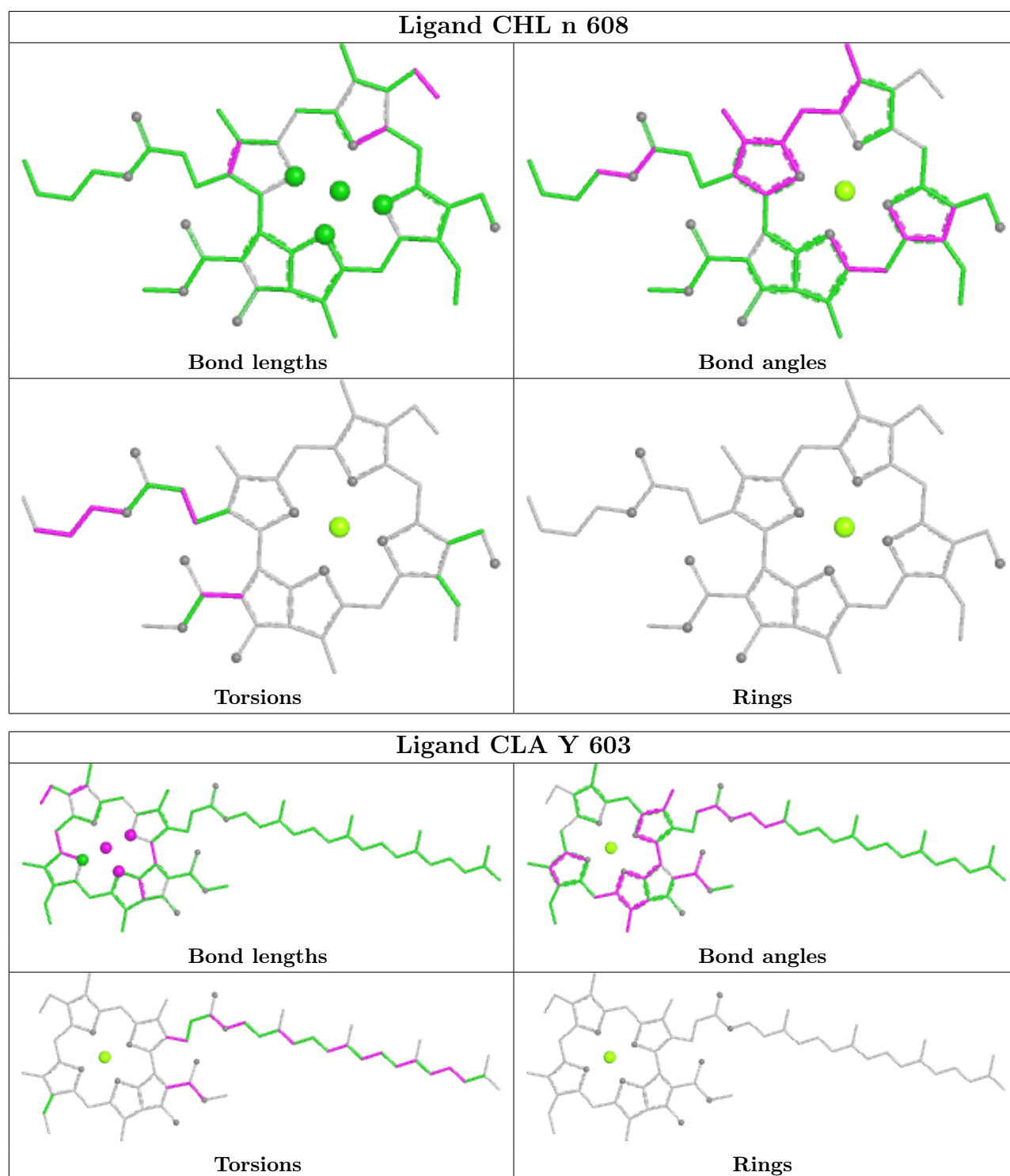


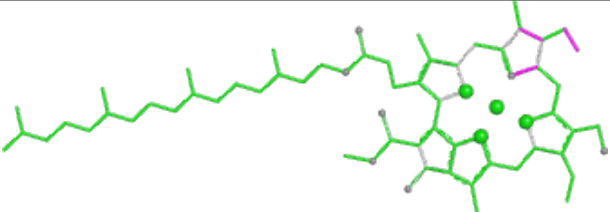
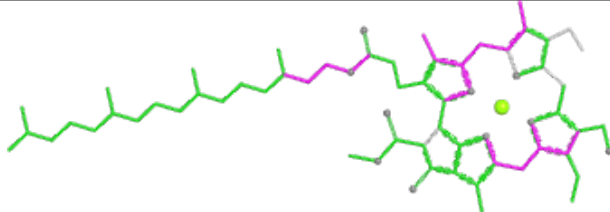
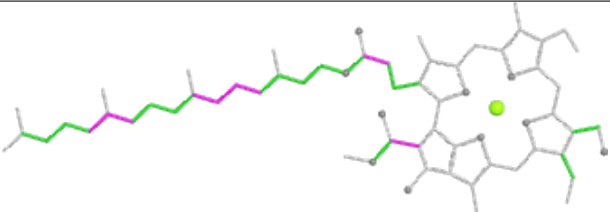
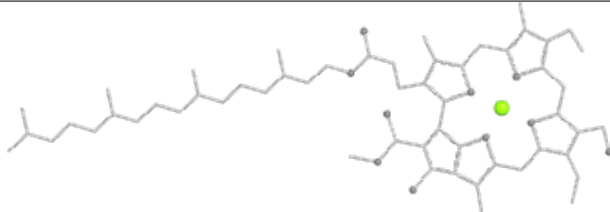
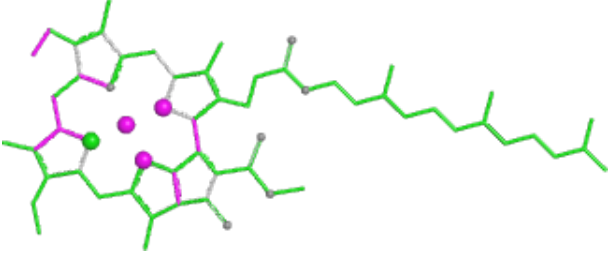
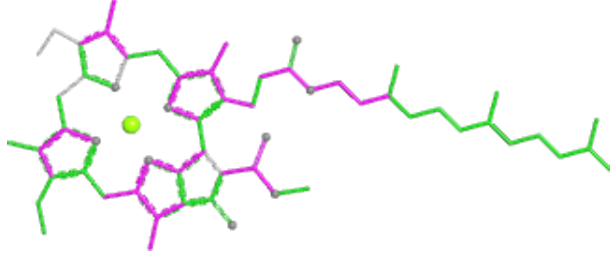
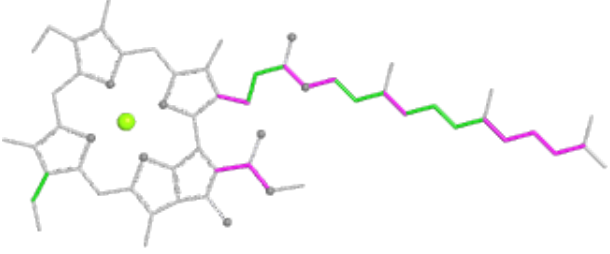
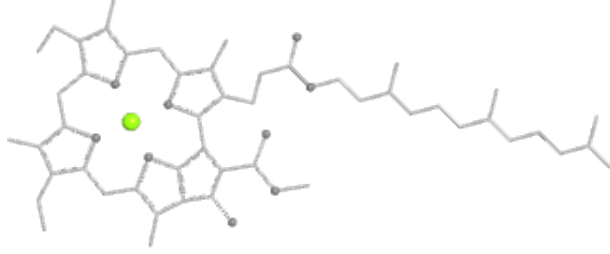


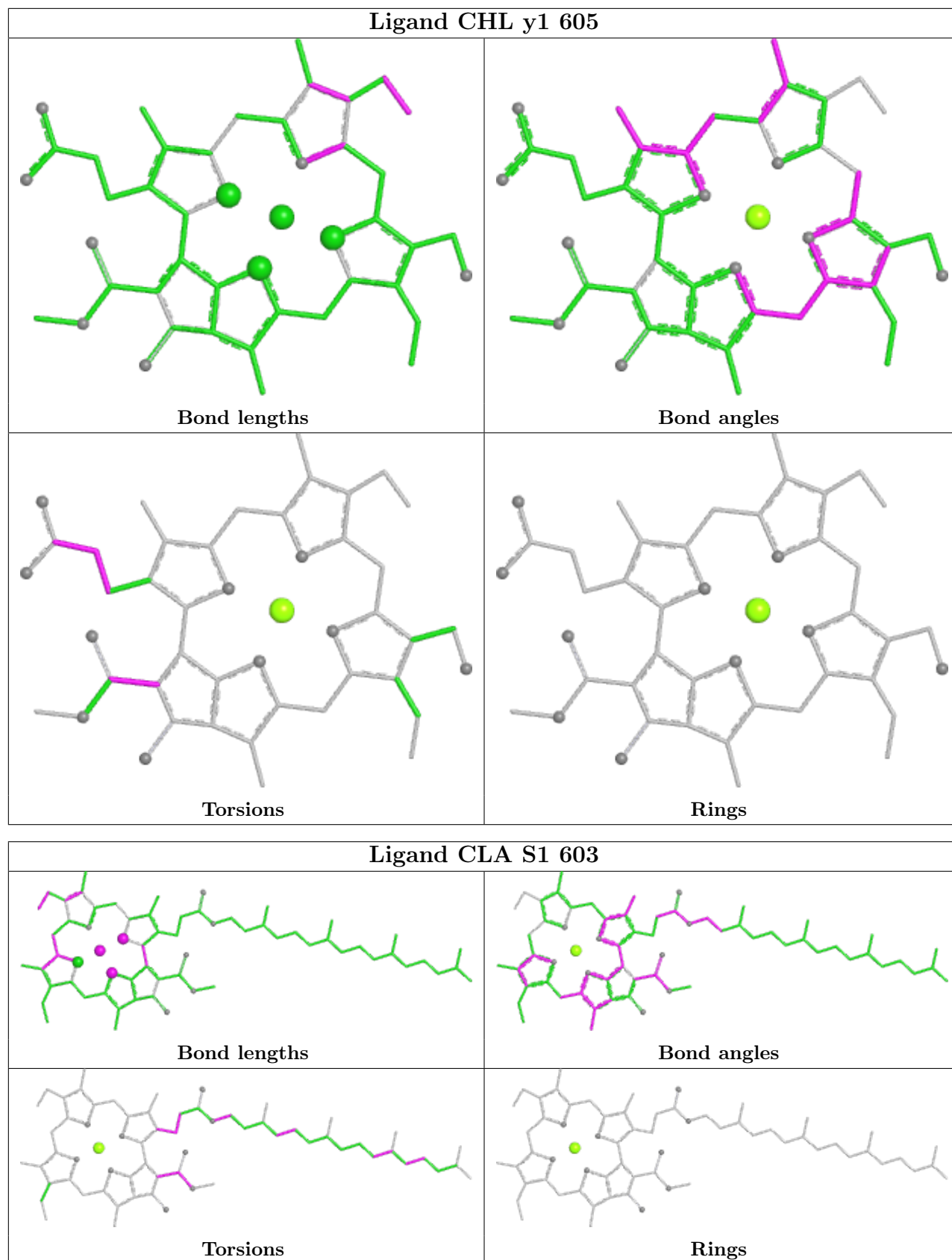




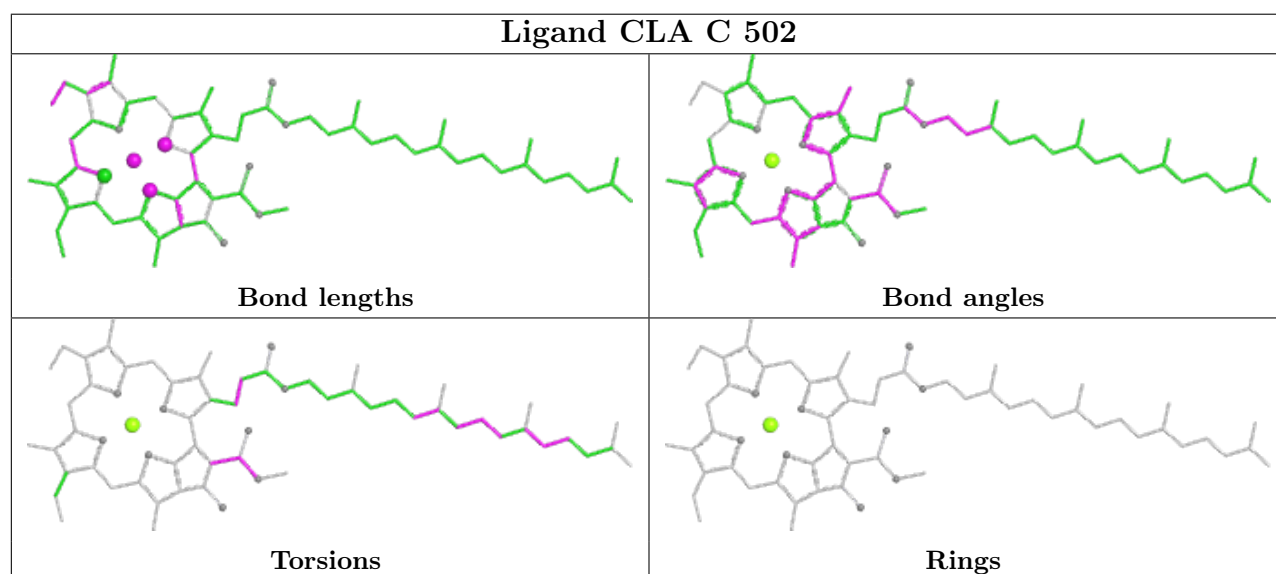
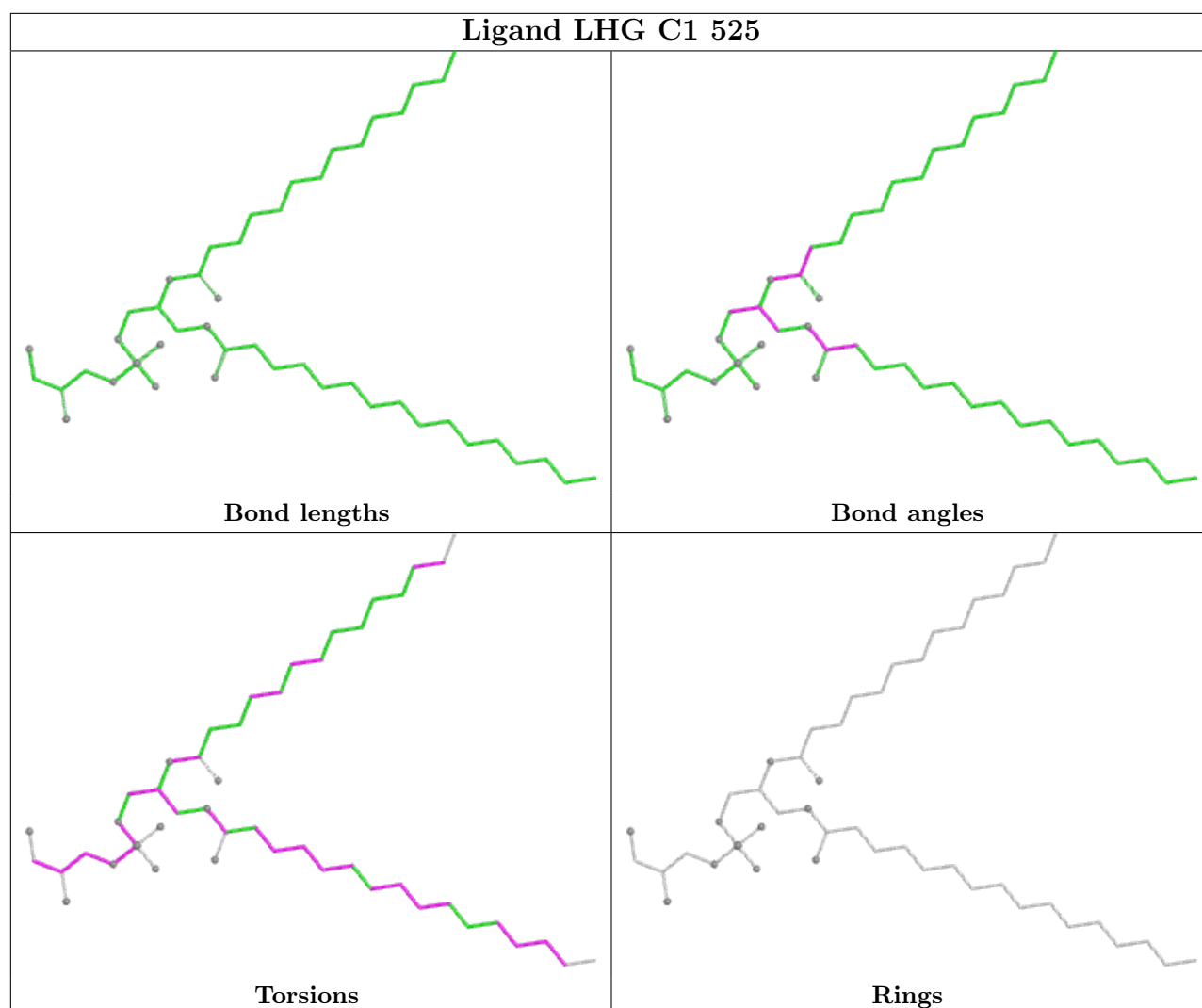


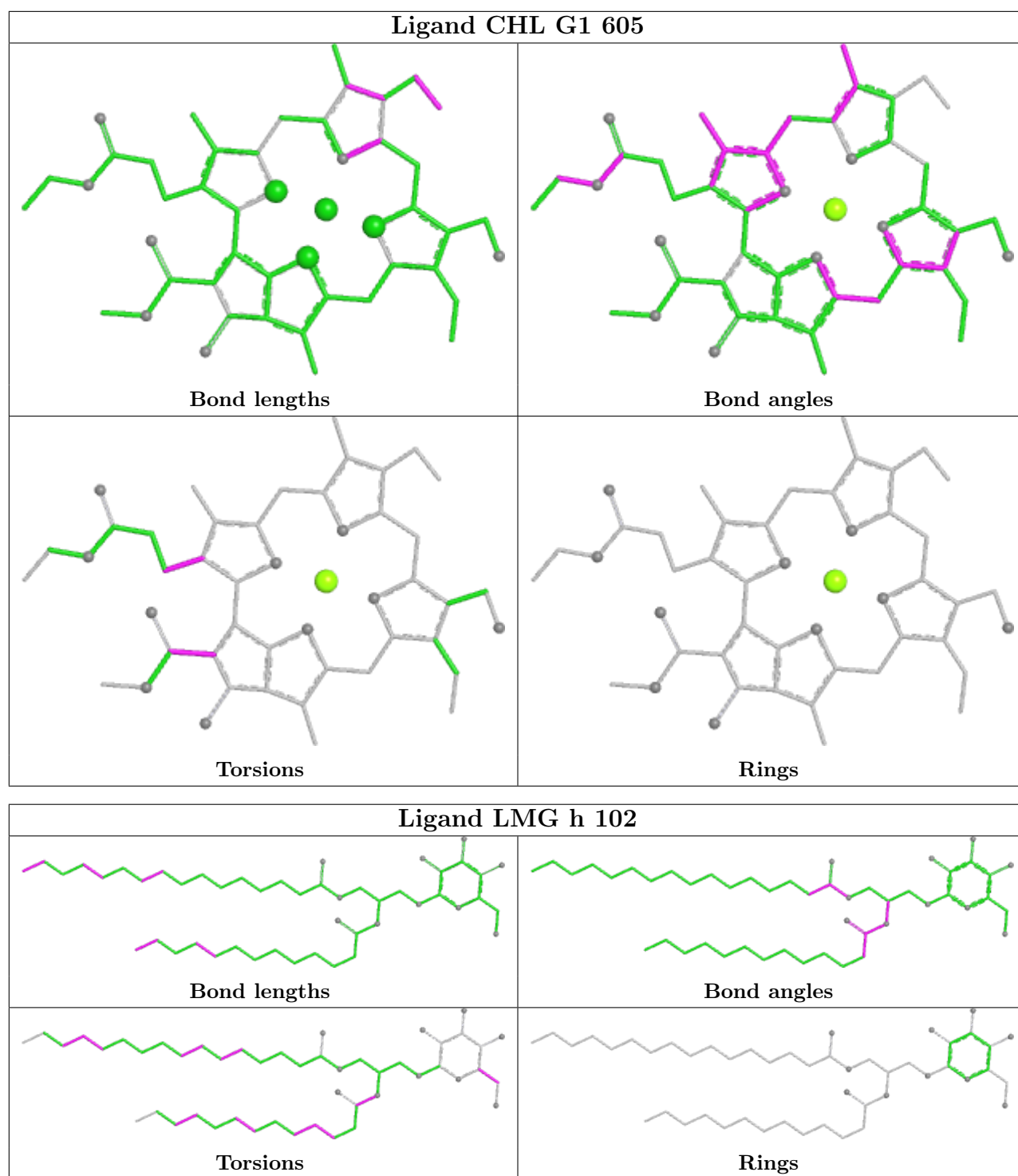


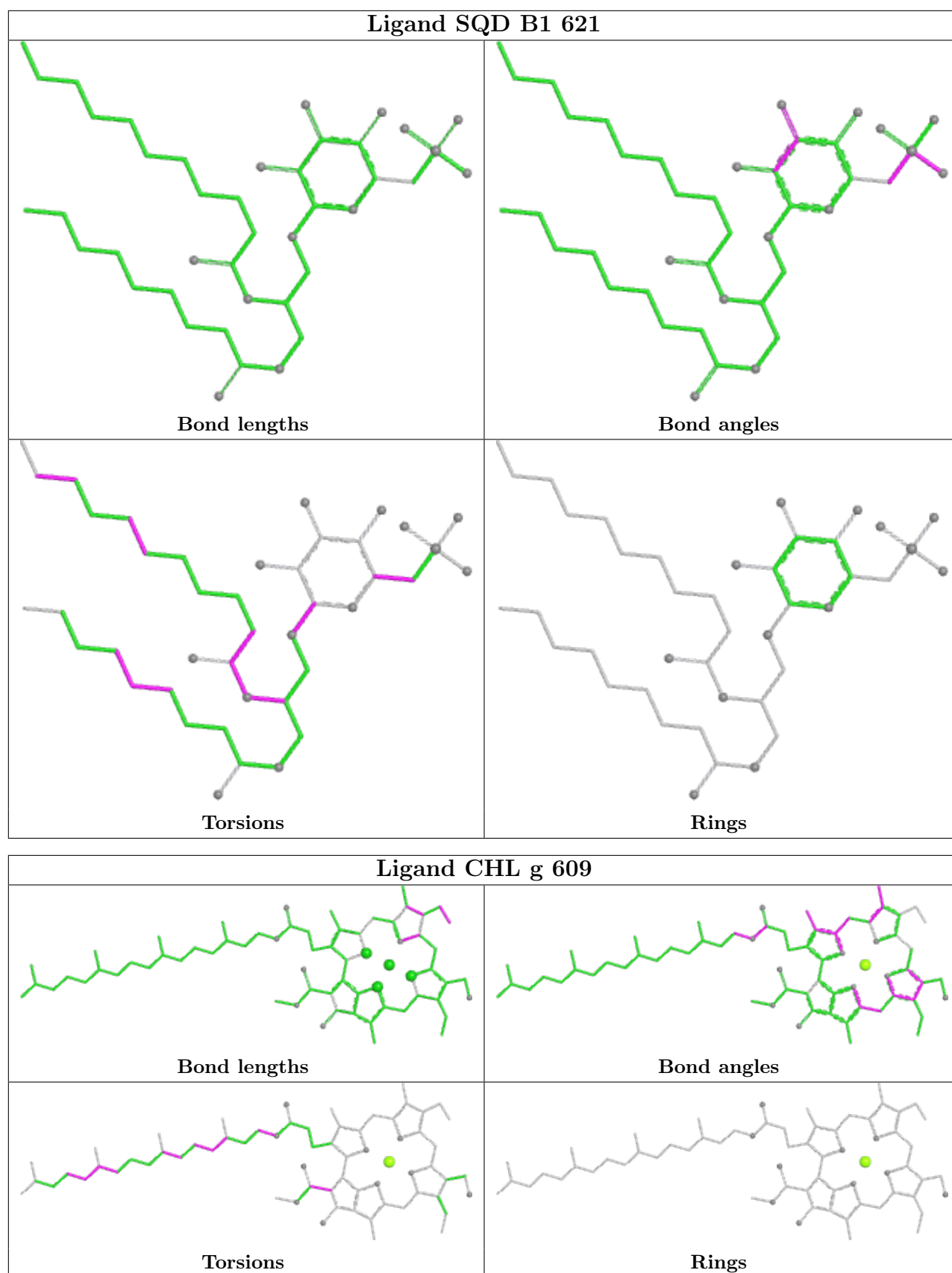
Ligand CHL G 601	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA A 410	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>

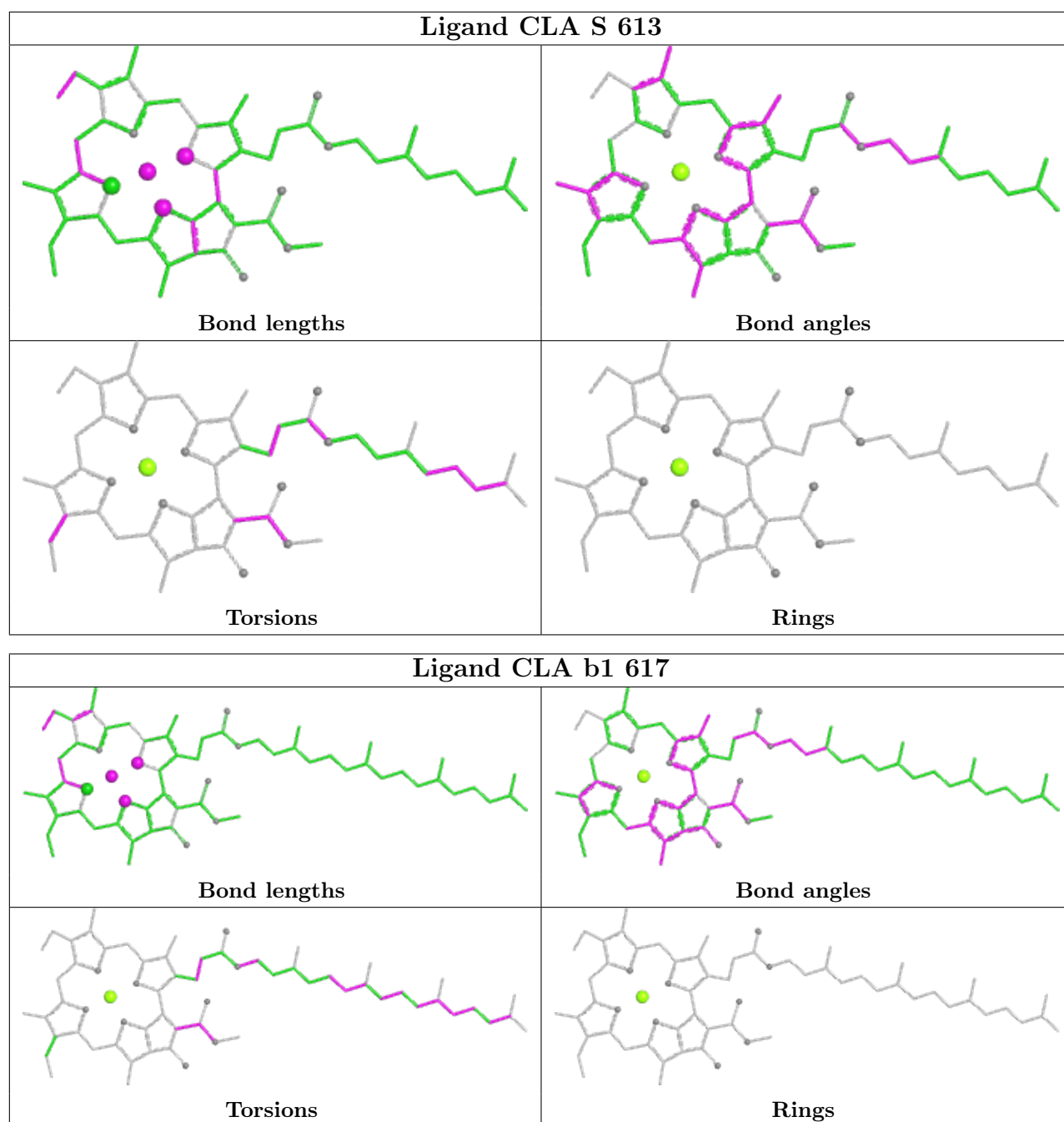


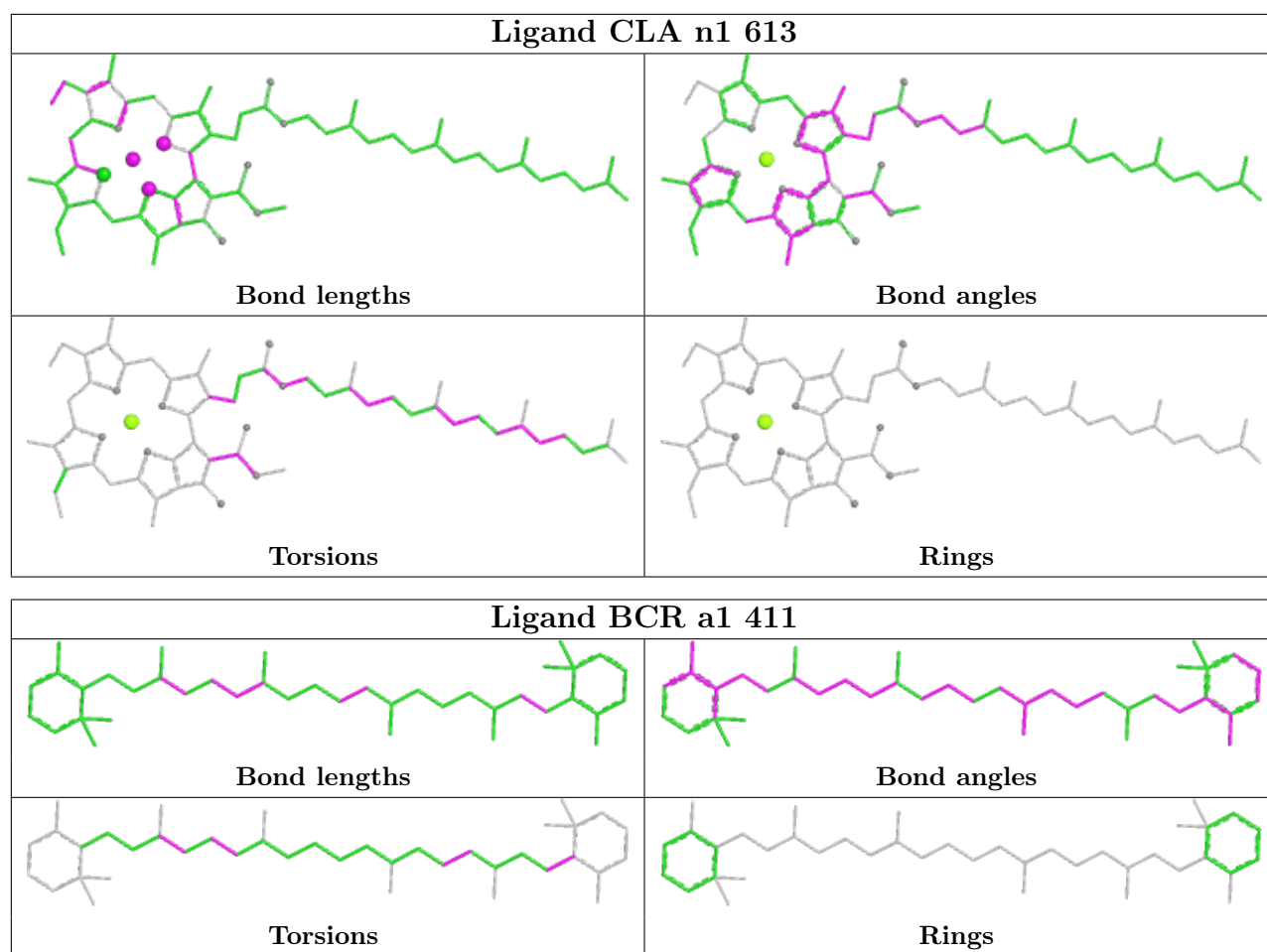


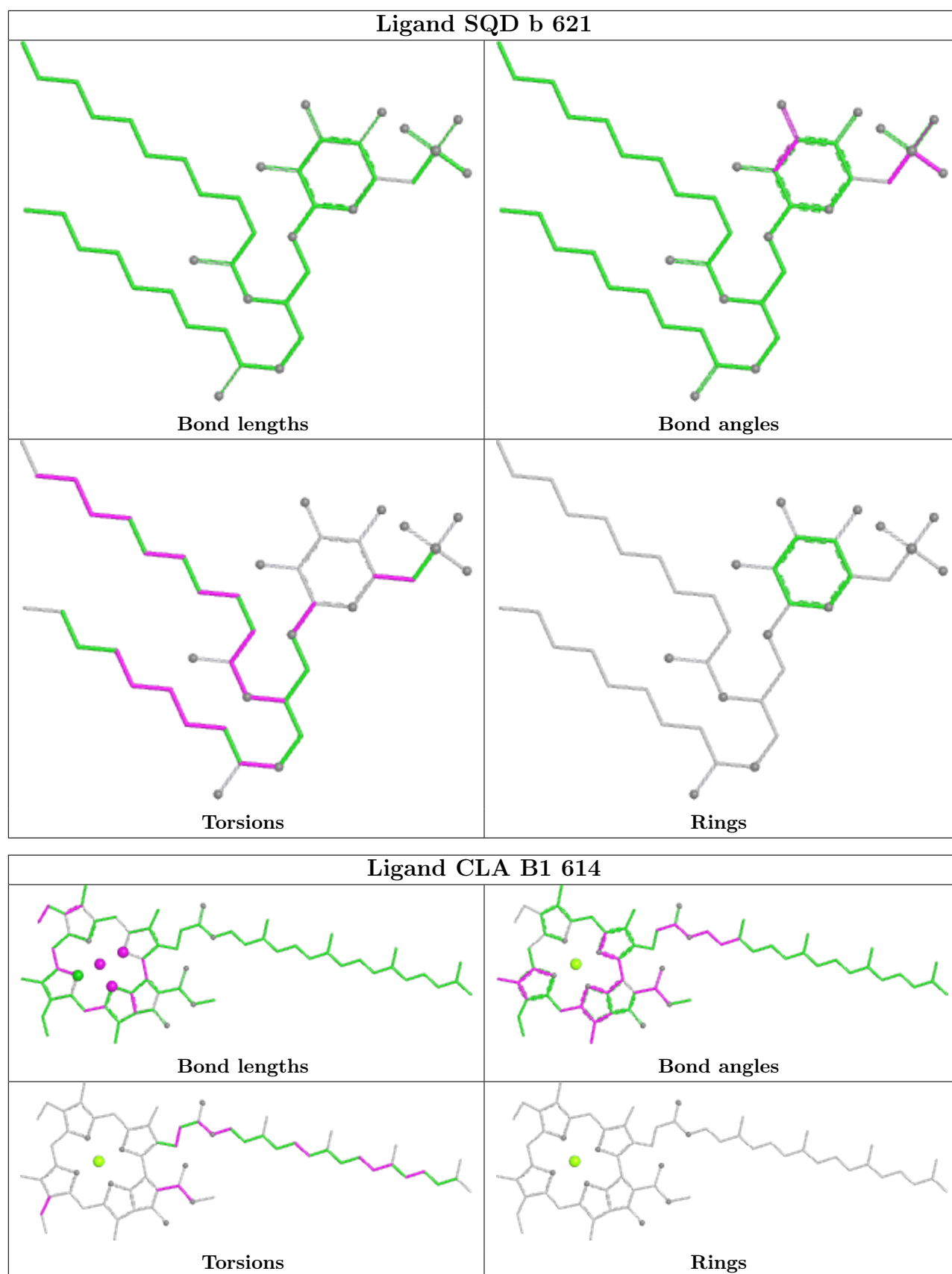




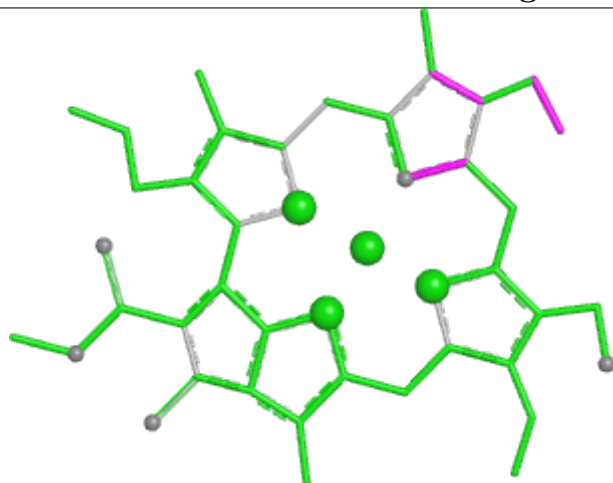




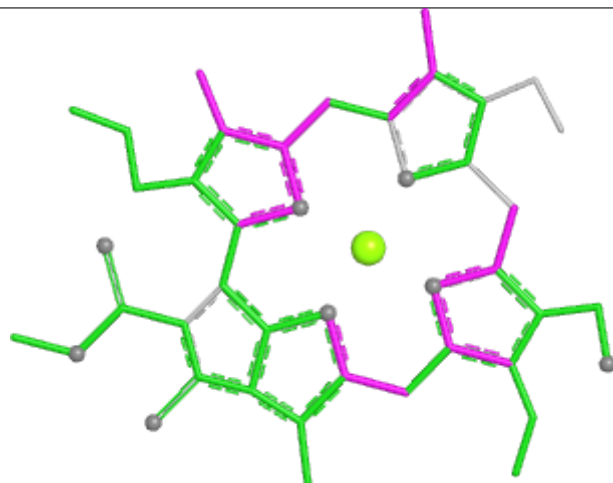




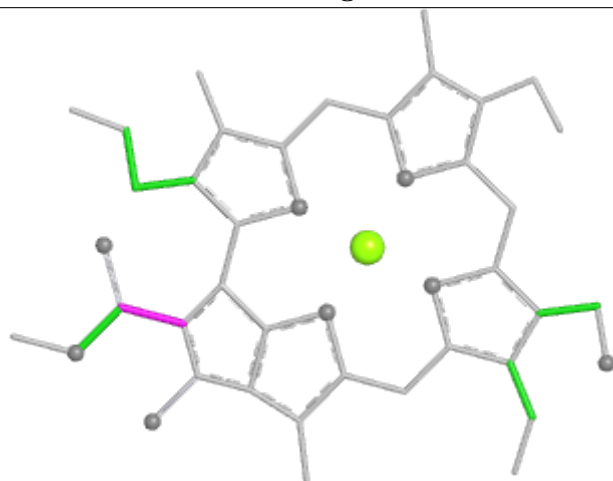
## Ligand CHL r 606



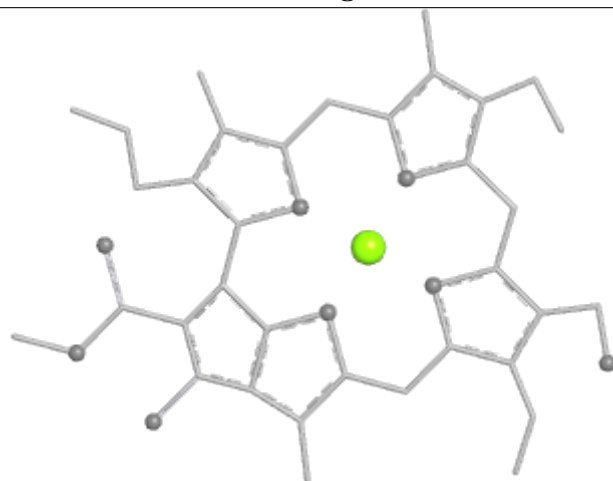
Bond lengths



Bond angles

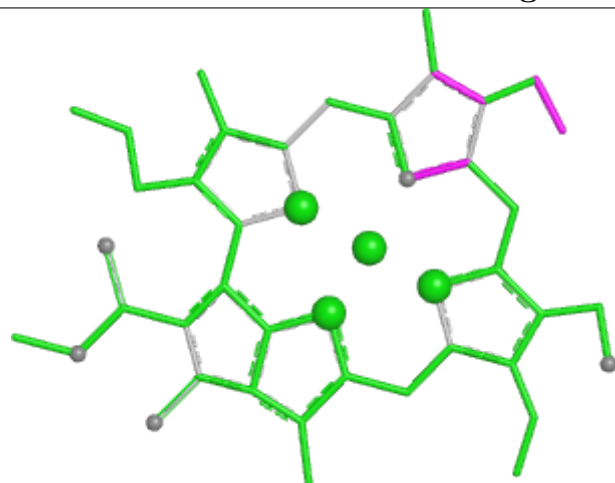


Torsions

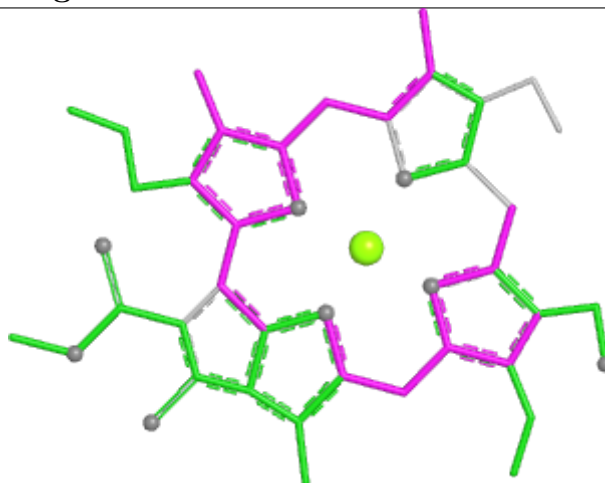


Rings

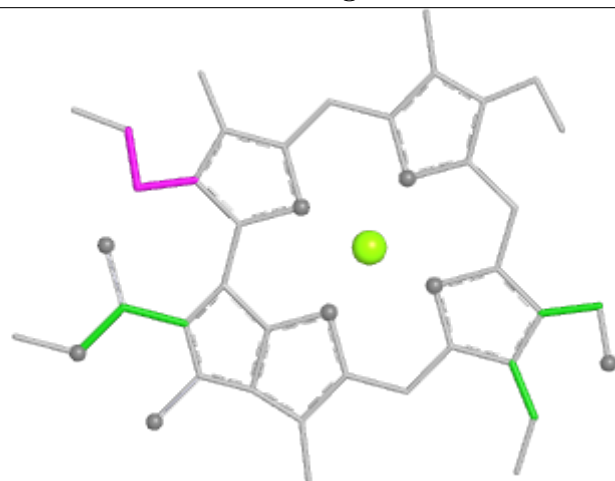
## Ligand CHL g 608



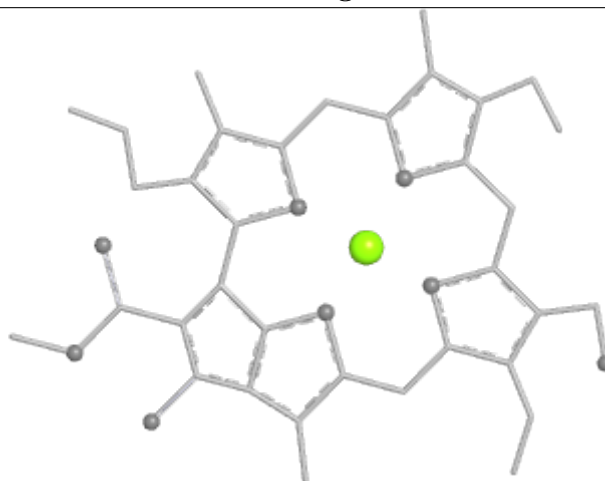
Bond lengths



Bond angles

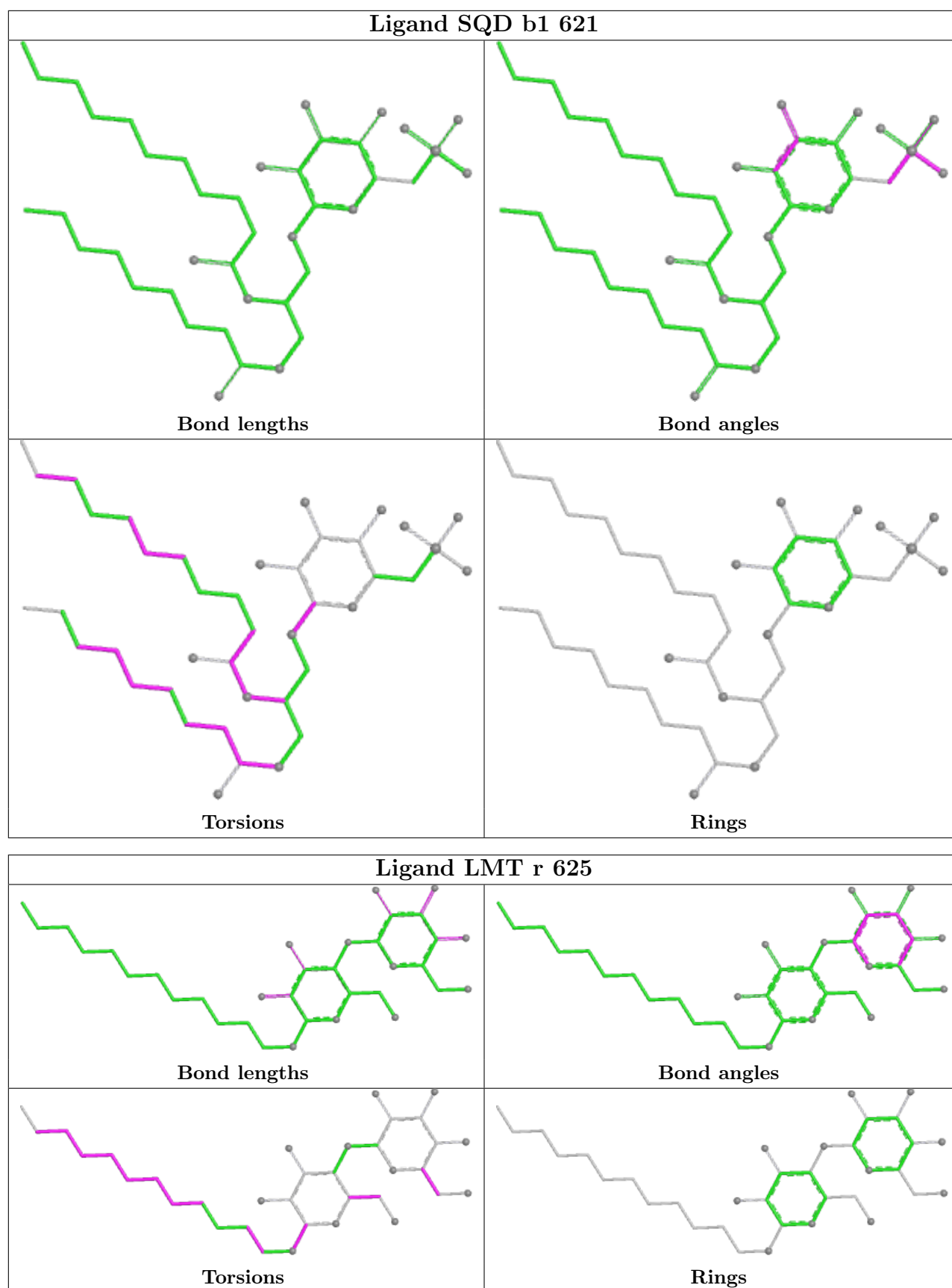


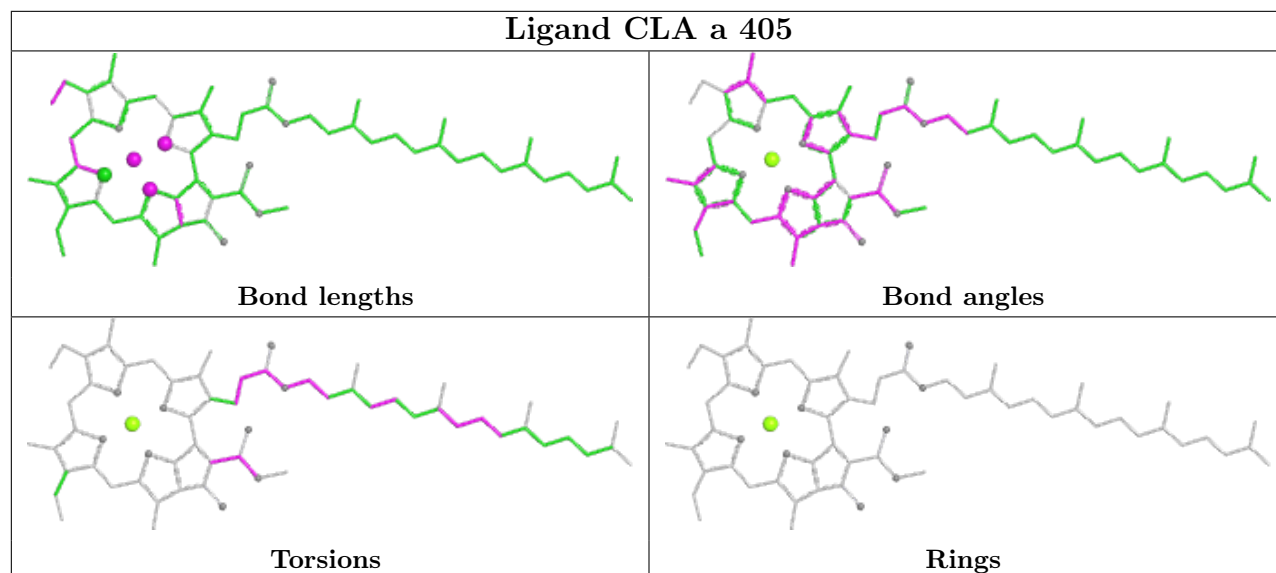
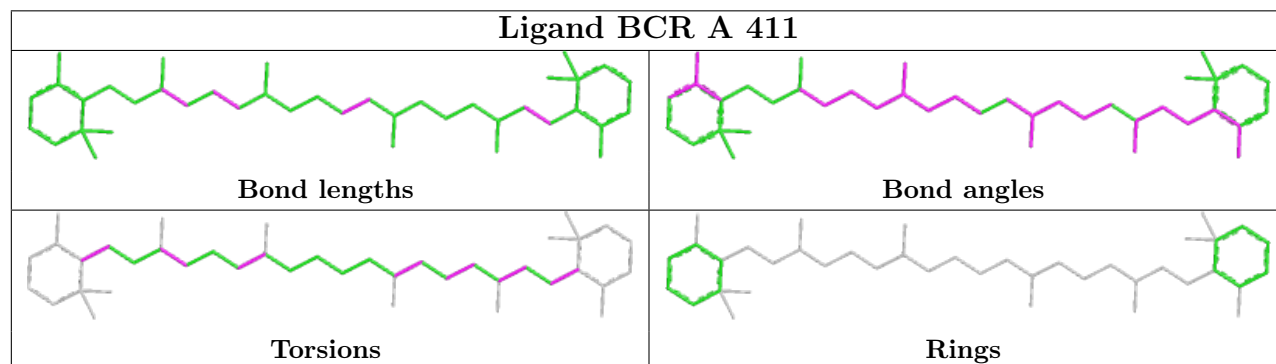
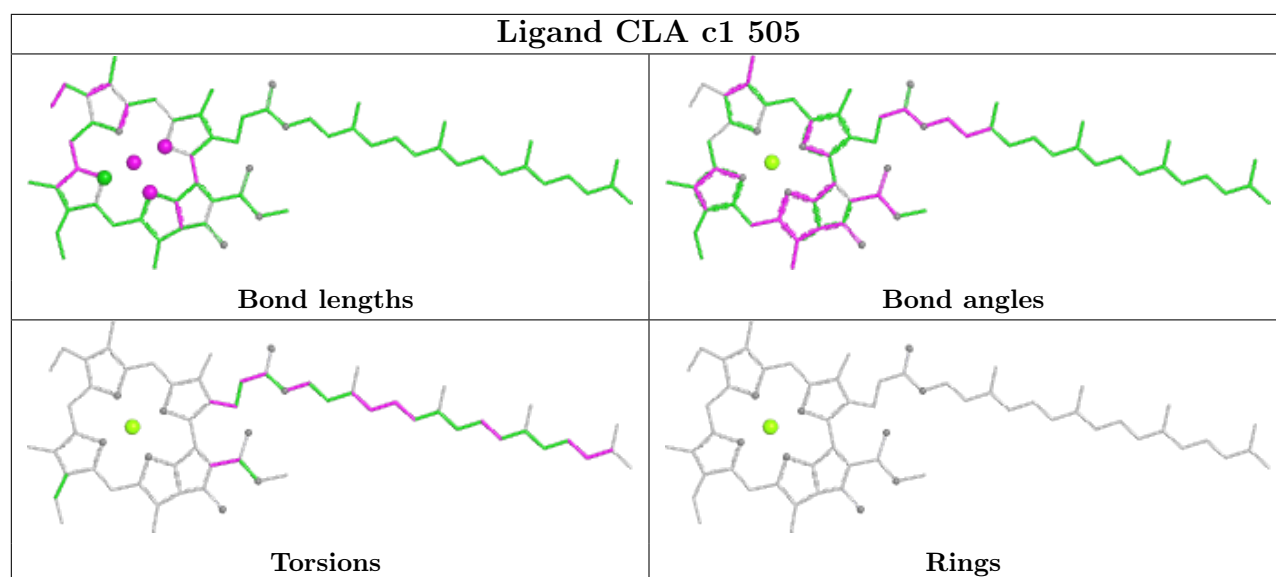
Torsions

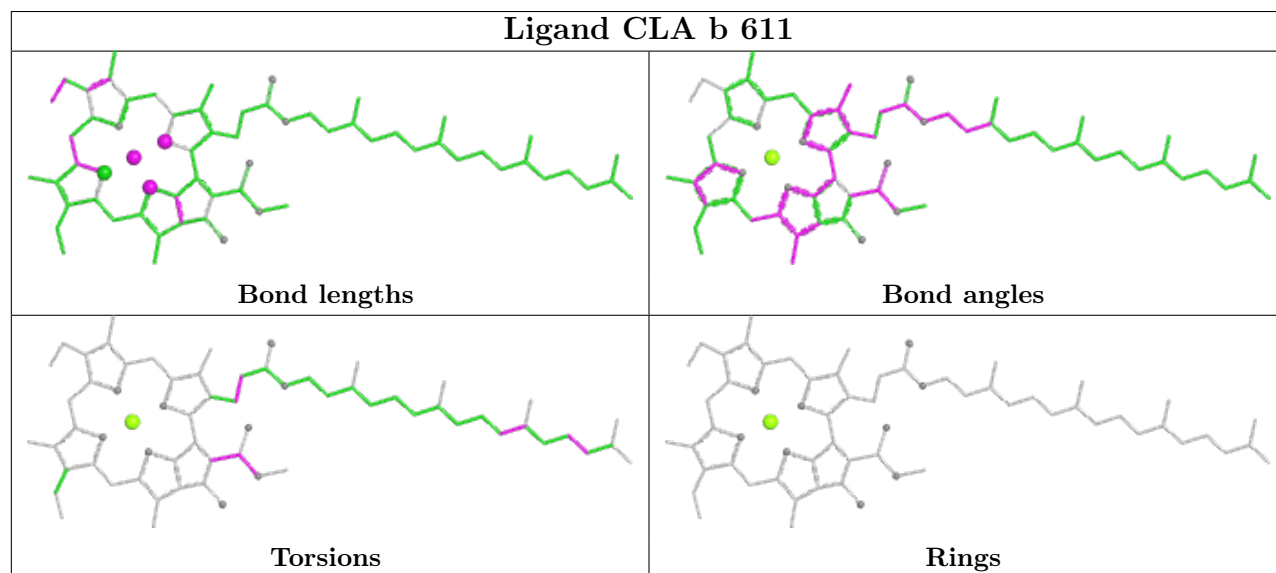
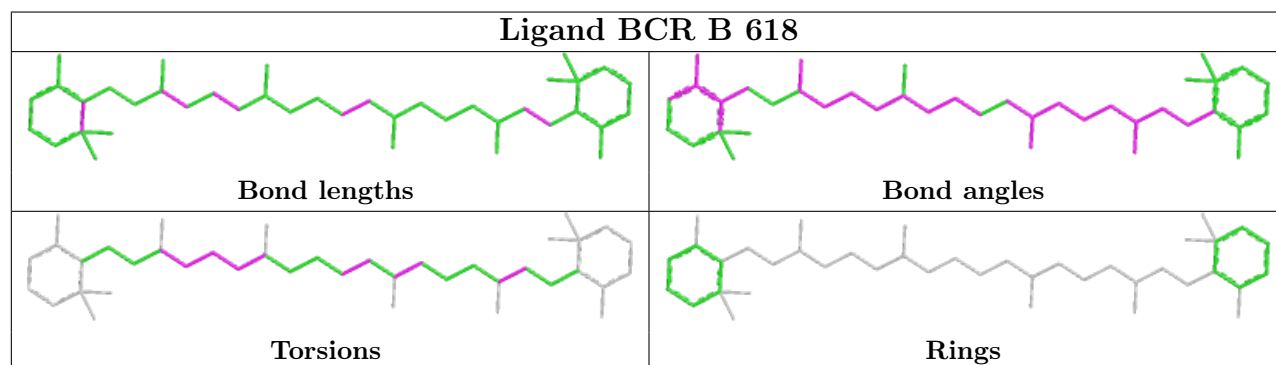
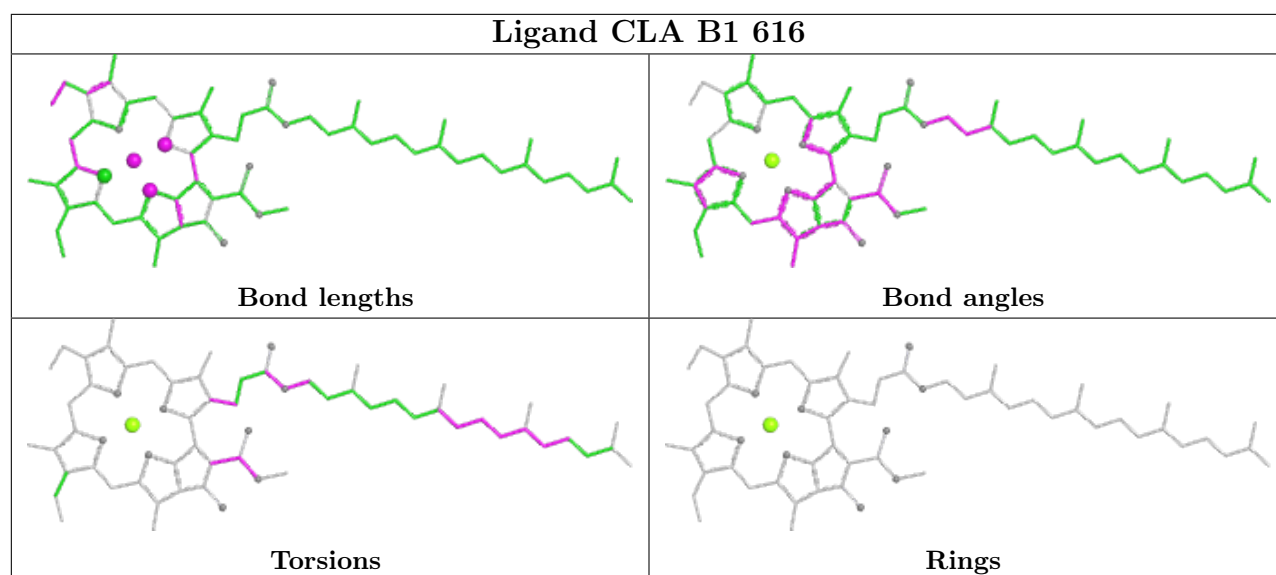


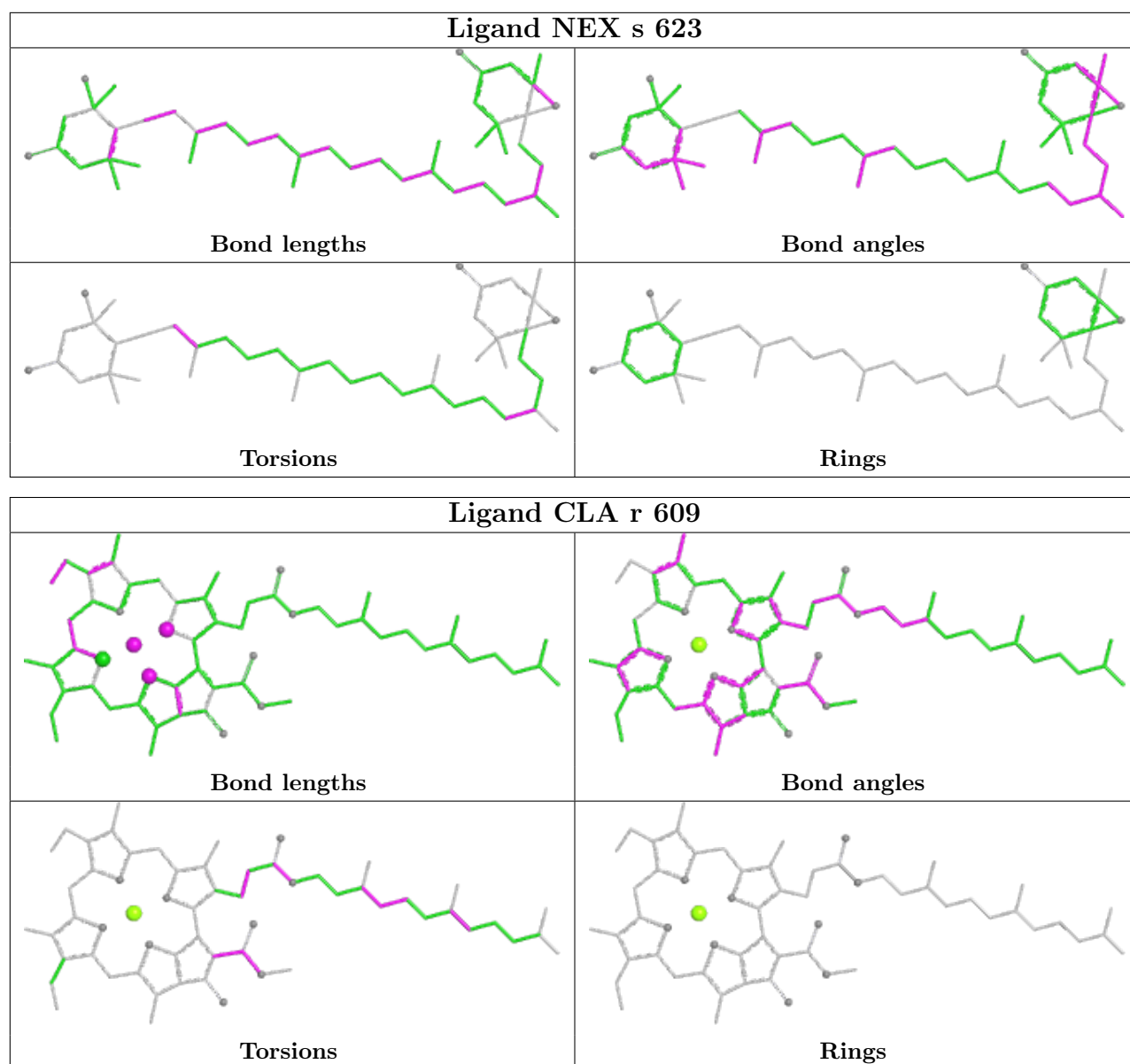
Rings

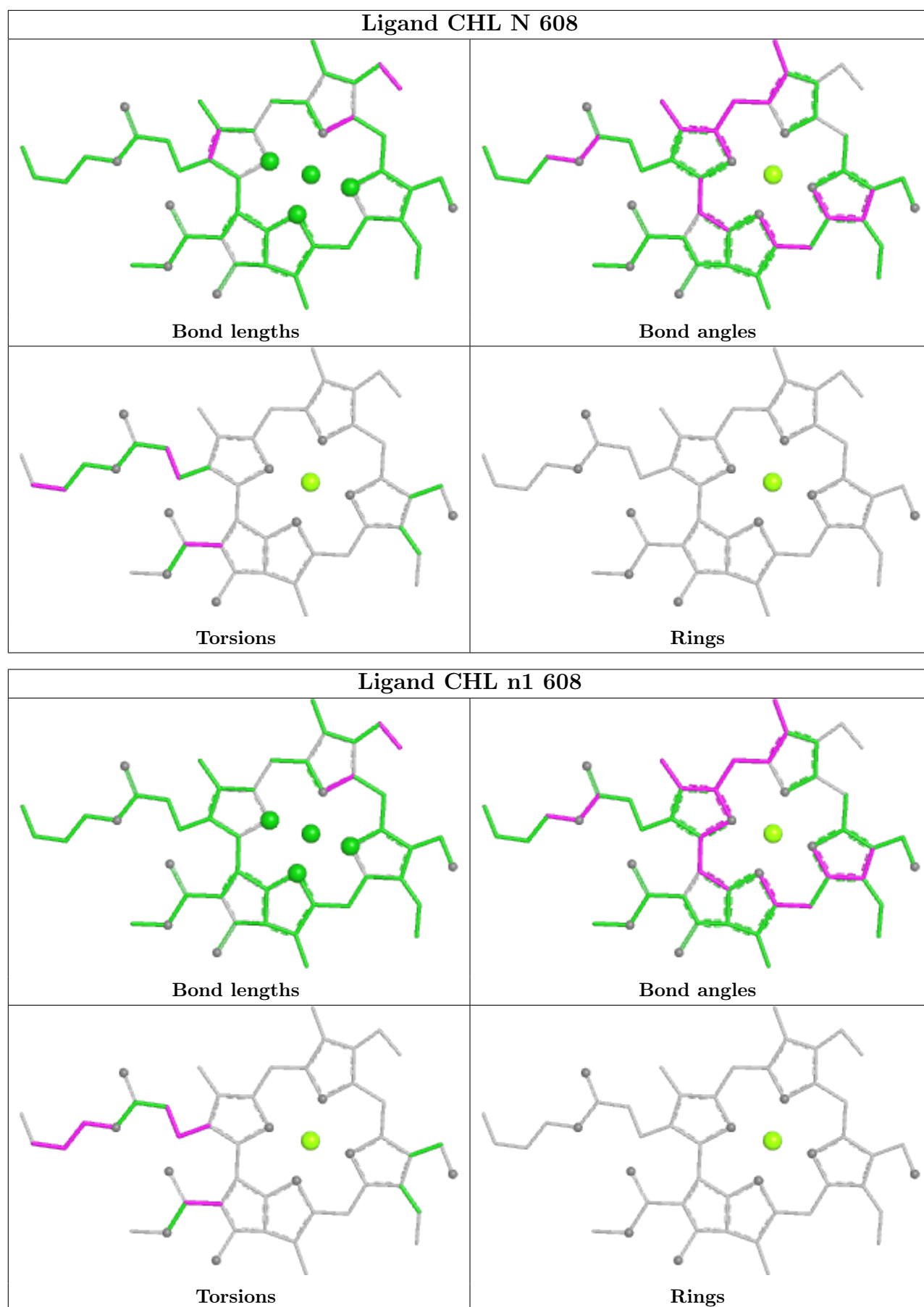


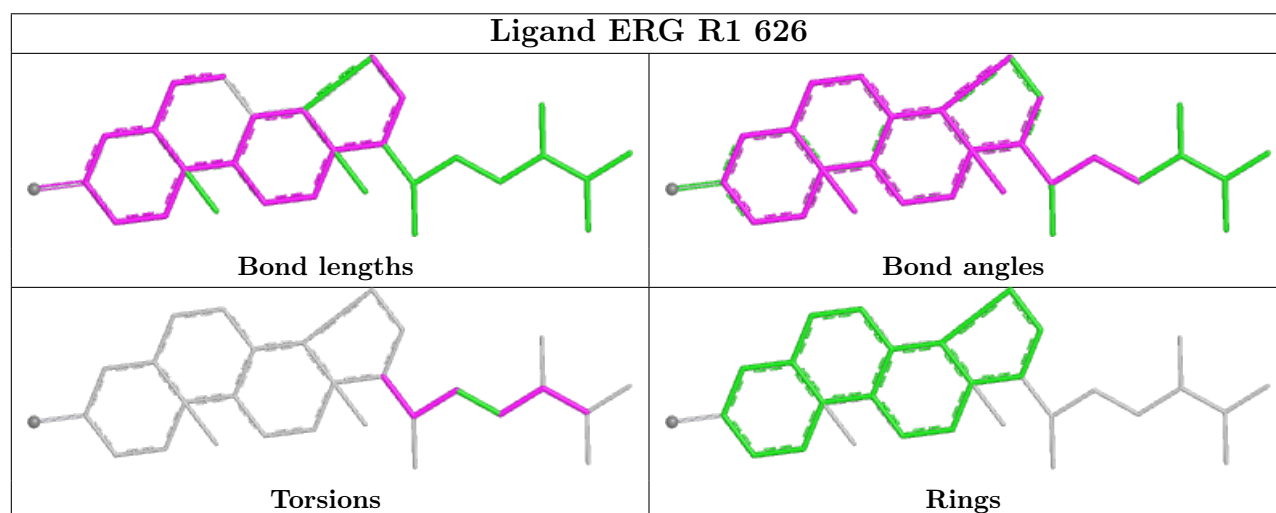
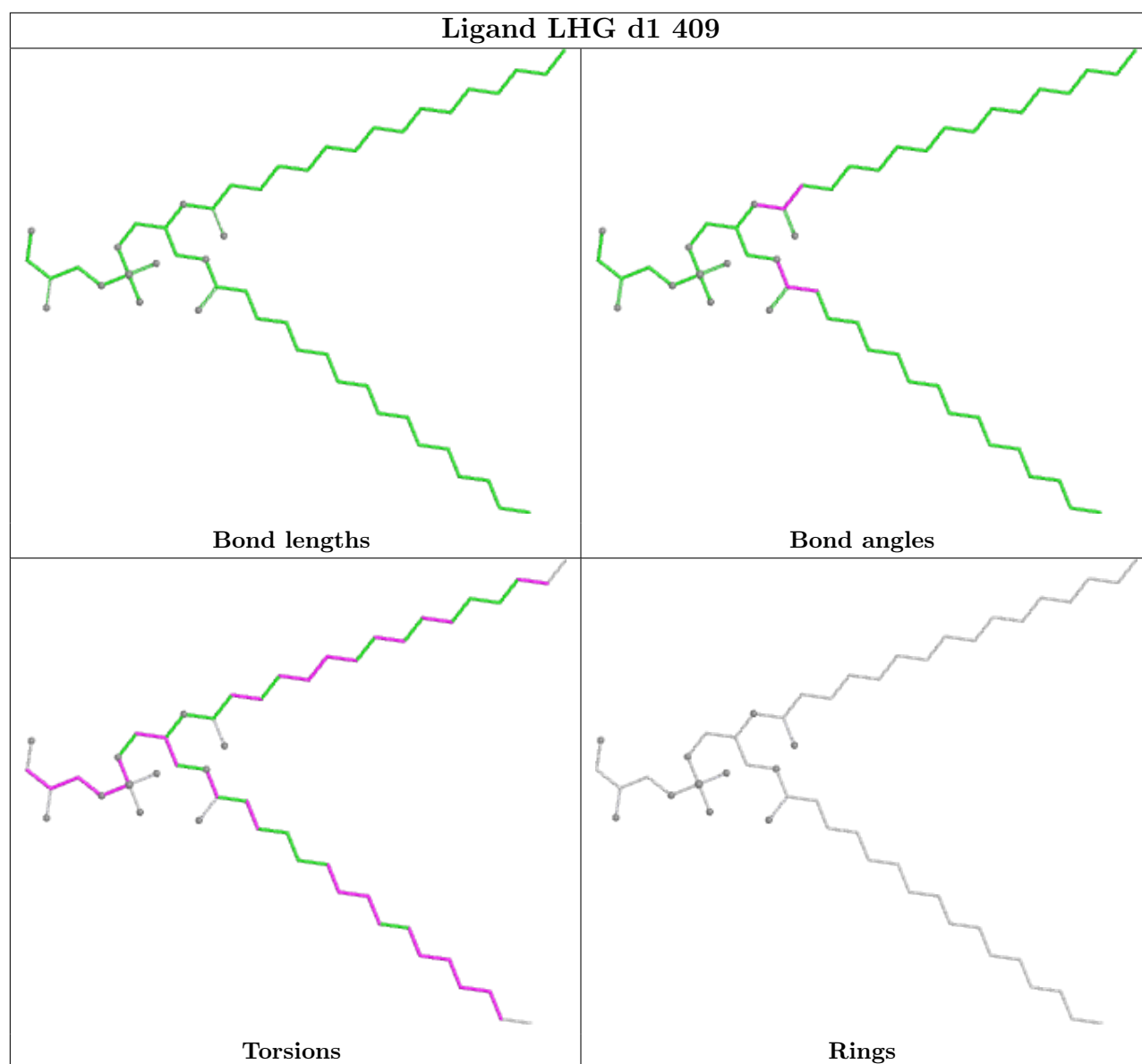


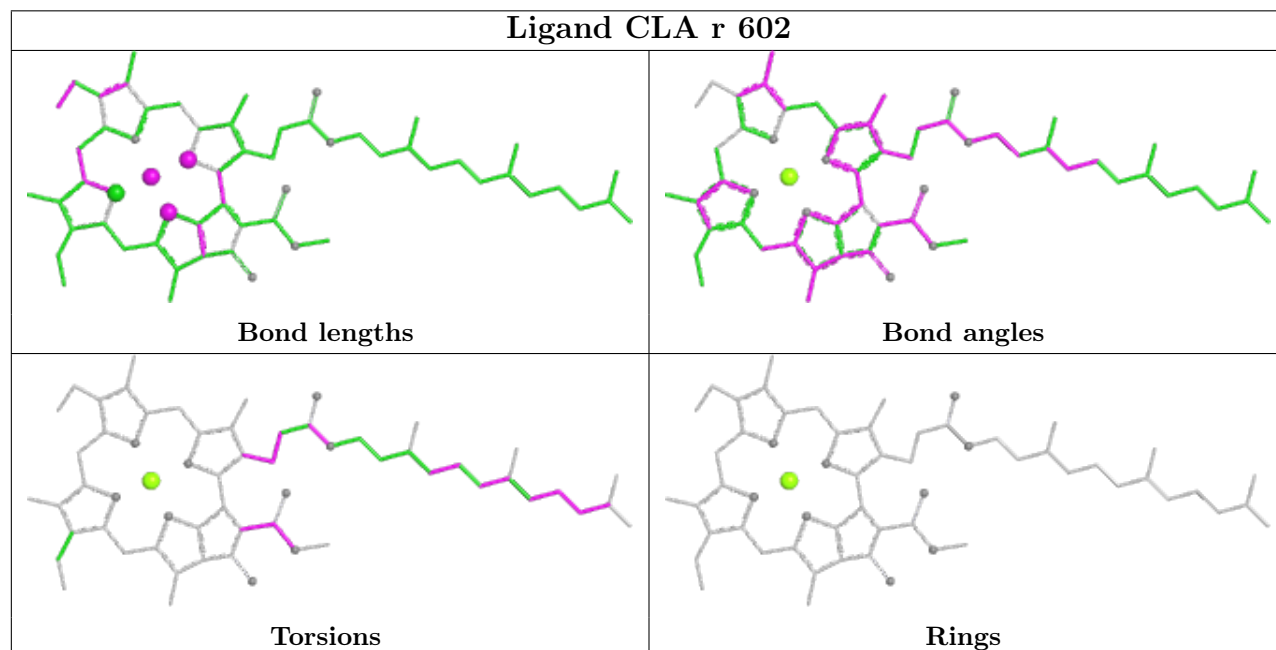
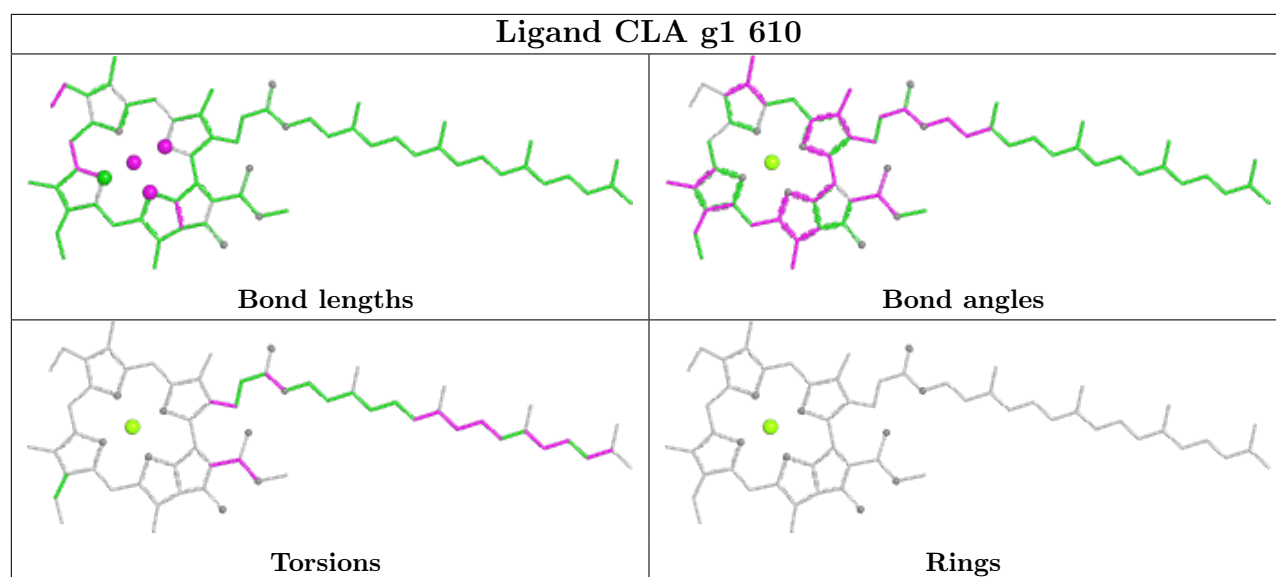


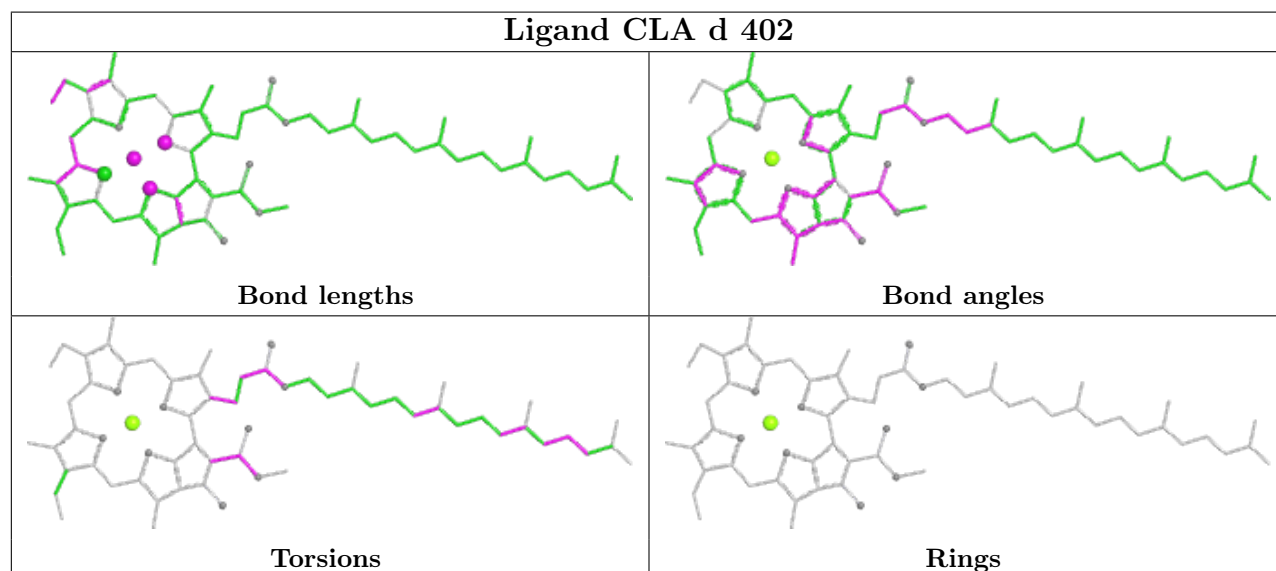
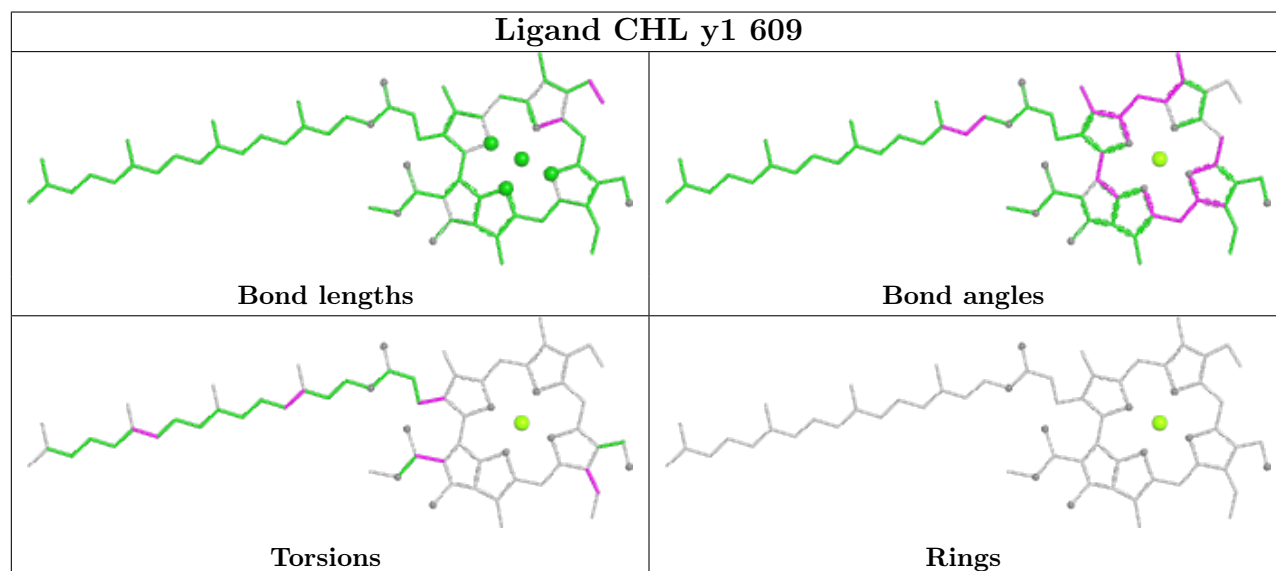
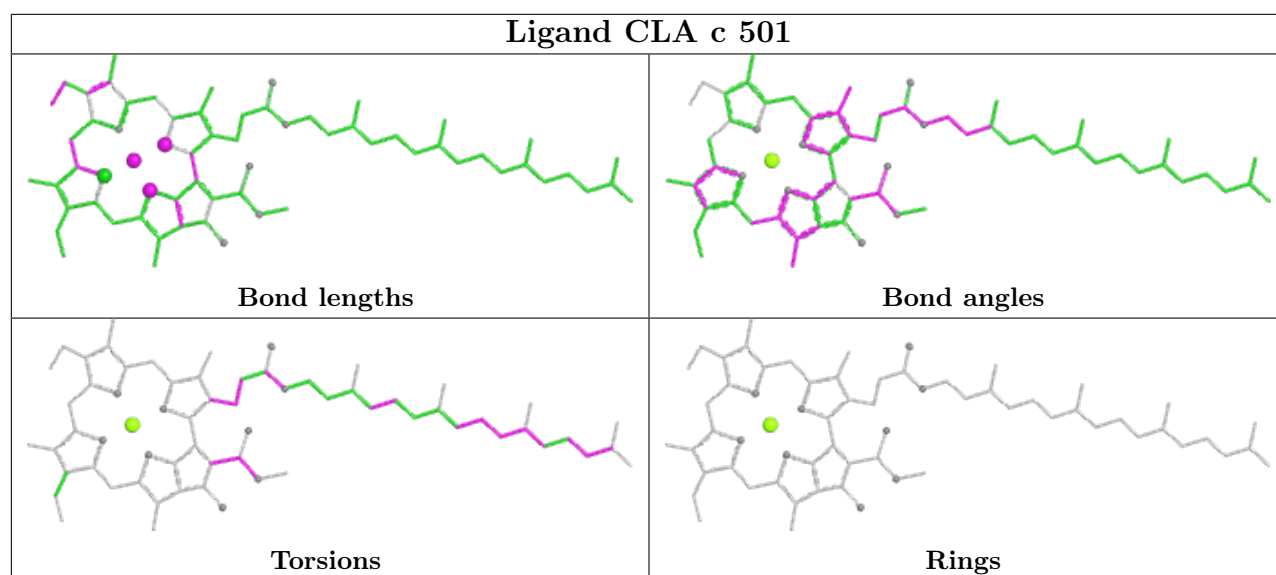




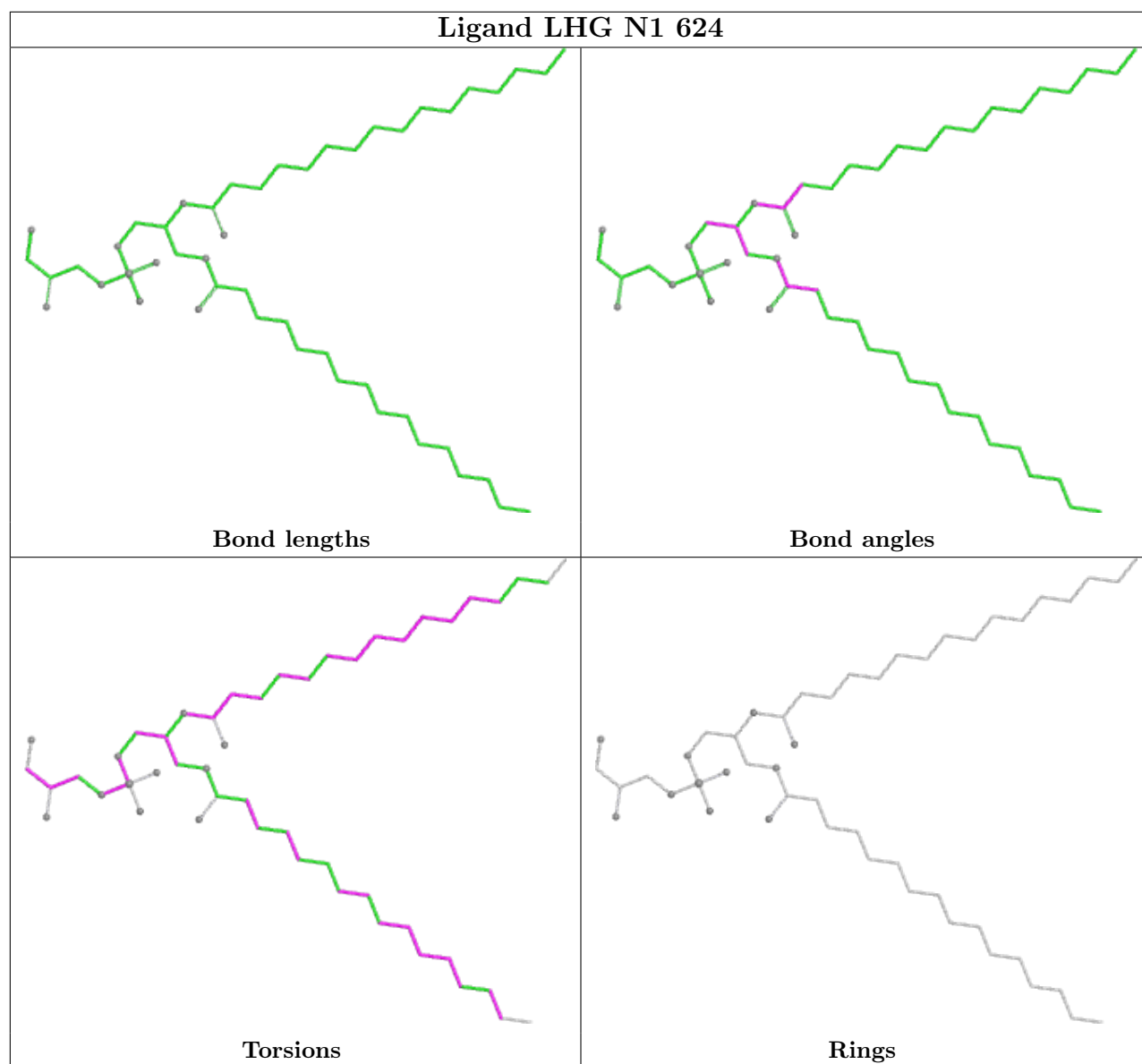
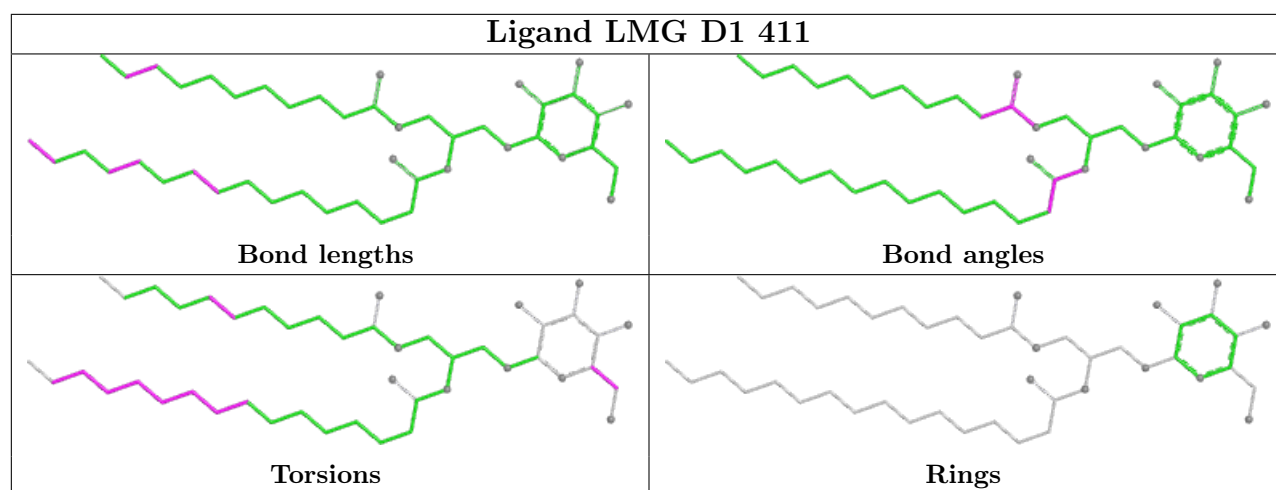


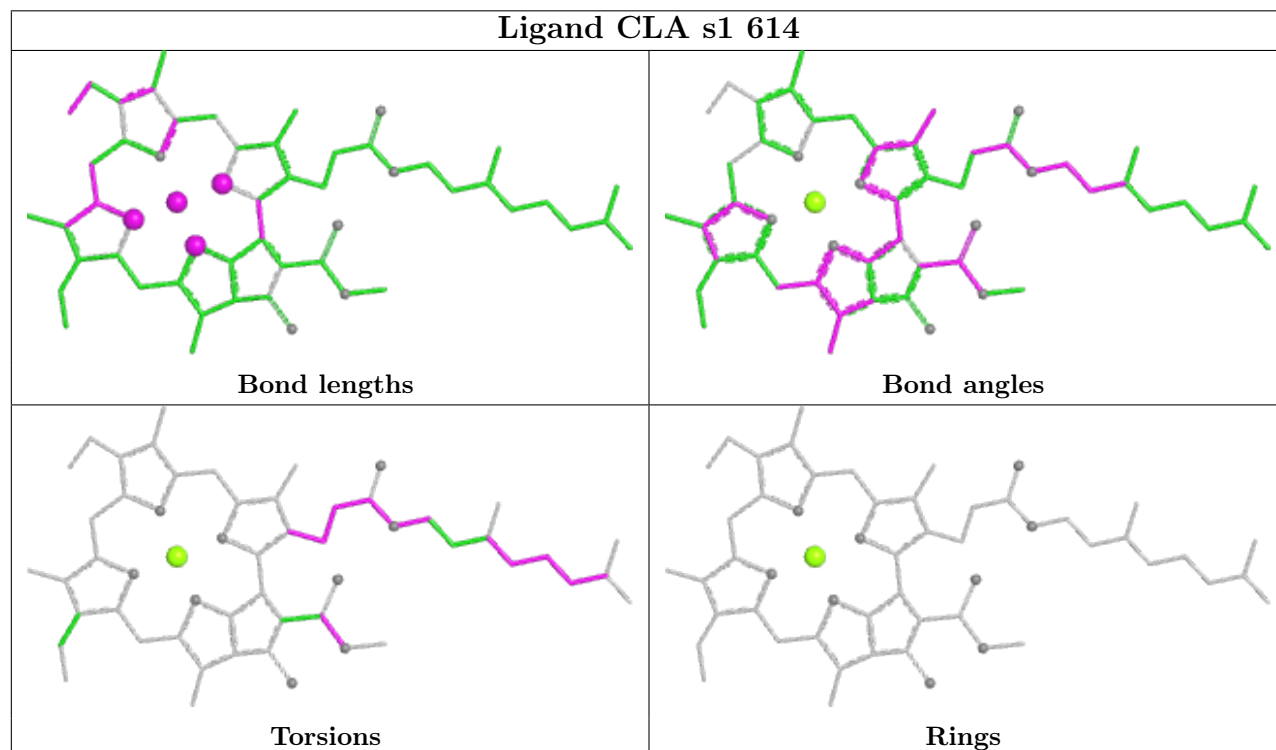
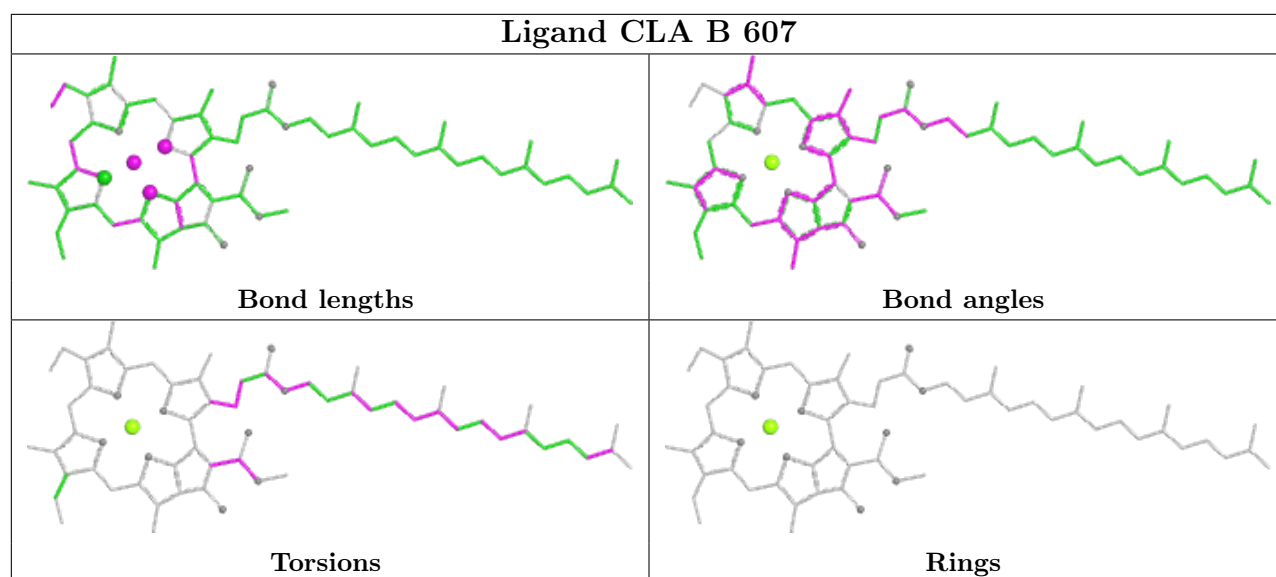


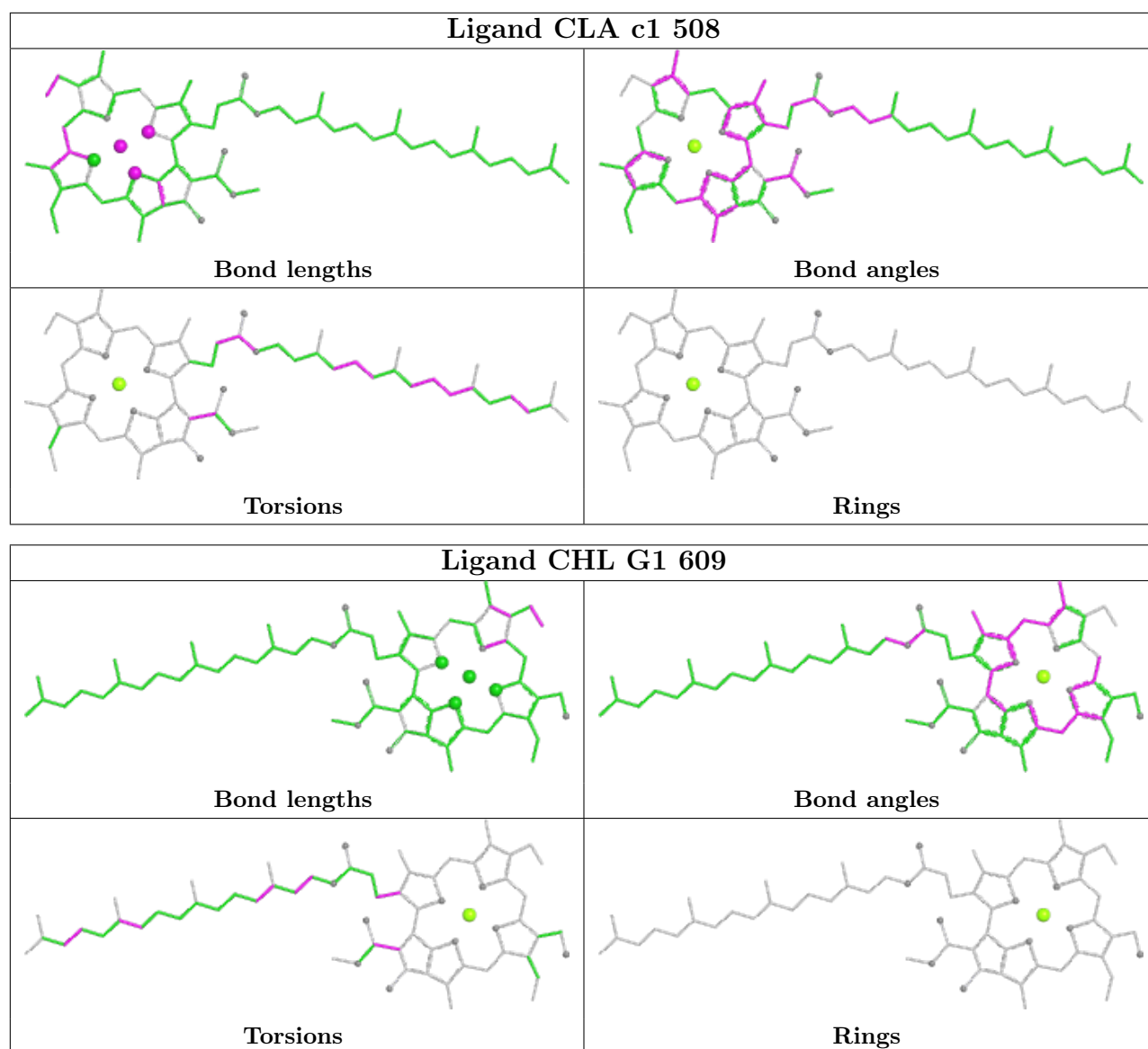


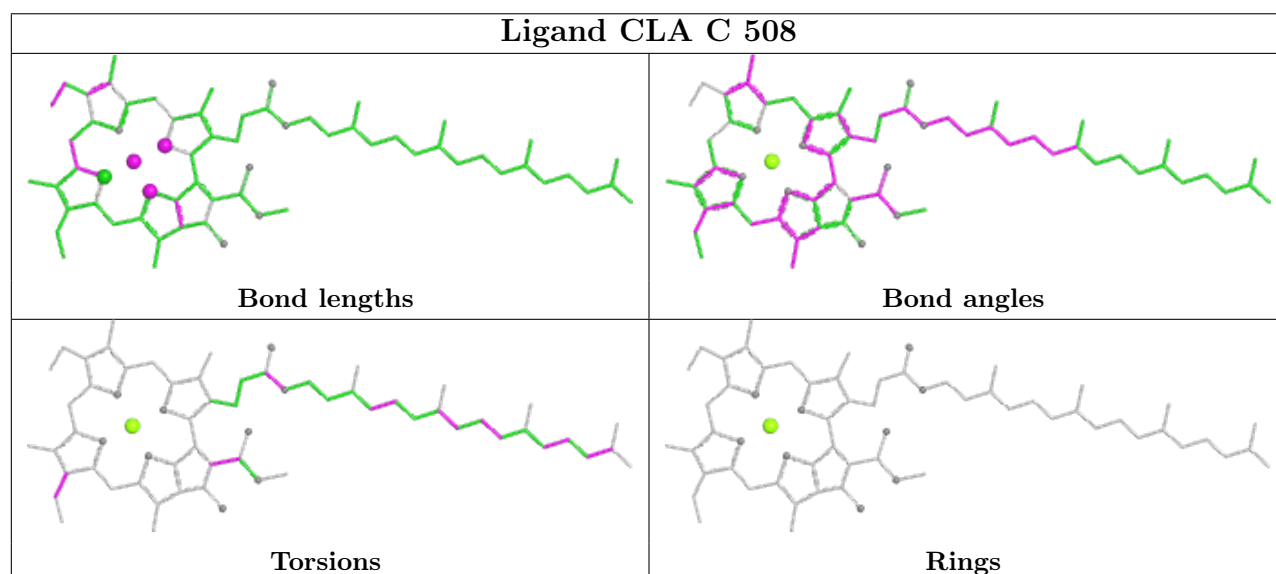
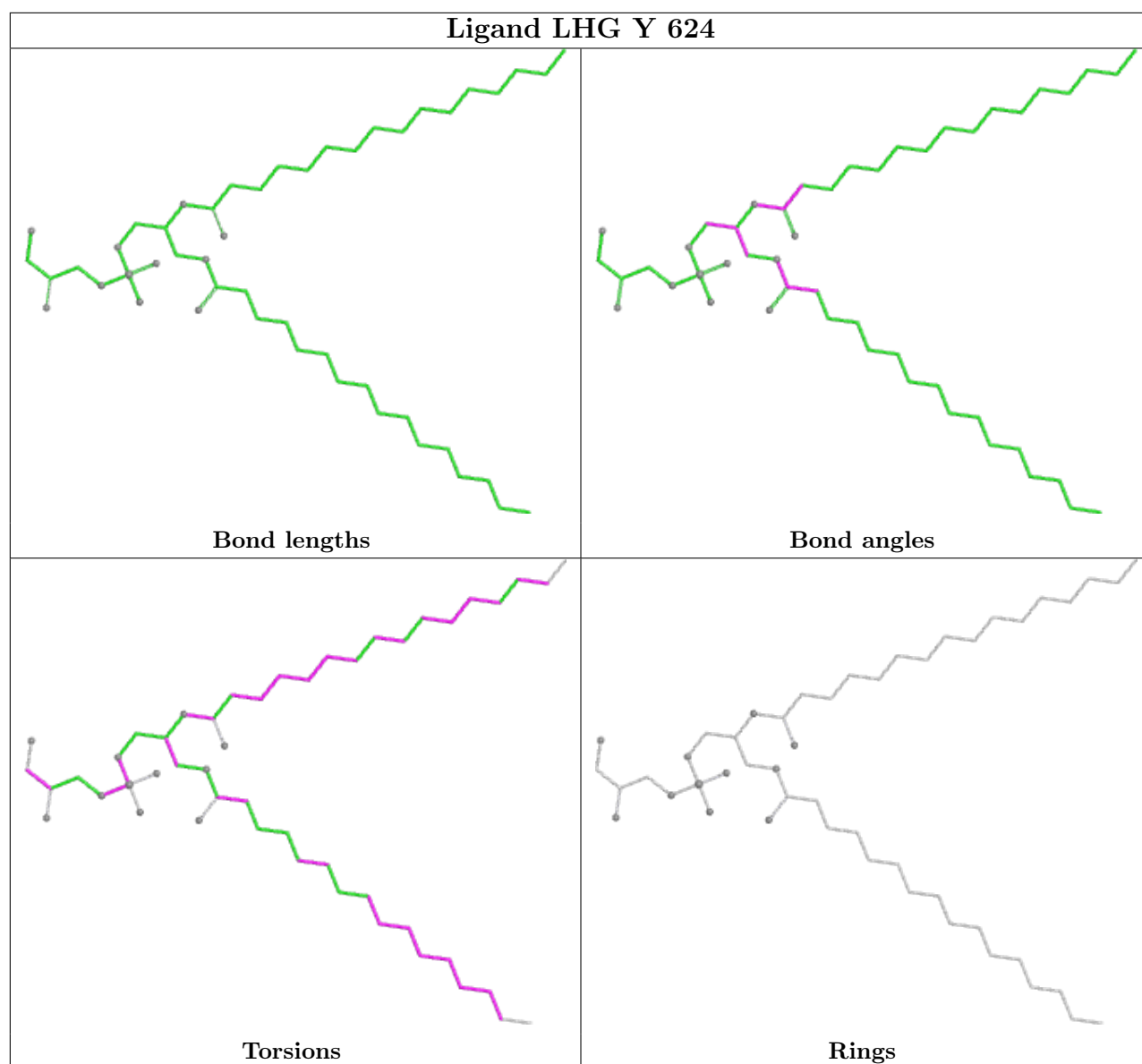


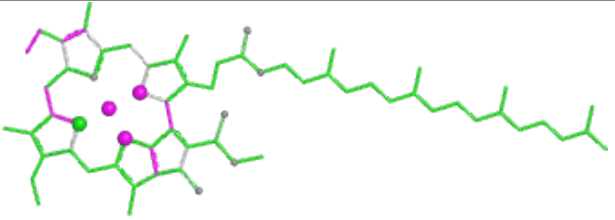
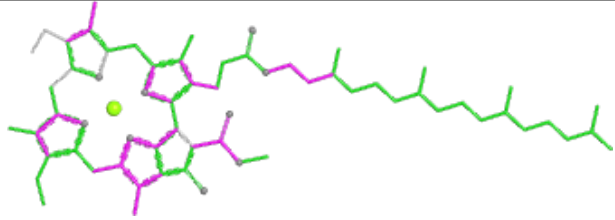
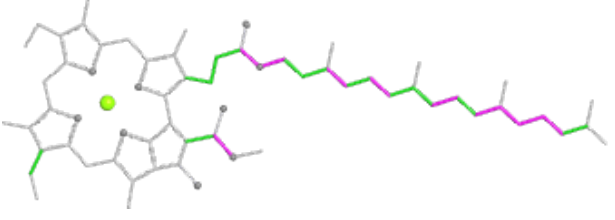
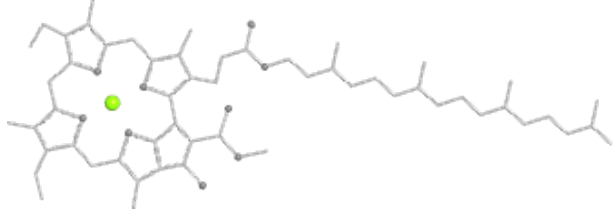
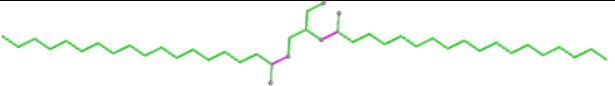
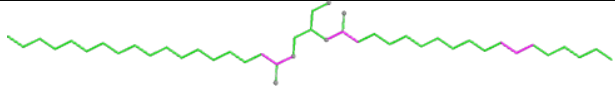
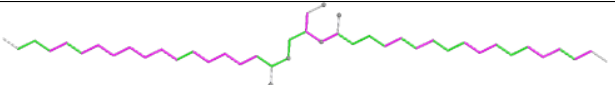
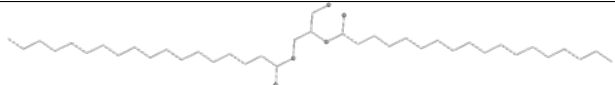
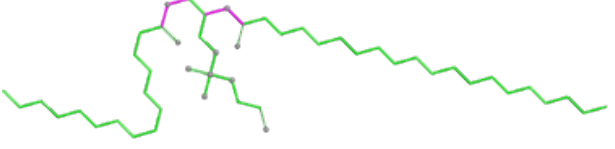
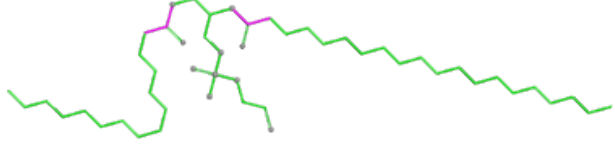
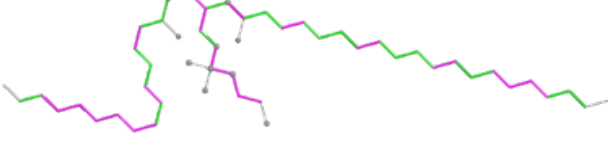
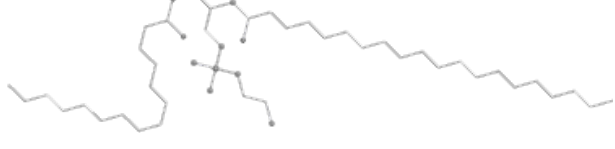
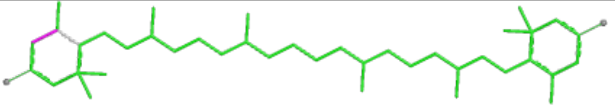
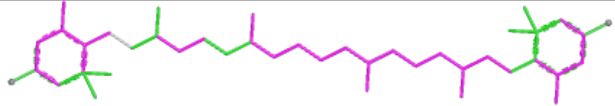
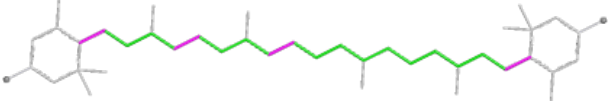
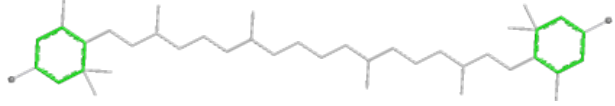


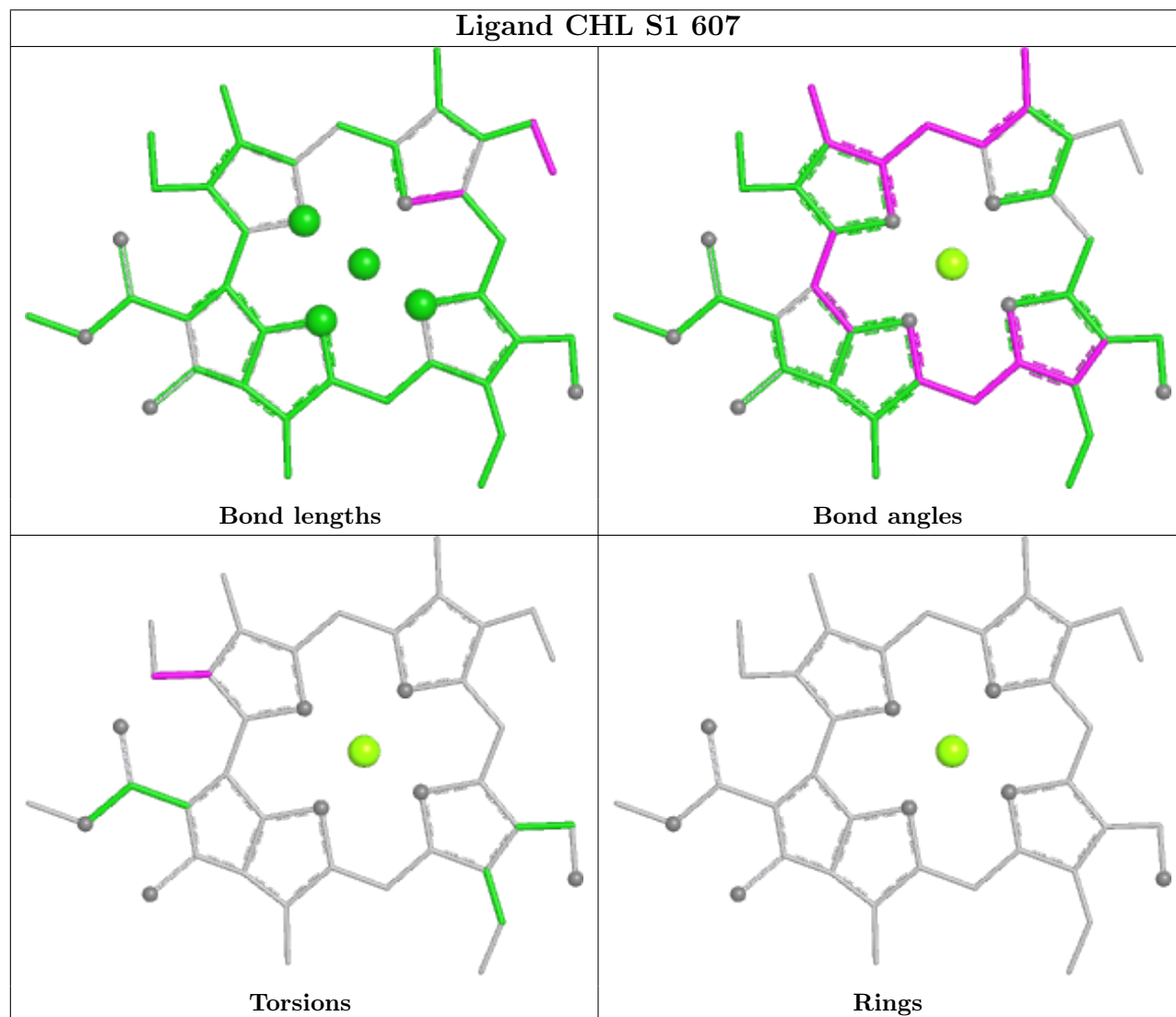
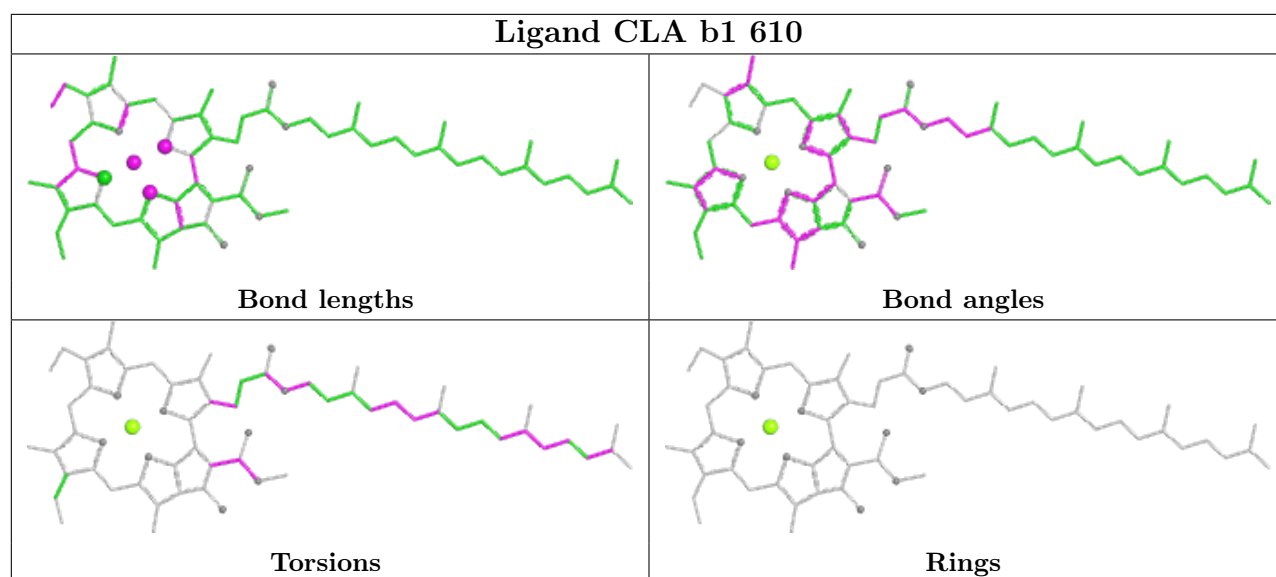


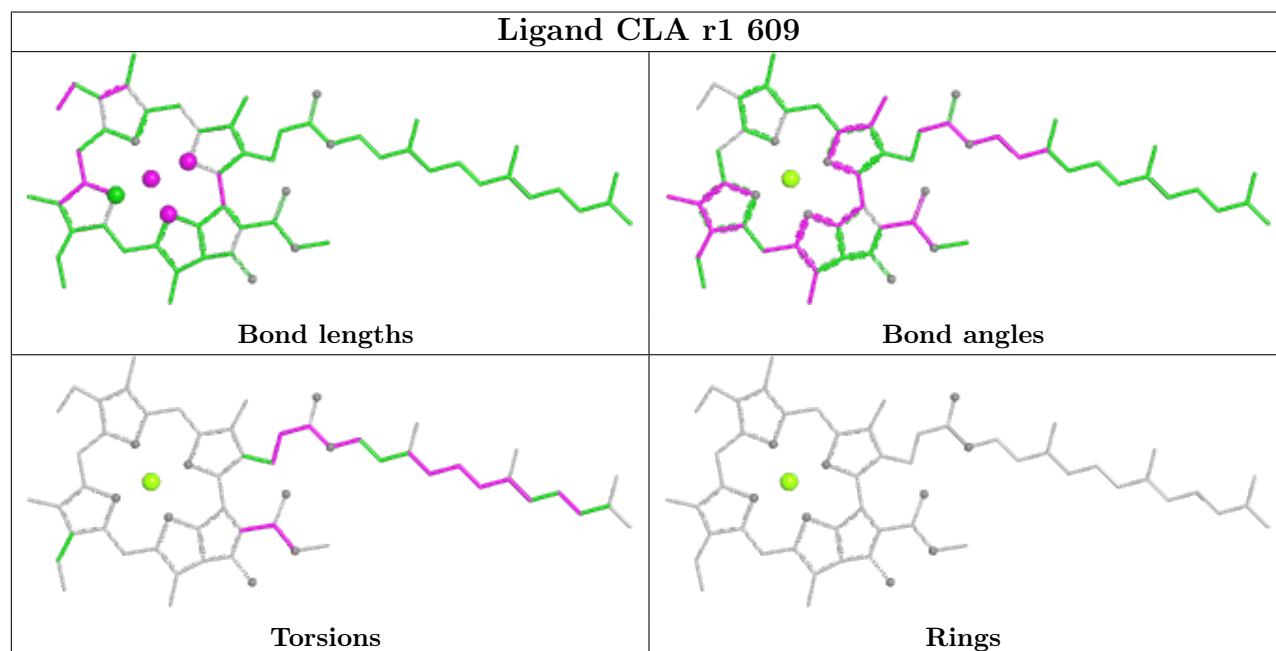
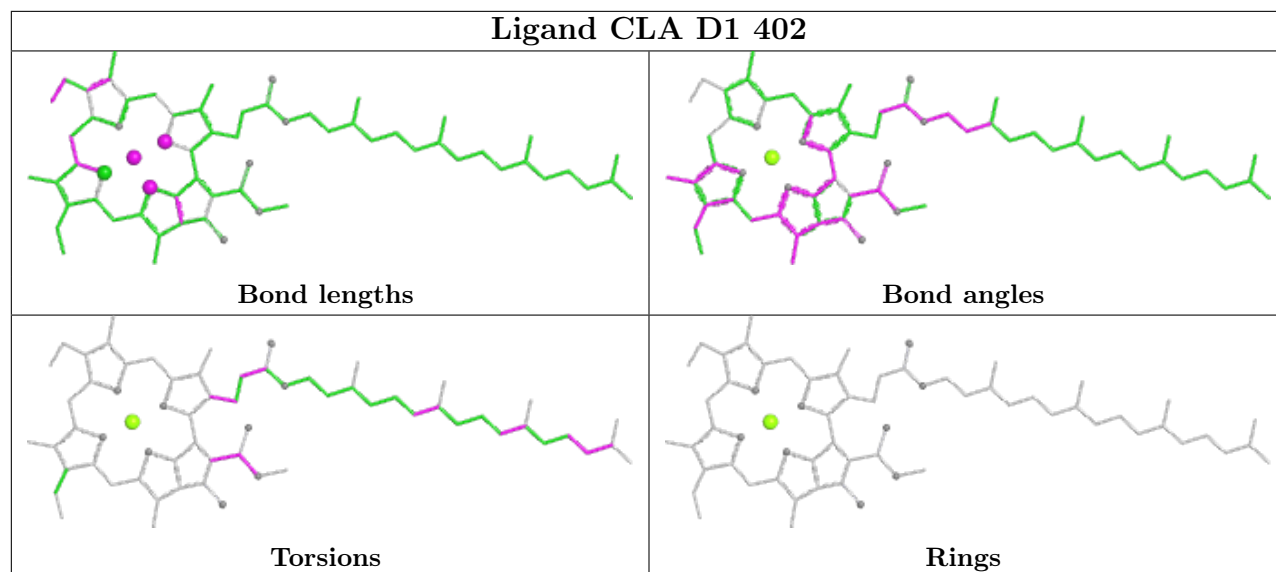


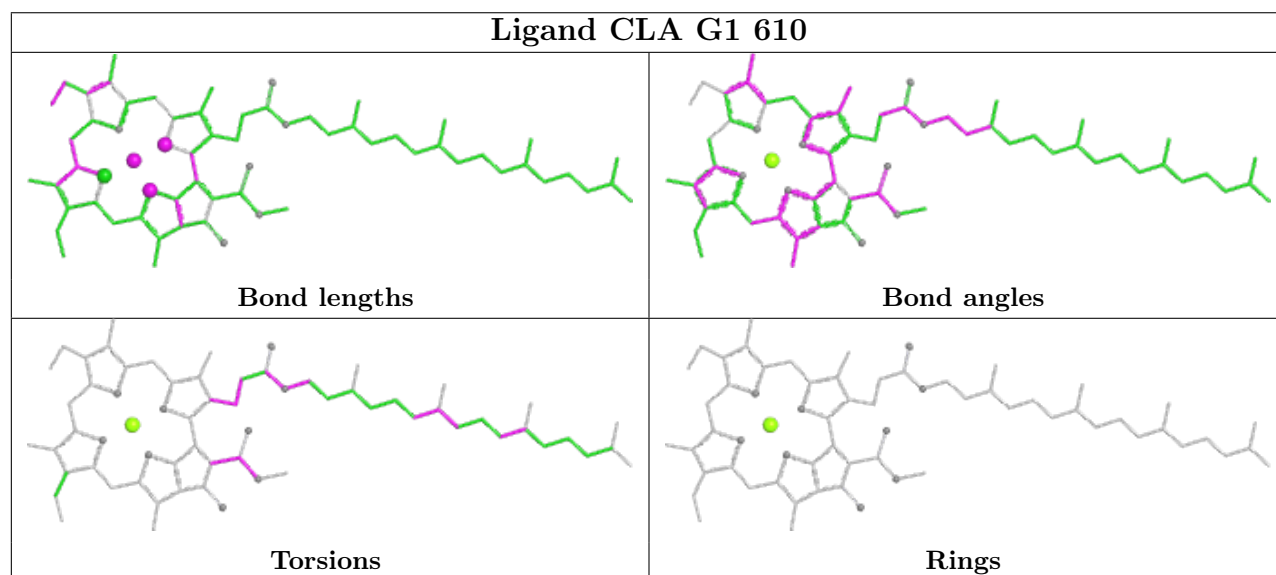
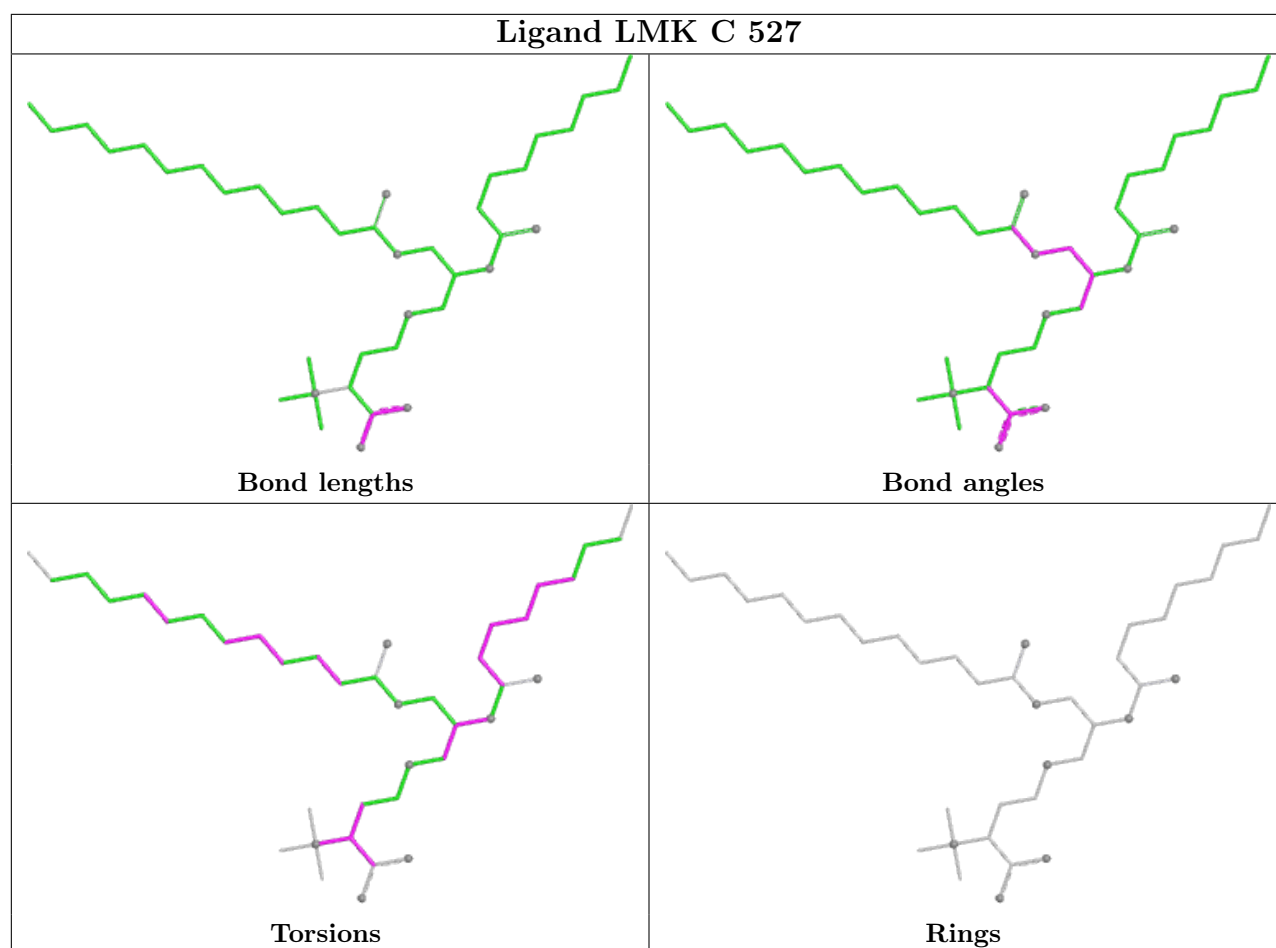




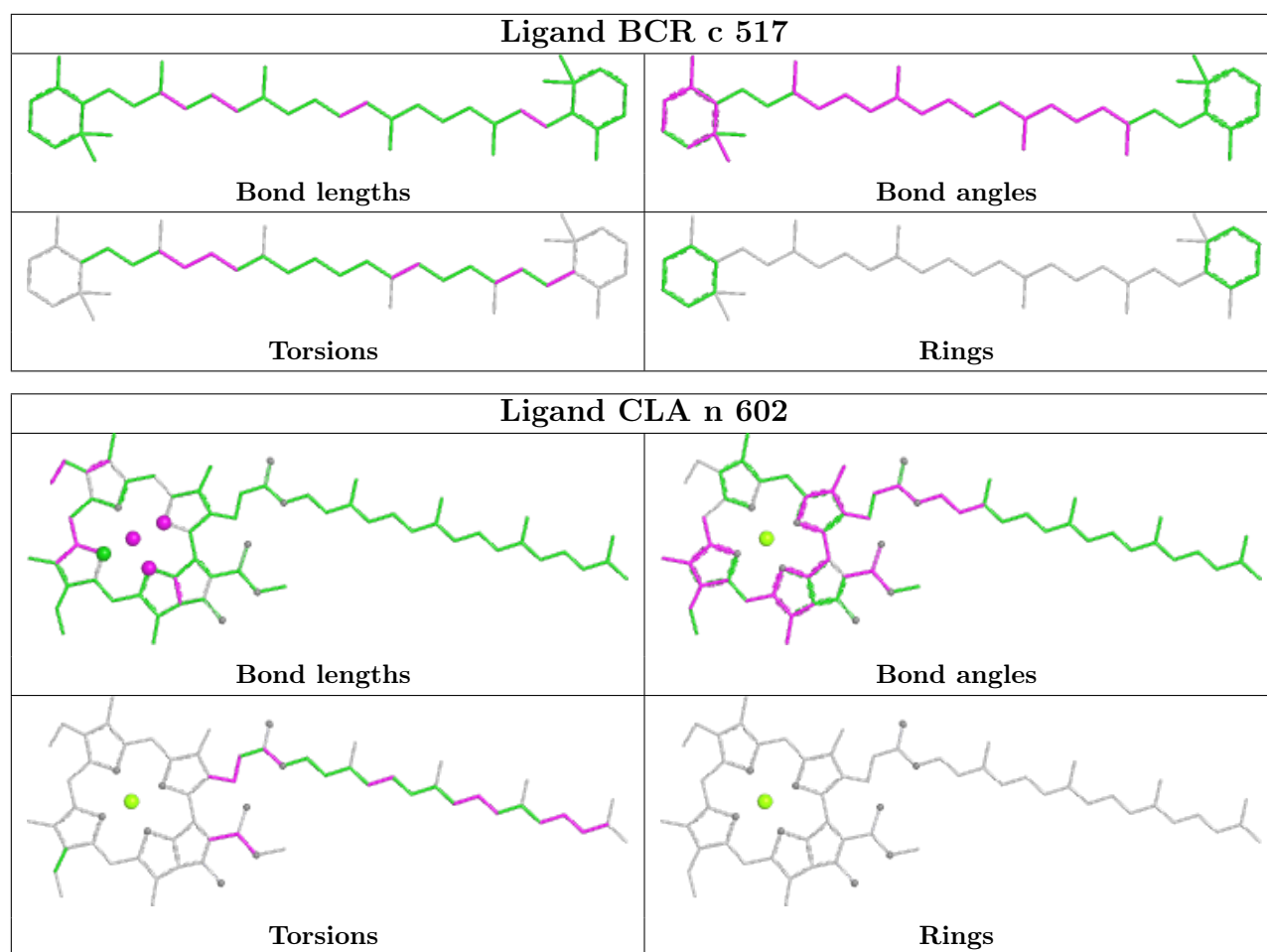
Ligand CLA b 614	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand DGA B 625	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand PTY Y1 626	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand LUT n1 621	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>



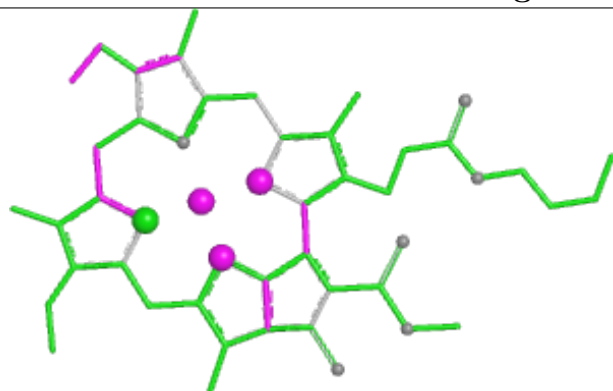




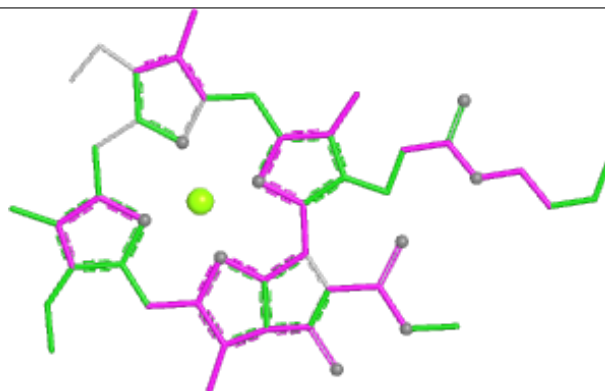




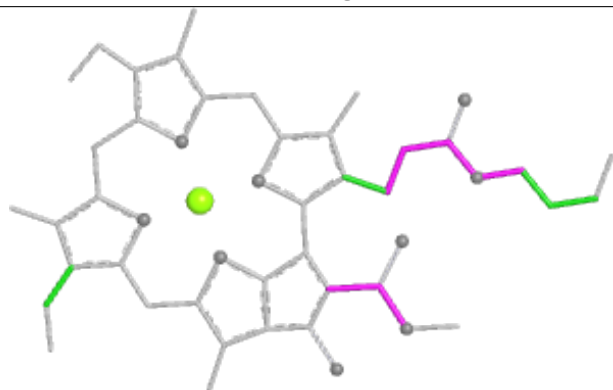
## Ligand CLA R 604



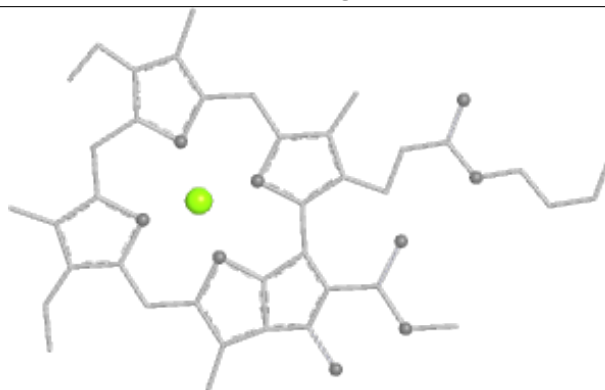
Bond lengths



Bond angles

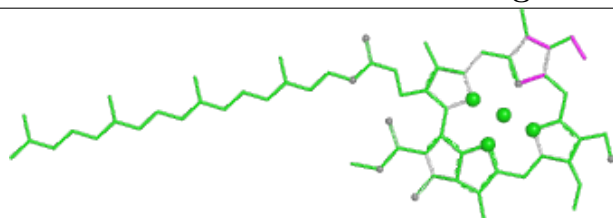


Torsions

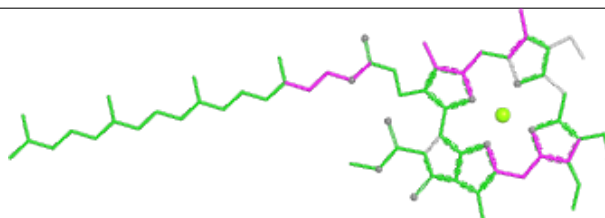


Rings

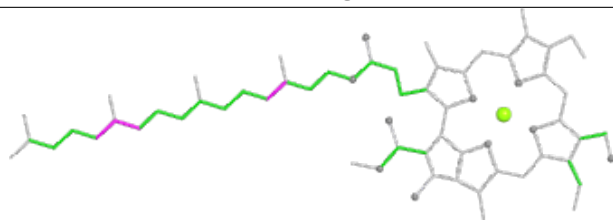
## Ligand CHL N 601



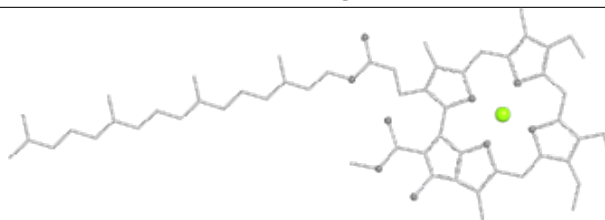
Bond lengths



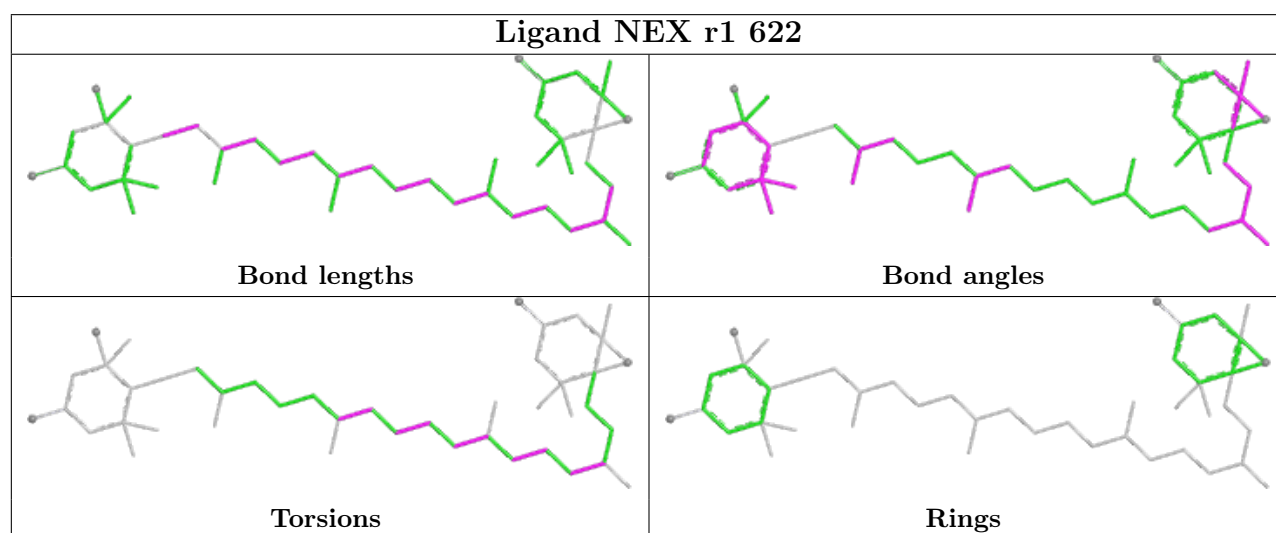
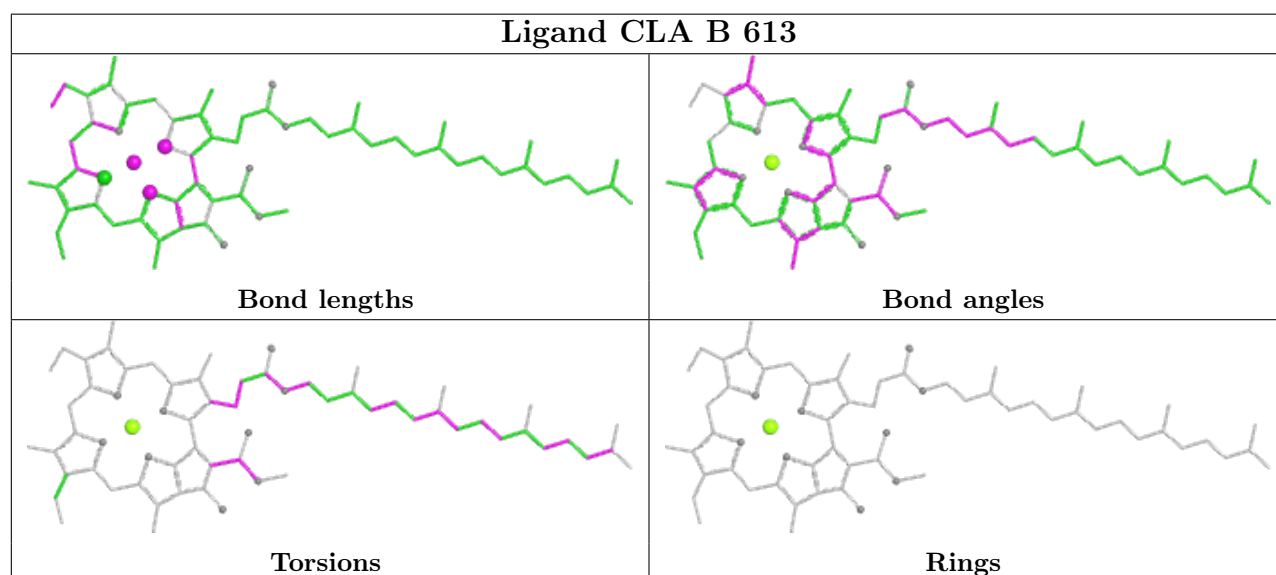
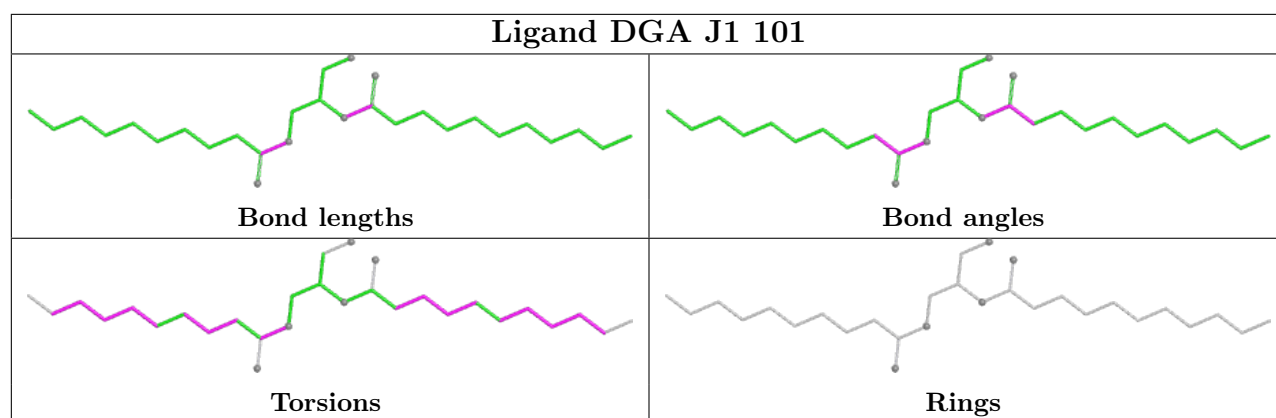
Bond angles

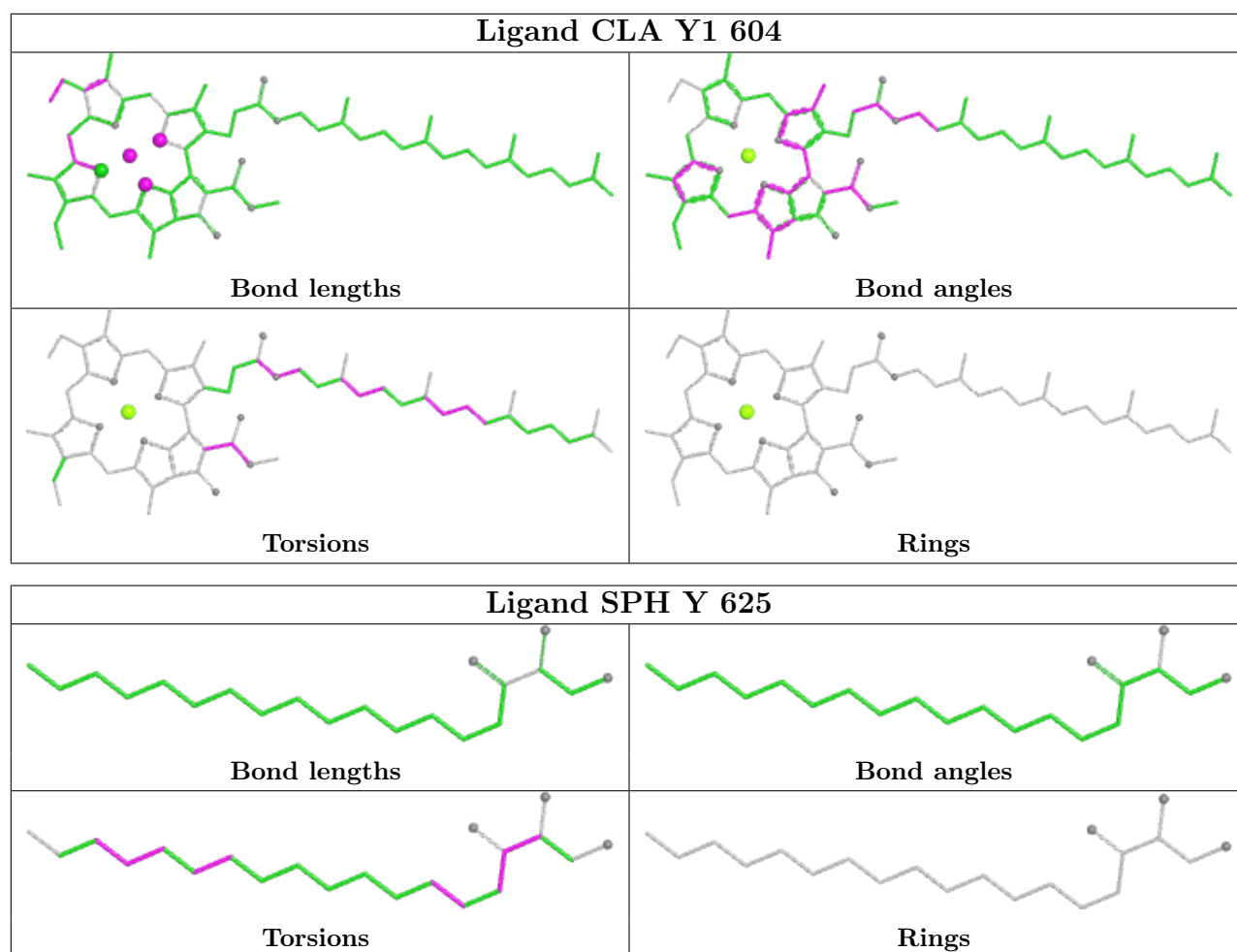


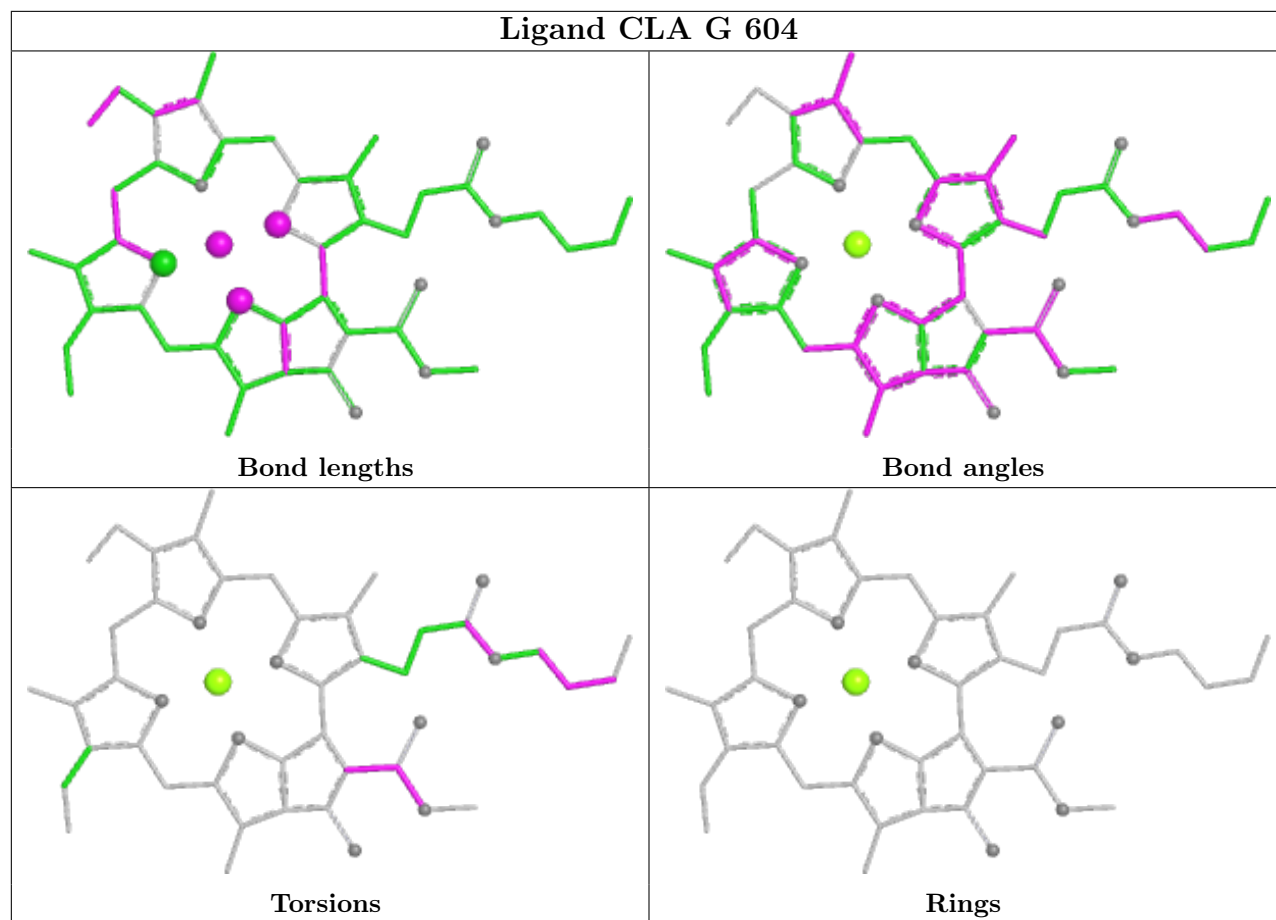
Torsions

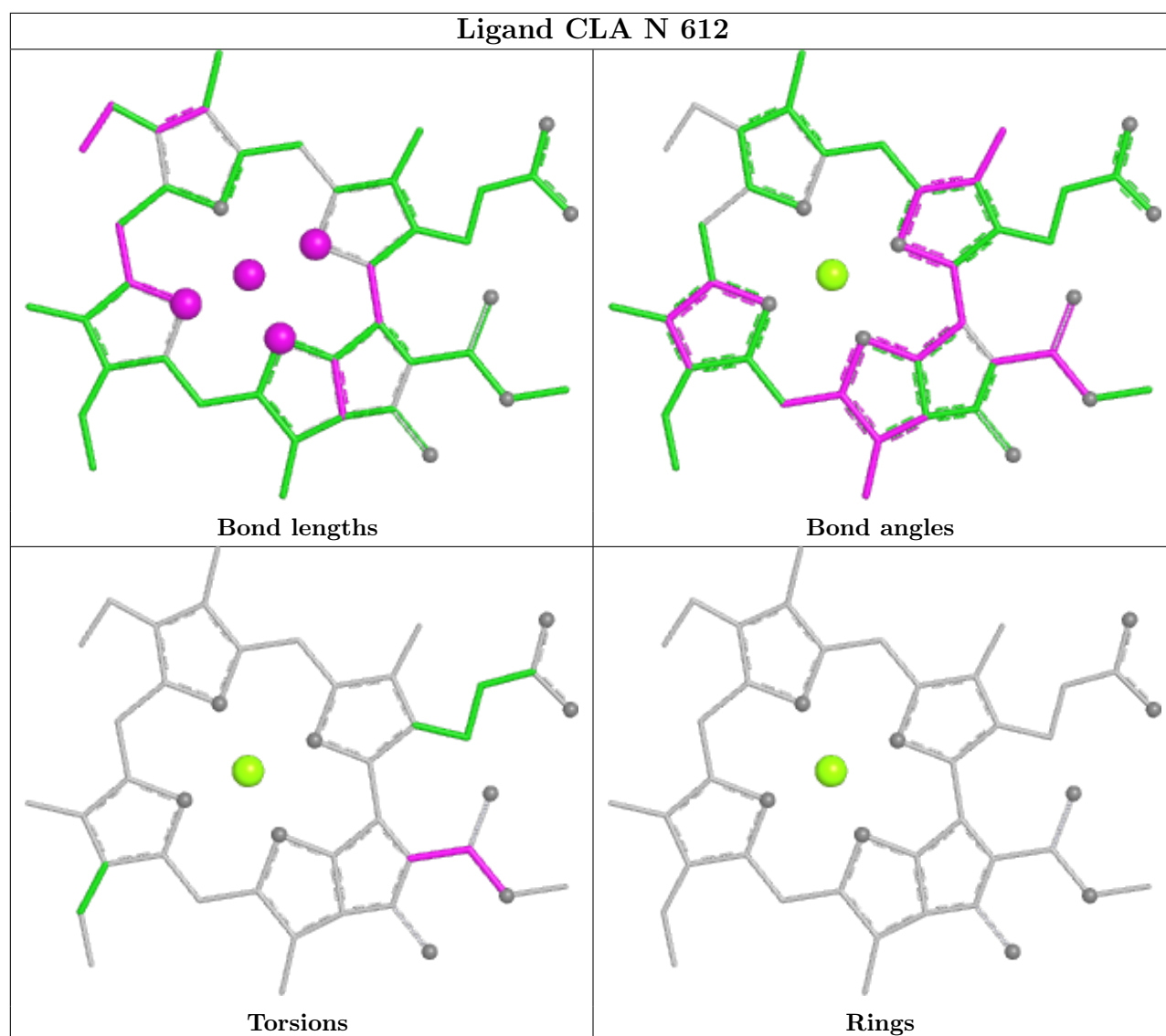


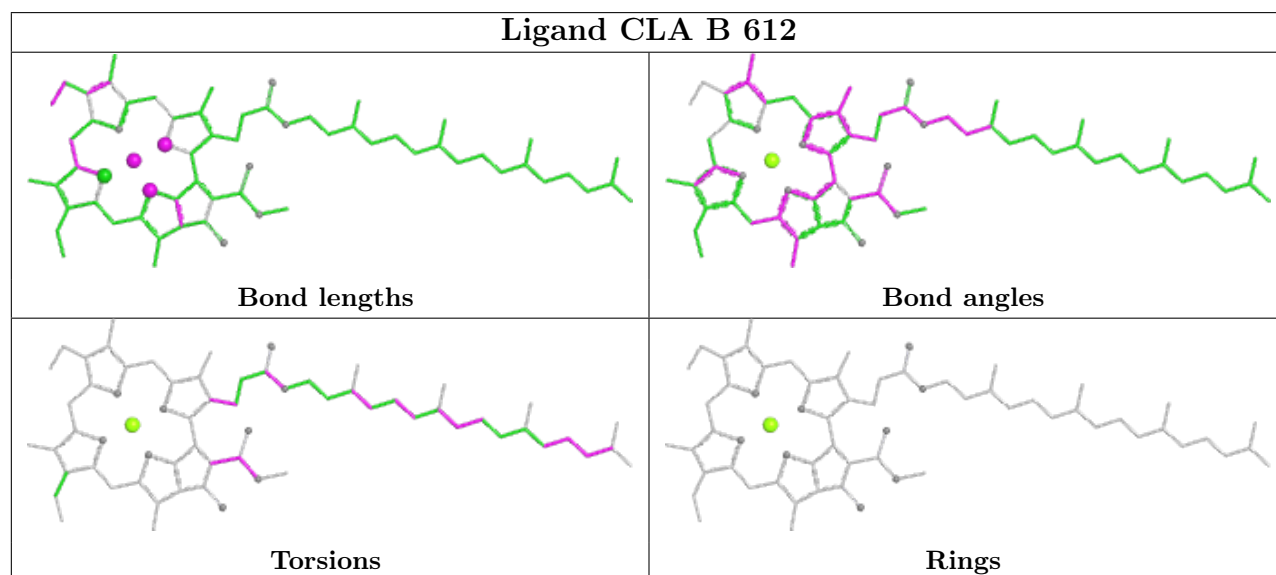
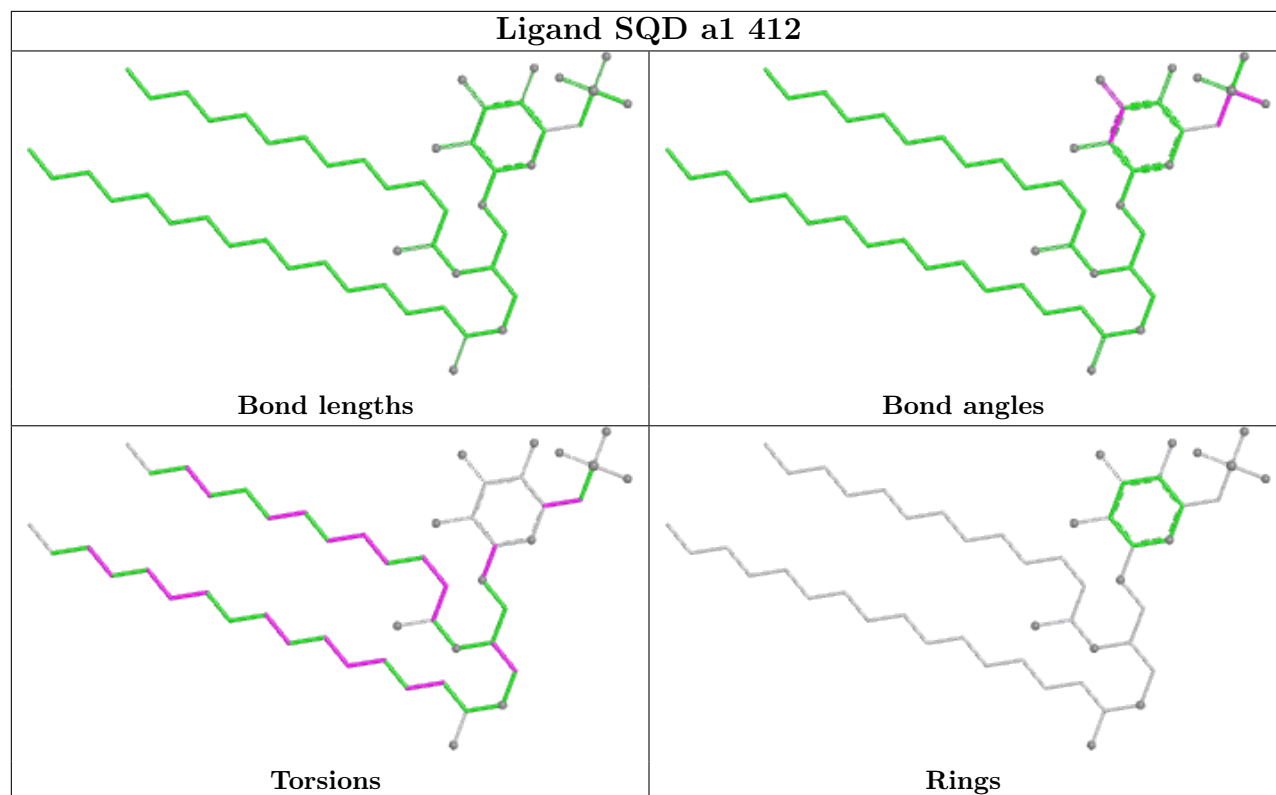
Rings

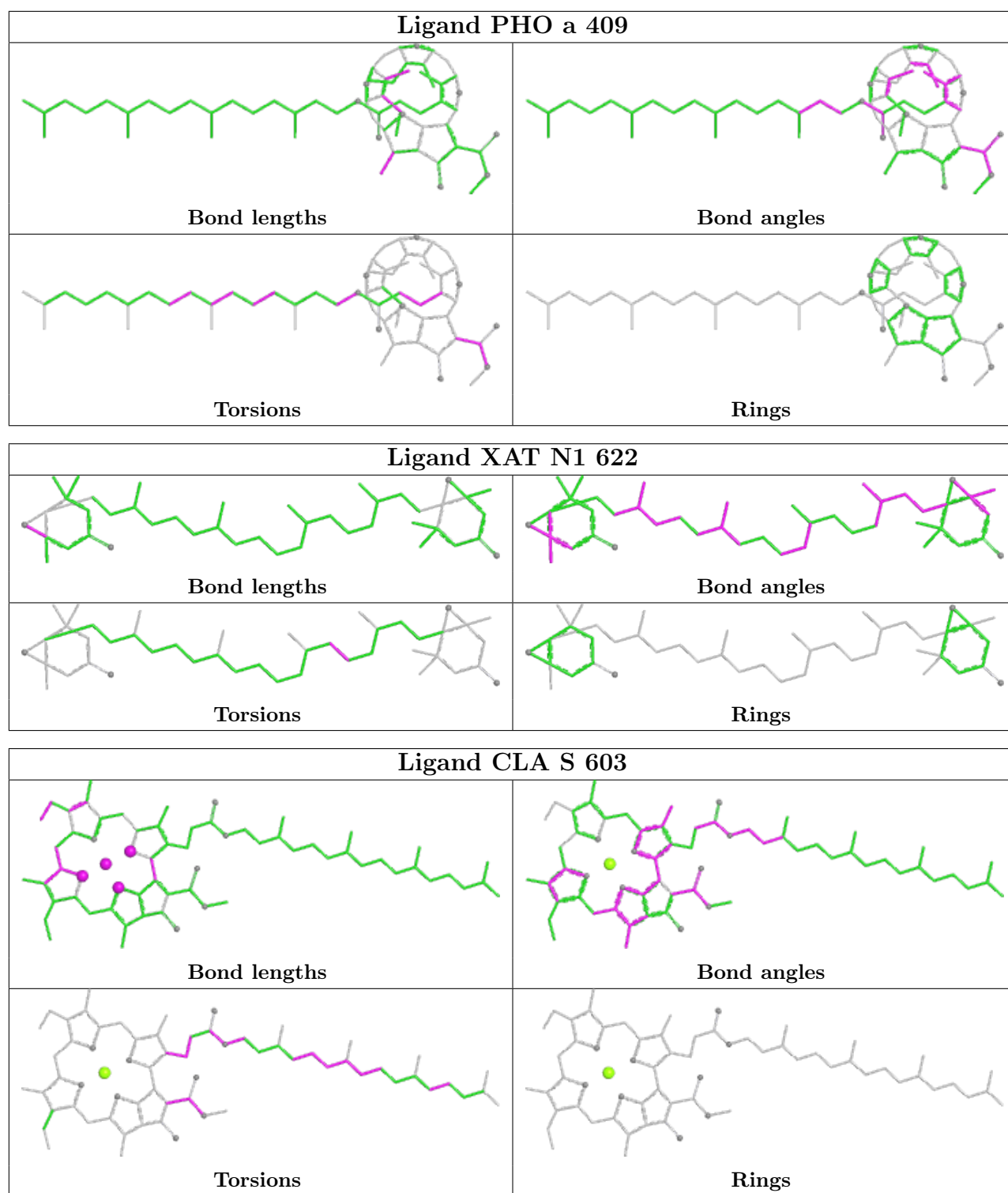




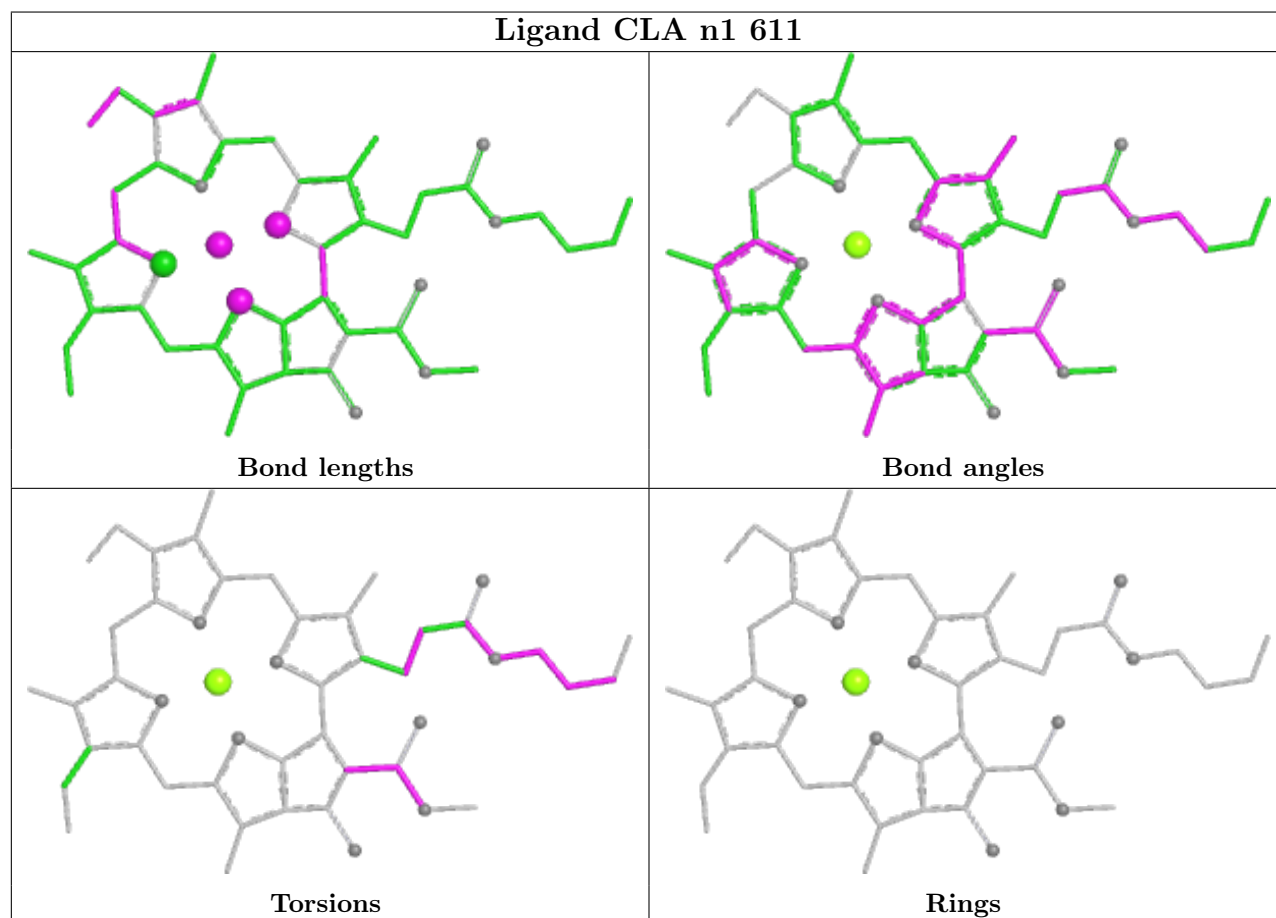
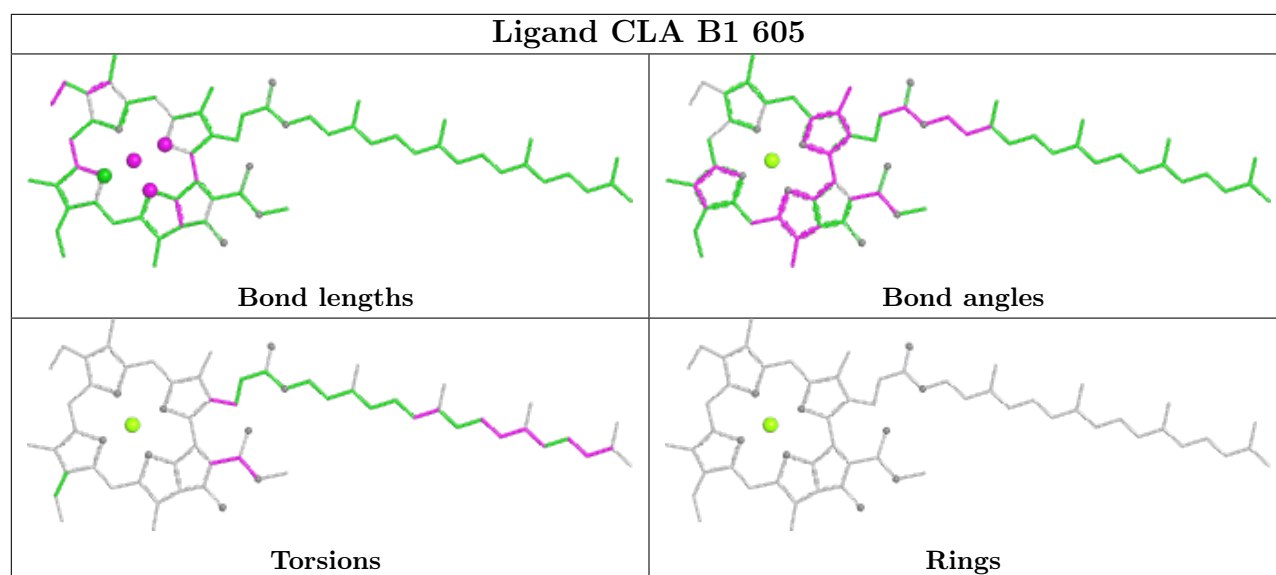


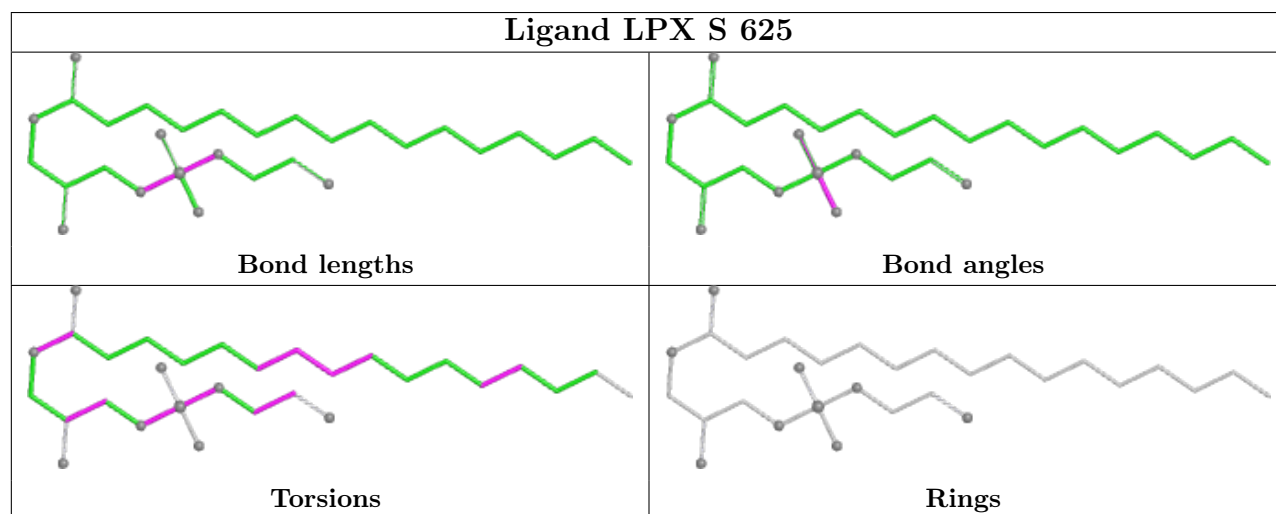
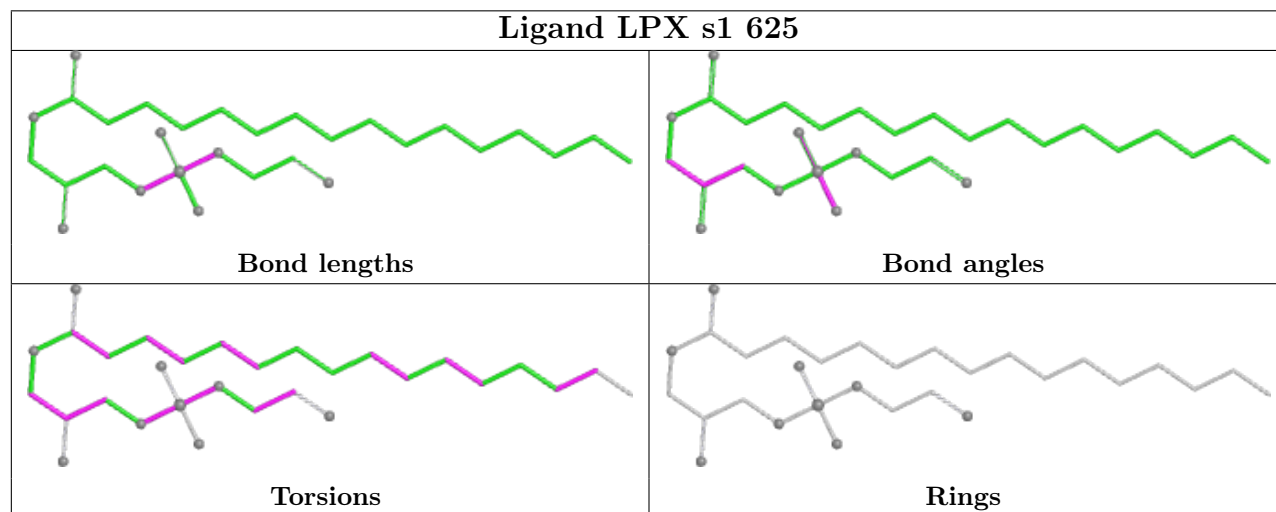
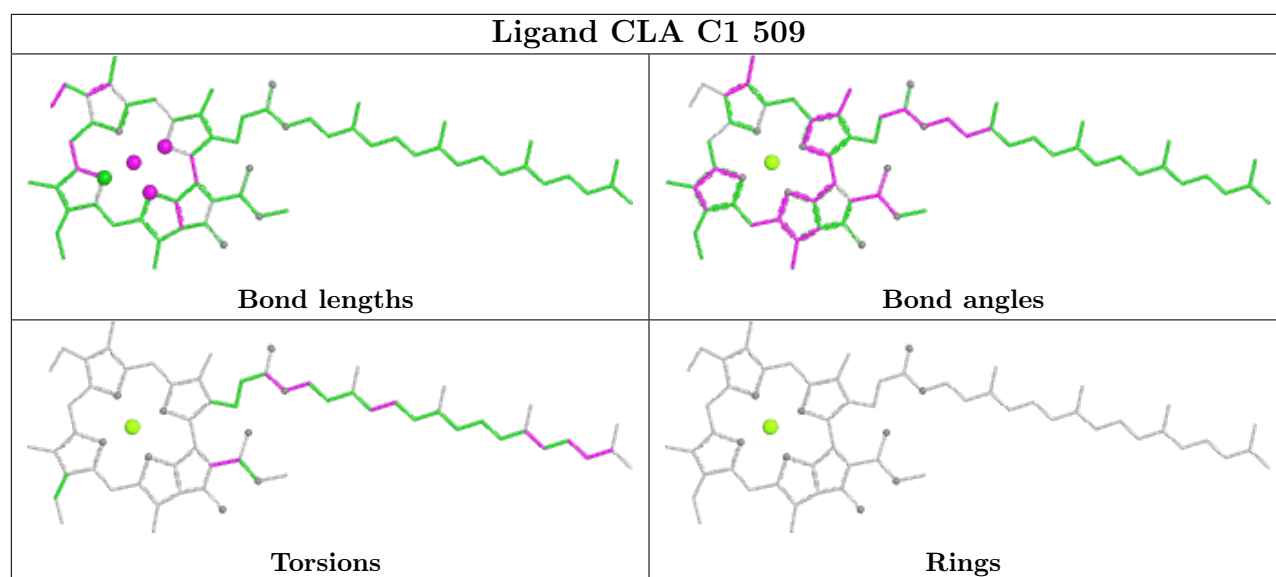


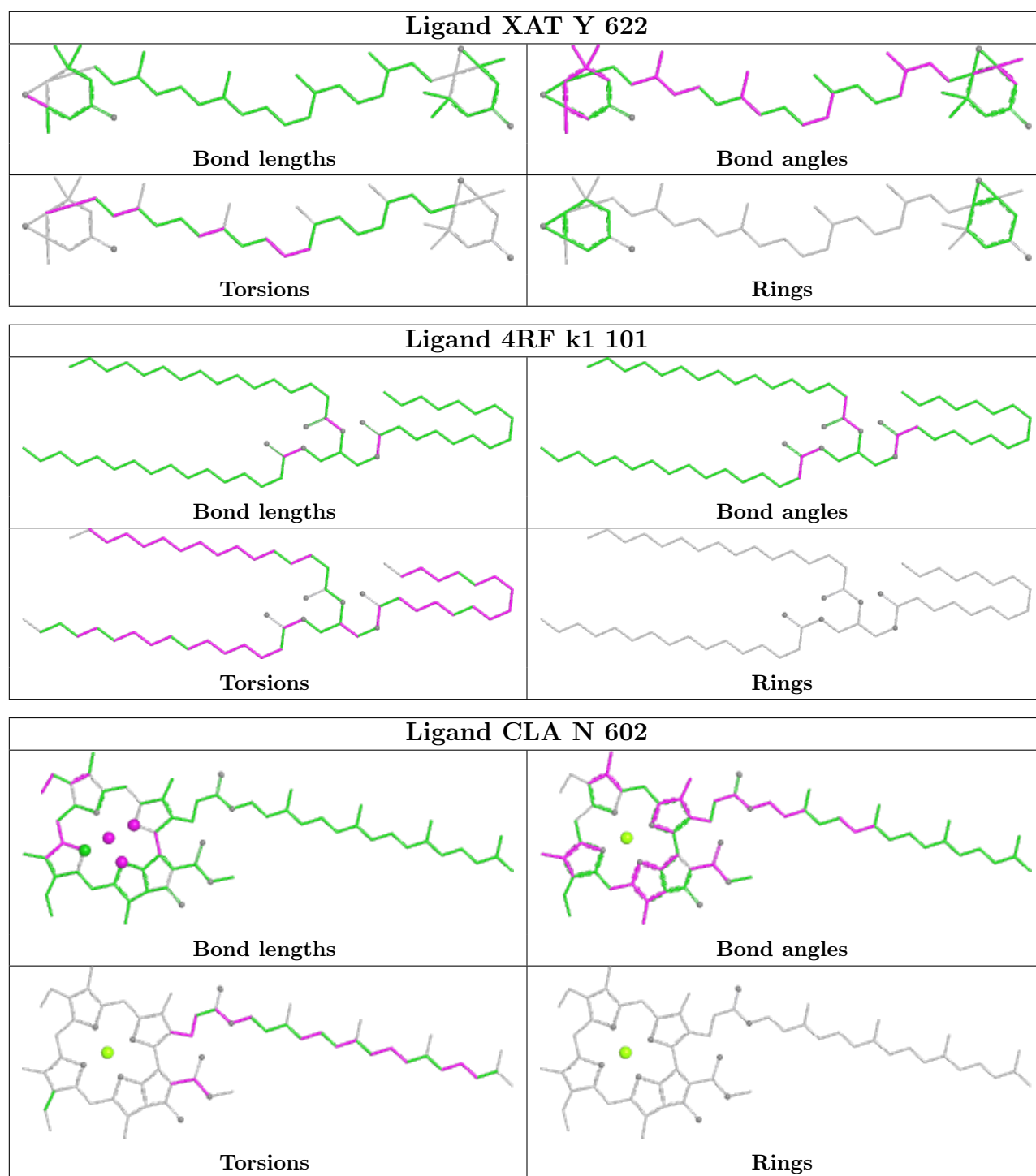


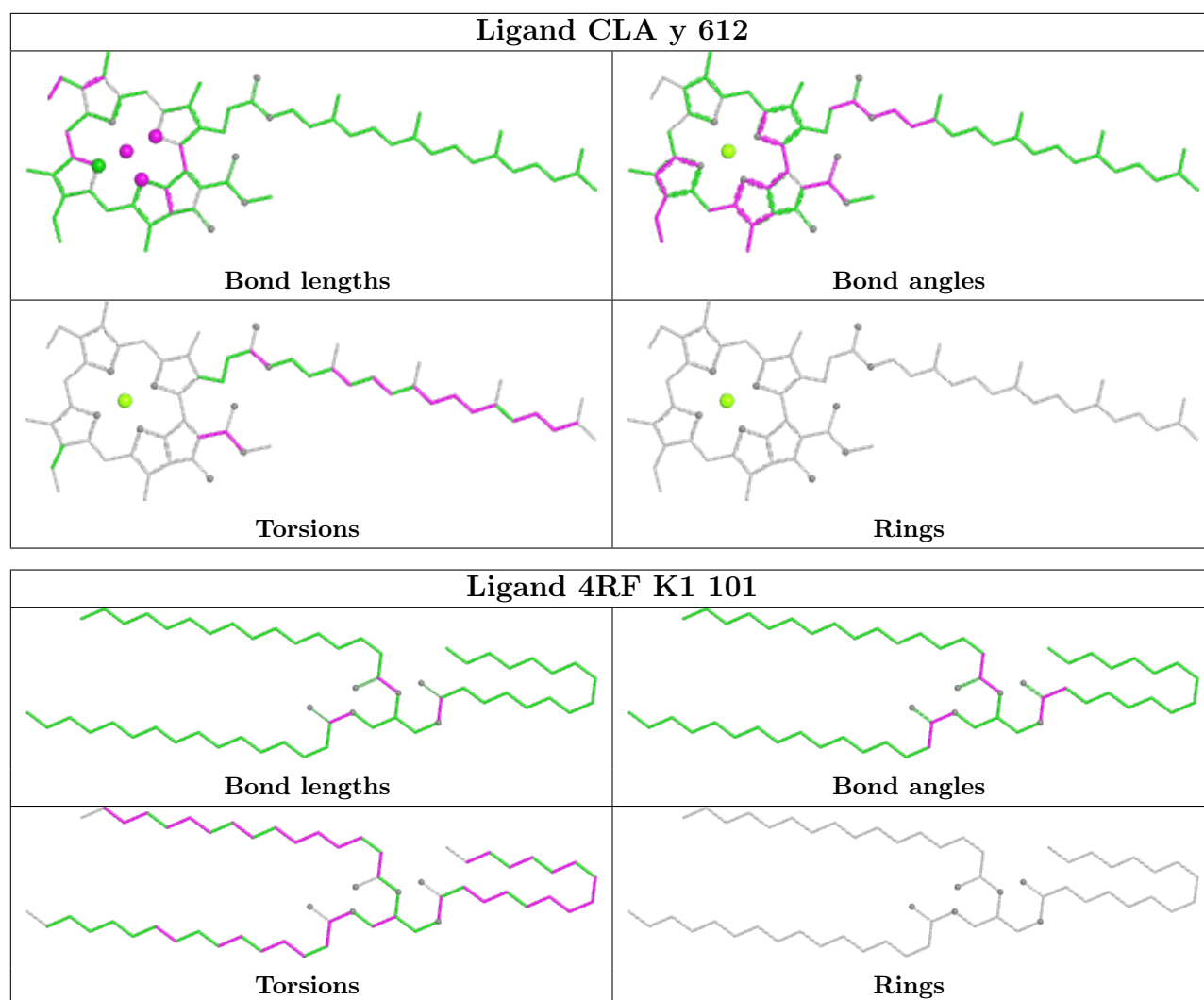


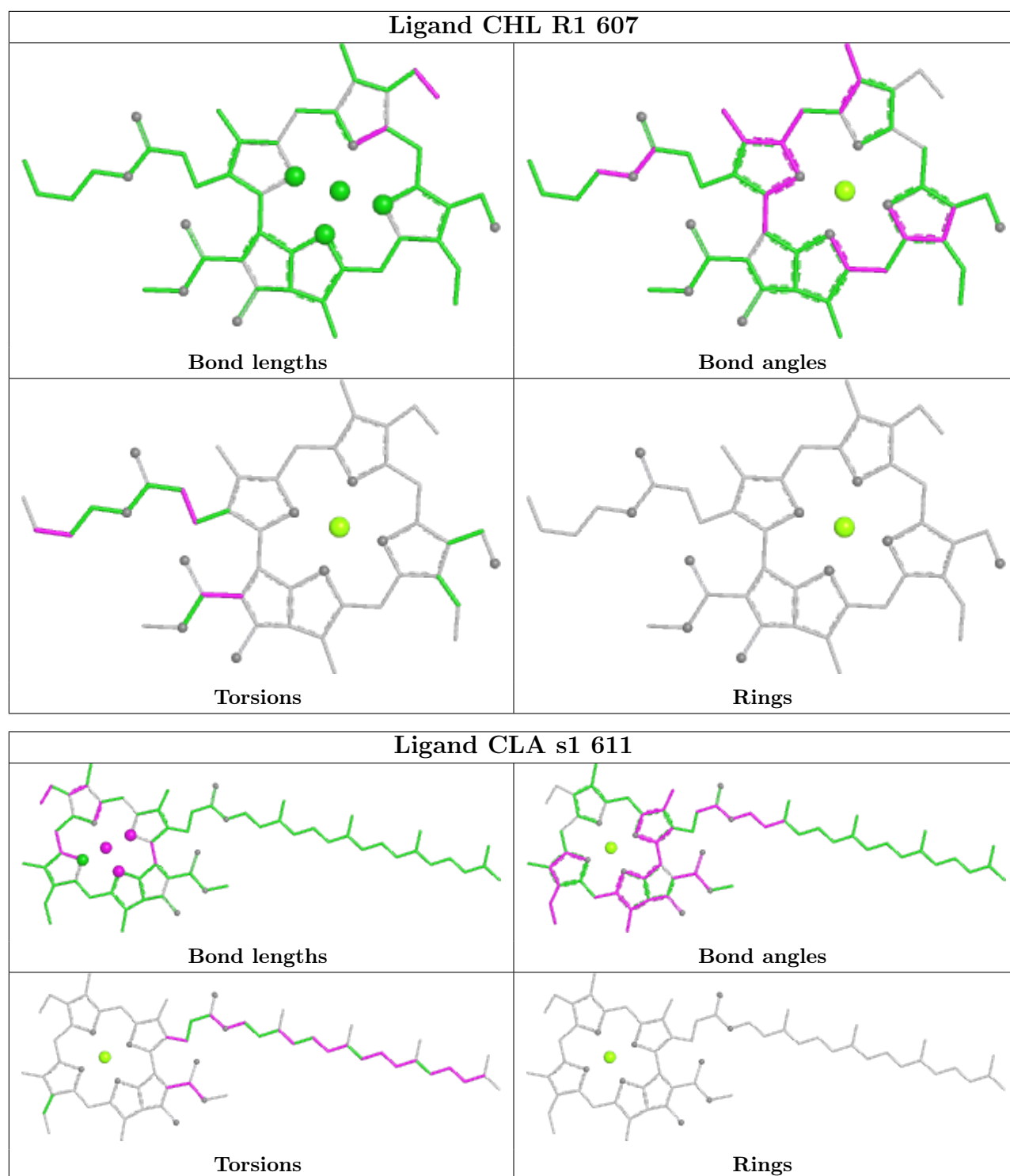


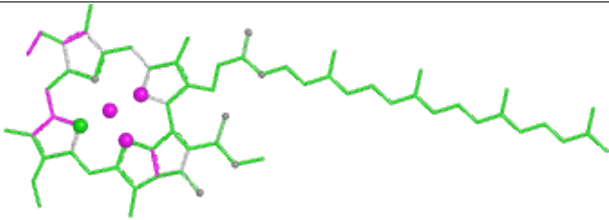
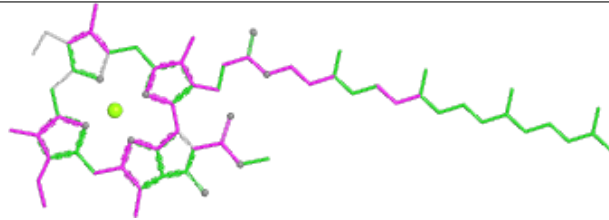
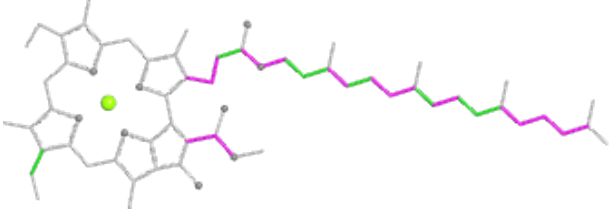
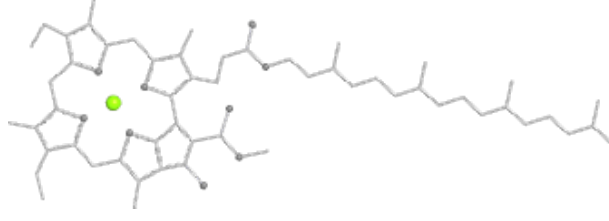


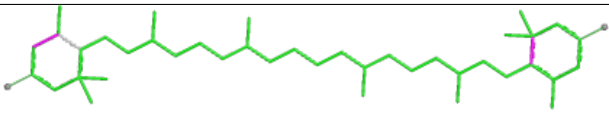
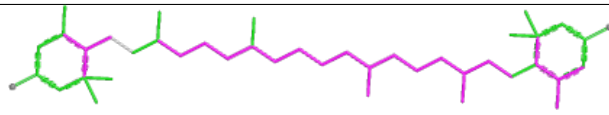
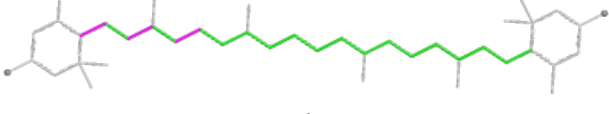
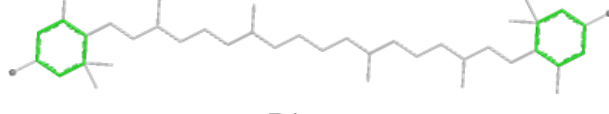


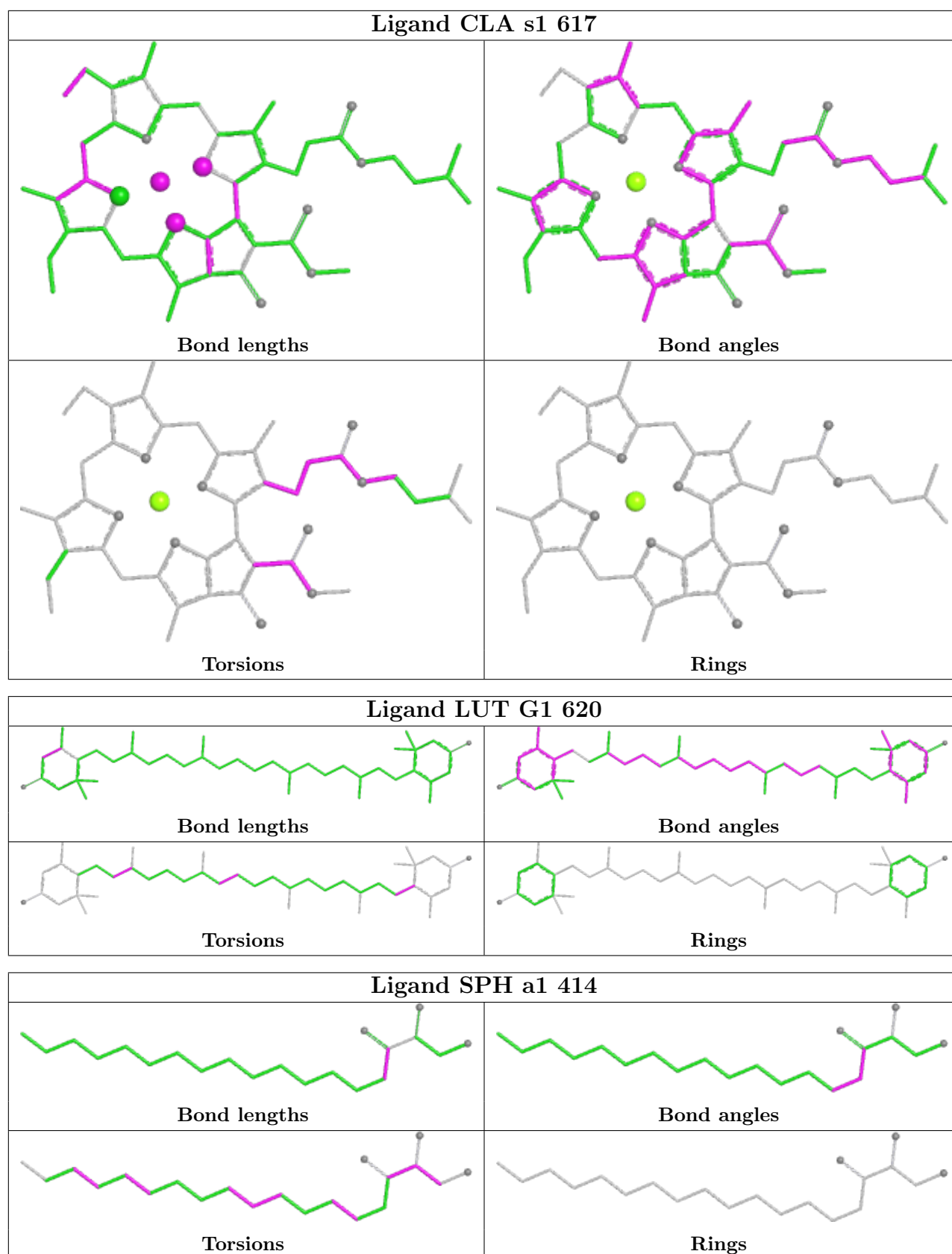




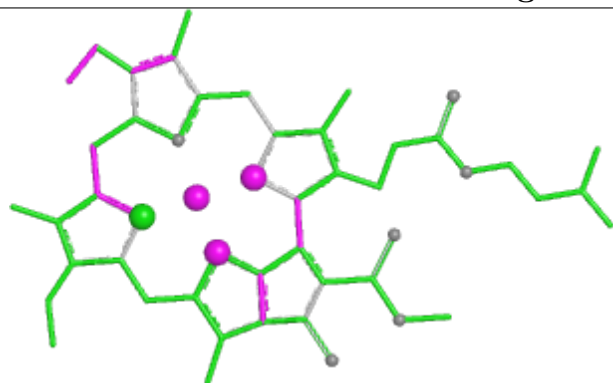


Ligand CLA g 602	
	
Bond lengths	Bond angles
	
Torsions	Rings

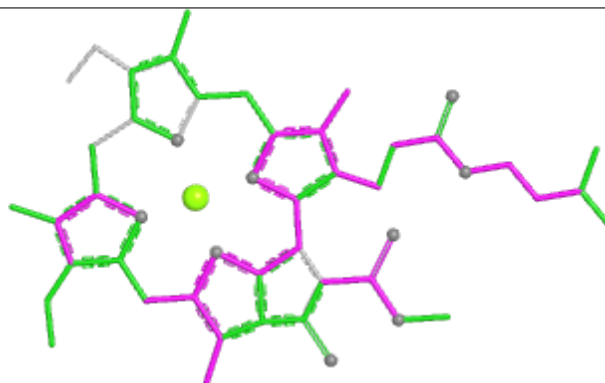
Ligand LUT r1 620	
	
Bond lengths	Bond angles
	
Torsions	Rings



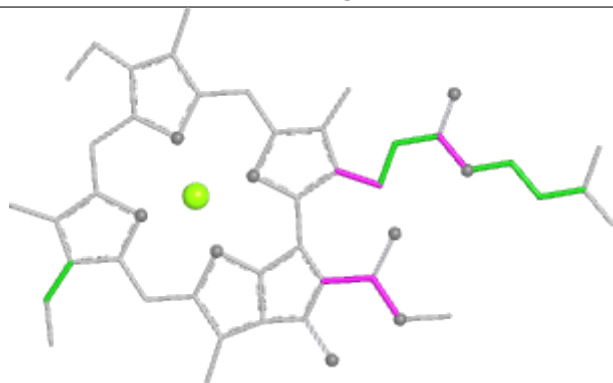
## Ligand CLA S 617



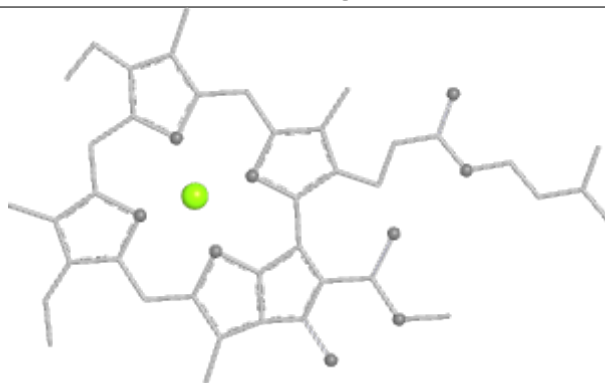
Bond lengths



Bond angles

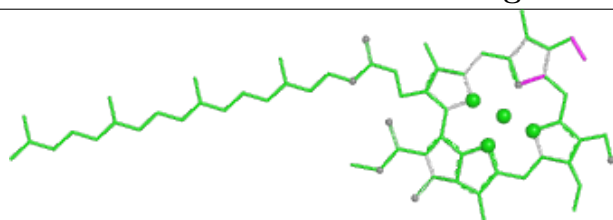


Torsions

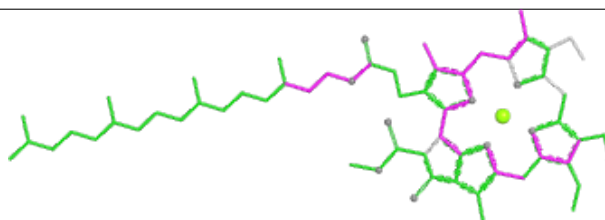


Rings

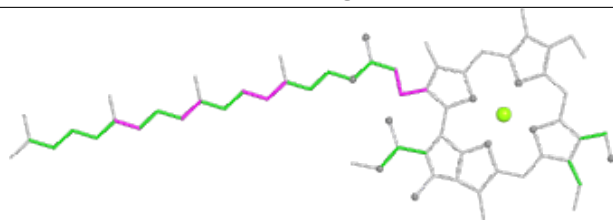
## Ligand CHL N1 607



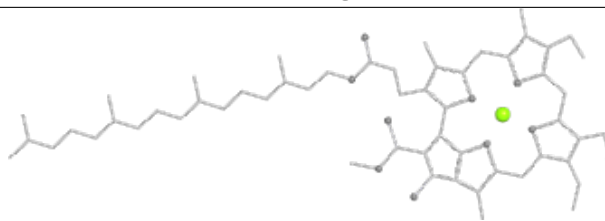
Bond lengths



Bond angles

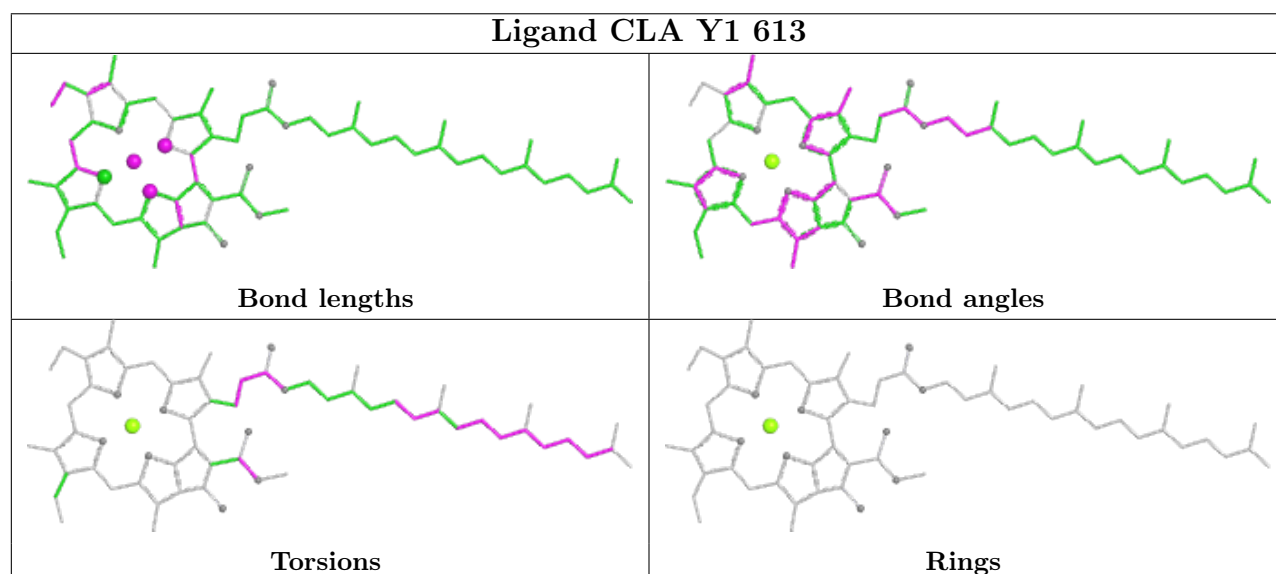
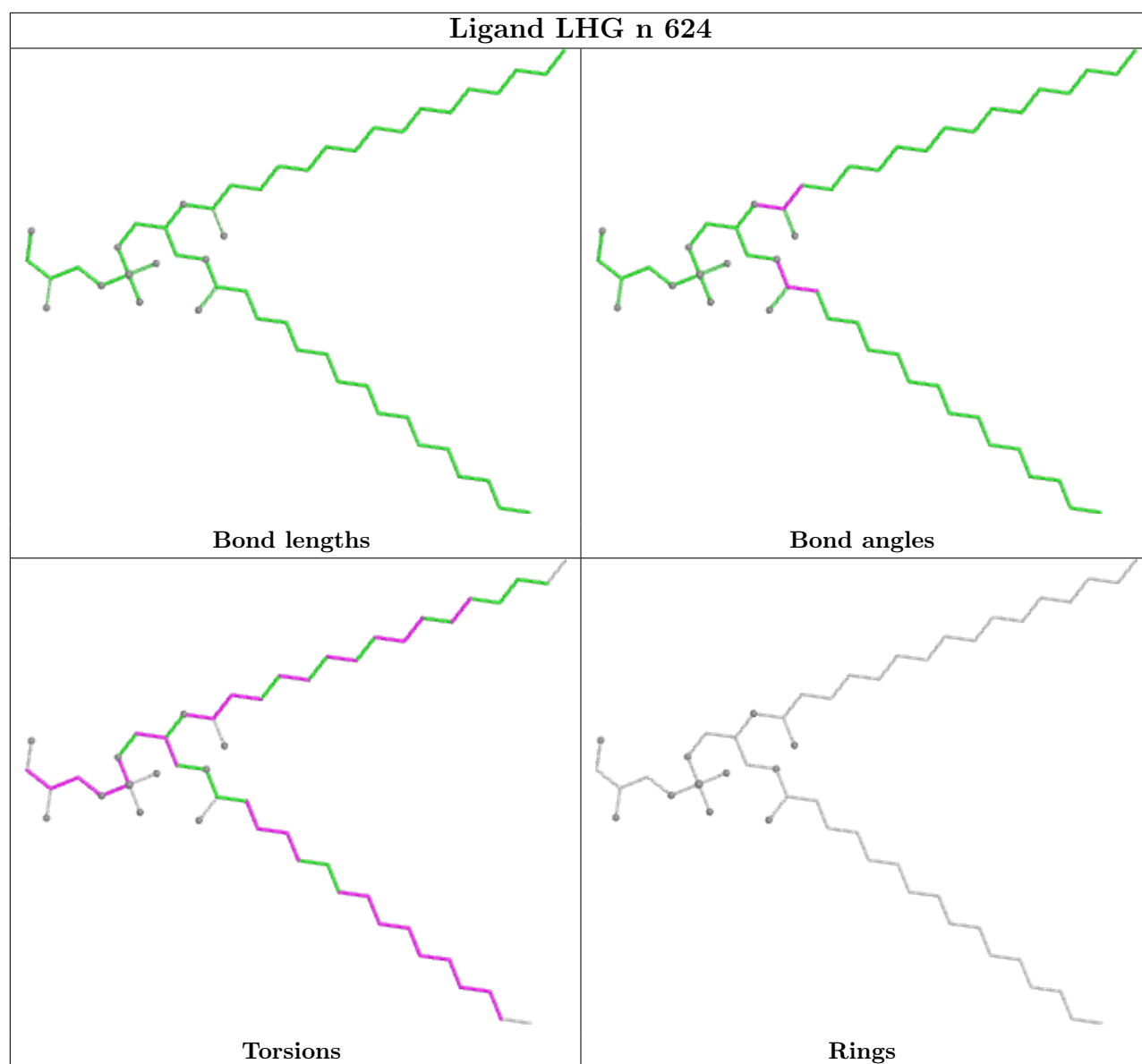


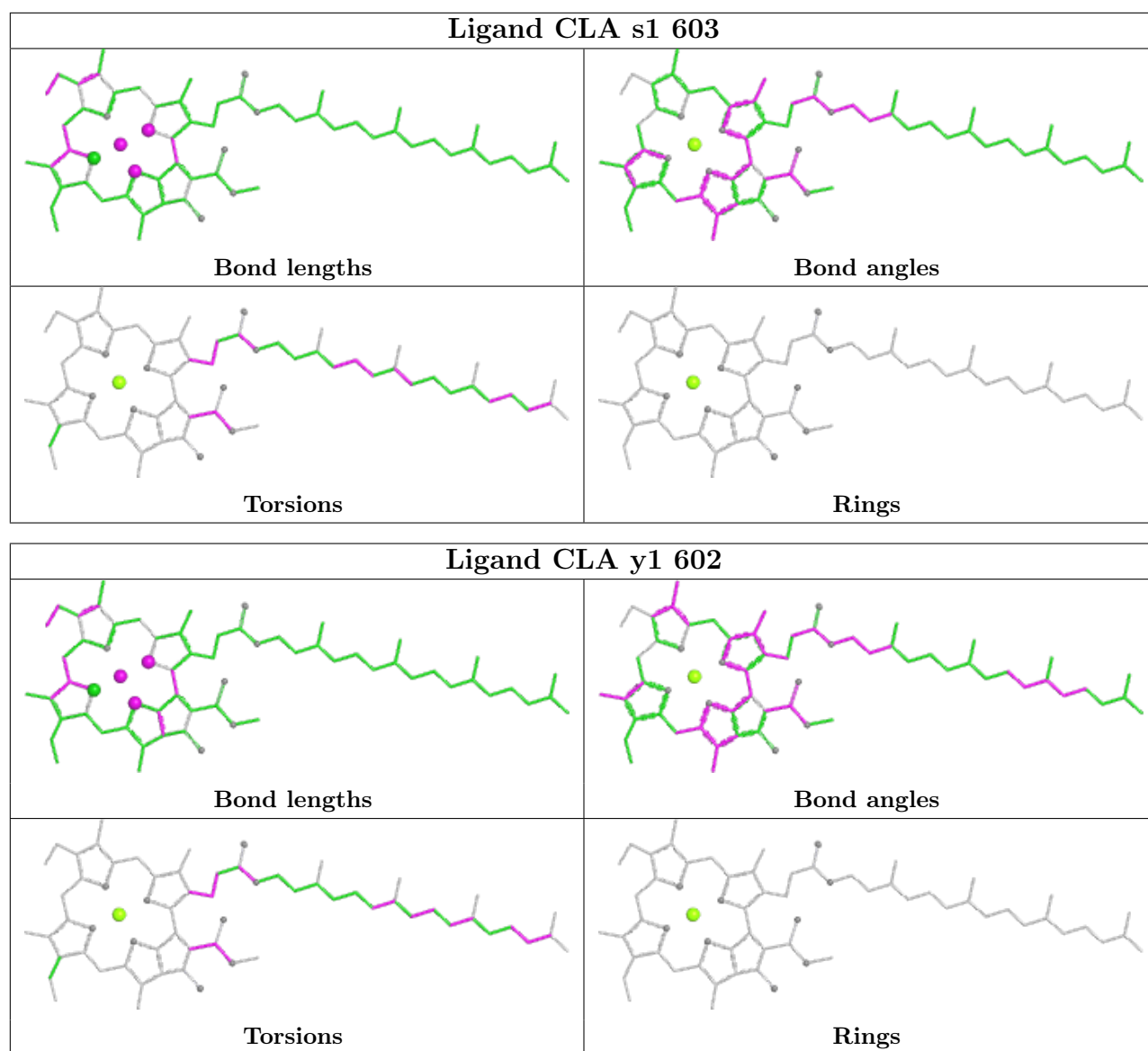
Torsions

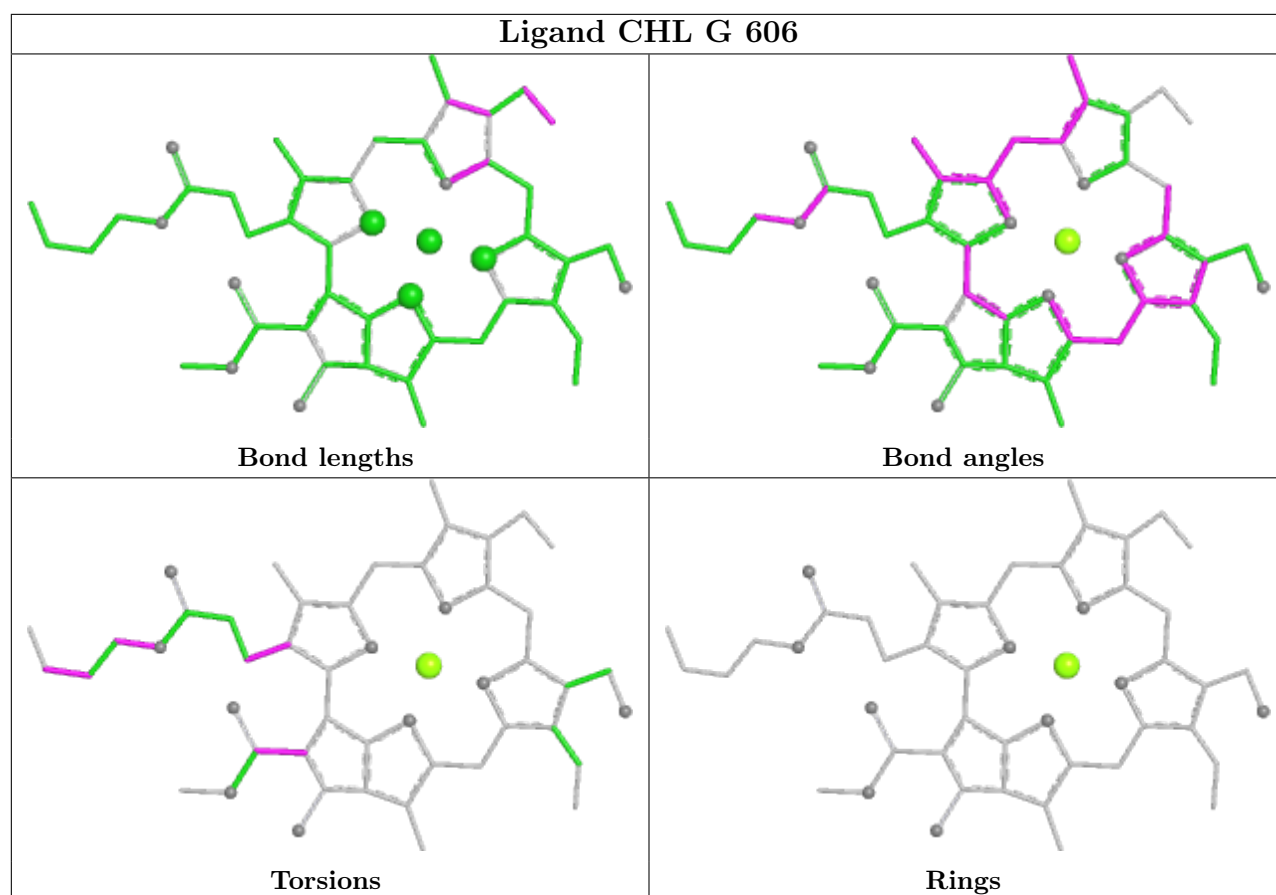


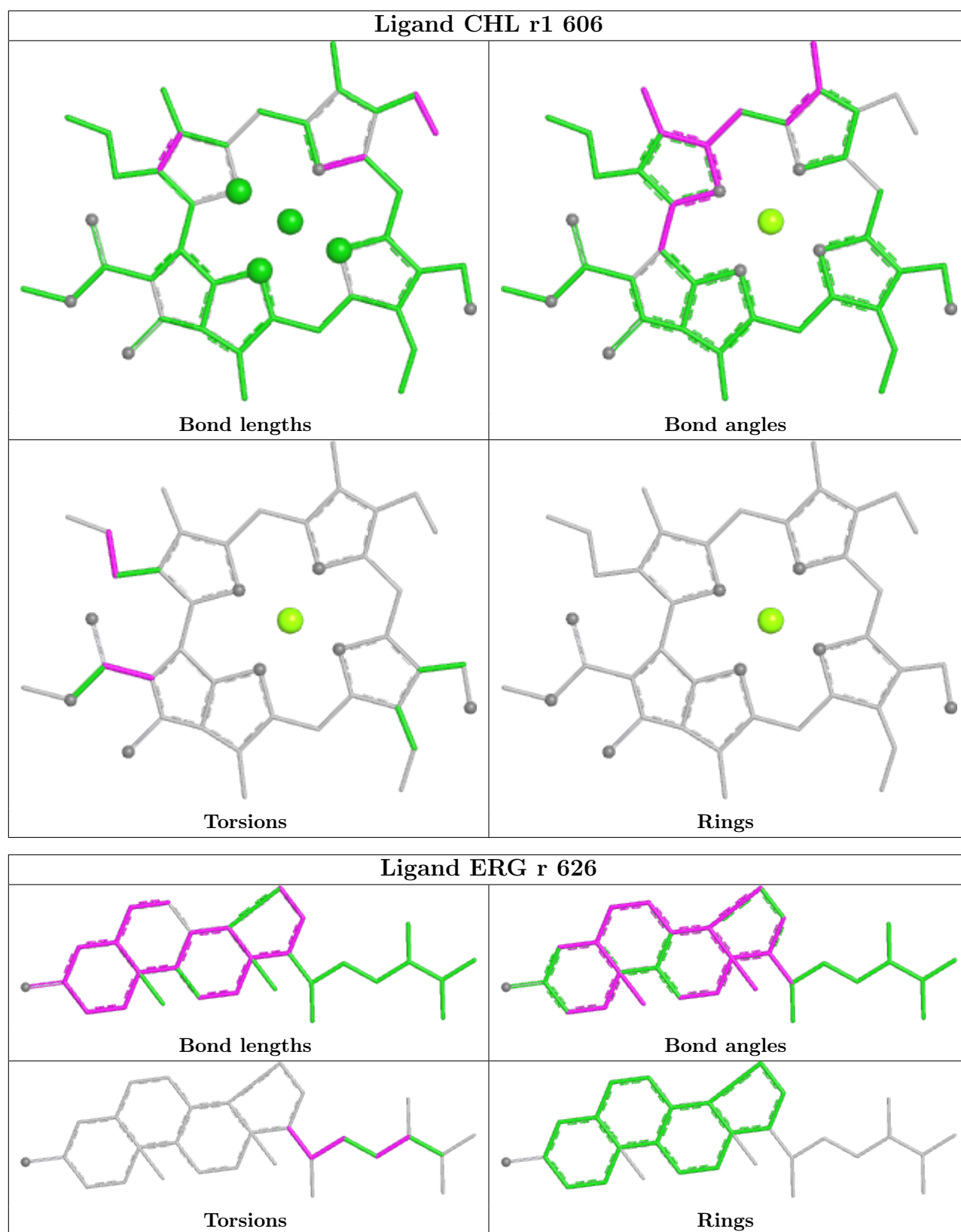
Rings



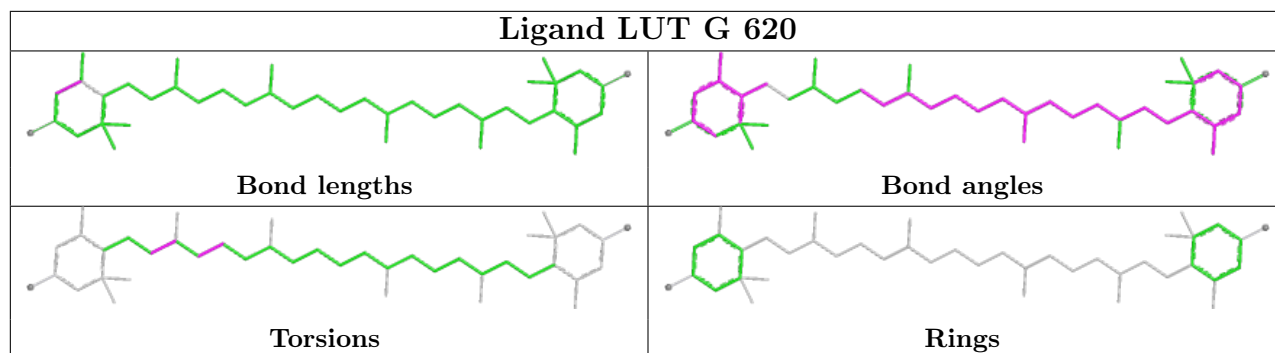




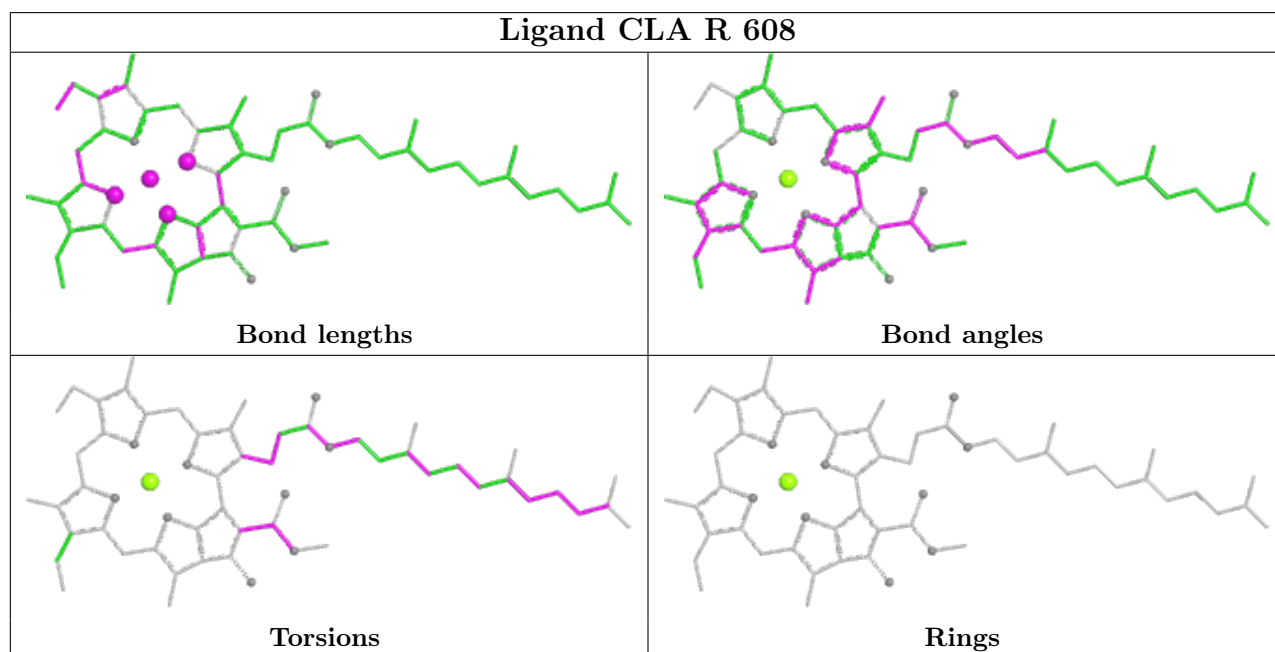




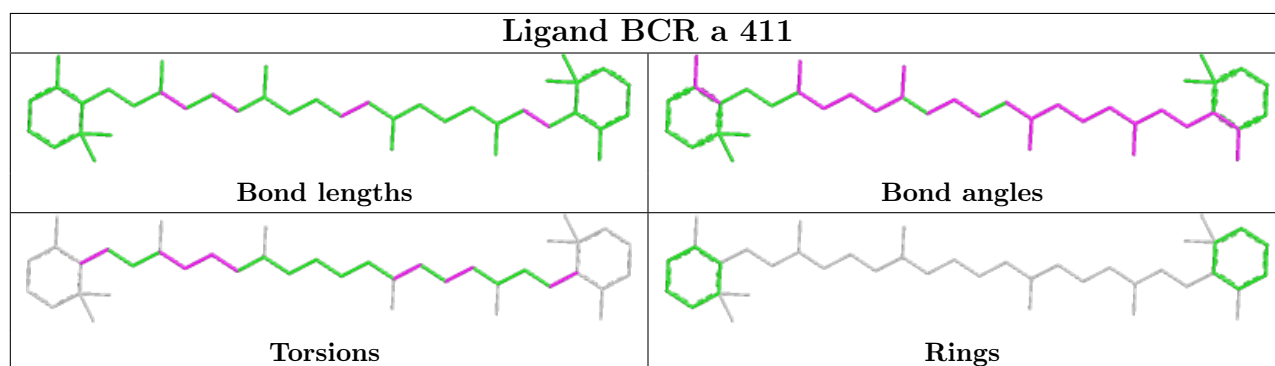
## Ligand LUT G 620



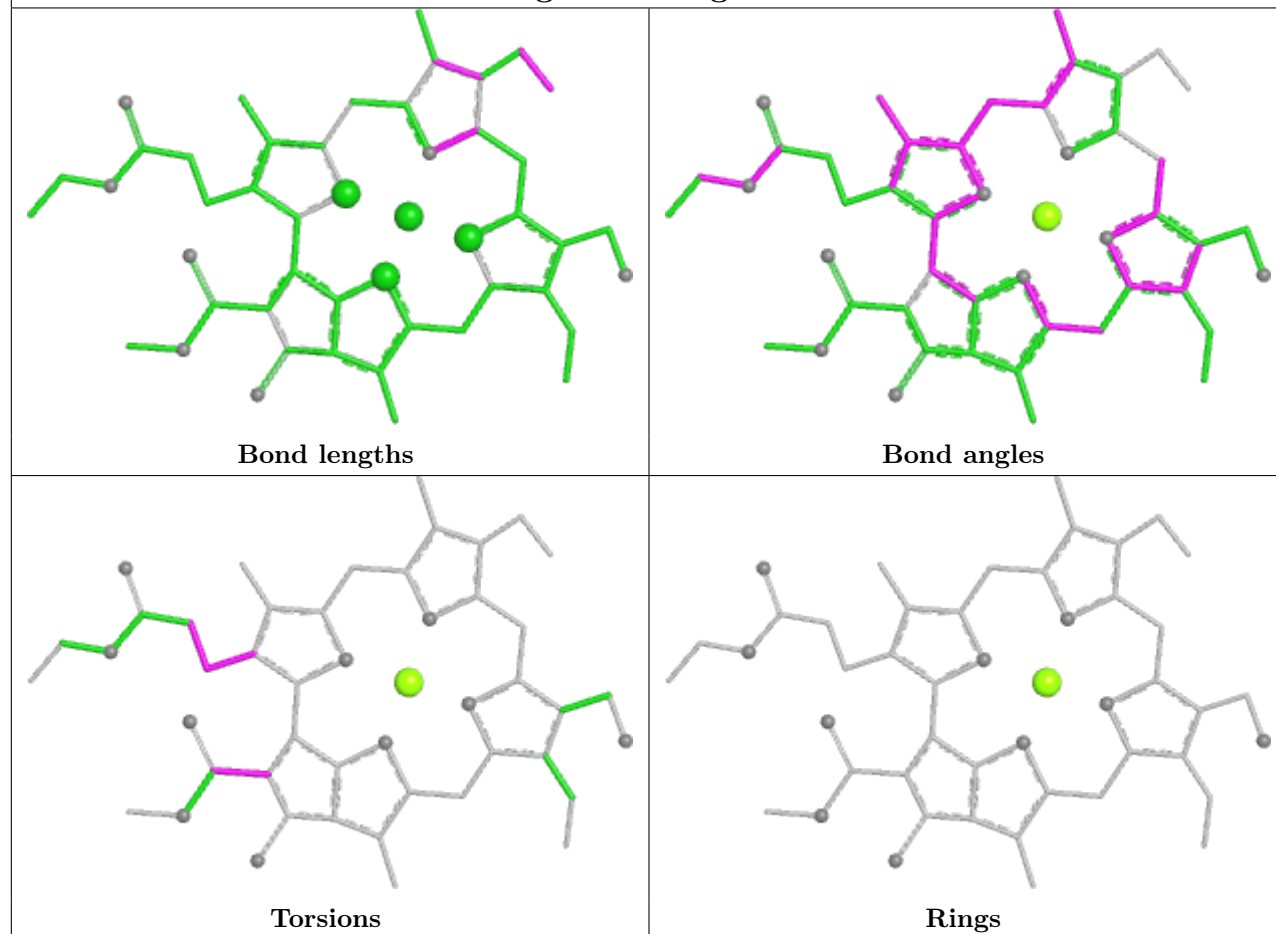
## Ligand CLA R 608



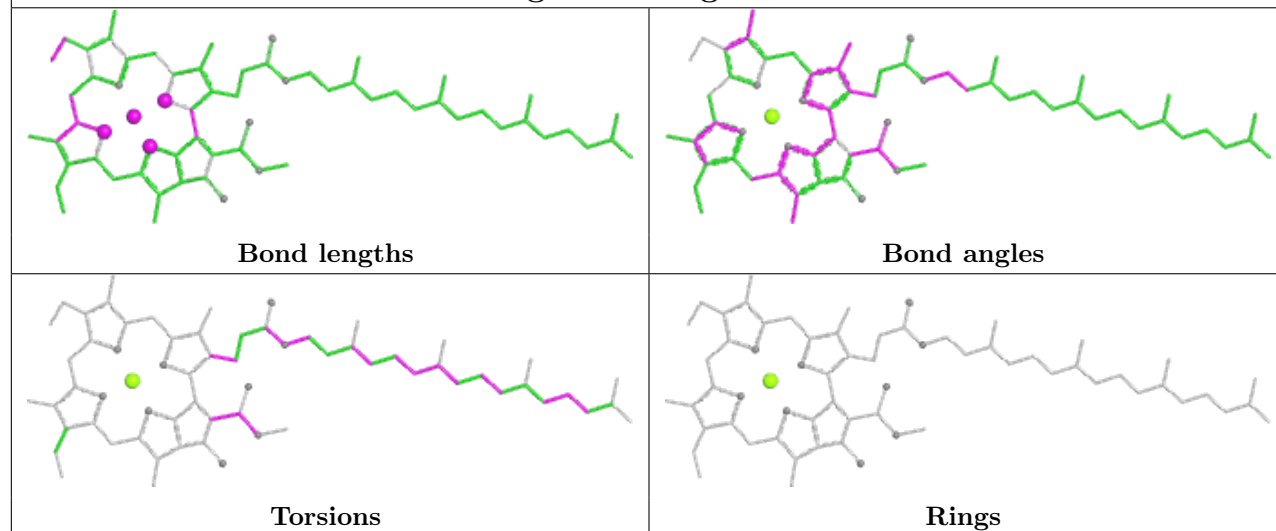
## Ligand BCR a 411

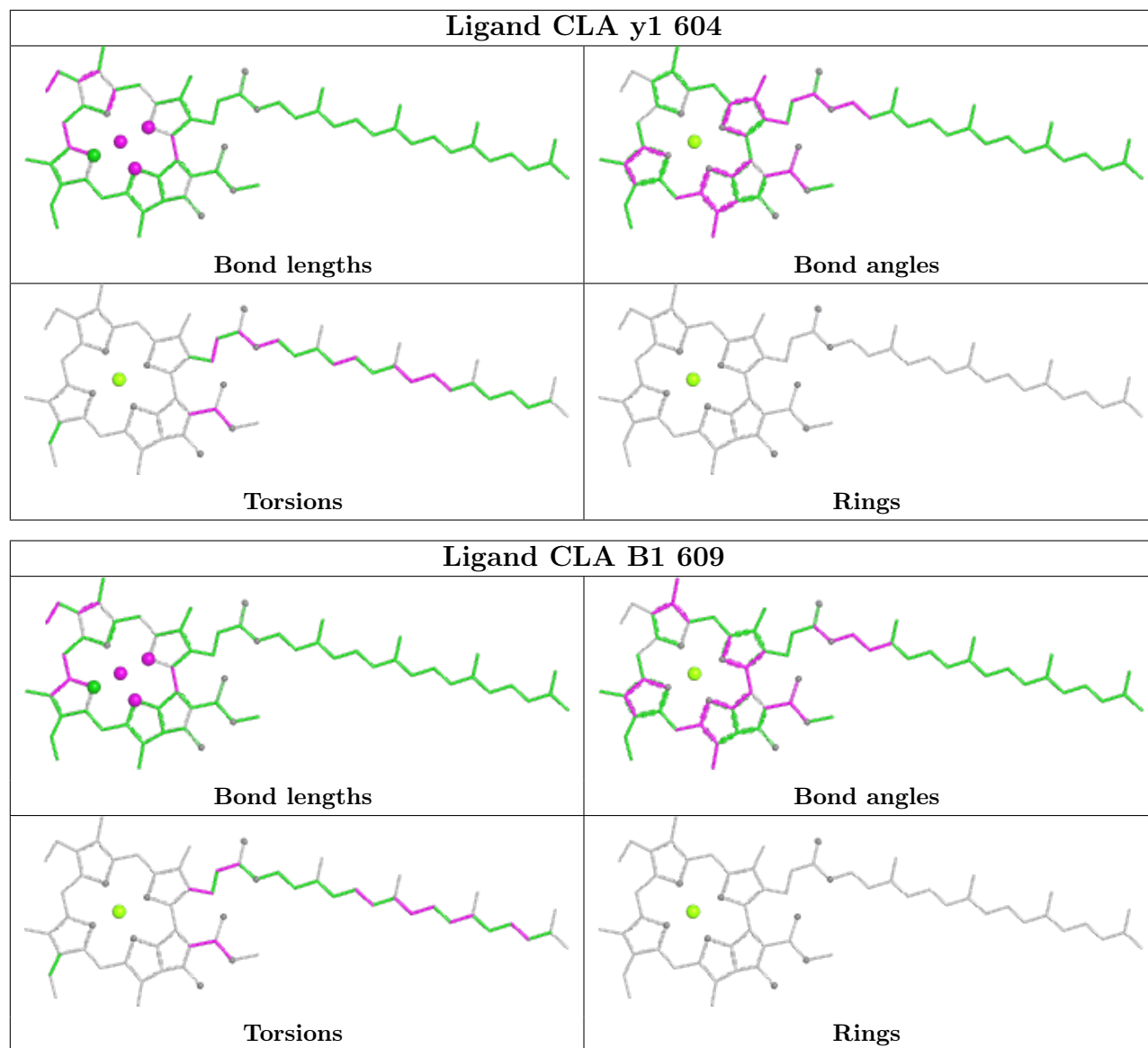


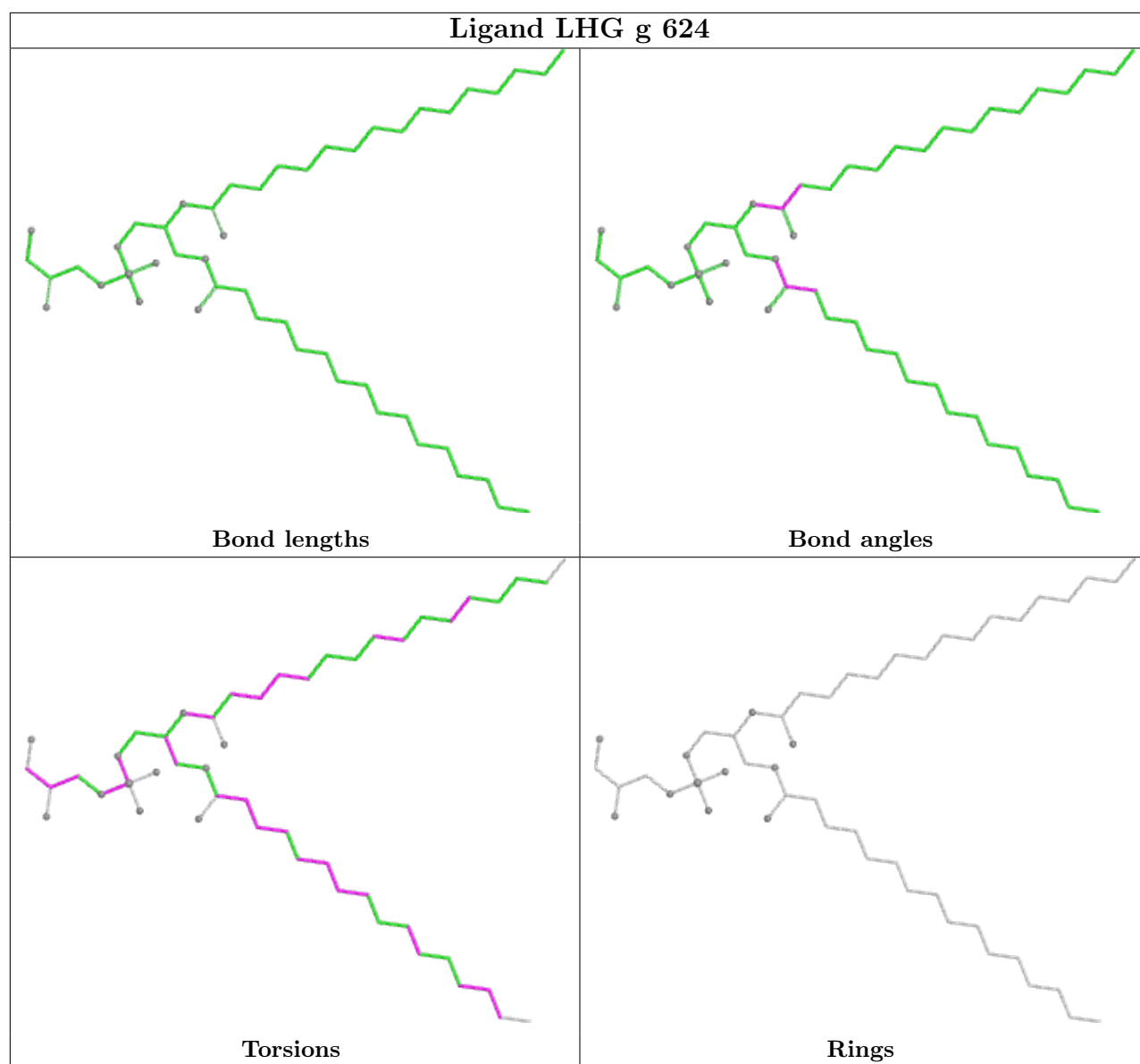
## Ligand CHL g 605



## Ligand CLA g1 611

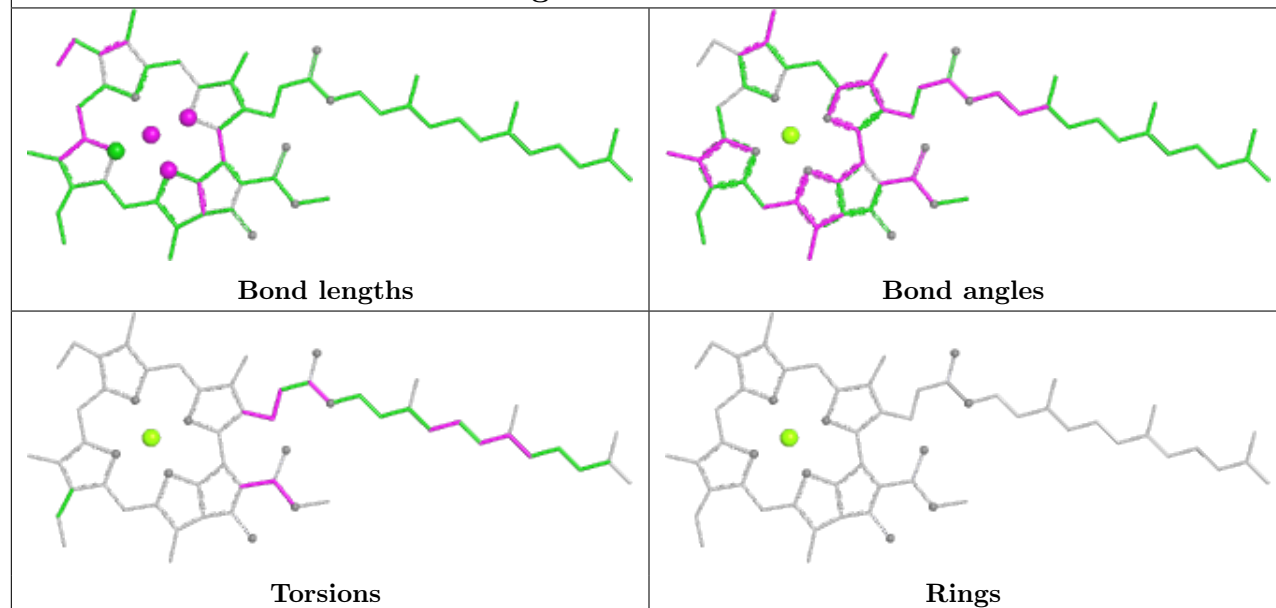




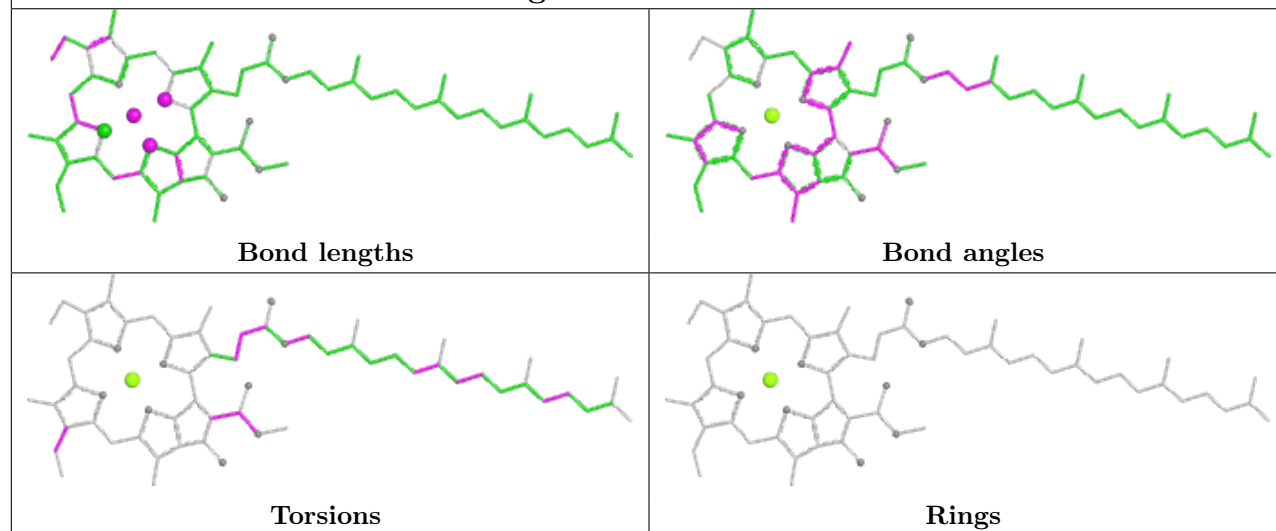


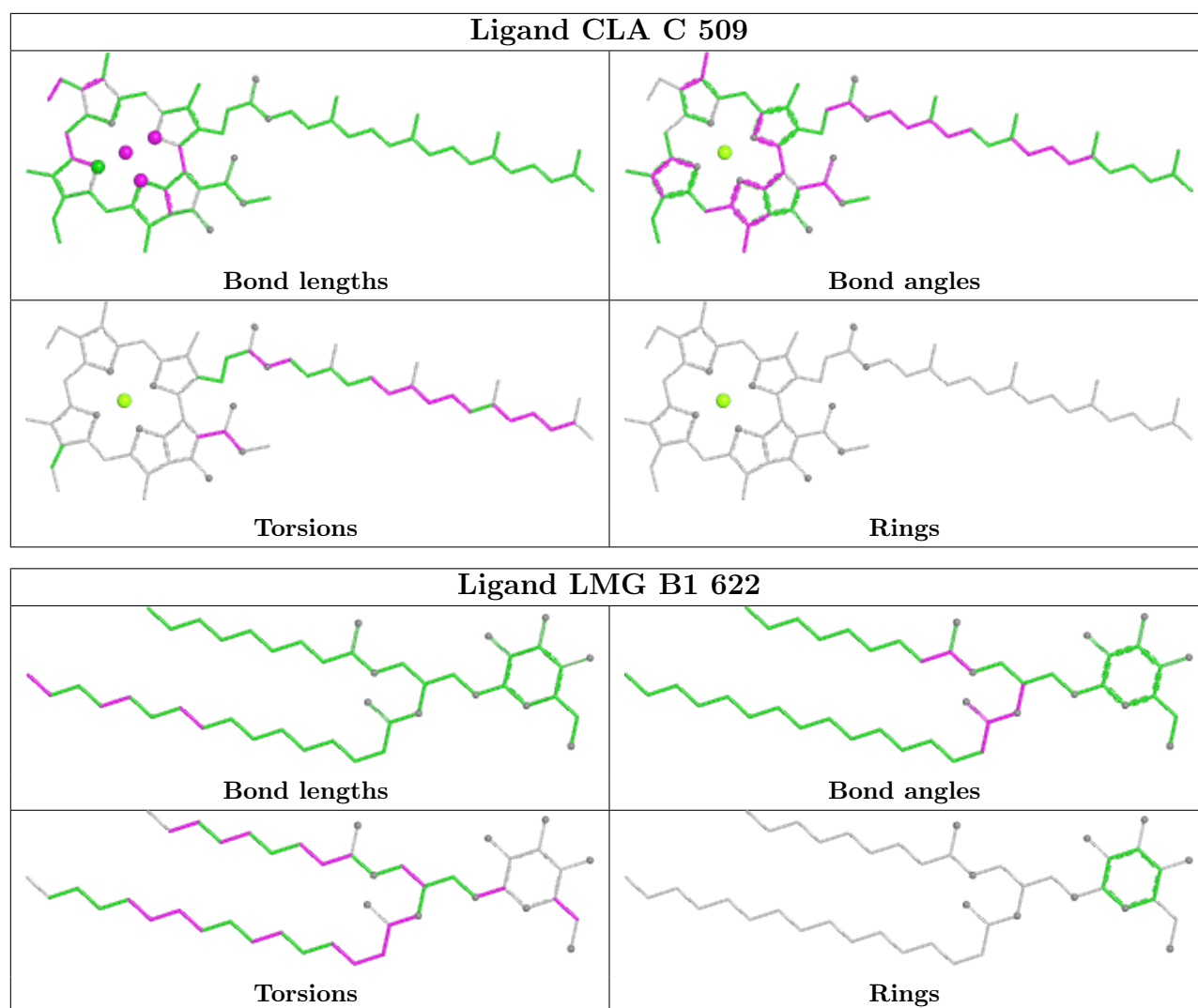


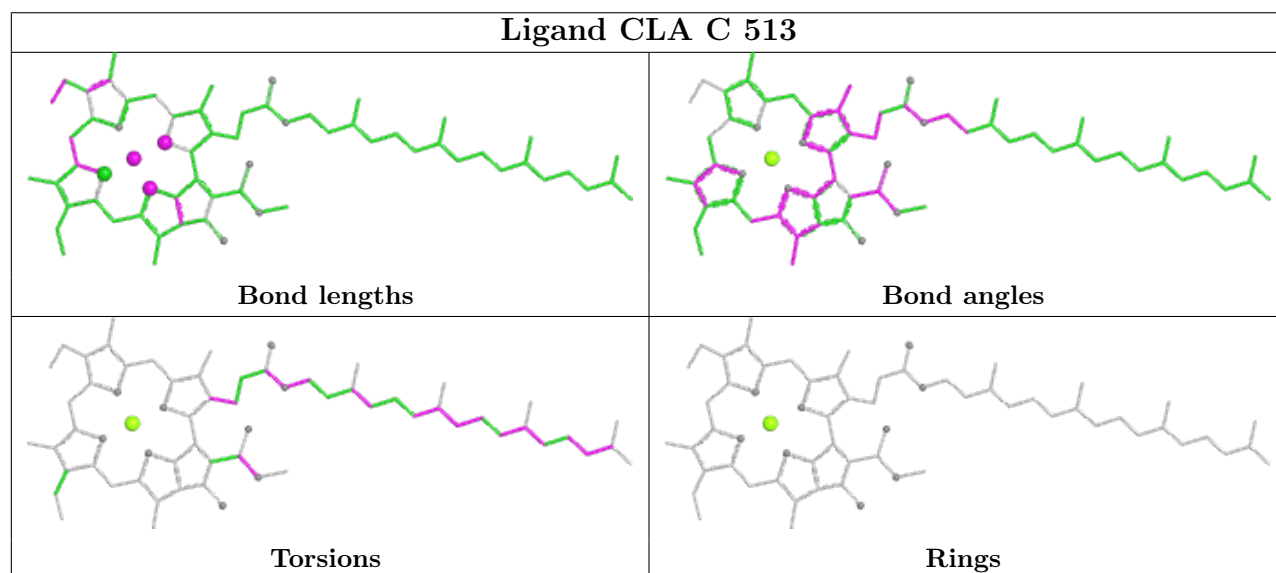
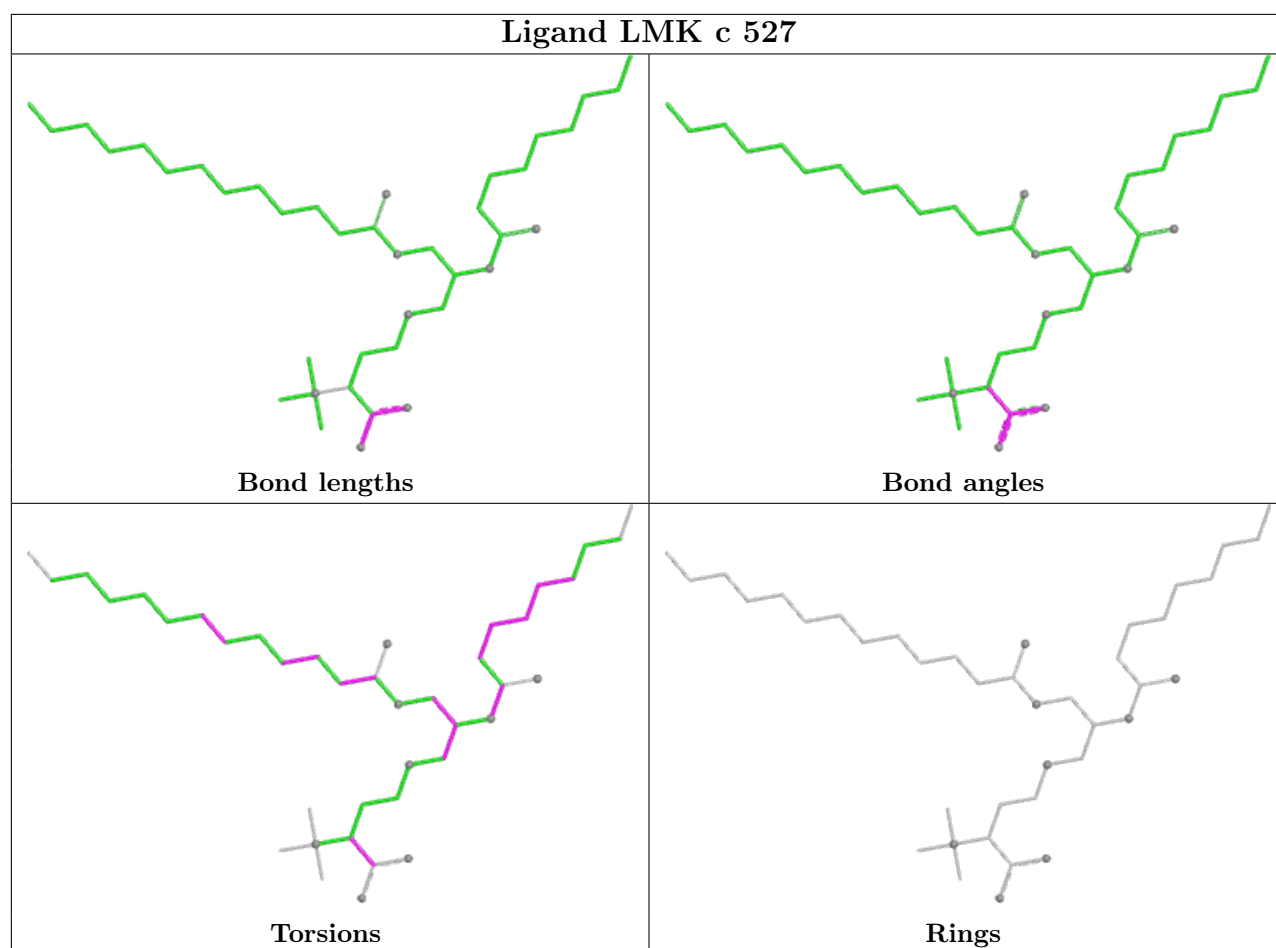
## Ligand CLA R 602

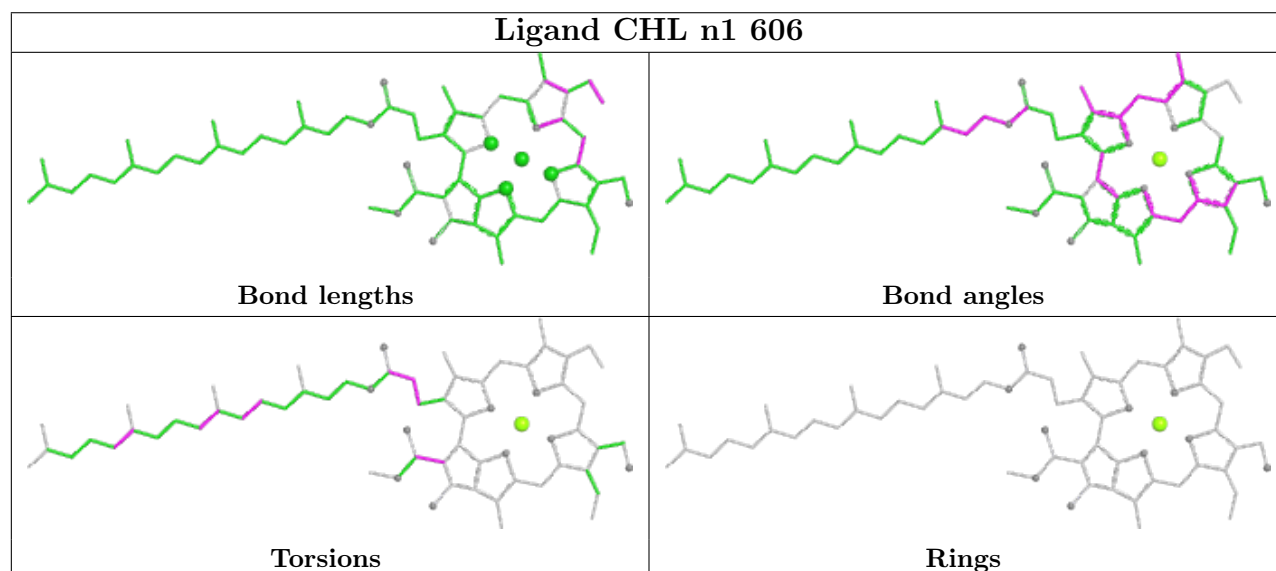
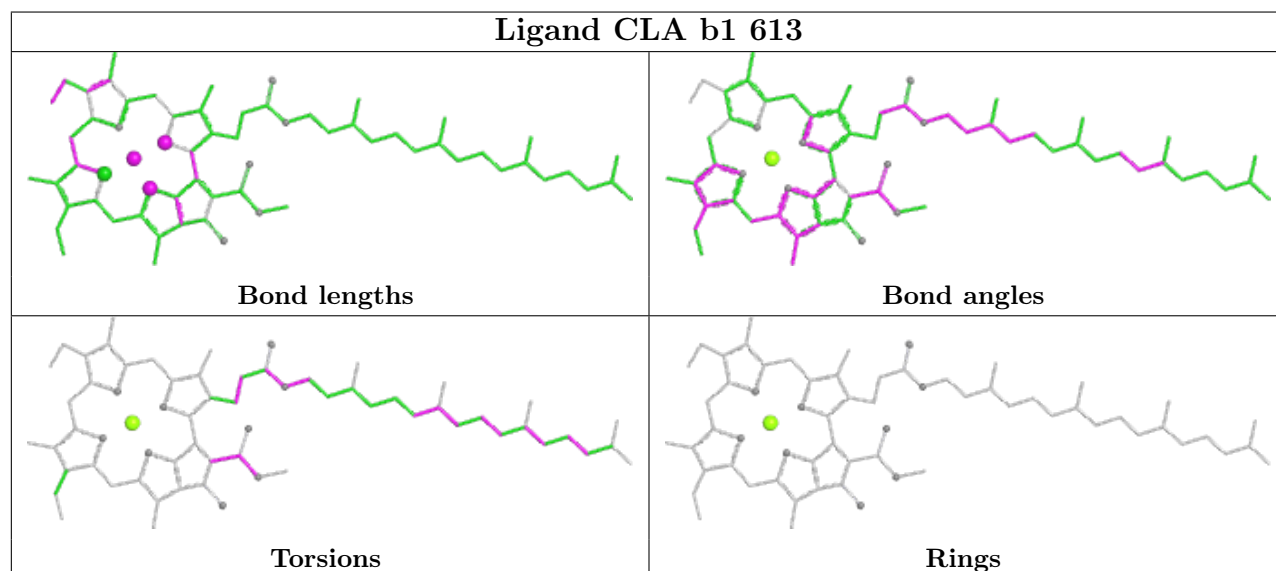
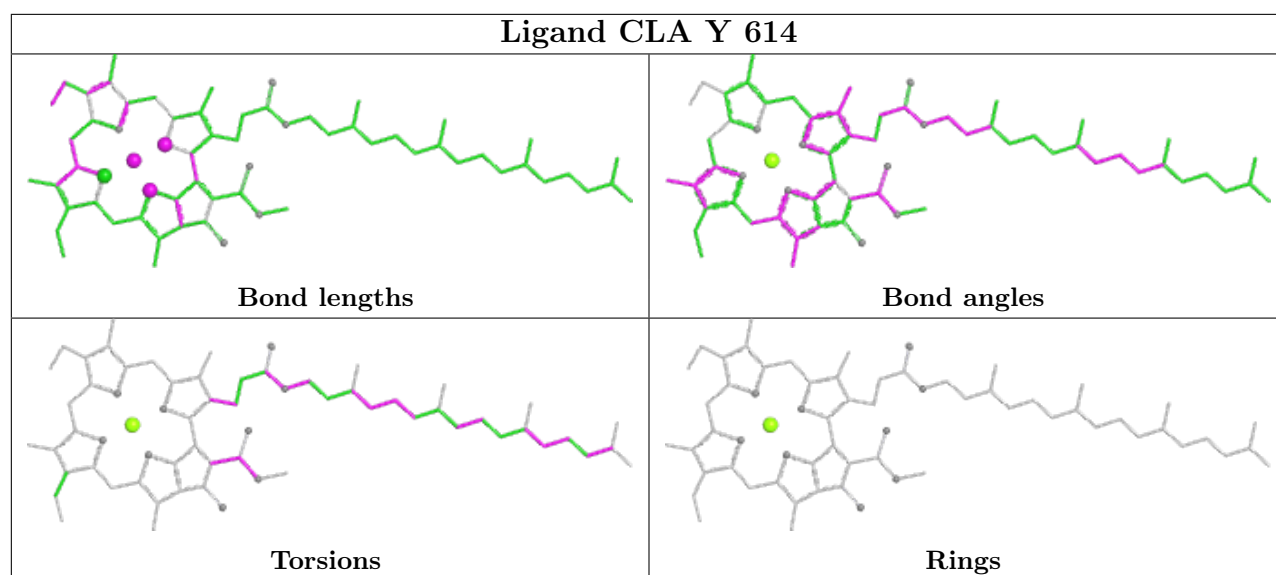


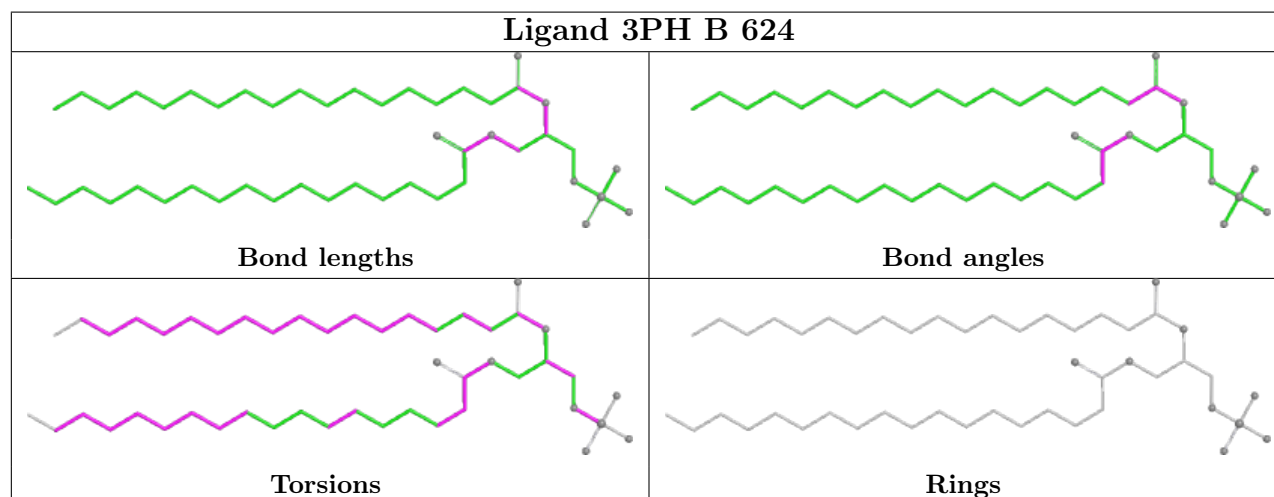
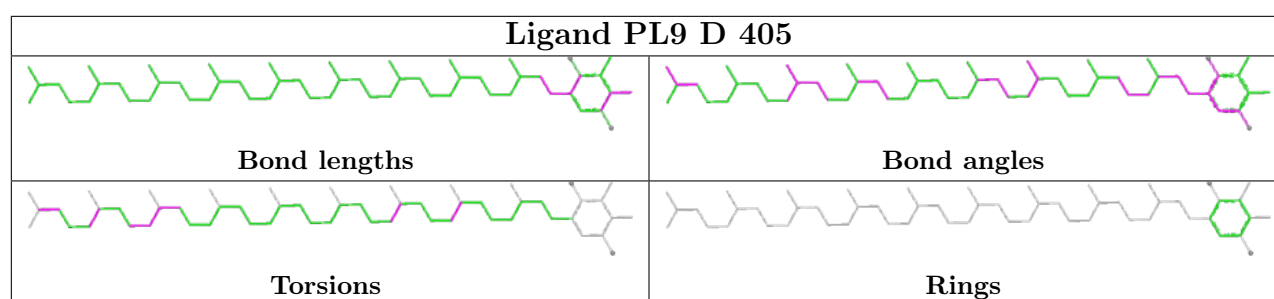
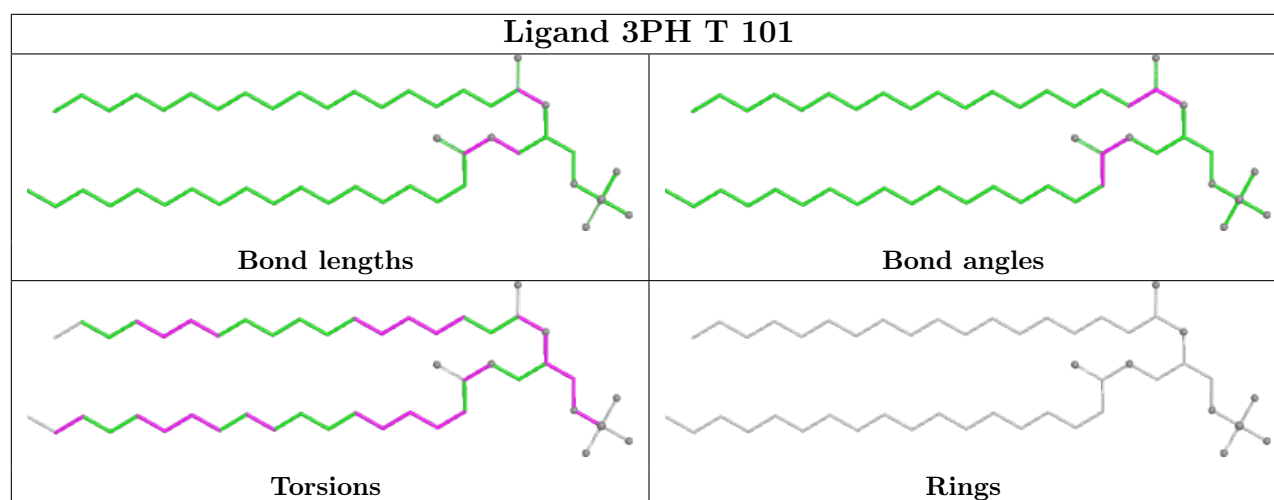
## Ligand CLA c1 502

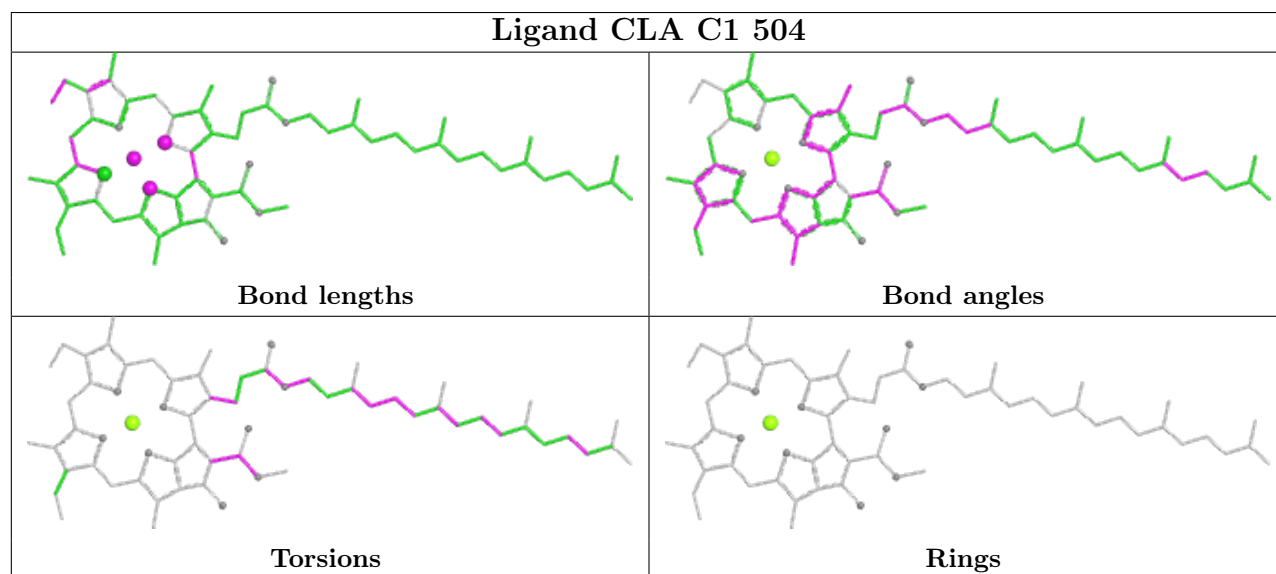
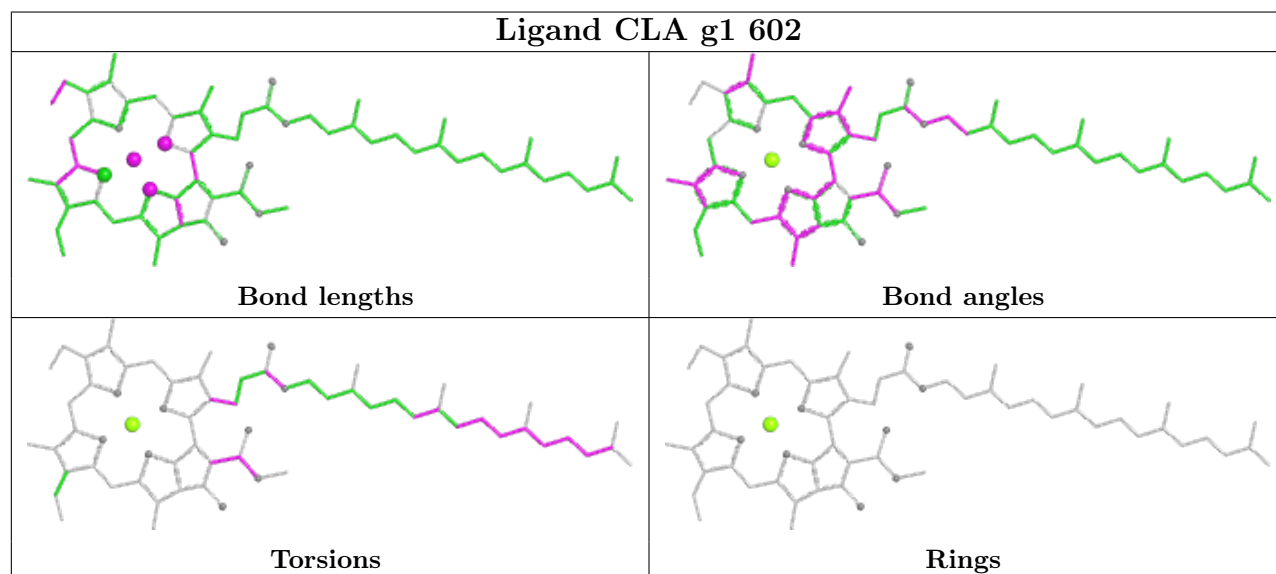
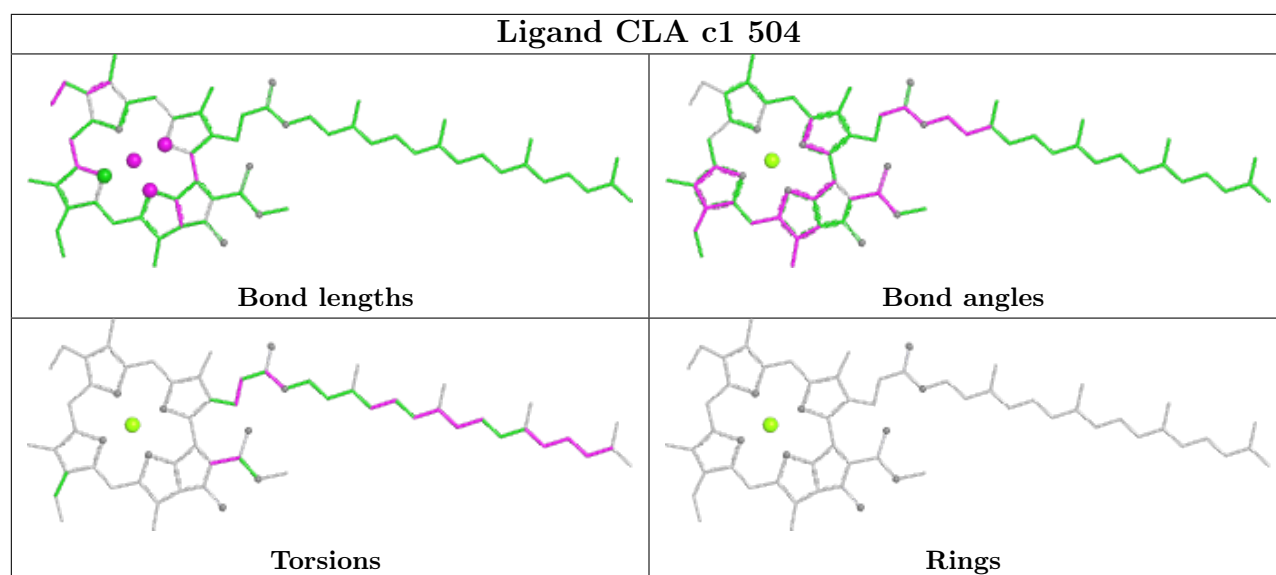


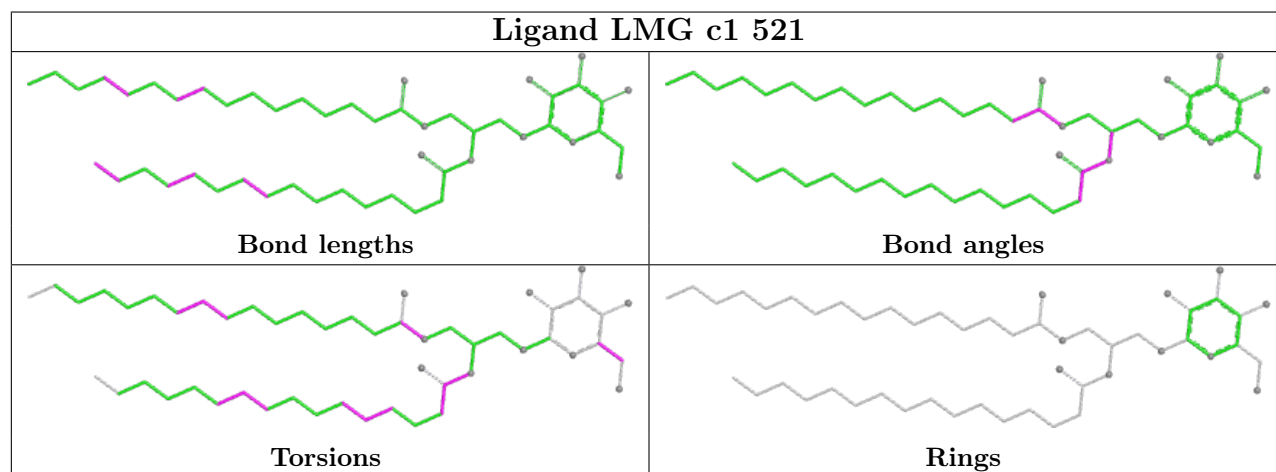
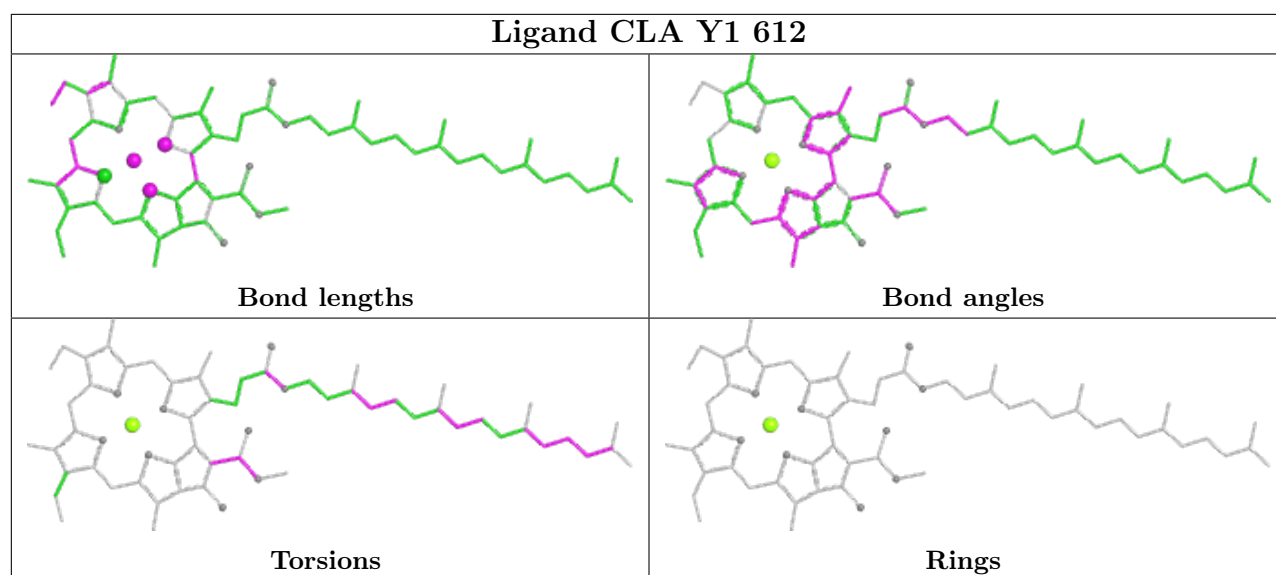




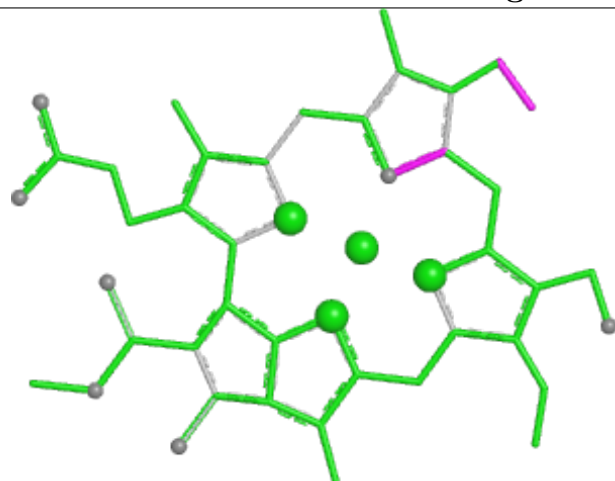




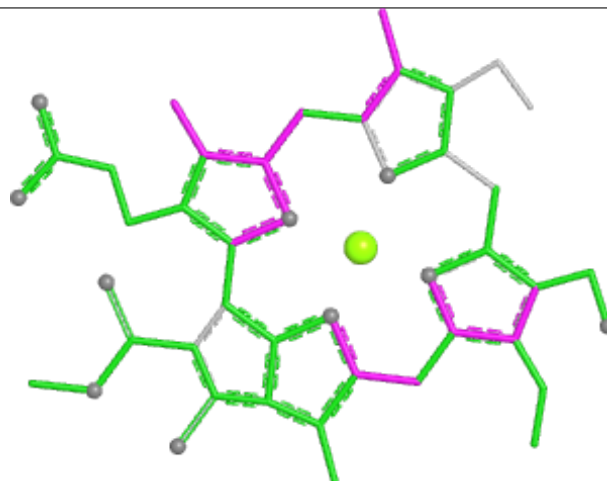




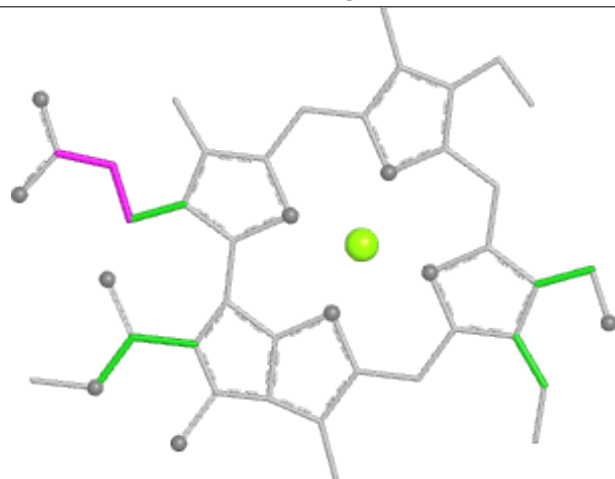
## Ligand CHL Y1 605



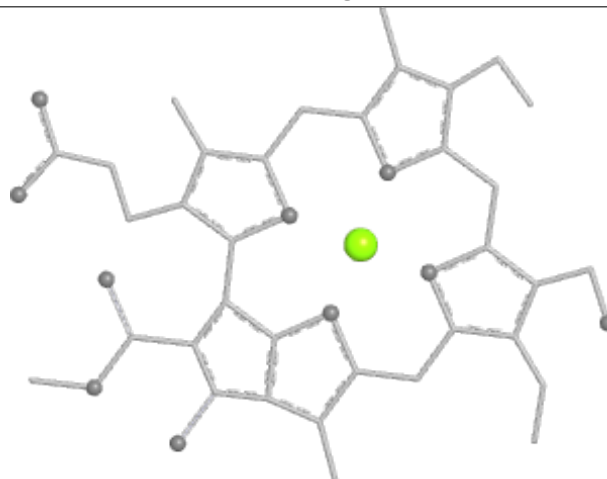
Bond lengths



Bond angles

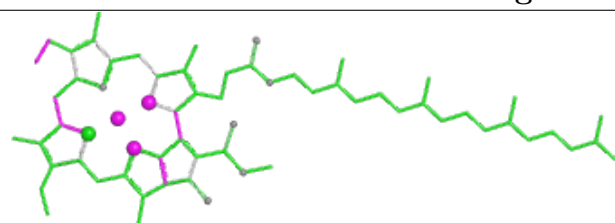


Torsions

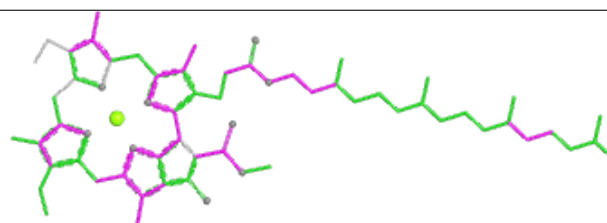


Rings

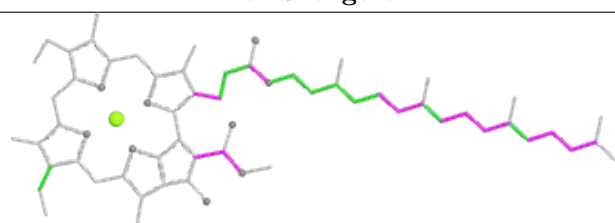
## Ligand CLA G 602



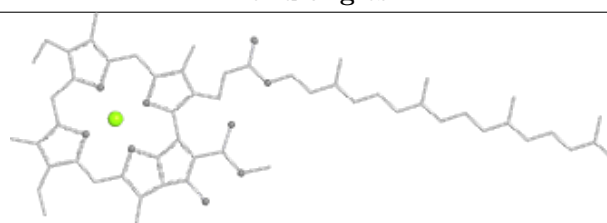
Bond lengths



Bond angles

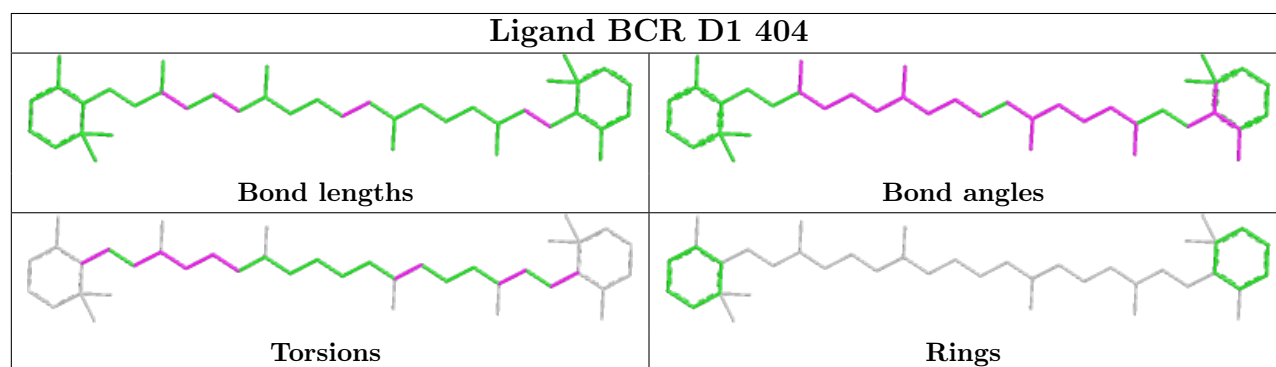
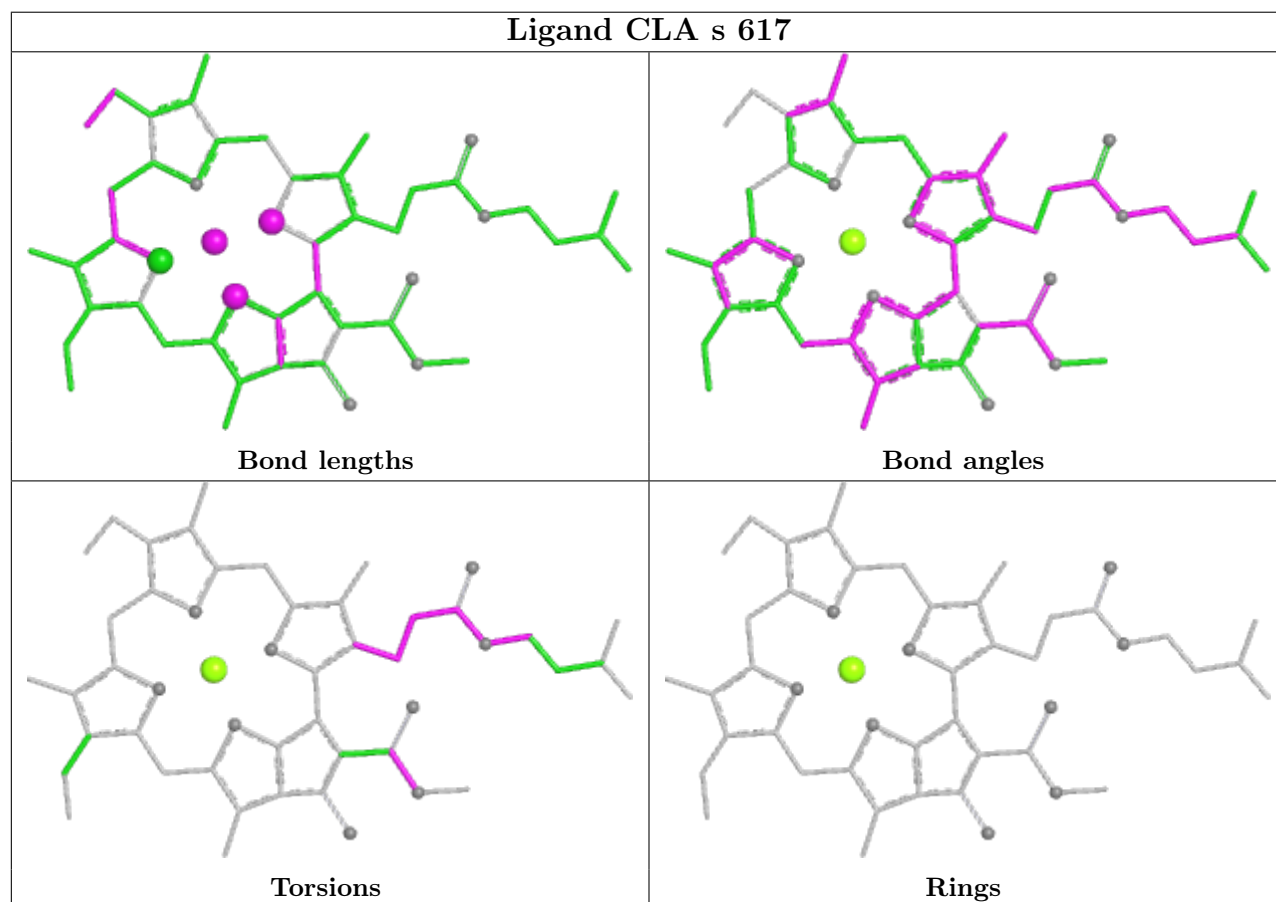
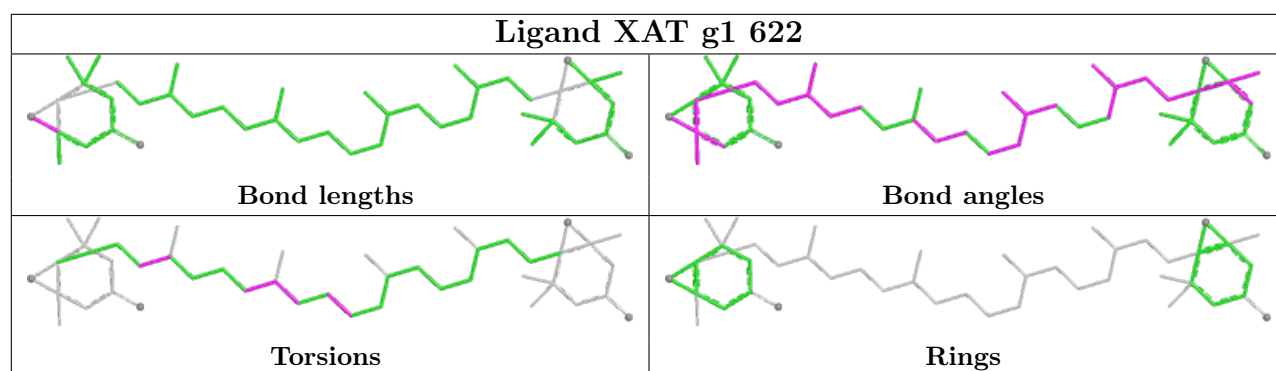


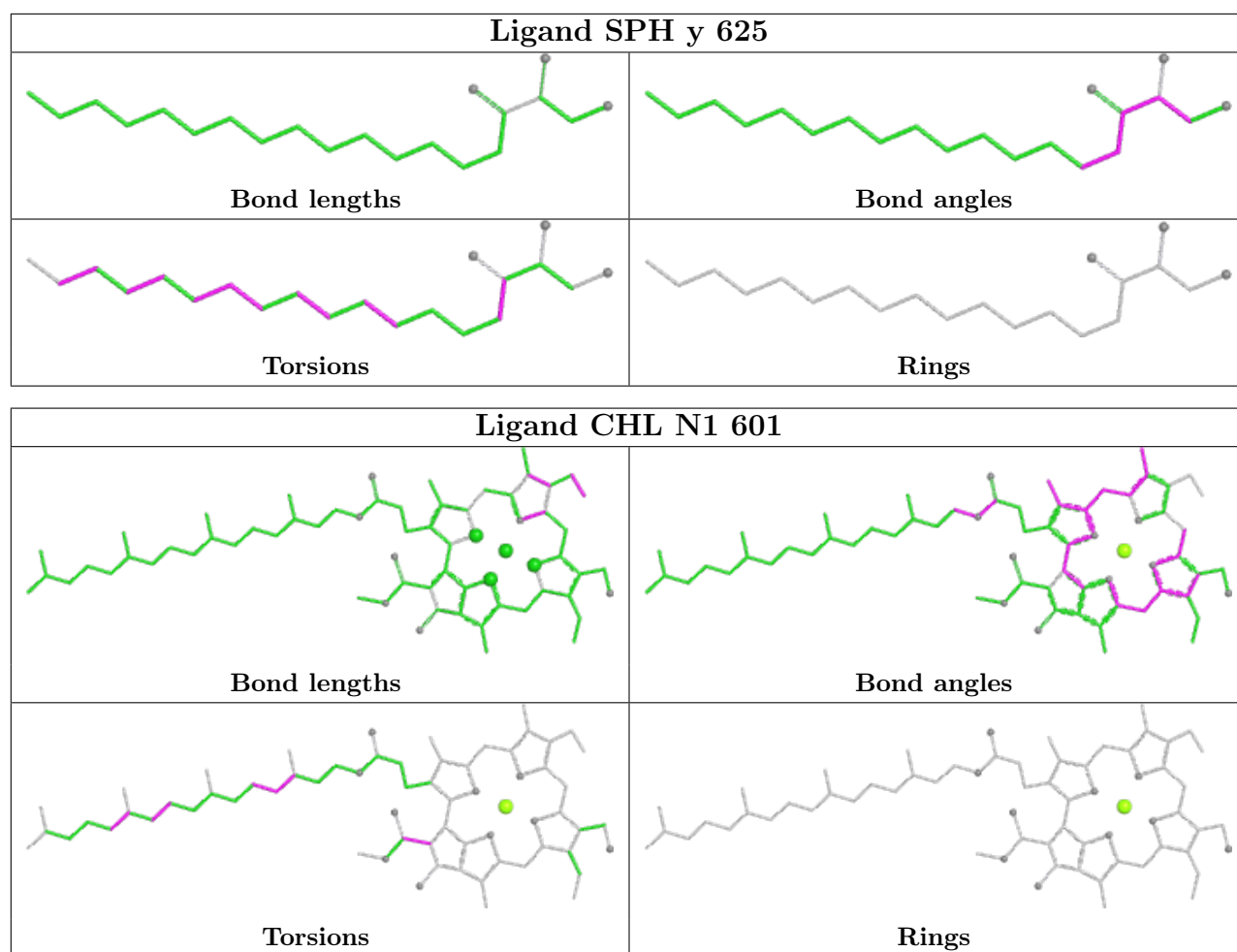
Torsions



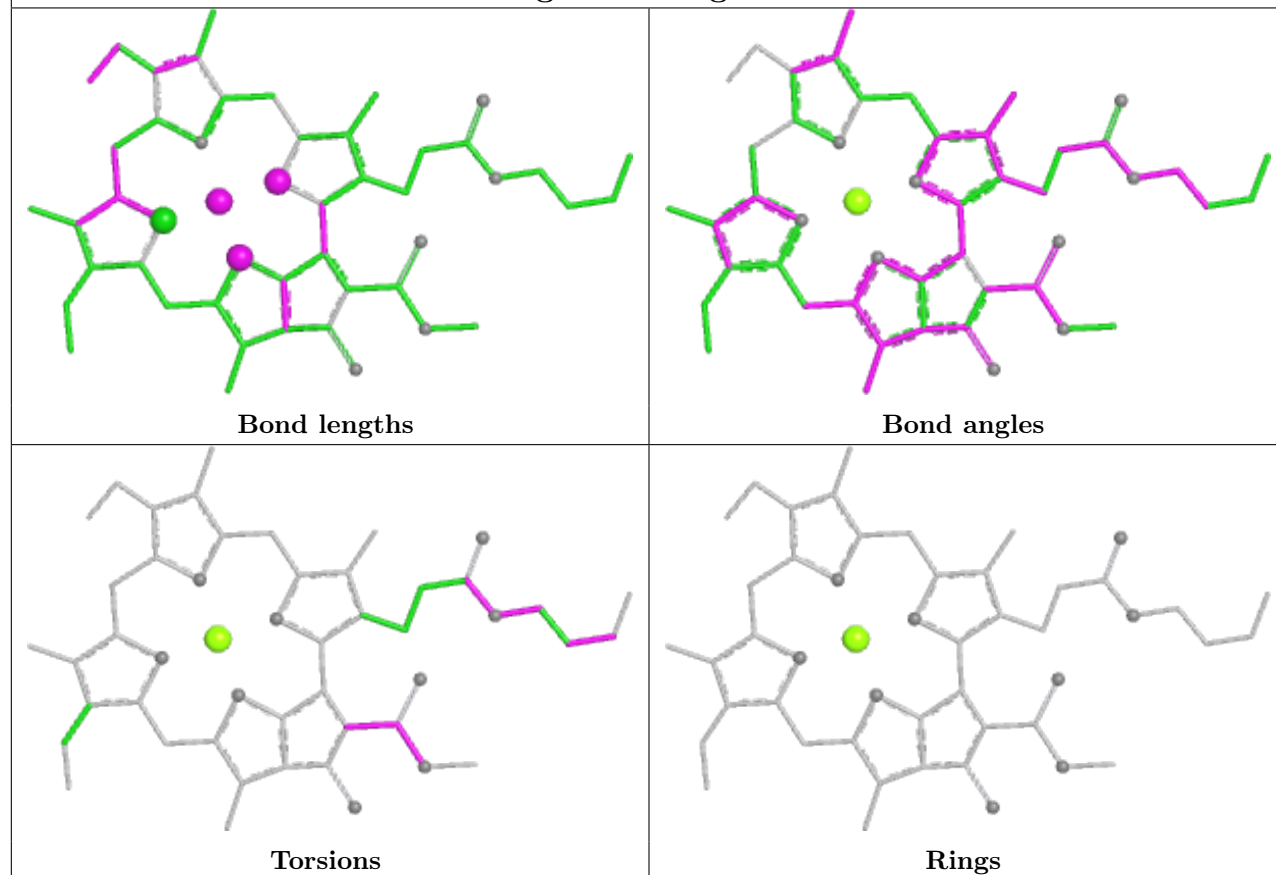
Rings



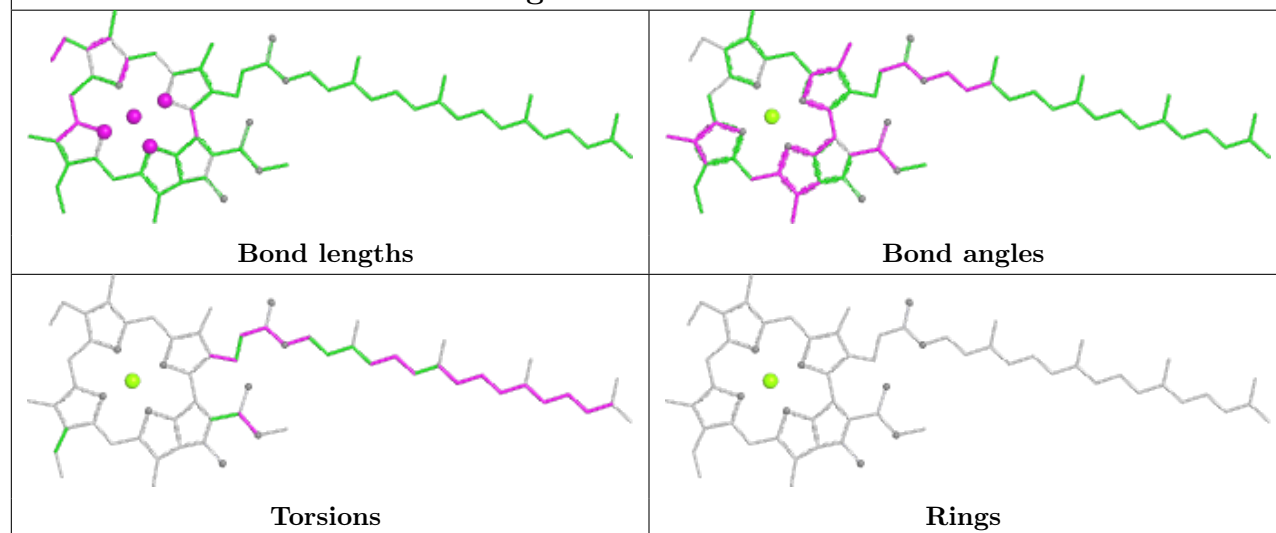


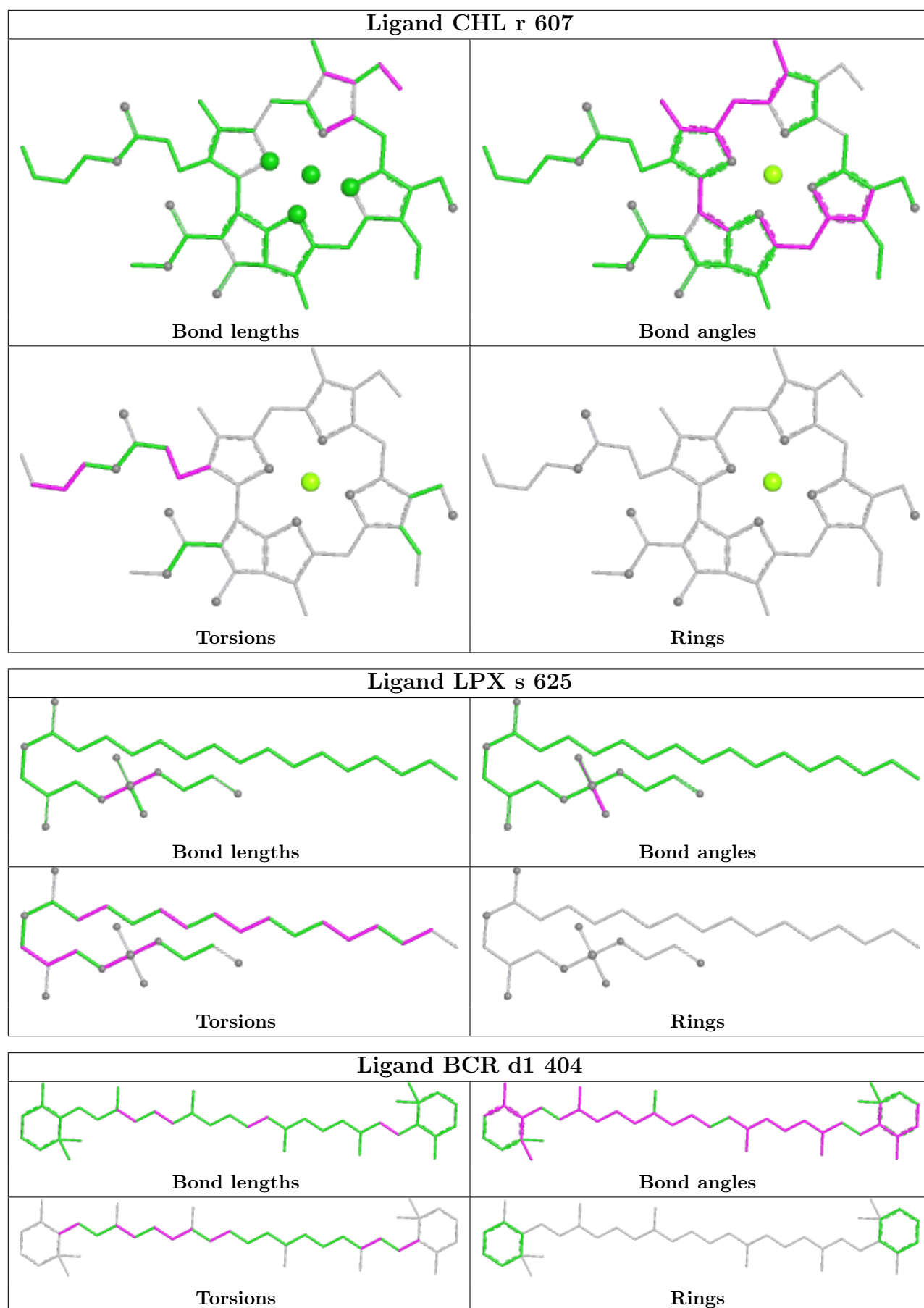


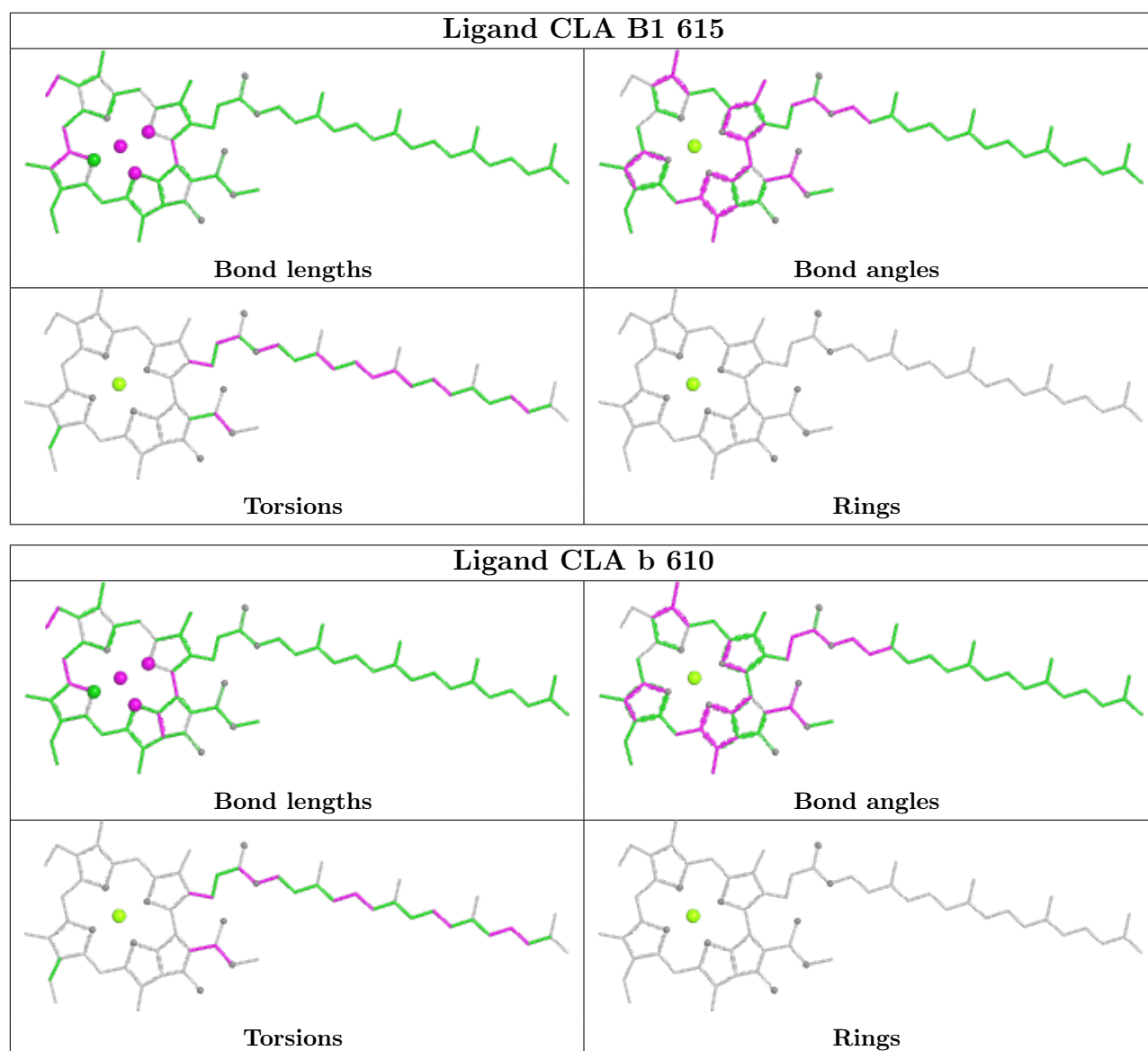
## Ligand CLA g 604

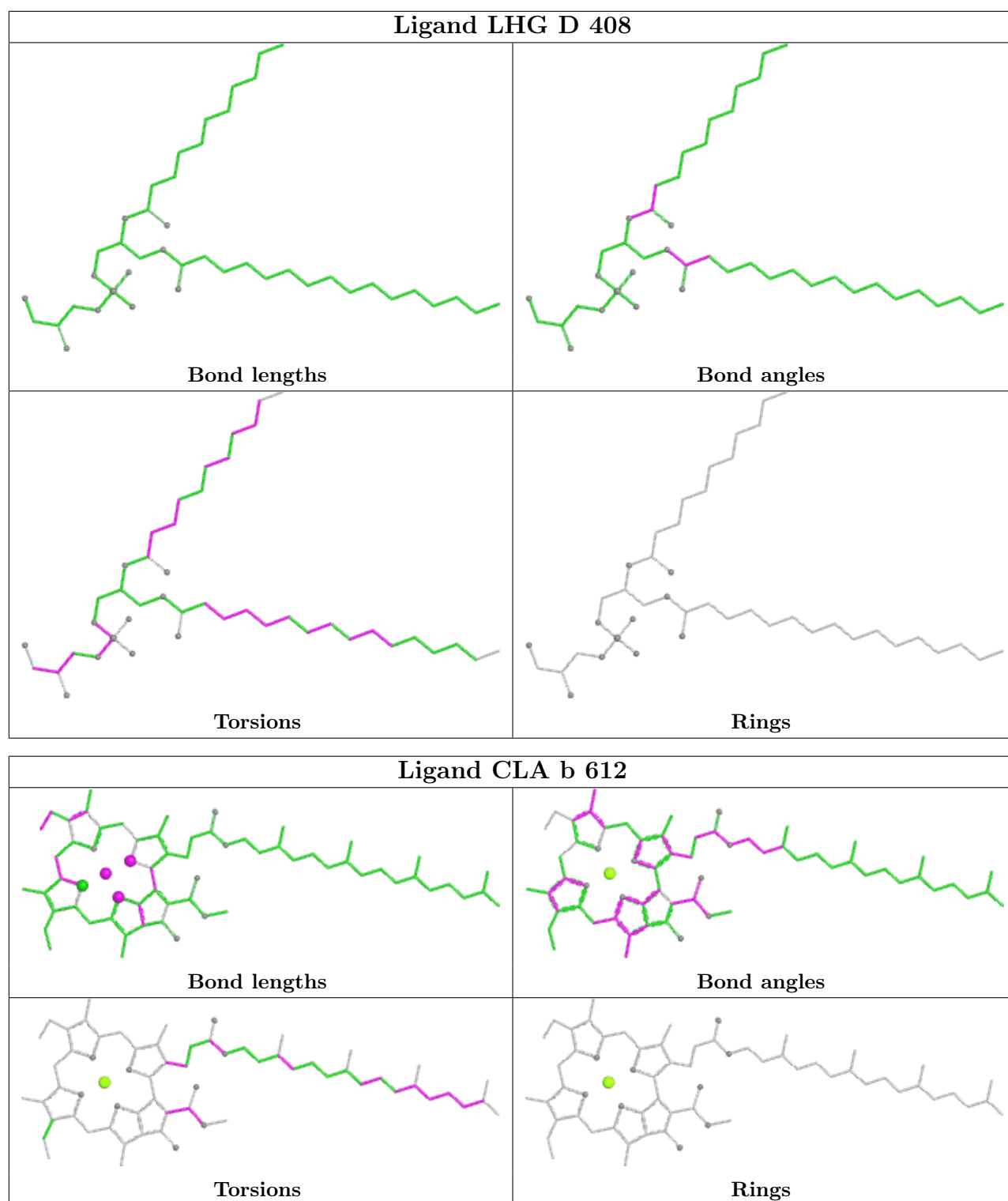


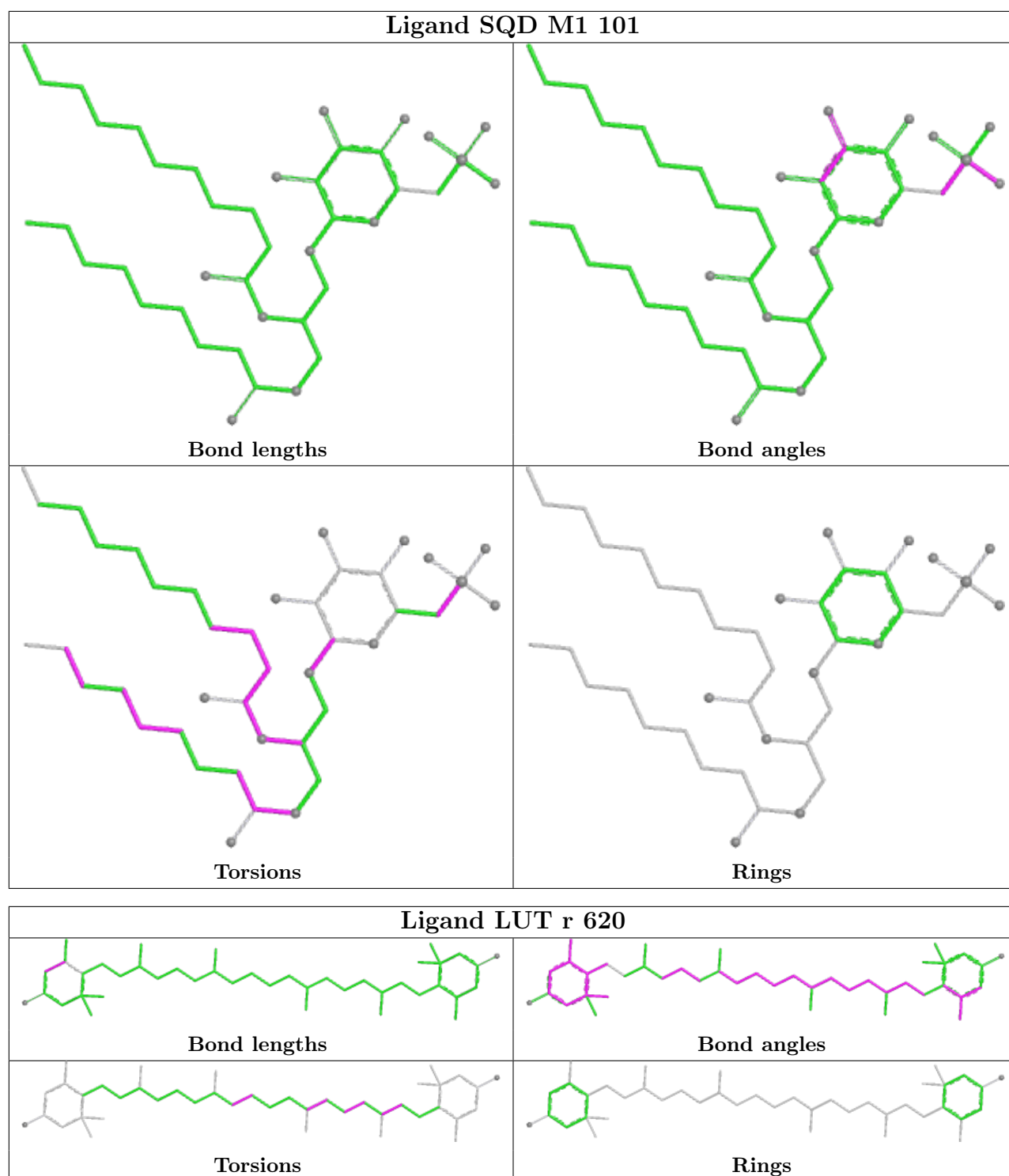
## Ligand CLA b1 602

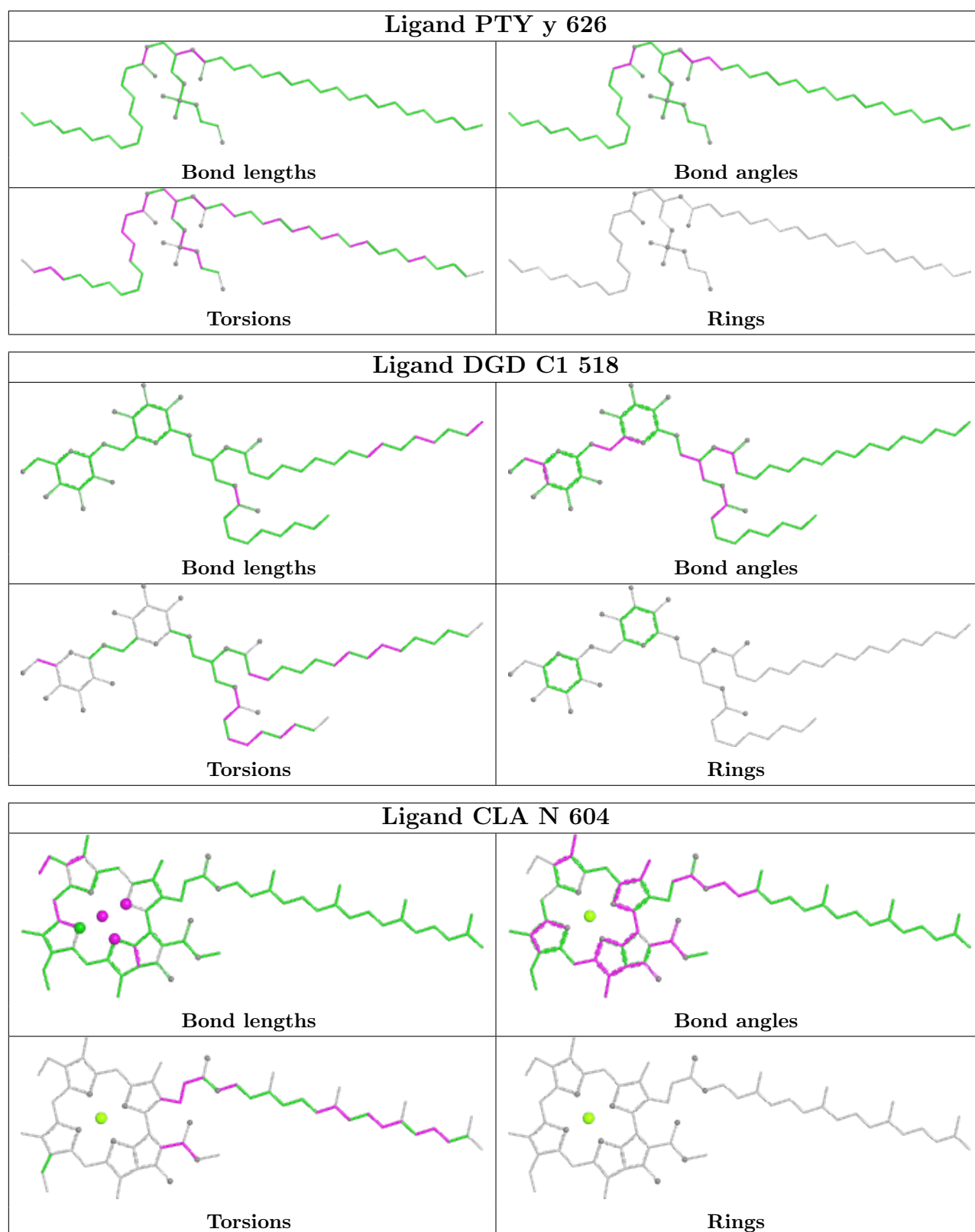




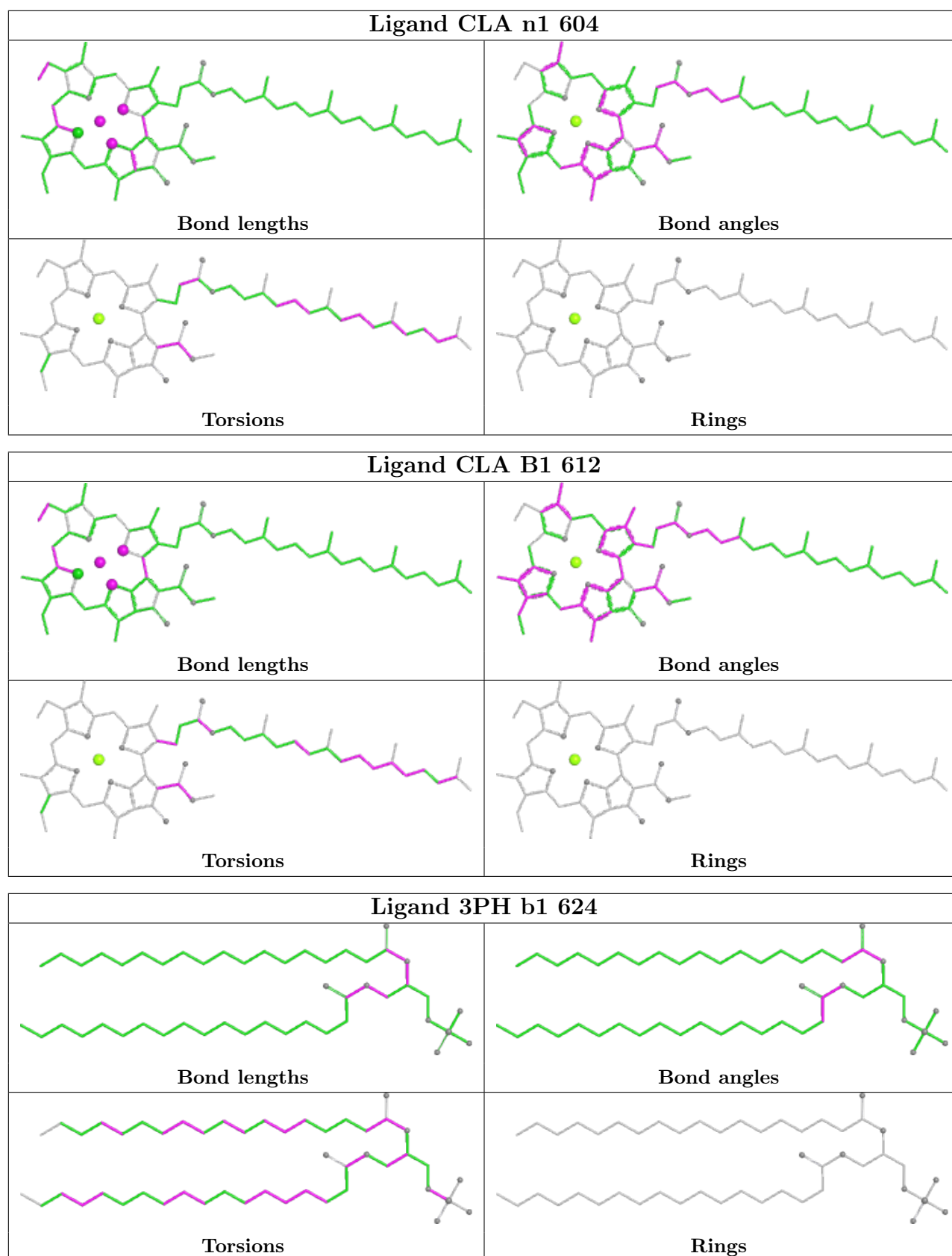


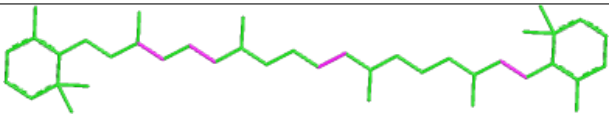
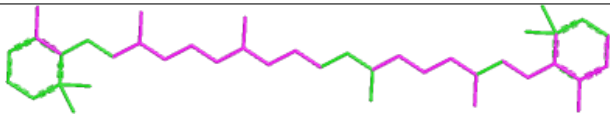
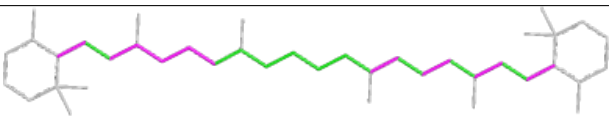
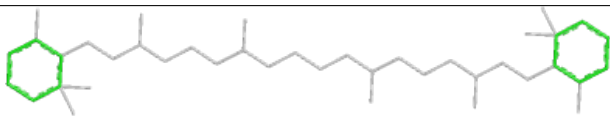


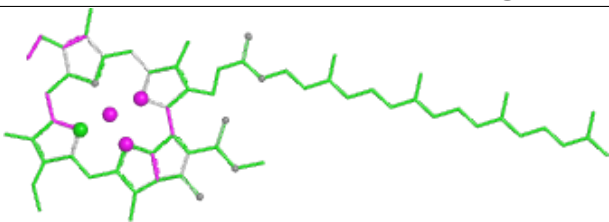
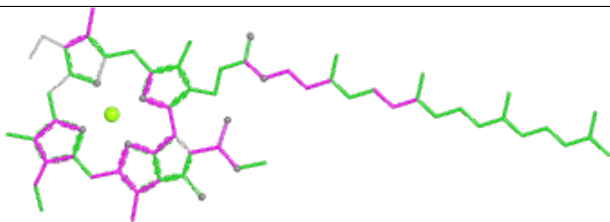
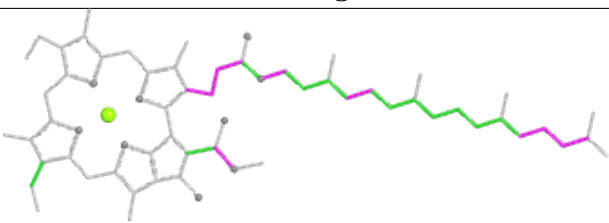
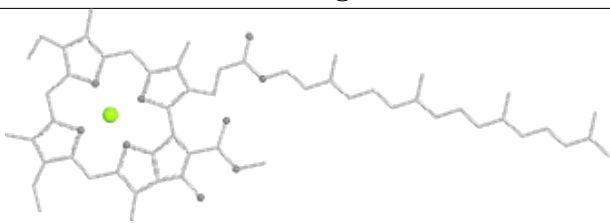


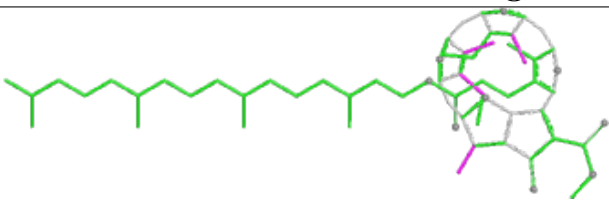
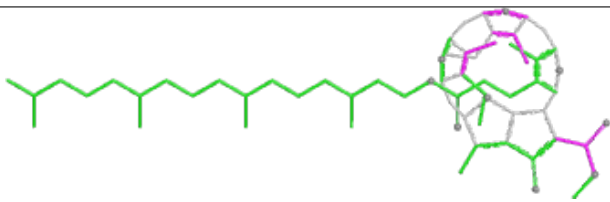
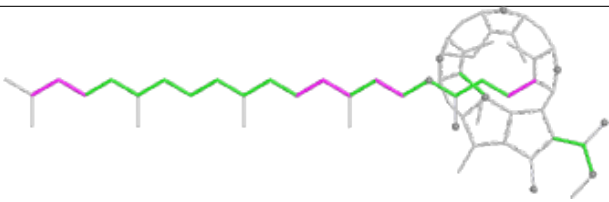
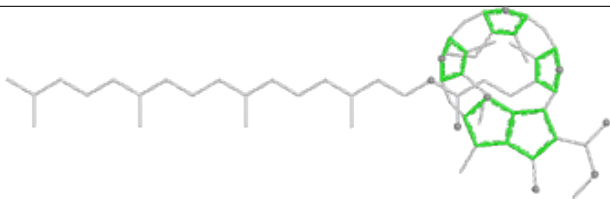


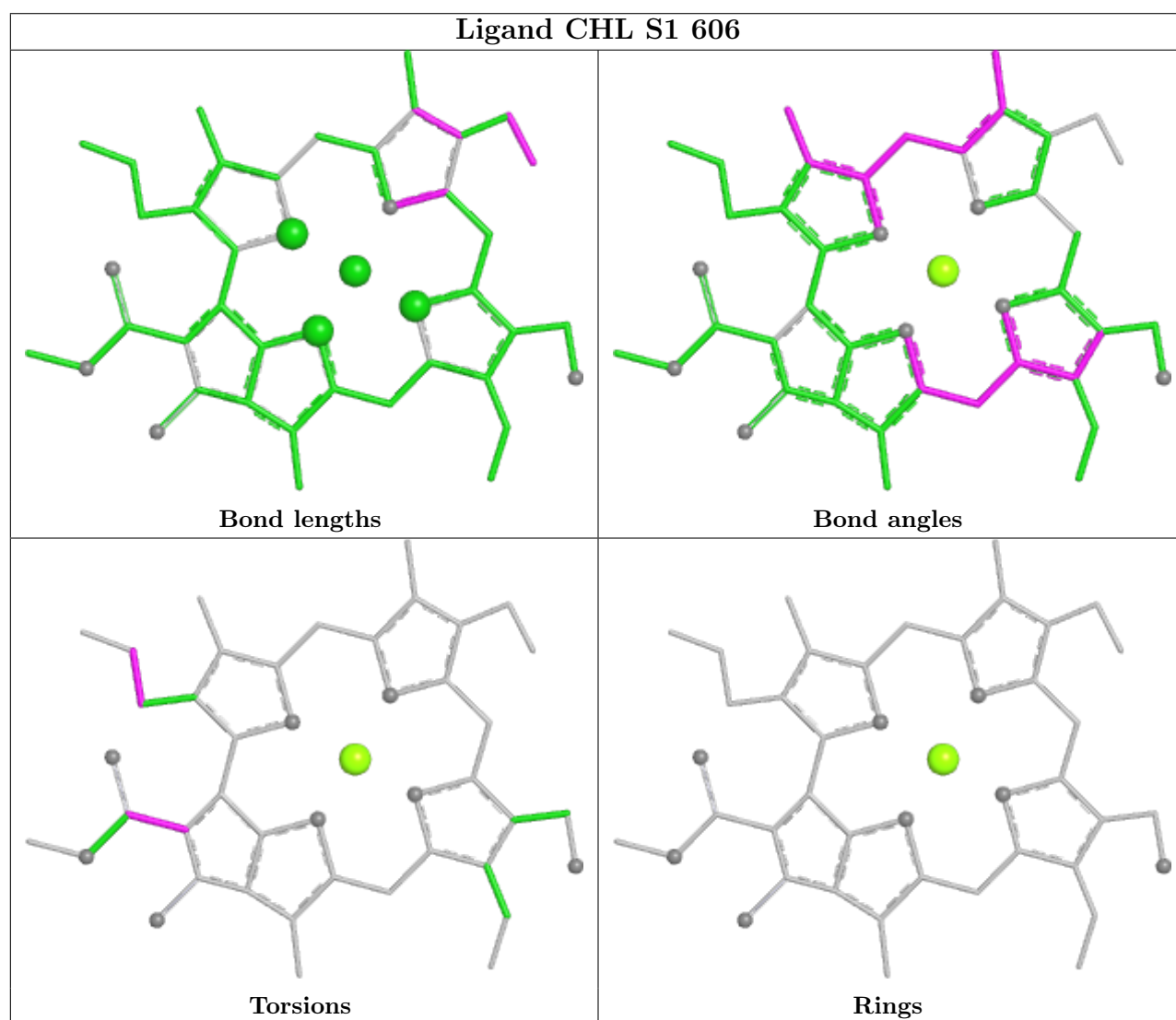
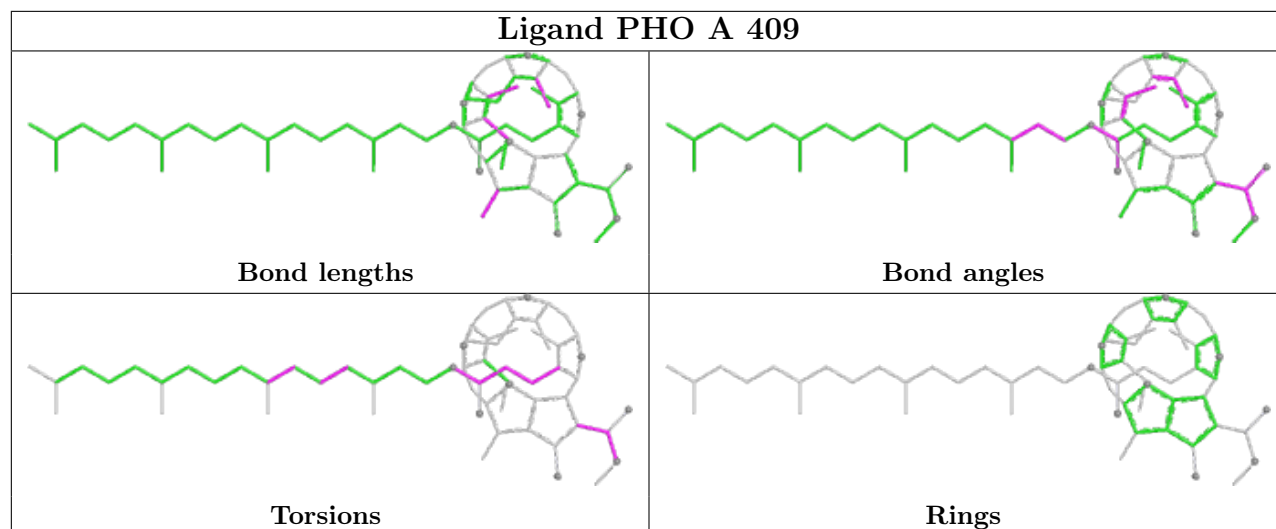


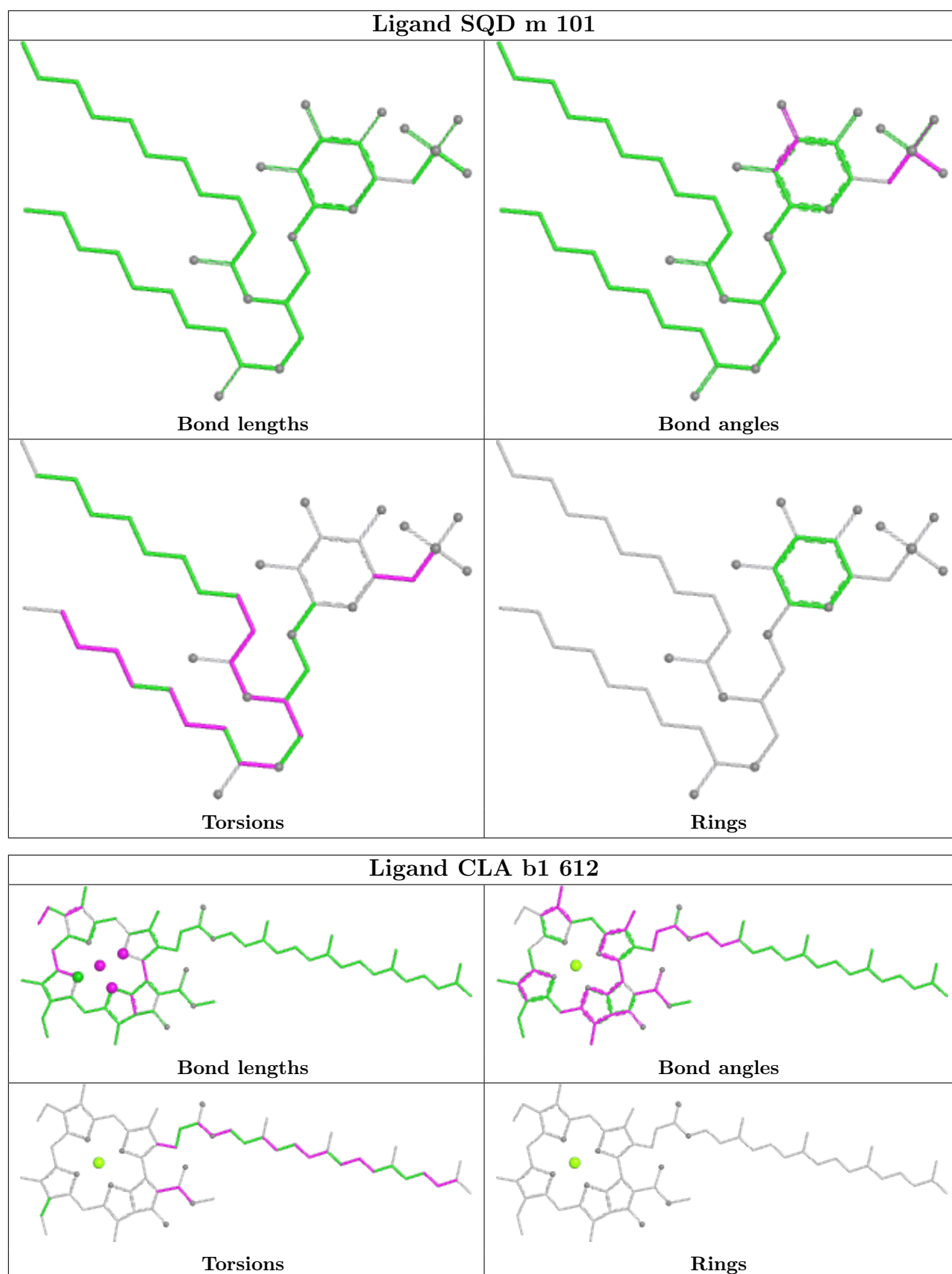


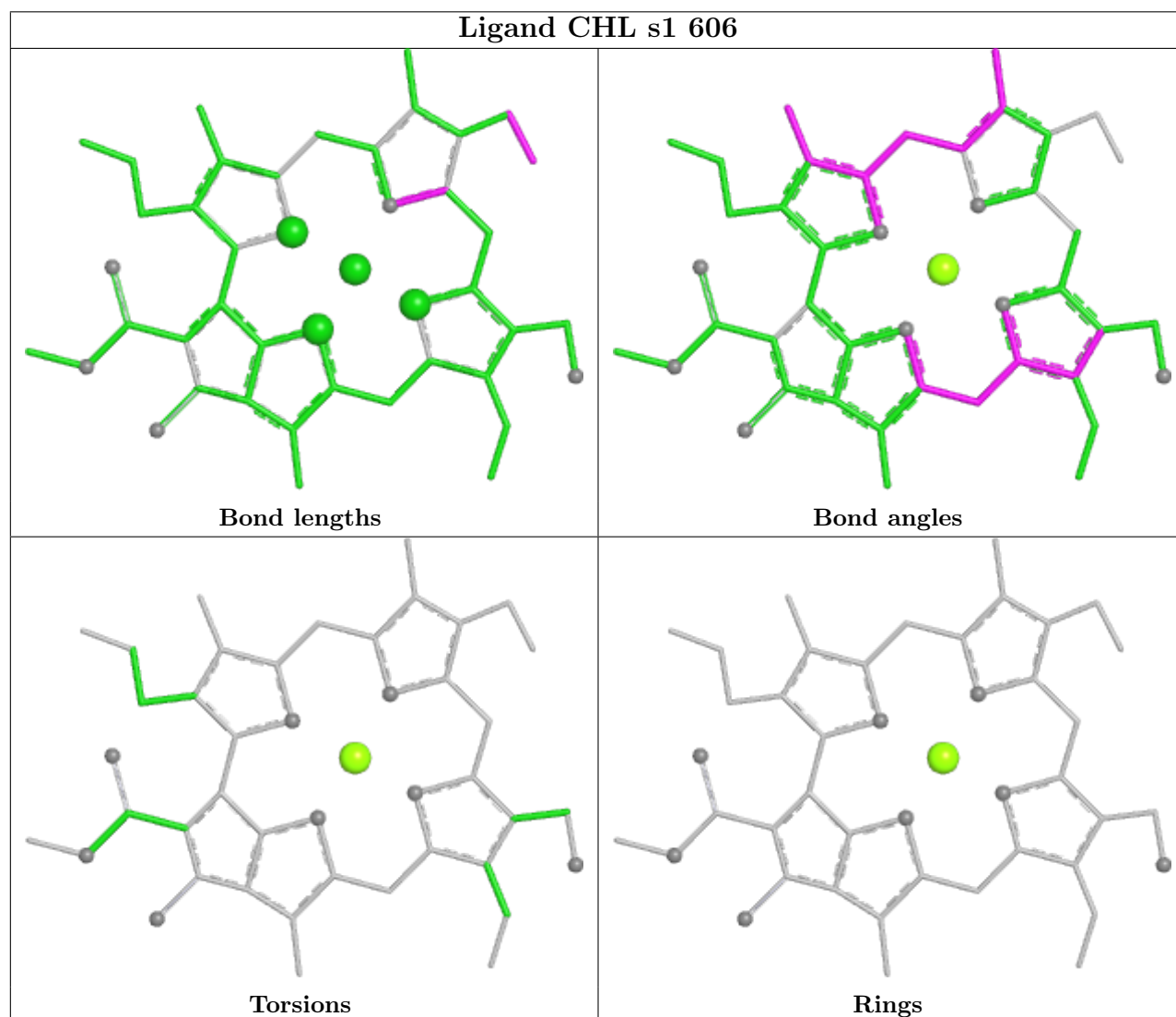
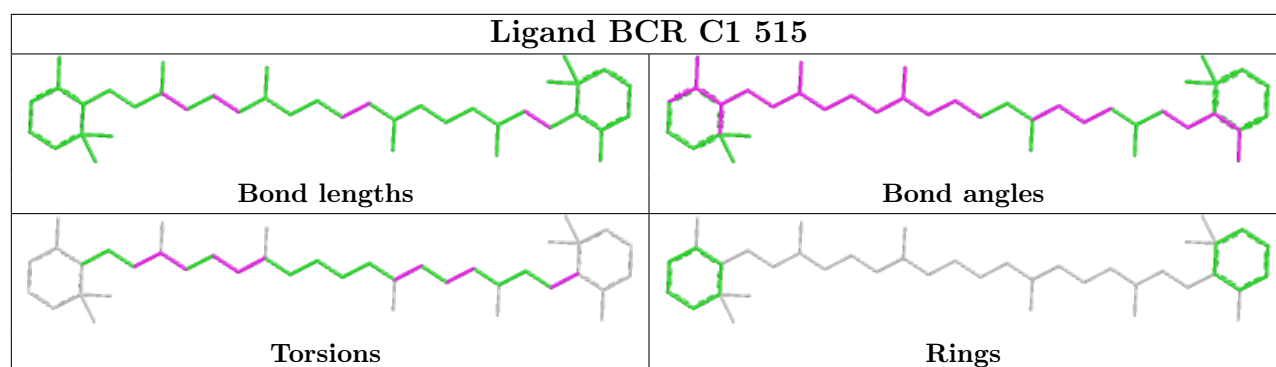
Ligand BCR C1 516	
	
Bond lengths	Bond angles
	
Torsions	Rings

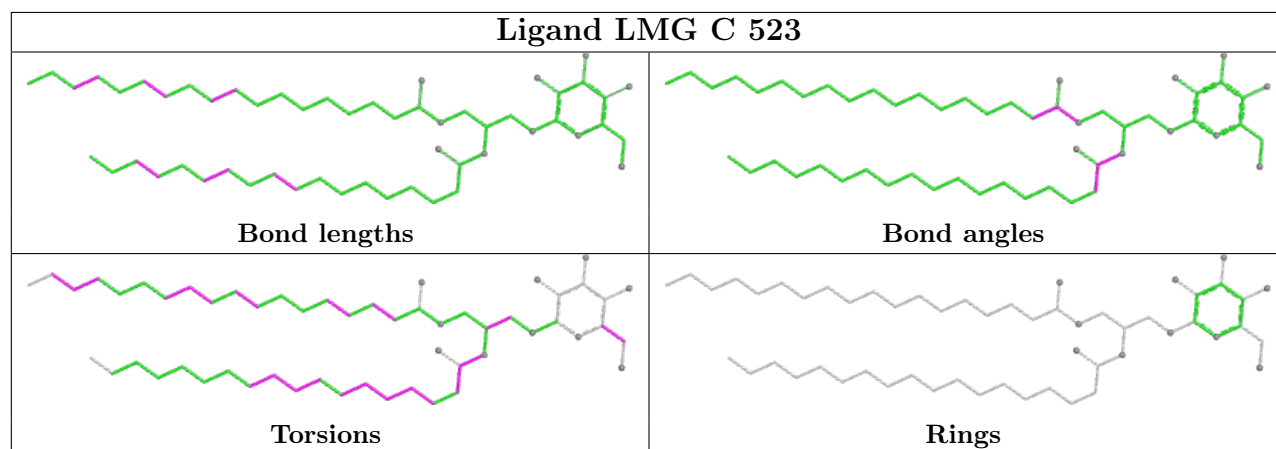
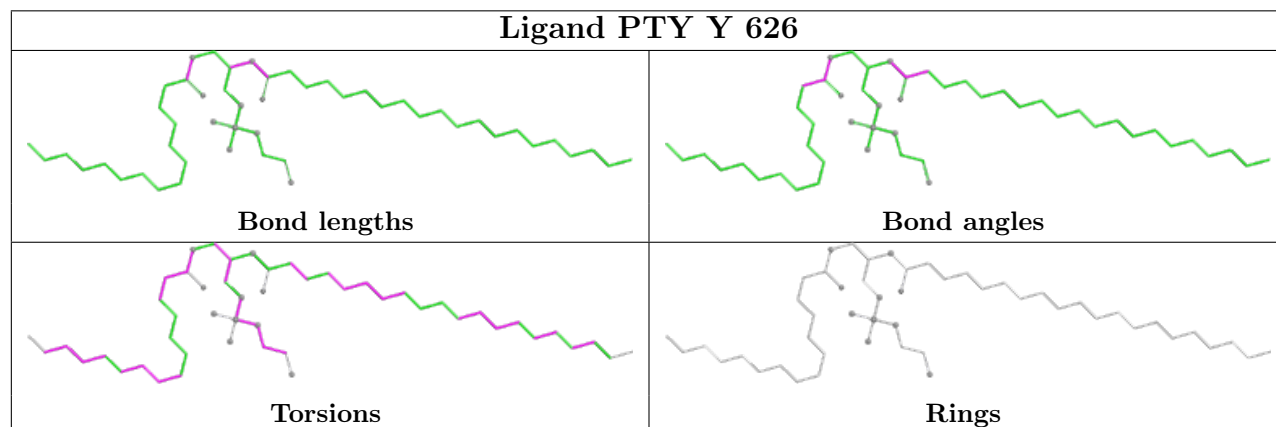
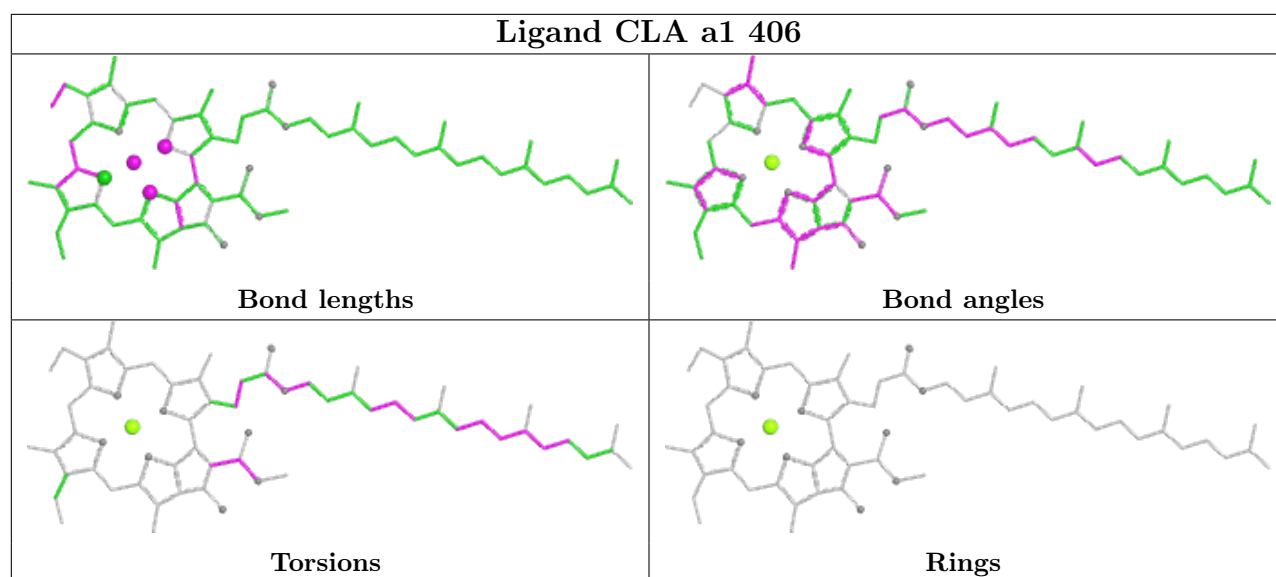
Ligand CLA A1 405	
	
Bond lengths	Bond angles
	
Torsions	Rings

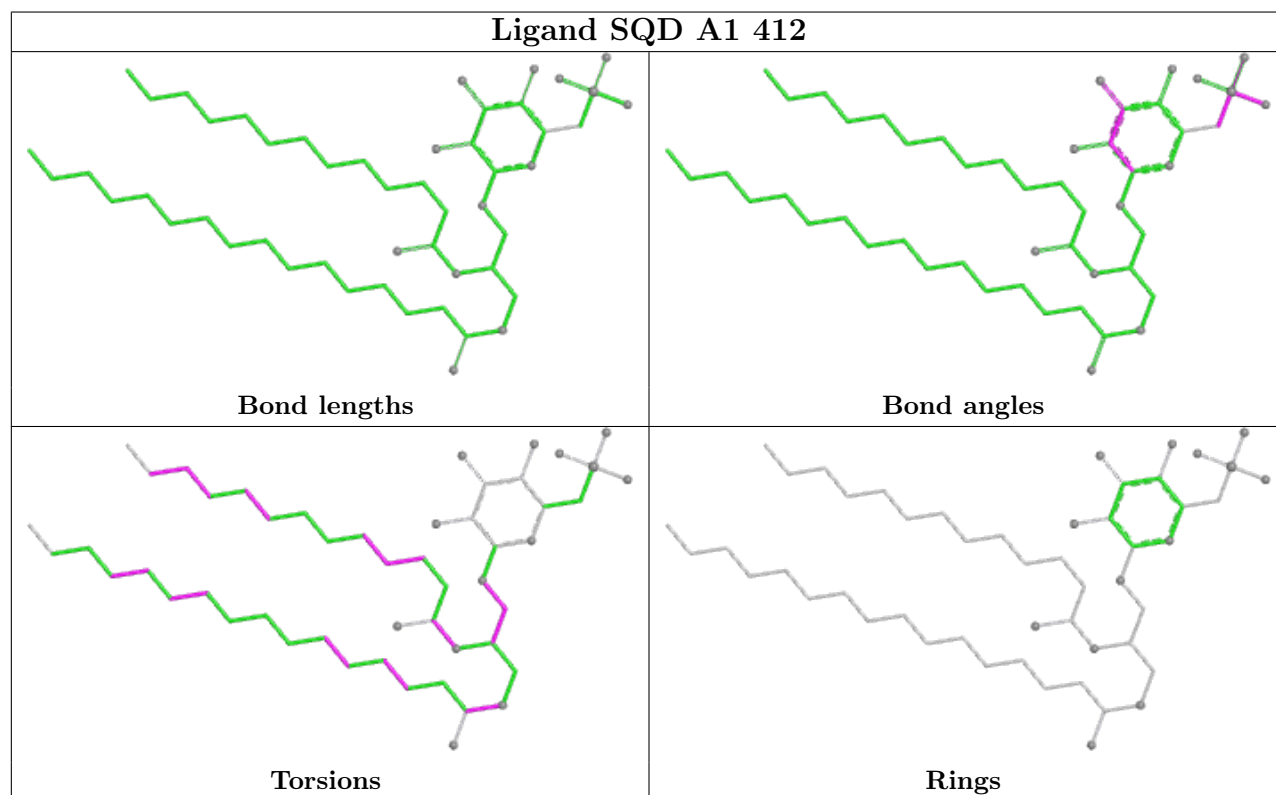
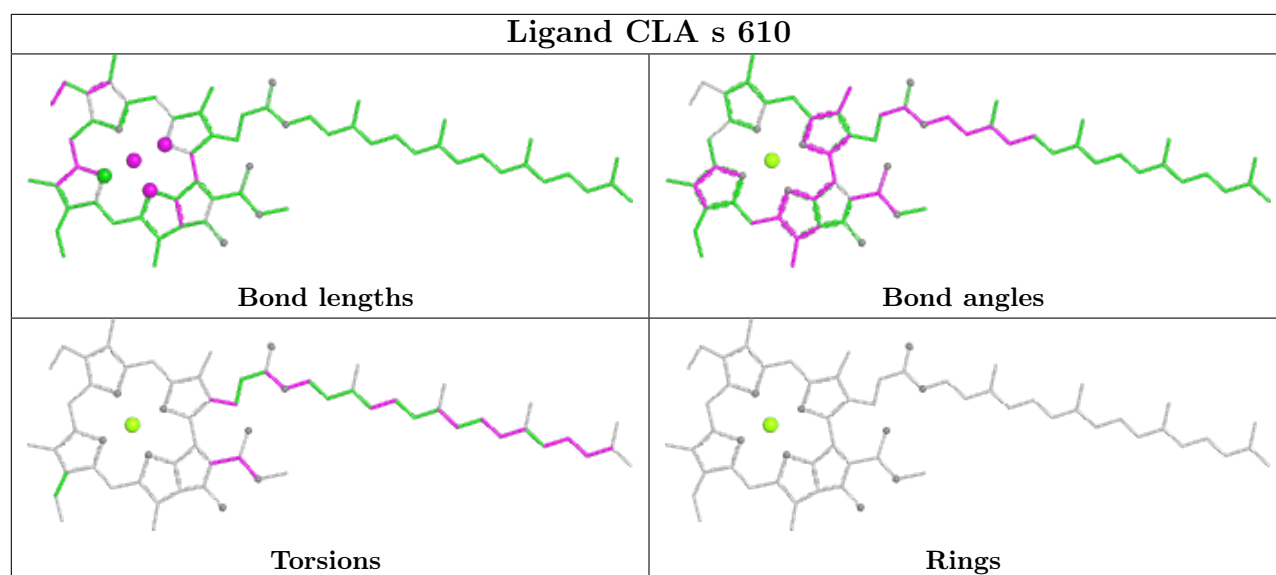
Ligand PHO A 408	
	
Bond lengths	Bond angles
	
Torsions	Rings

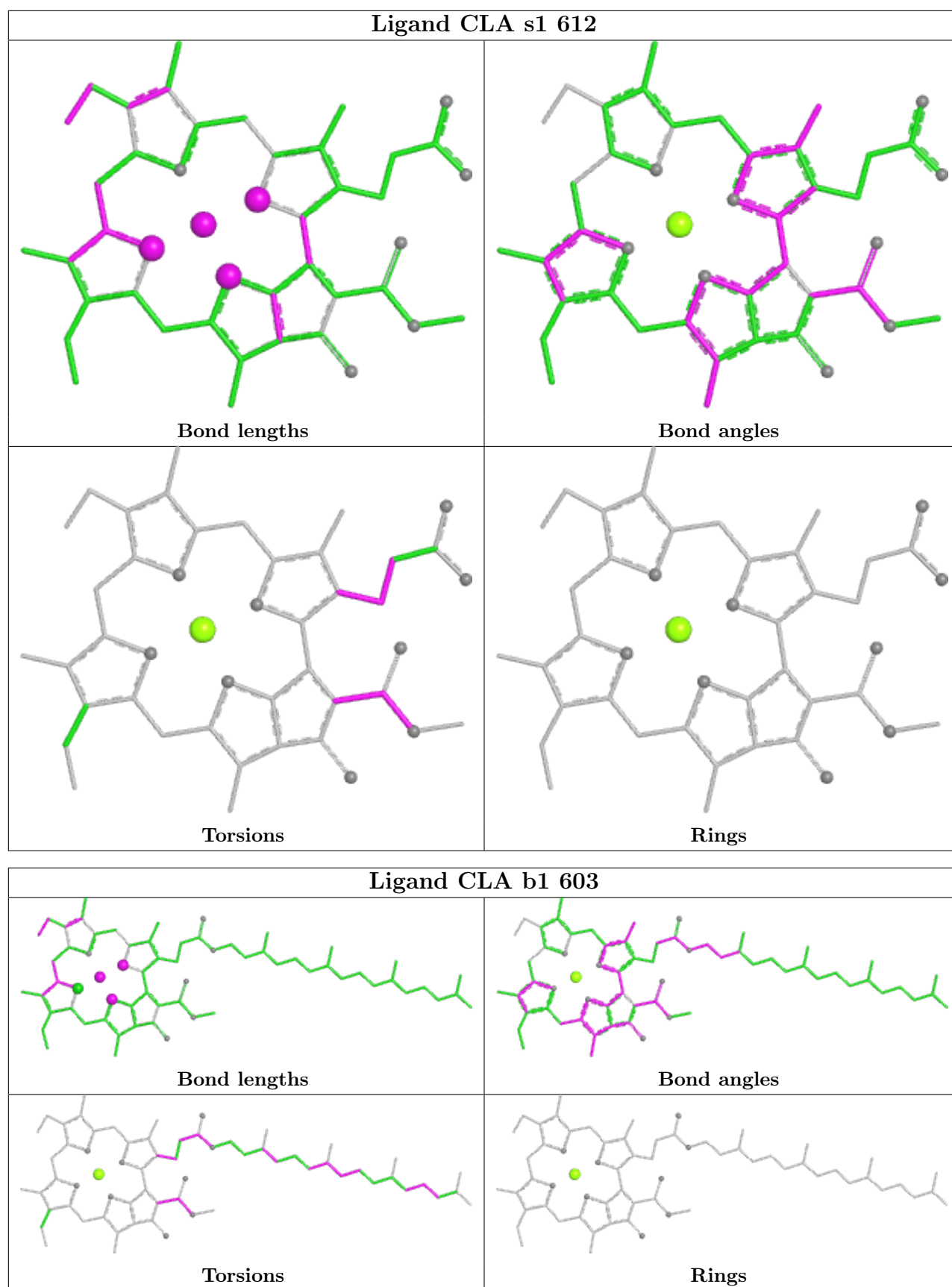






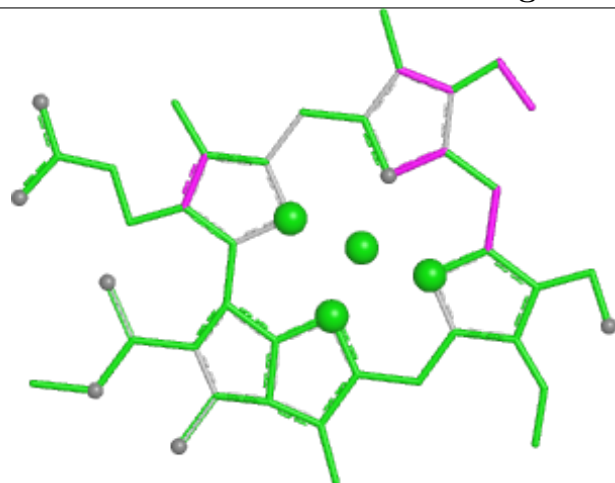




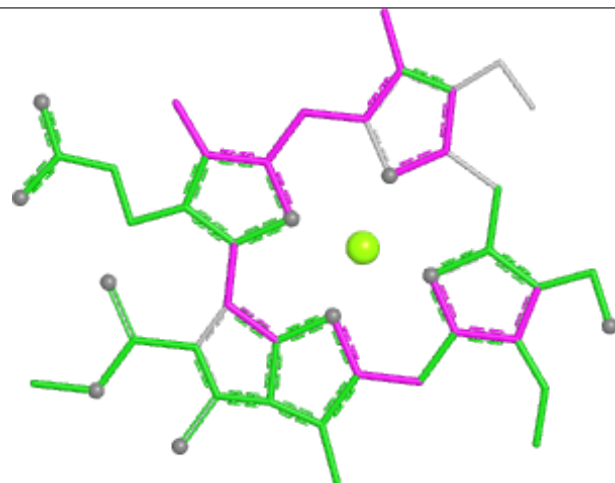




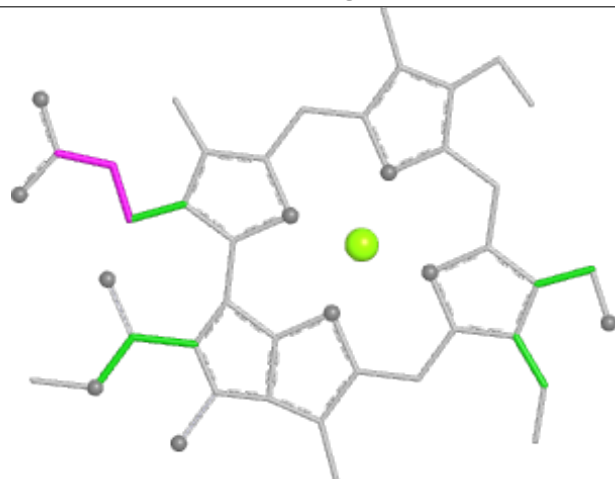
## Ligand CHL S 601



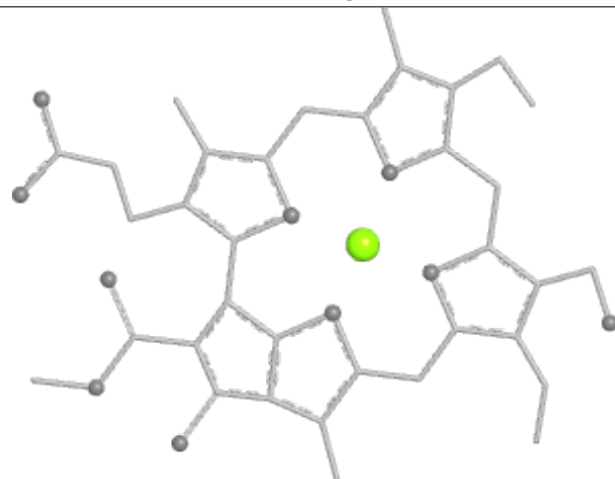
Bond lengths



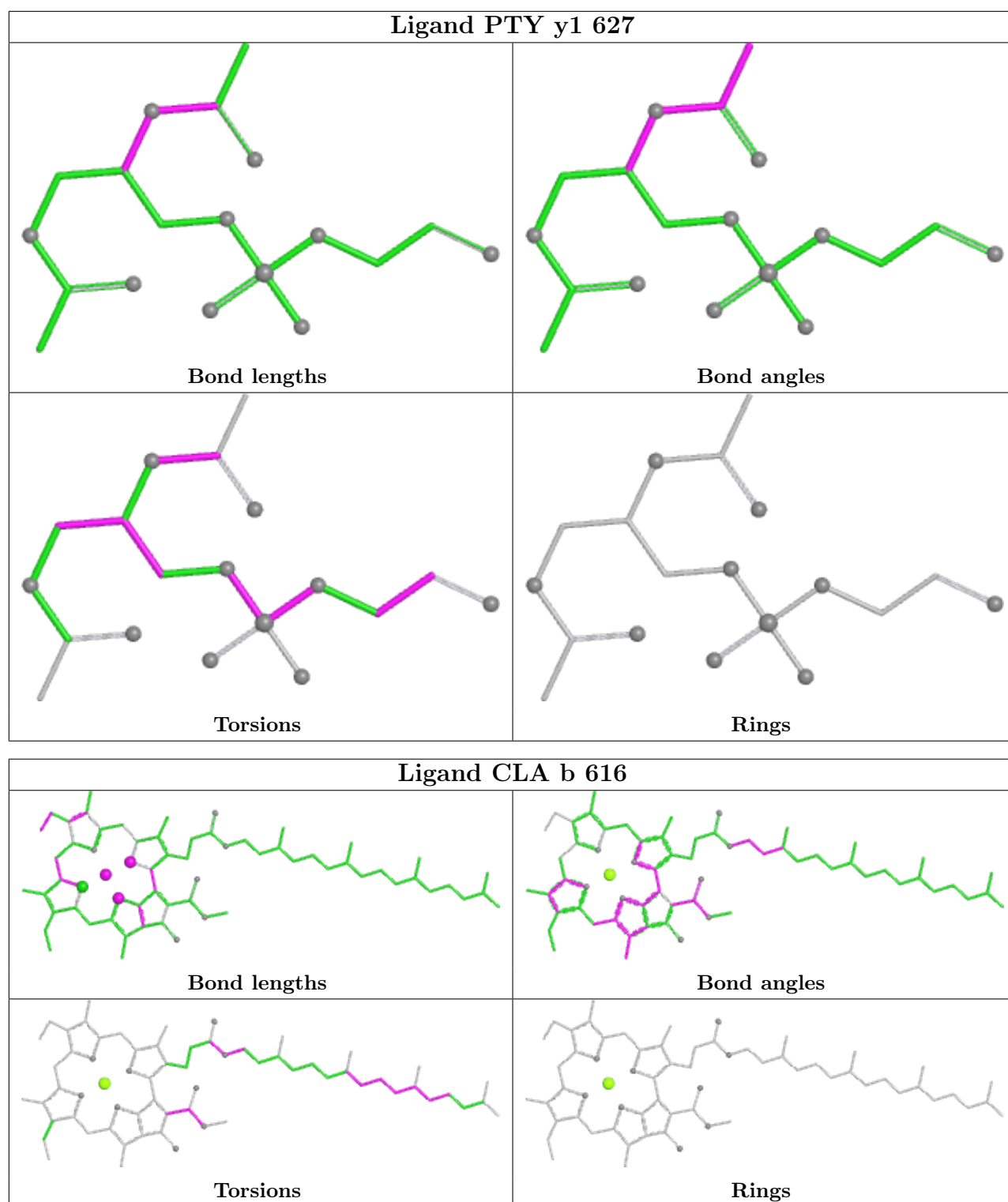
Bond angles

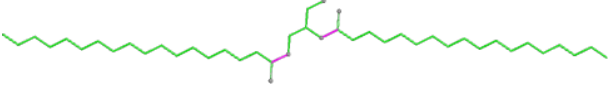
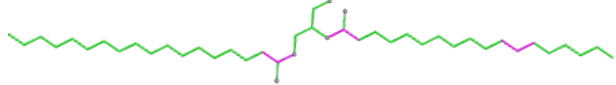
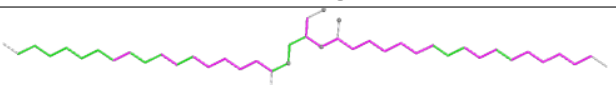
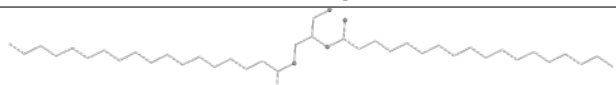
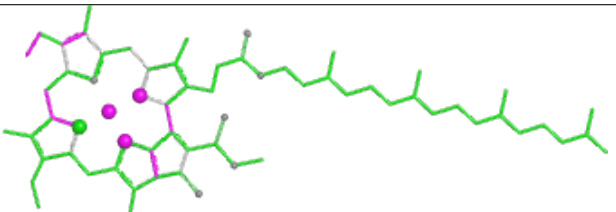
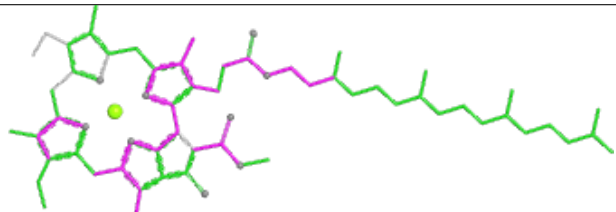
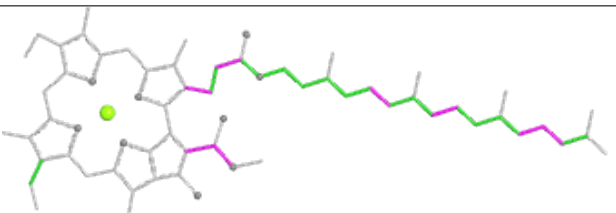
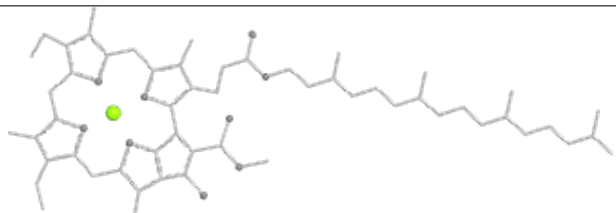
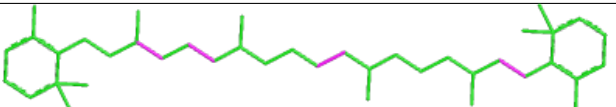
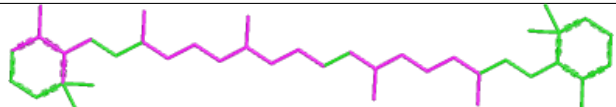
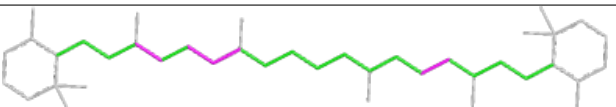
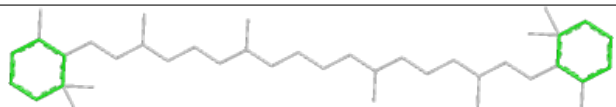


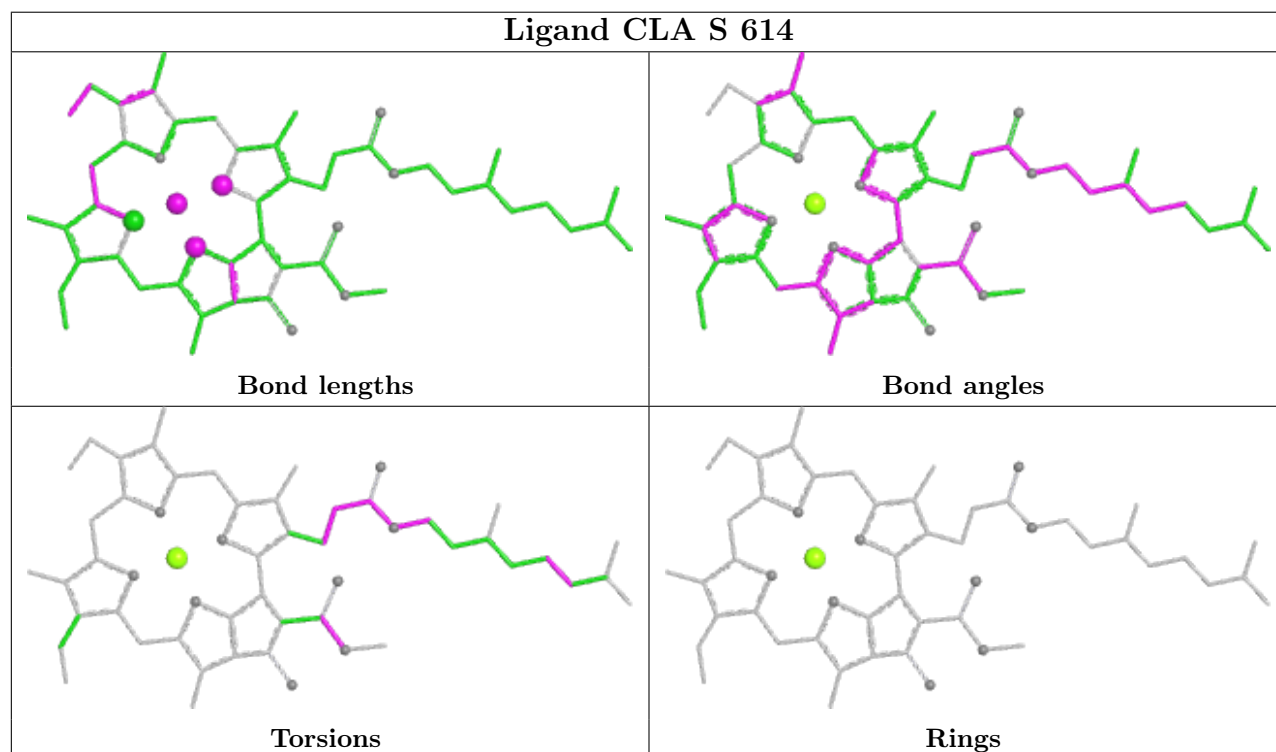
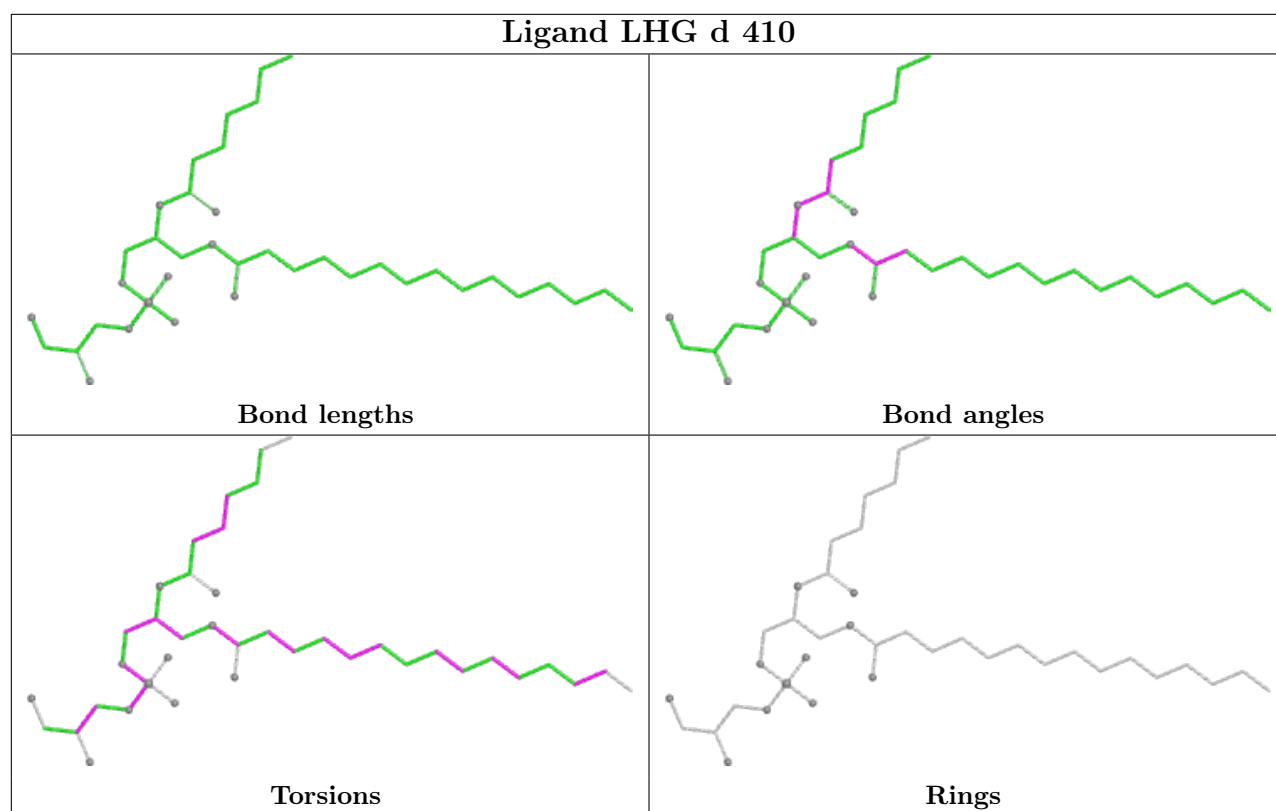
Torsions

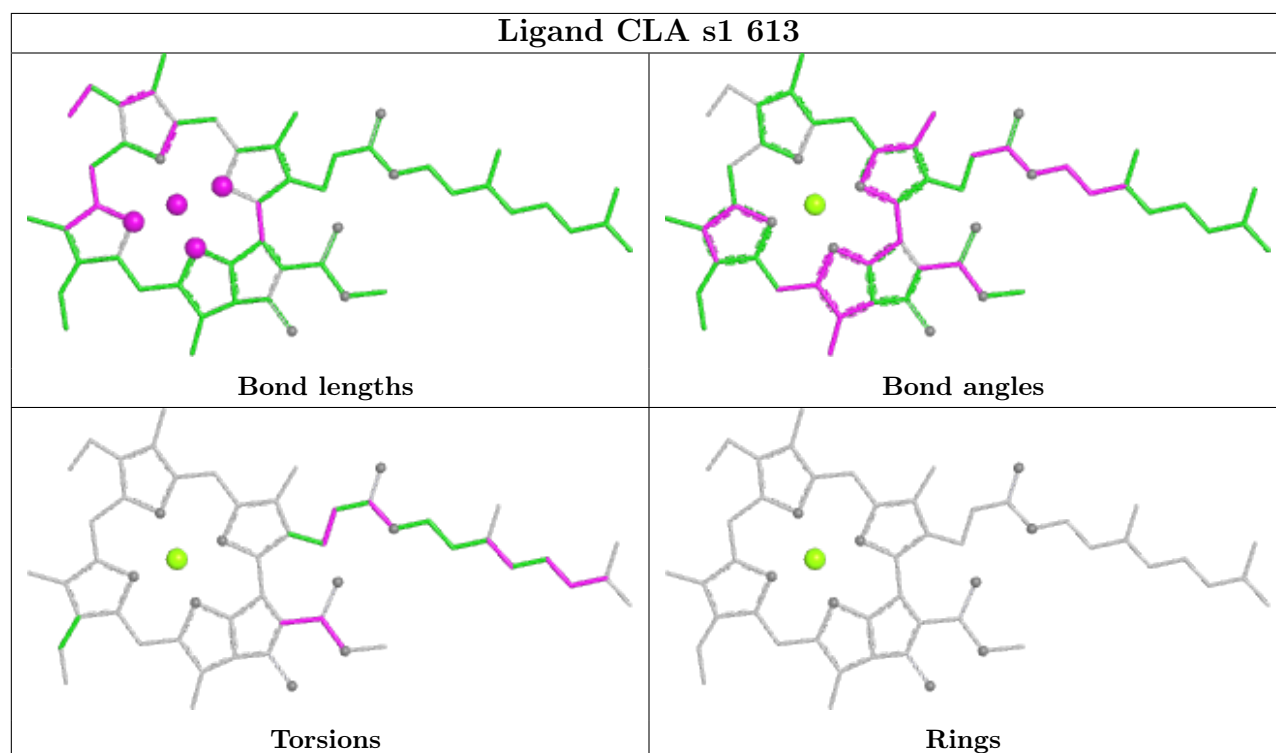
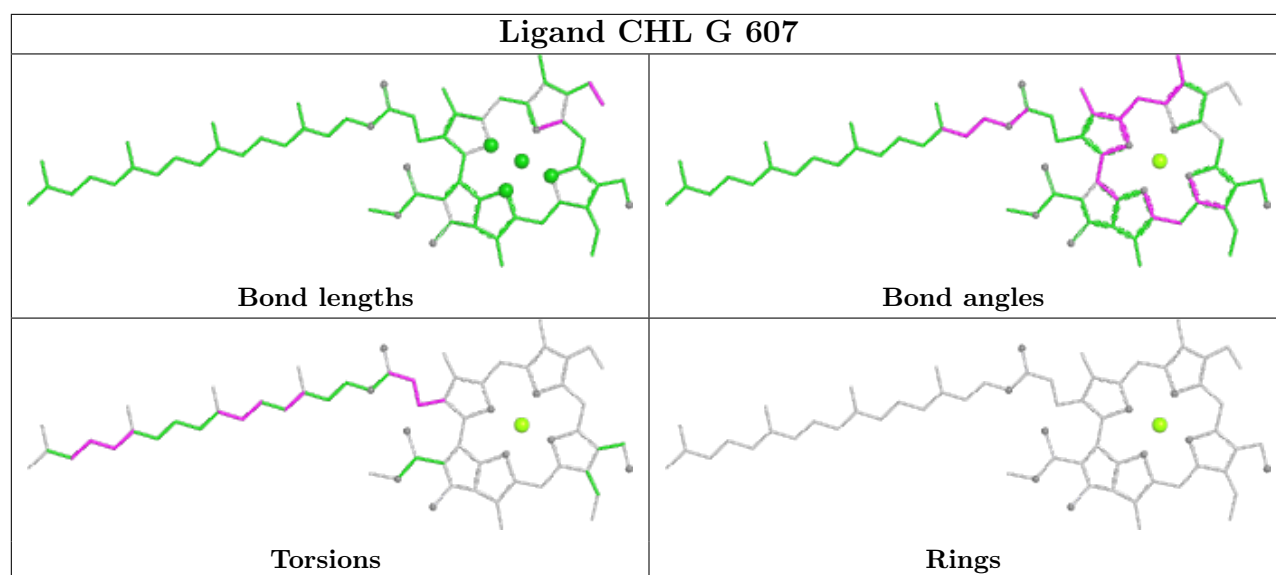


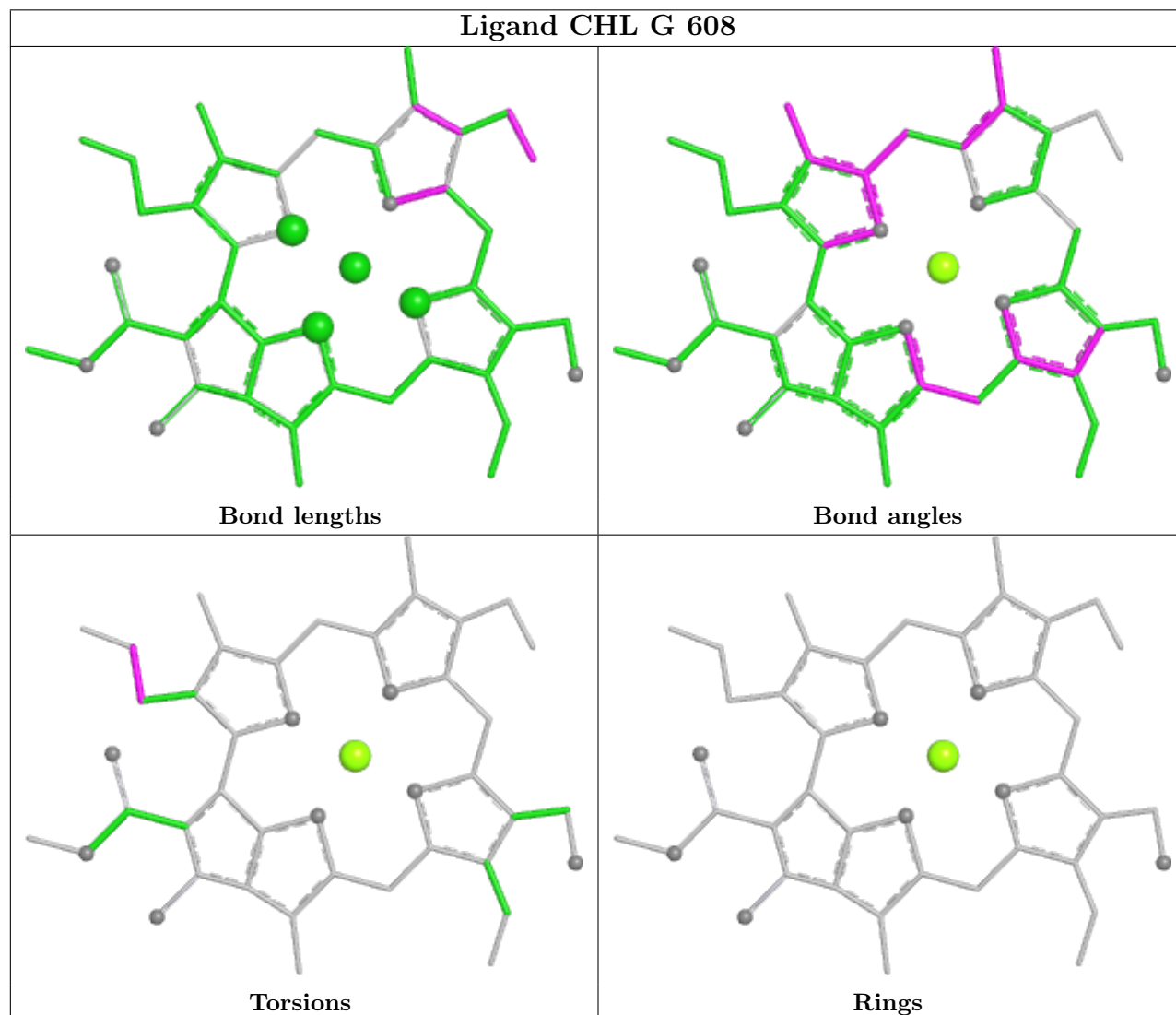
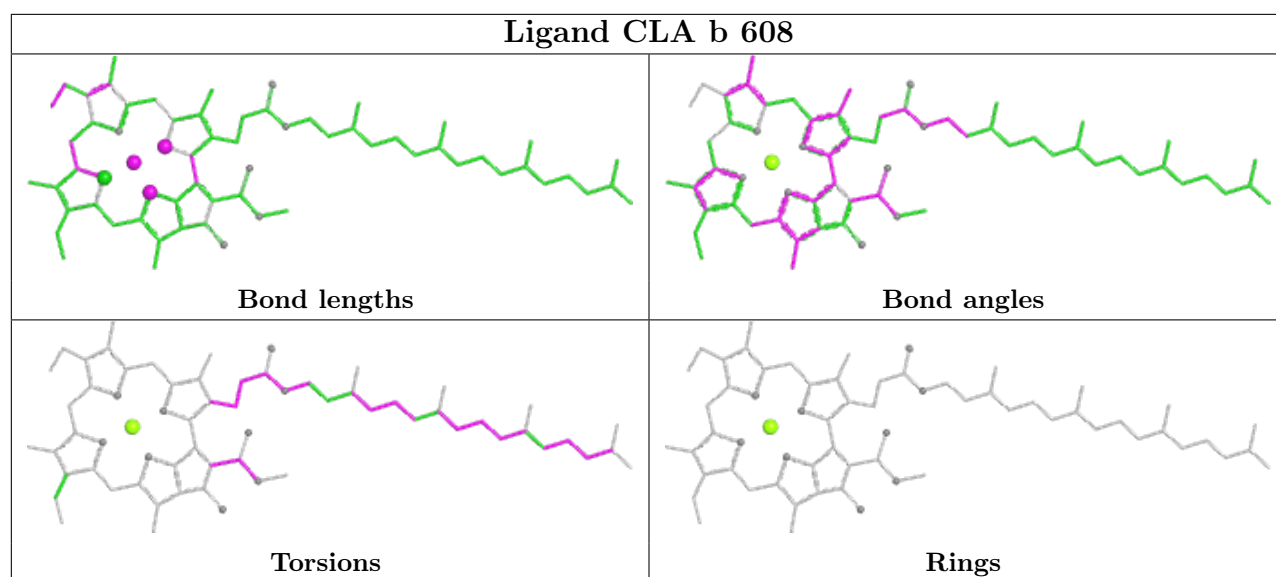
Rings

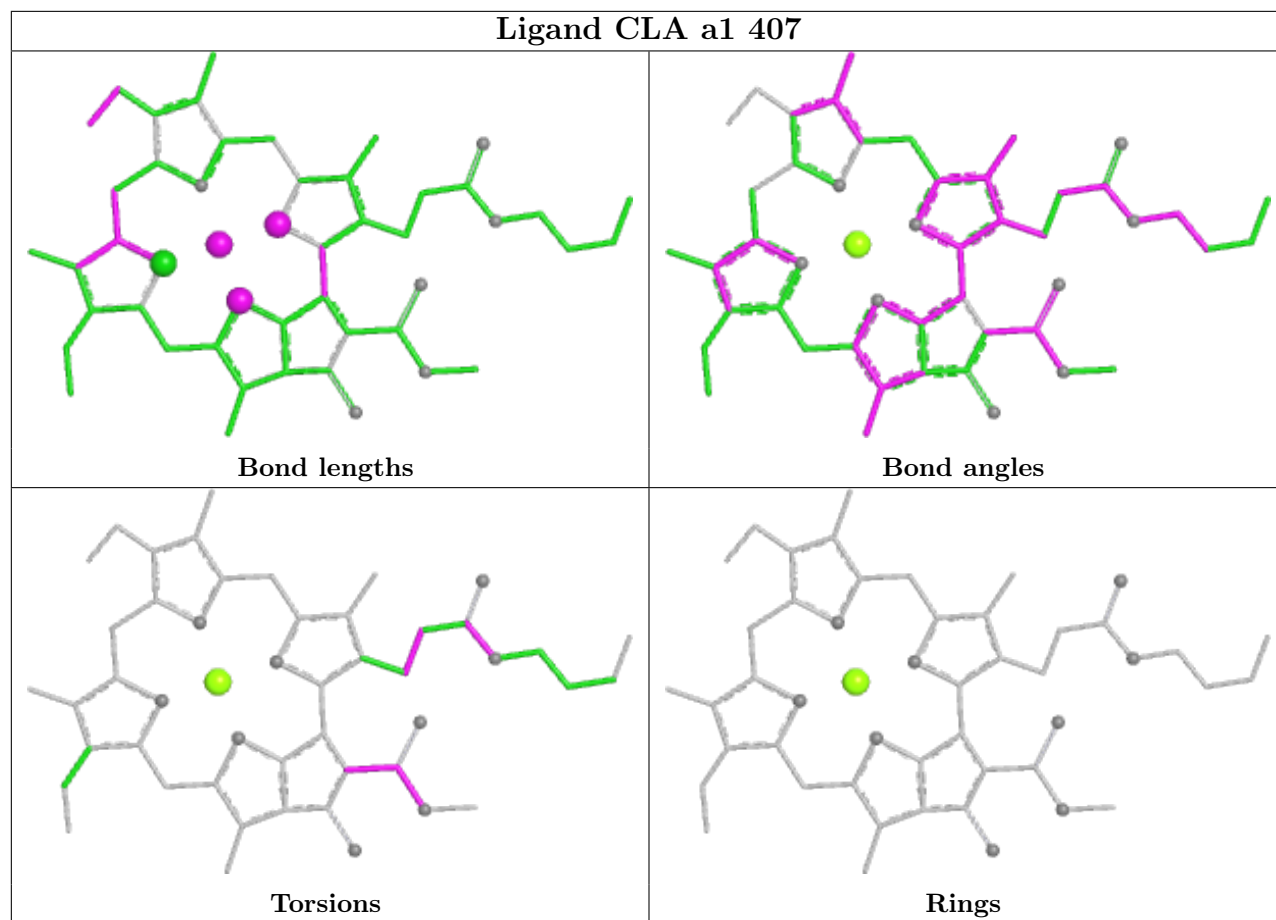


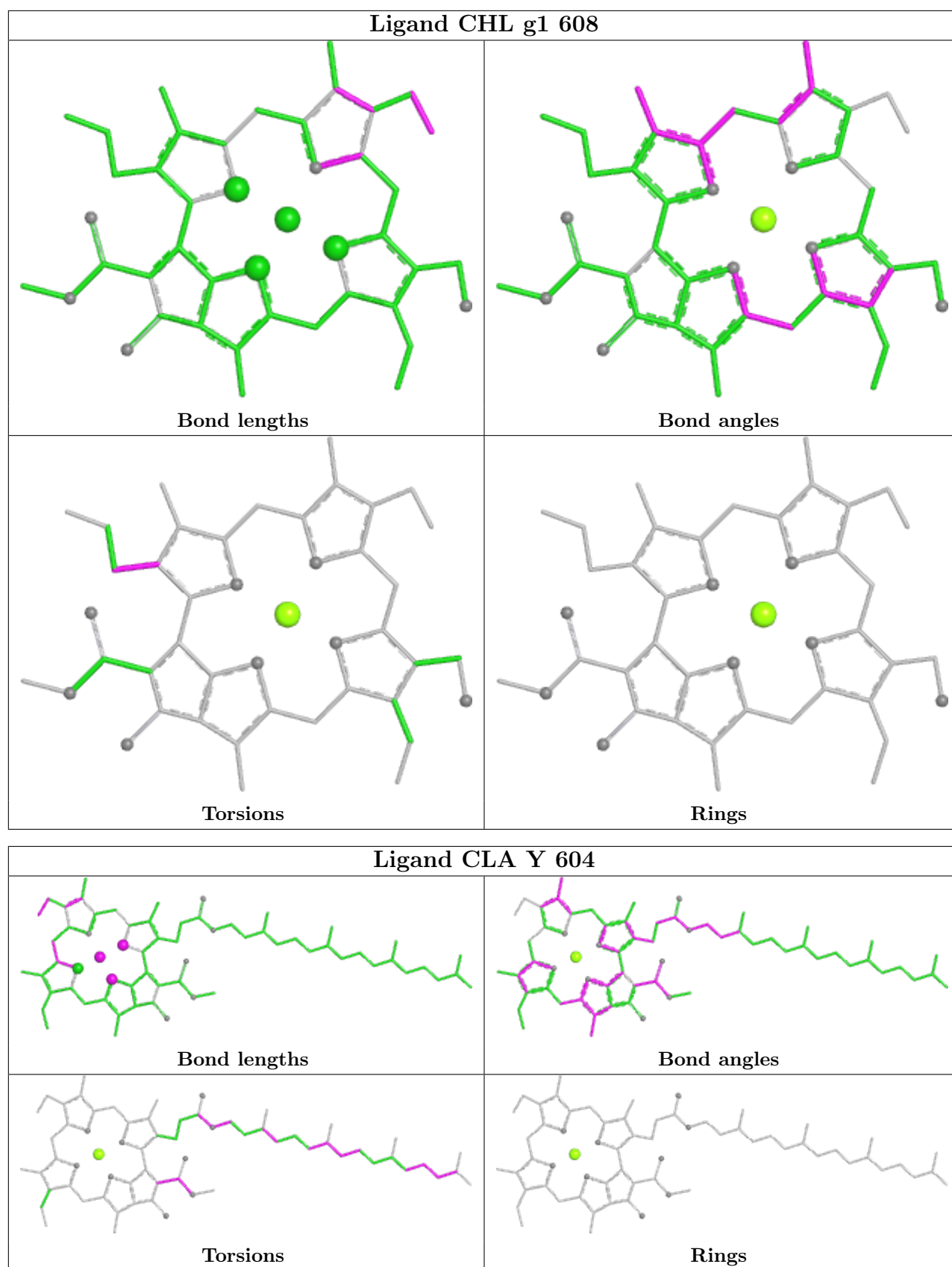
Ligand DGA b 625	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand CLA b1 607	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>
Ligand BCR B1 619	
 <p>Bond lengths</p>	 <p>Bond angles</p>
 <p>Torsions</p>	 <p>Rings</p>





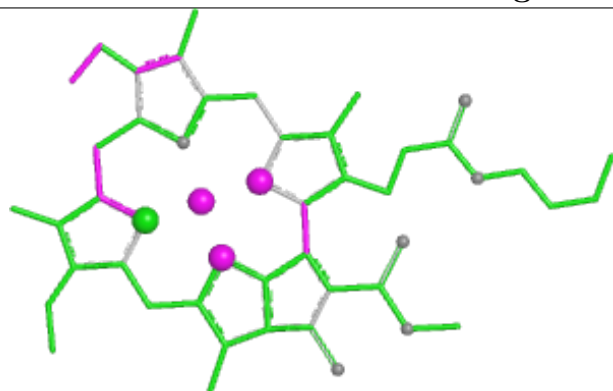




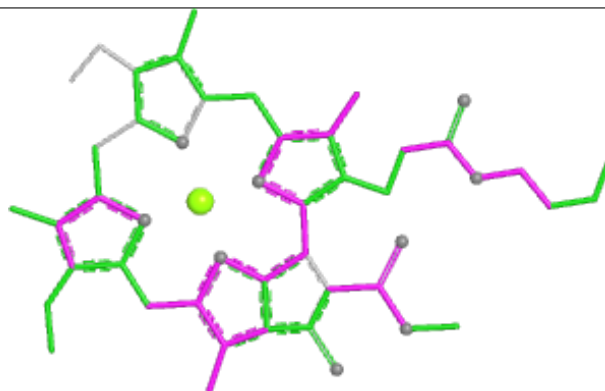




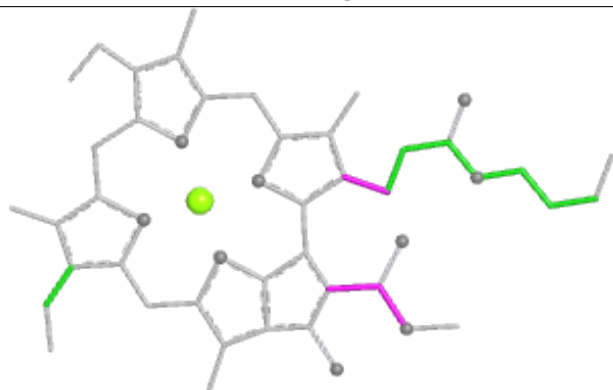
## Ligand CLA N 614



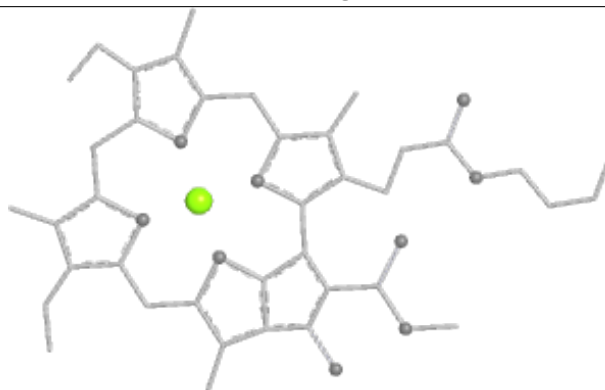
Bond lengths



Bond angles

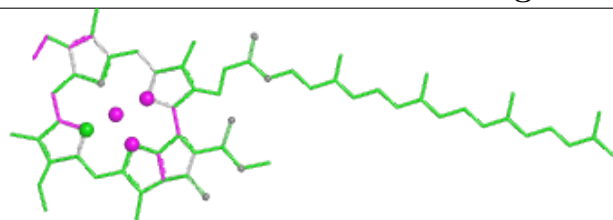


Torsions

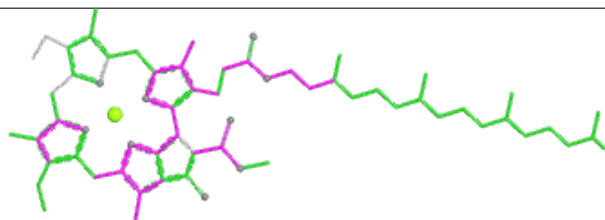


Rings

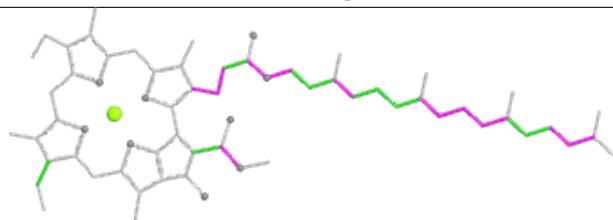
## Ligand CLA C 501



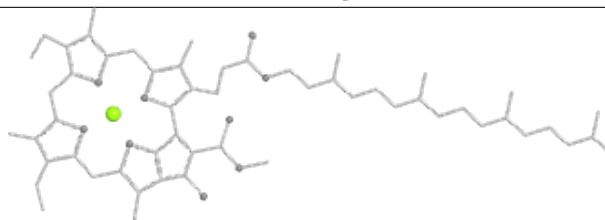
Bond lengths



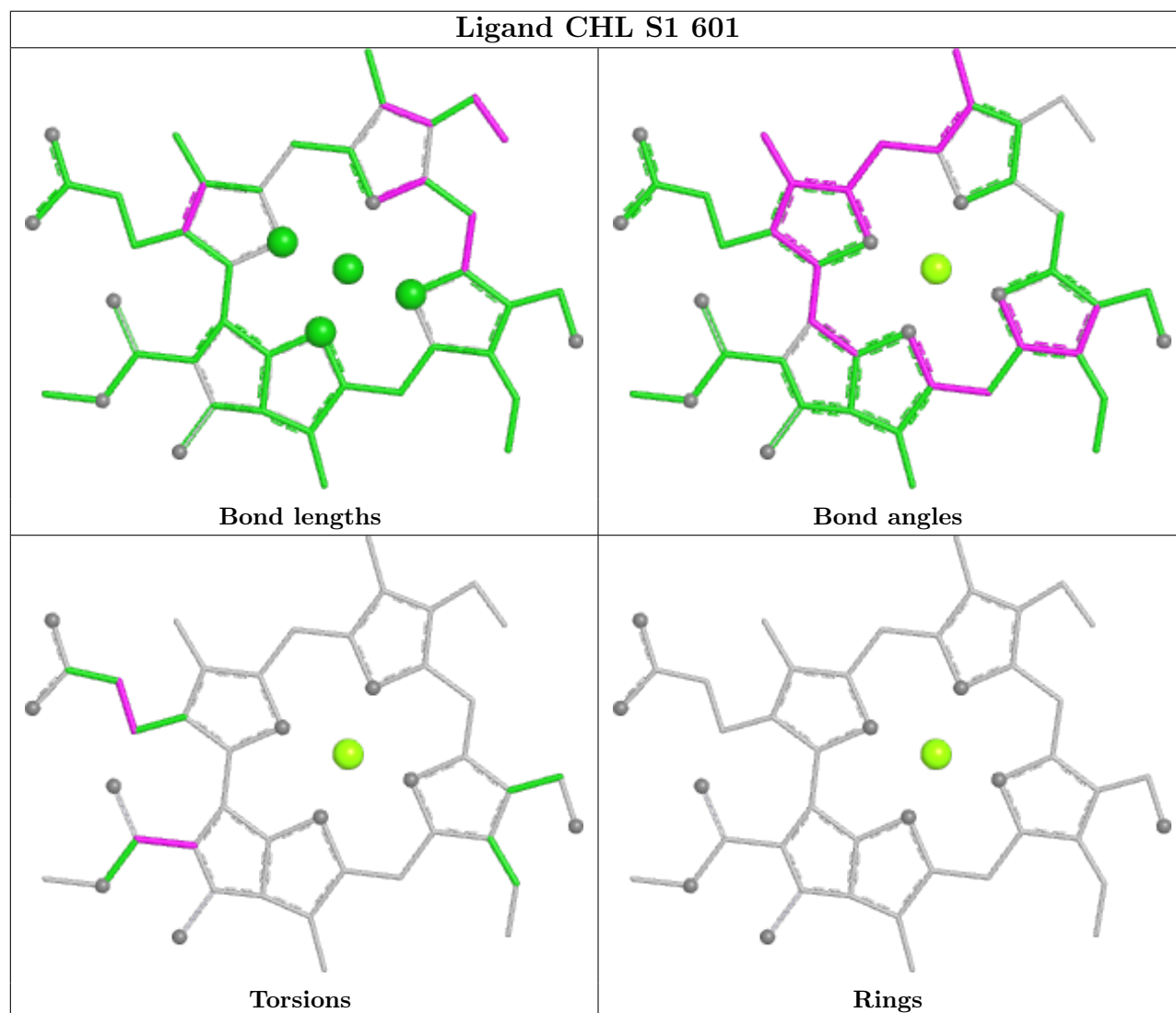
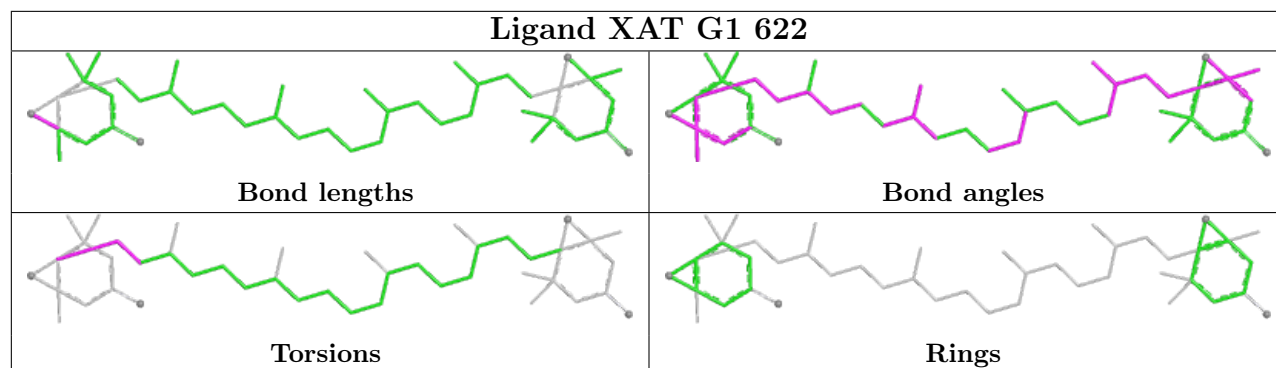
Bond angles

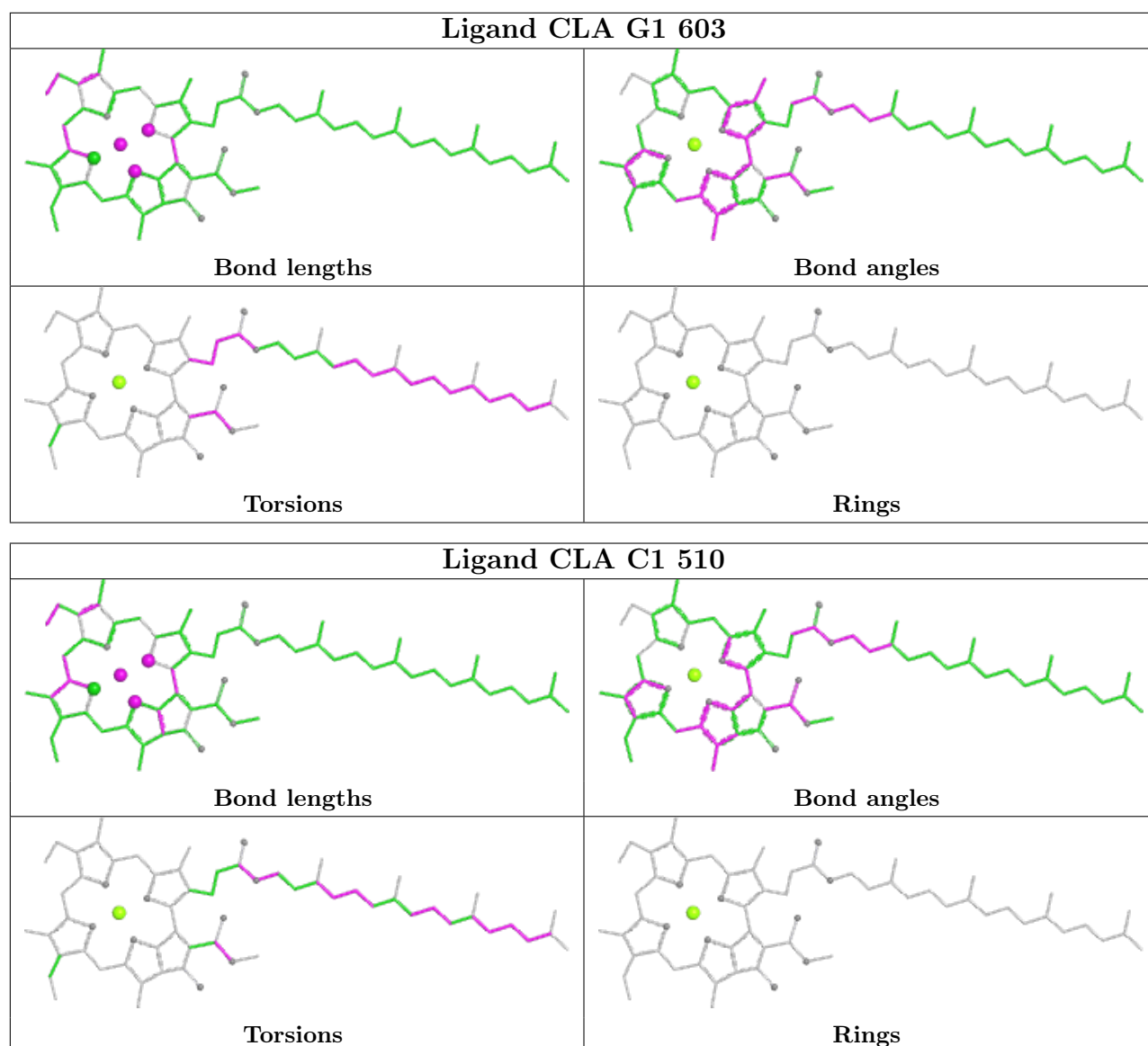


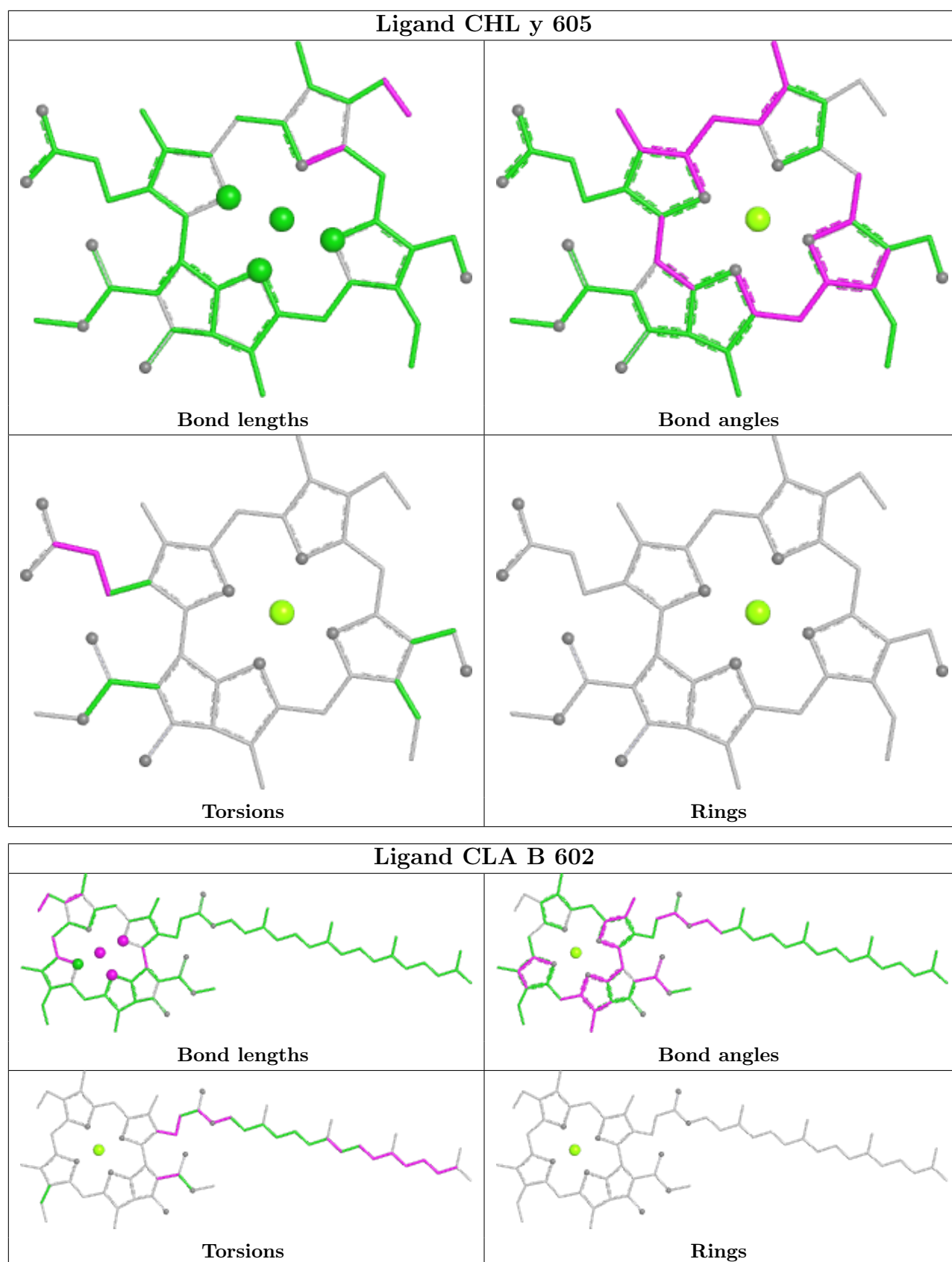
Torsions

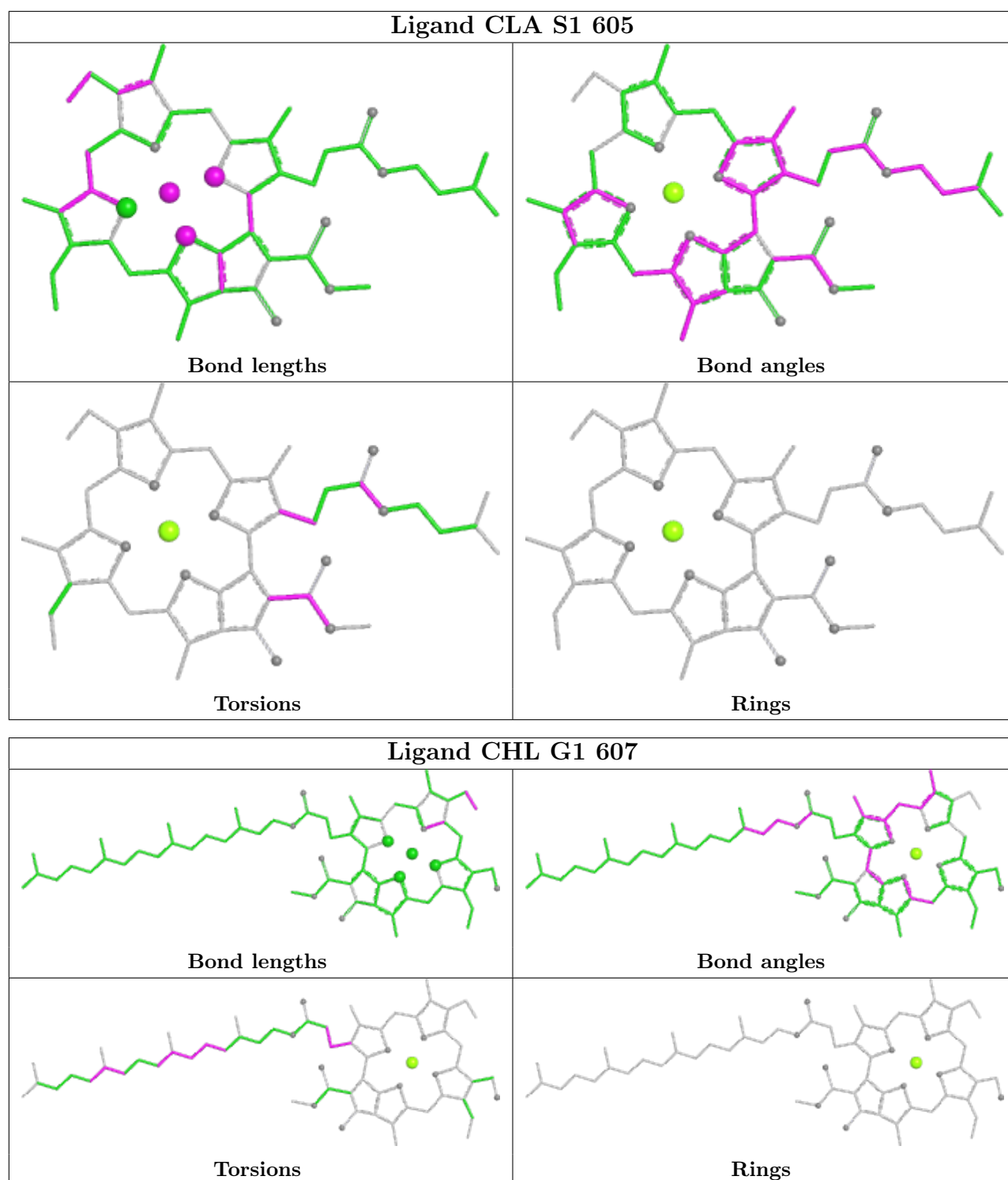


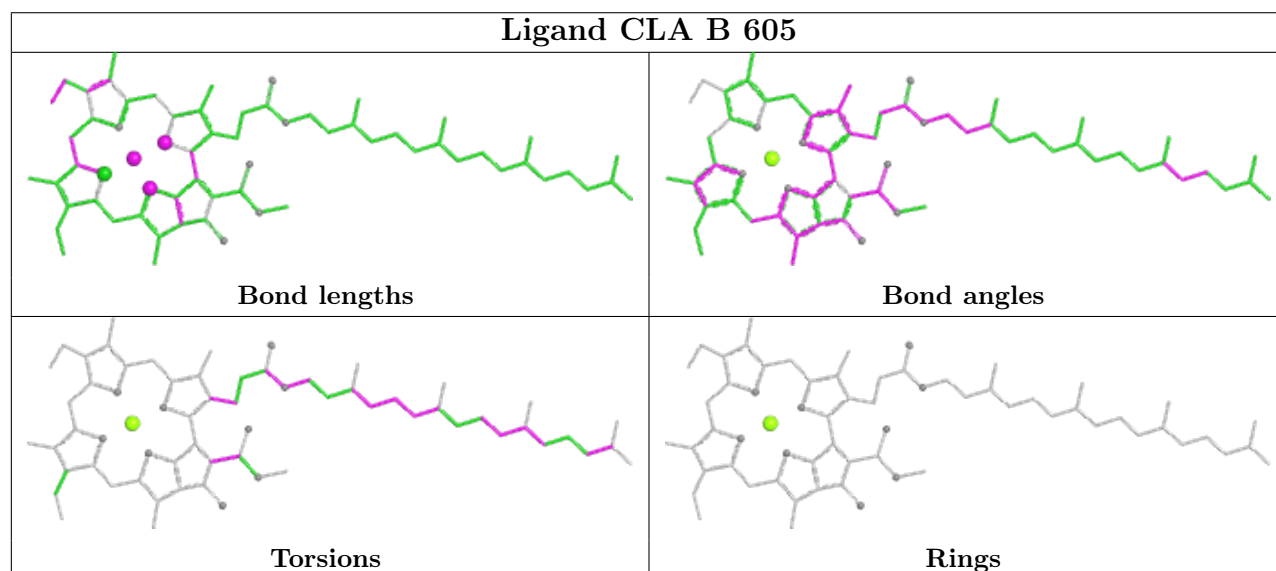
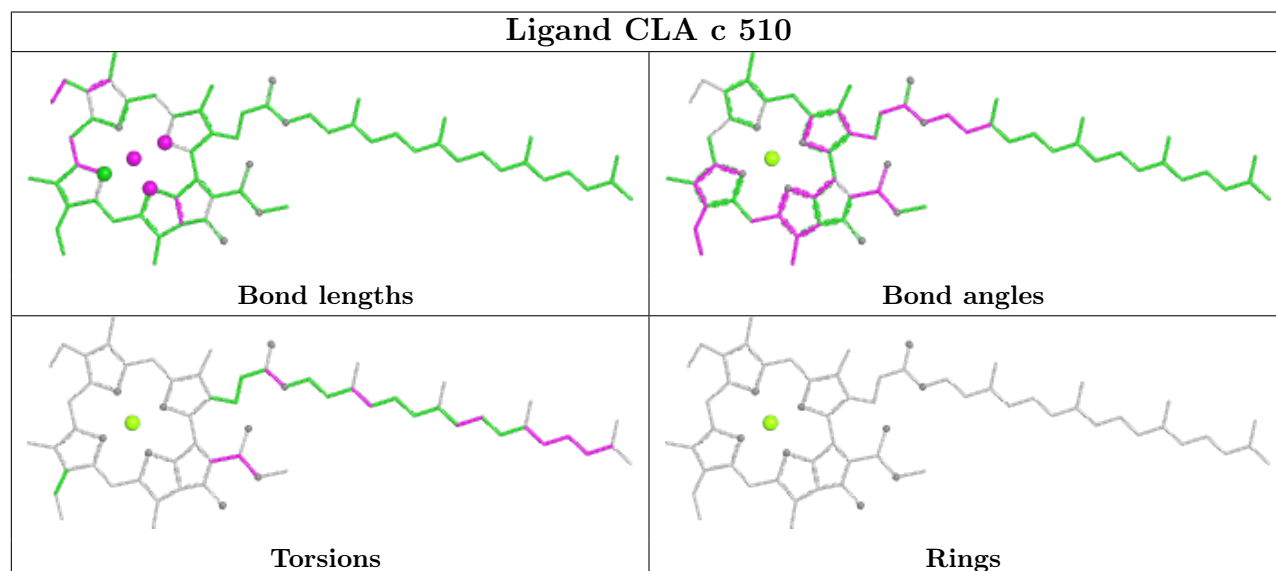
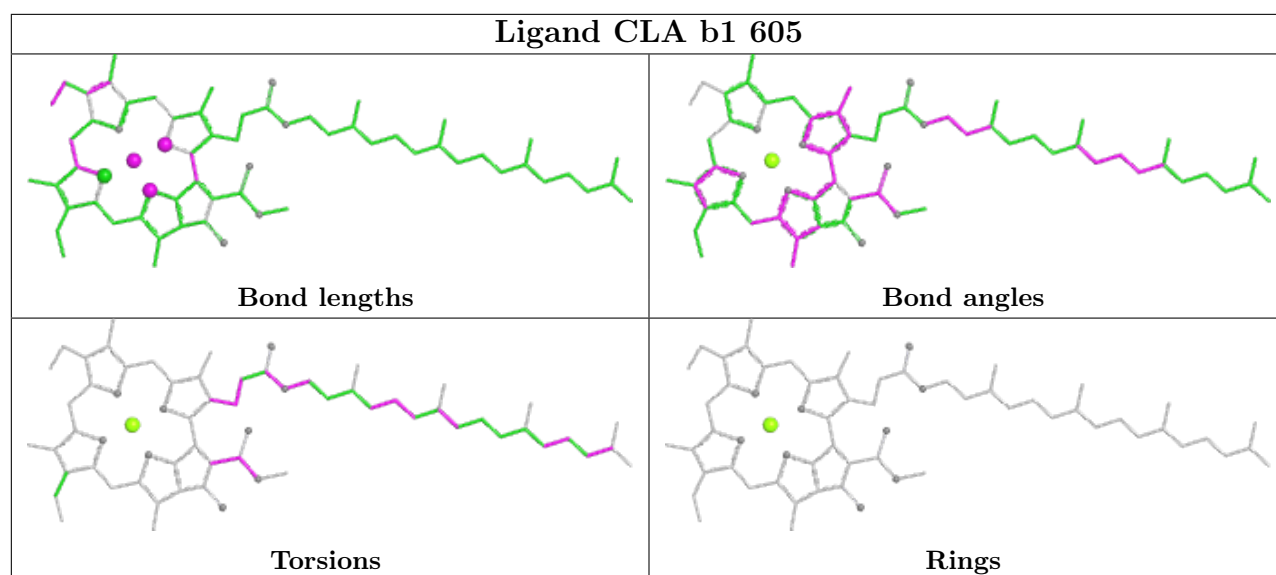
Rings

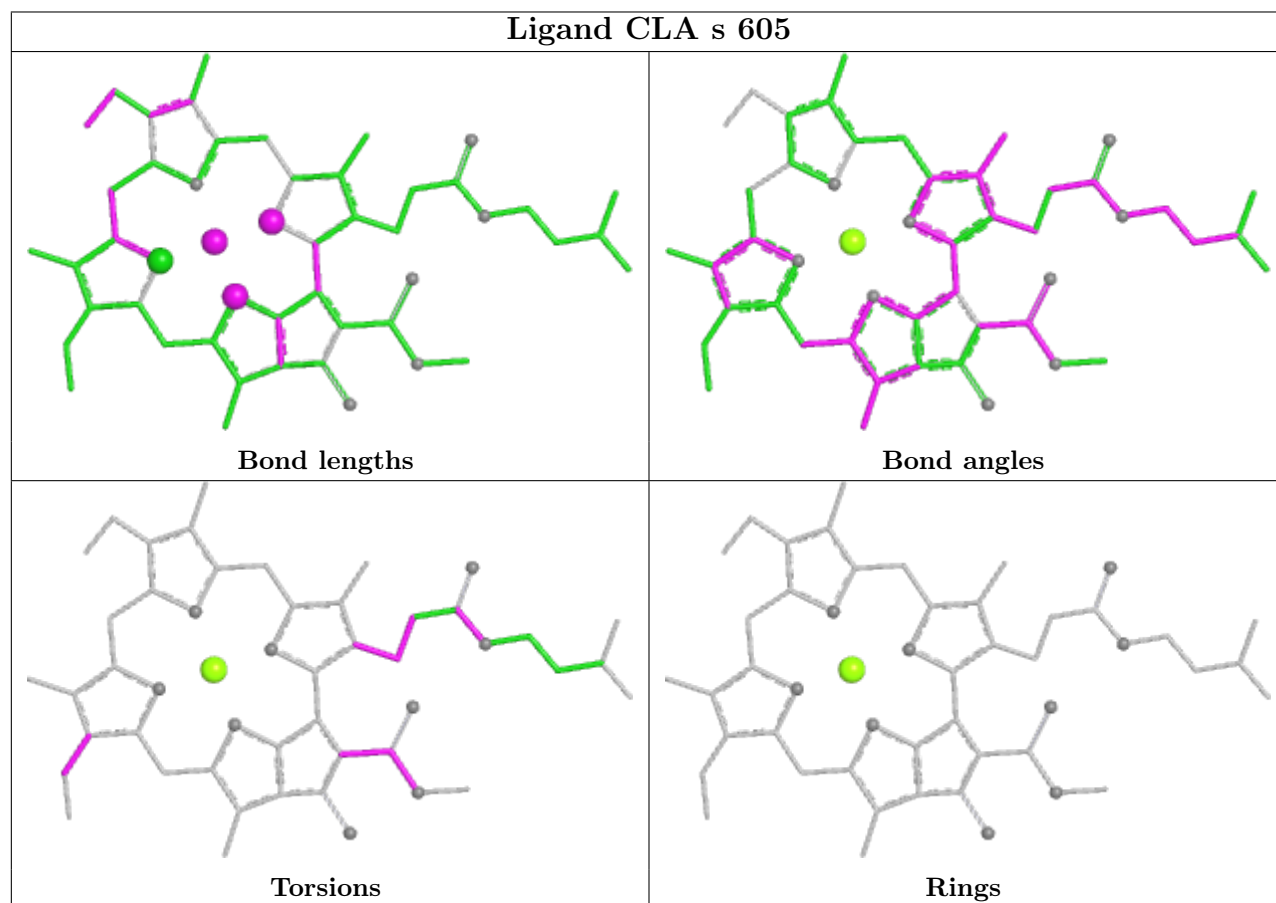
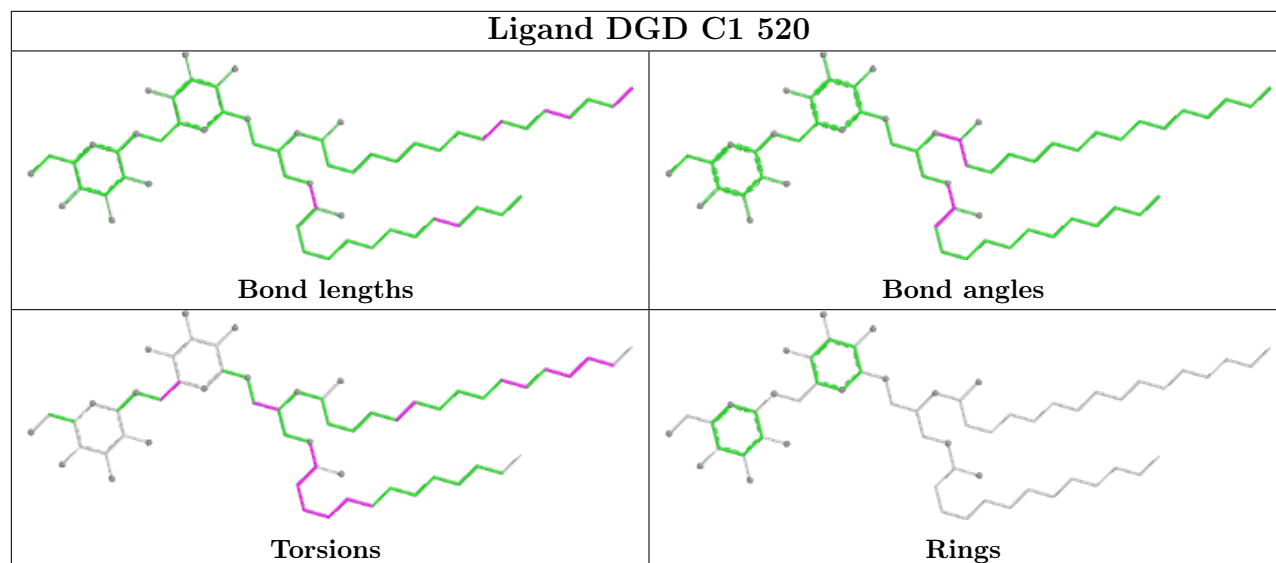


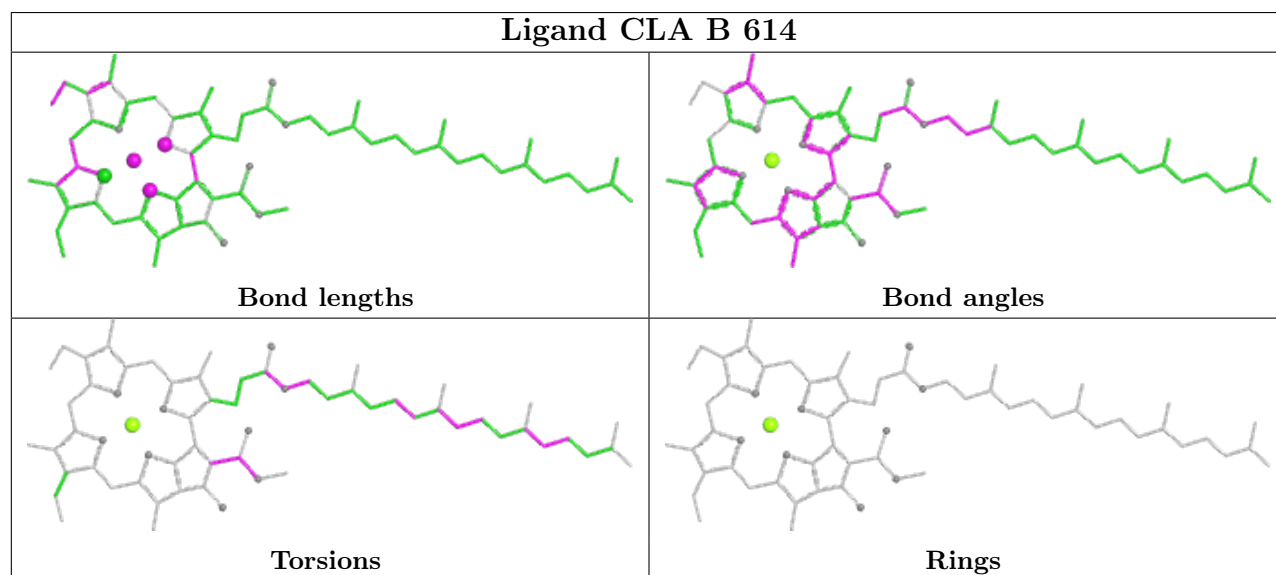
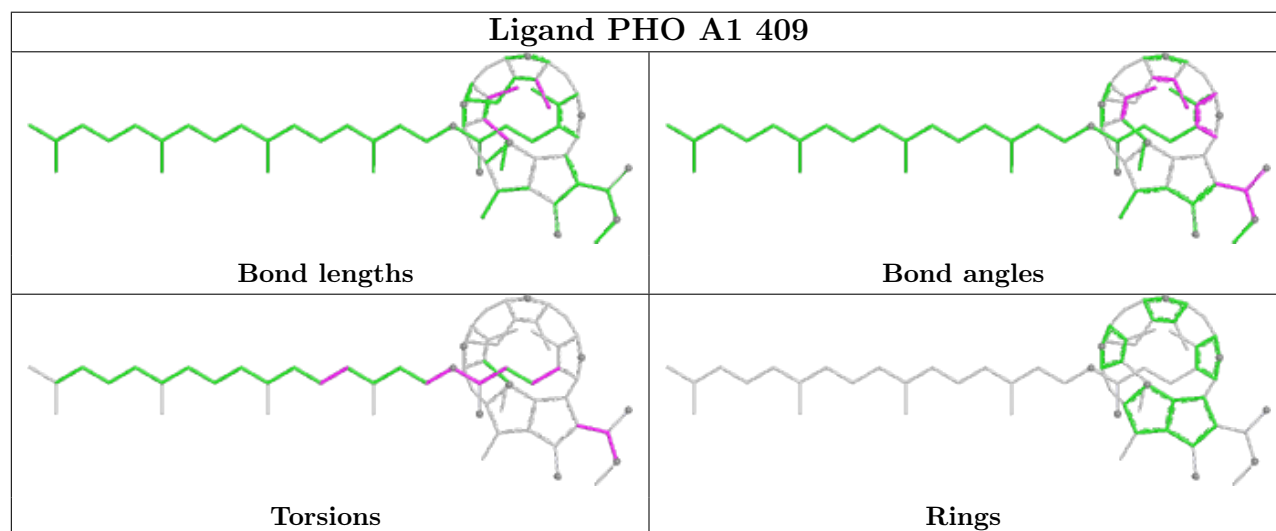
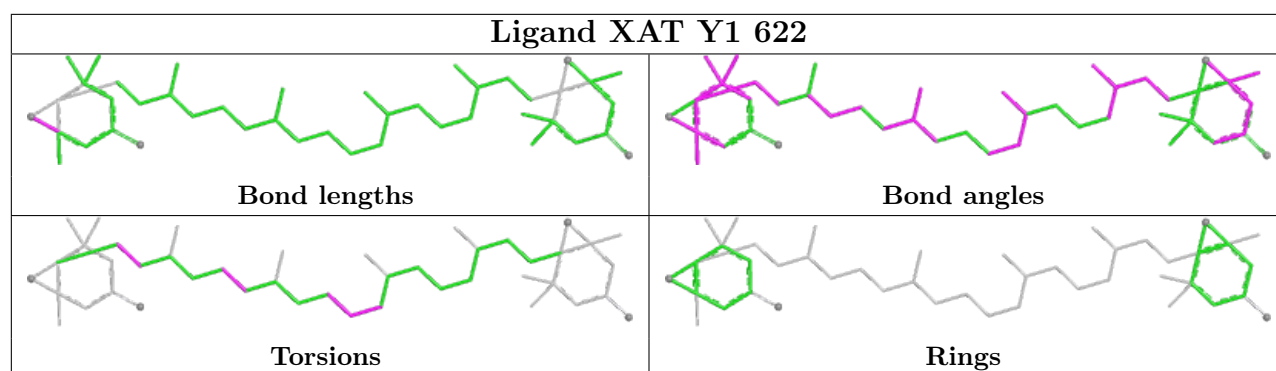




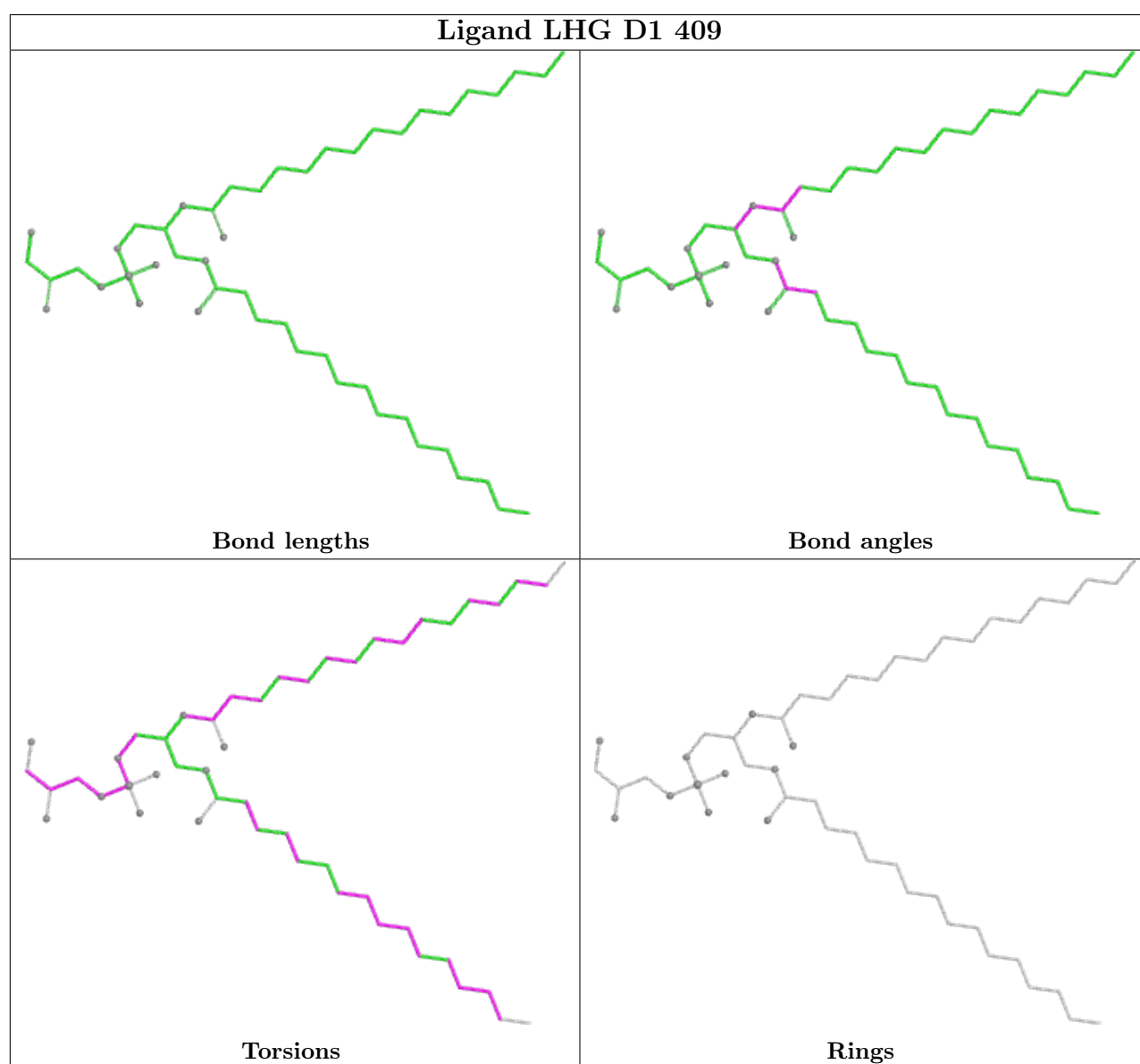
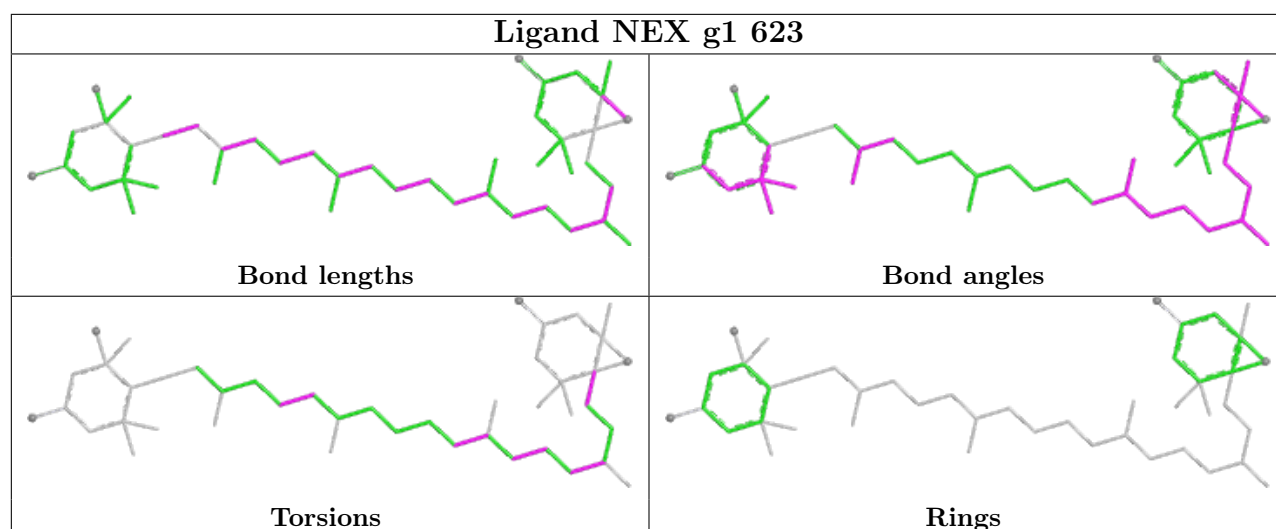


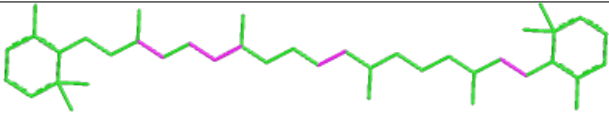
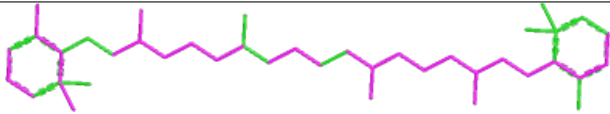
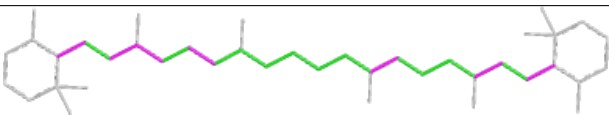
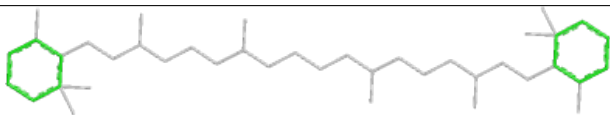


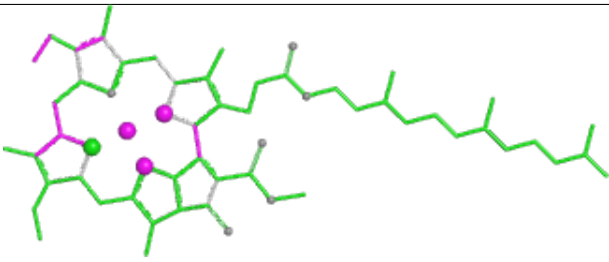
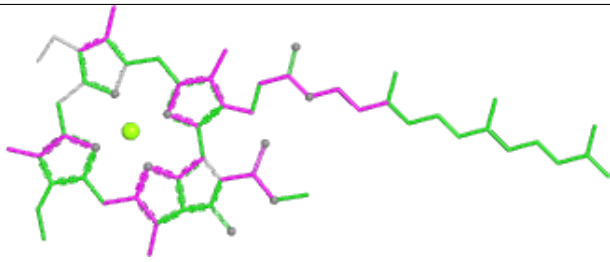
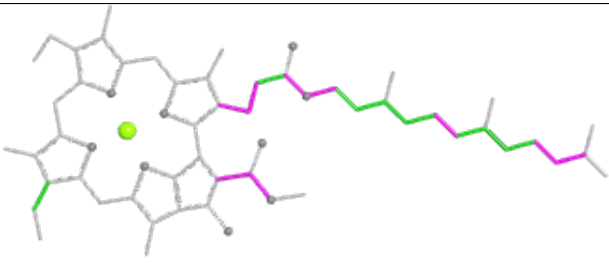
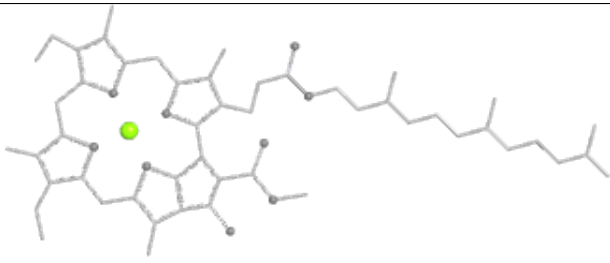


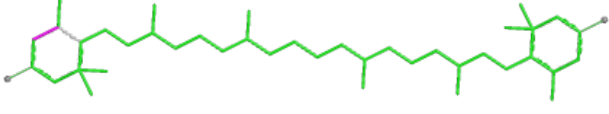
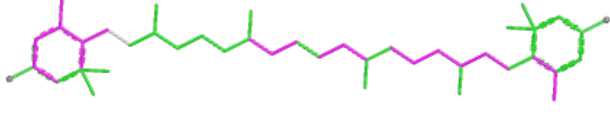
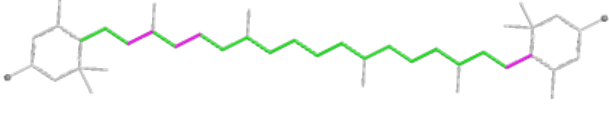
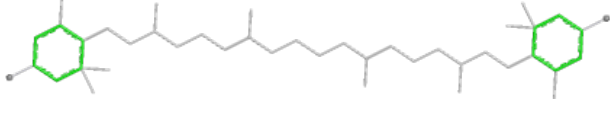


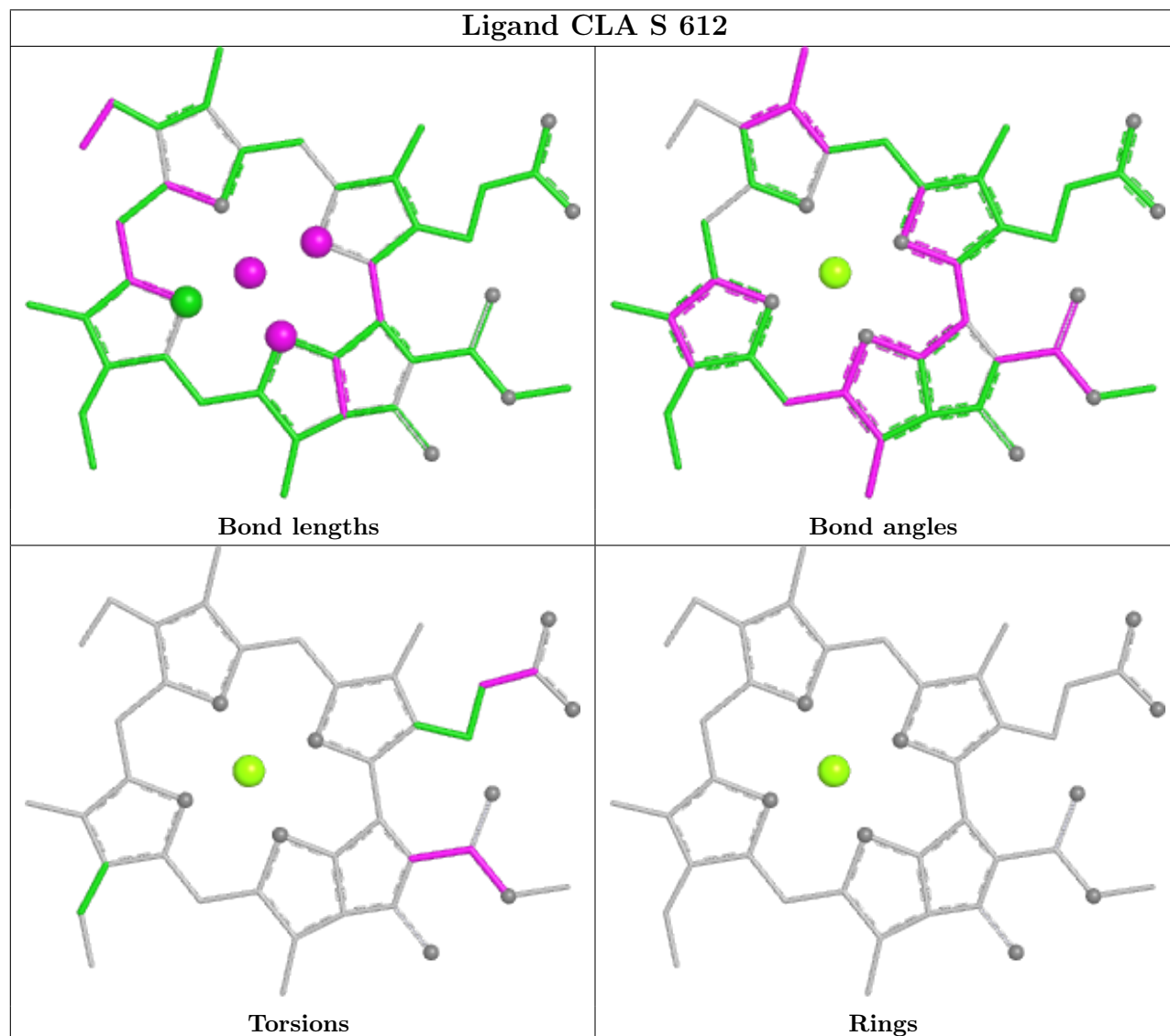
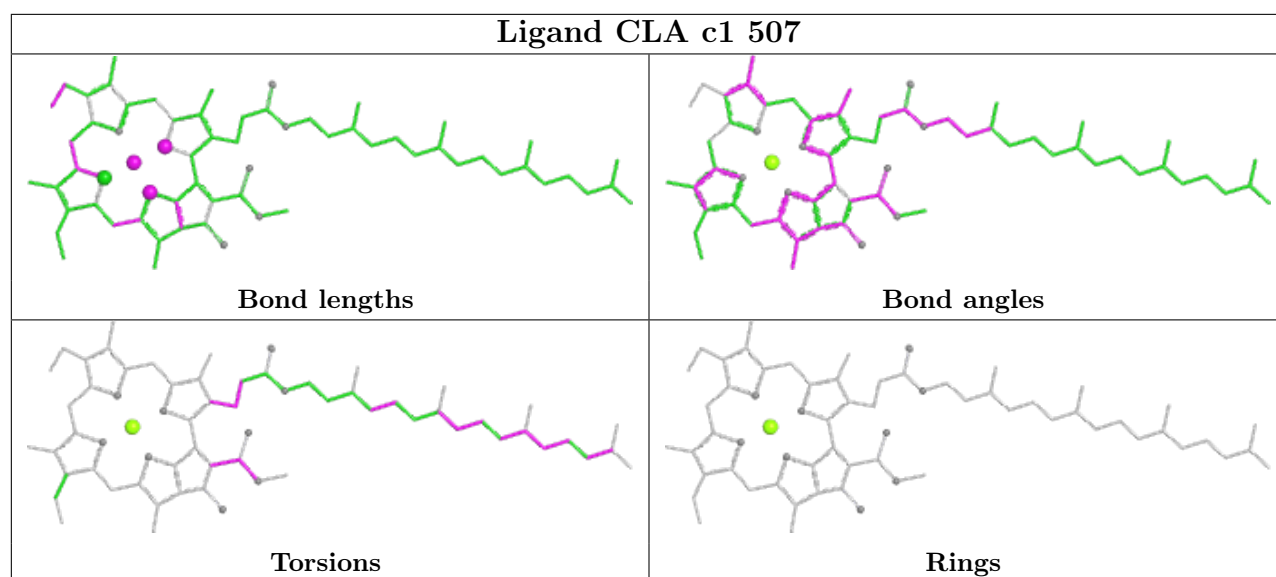




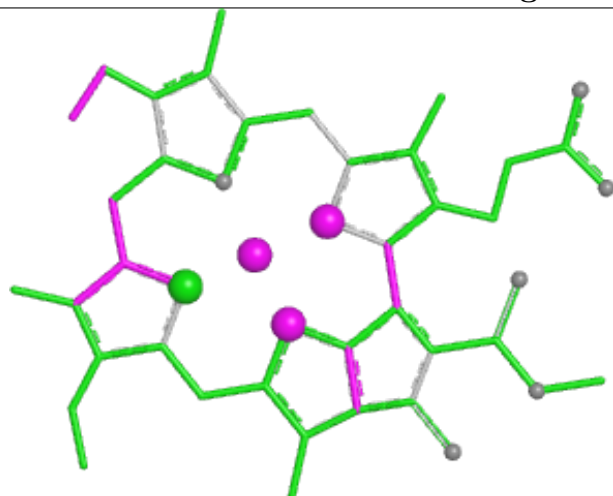
Ligand BCR C 517	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA r1 610	
	
Bond lengths	Bond angles
	
Torsions	Rings

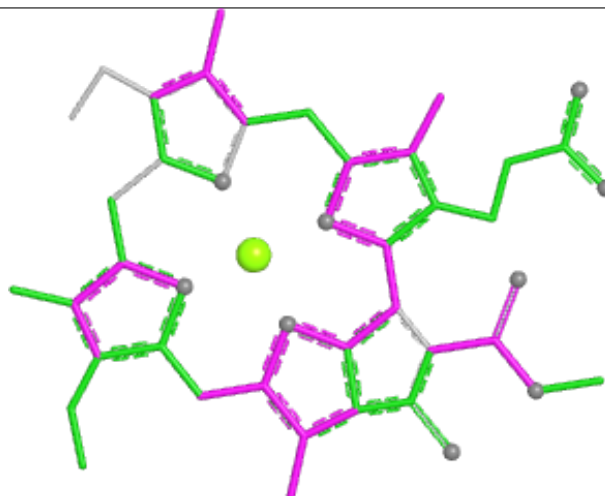
Ligand LUT n1 620	
	
Bond lengths	Bond angles
	
Torsions	Rings



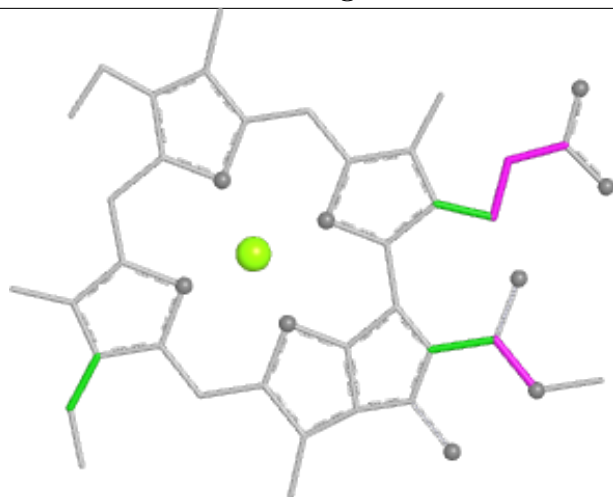
## Ligand CLA s 612



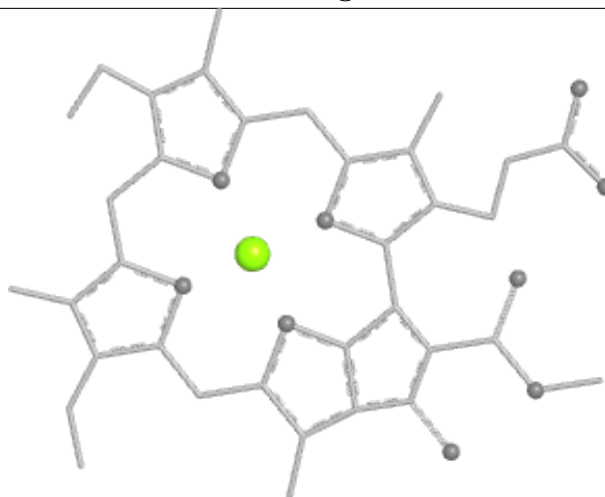
Bond lengths



Bond angles

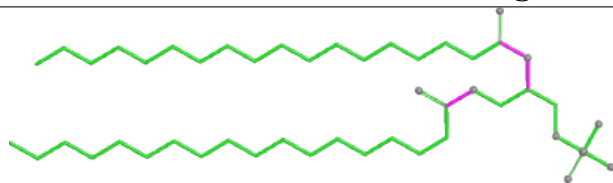


Torsions

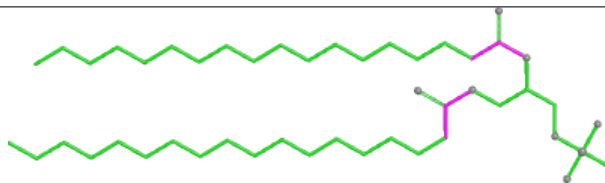


Rings

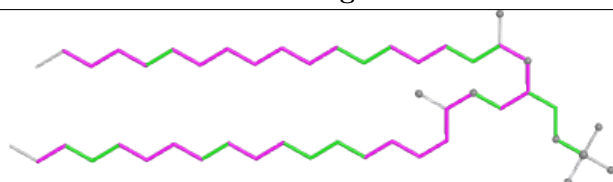
## Ligand 3PH t1 101



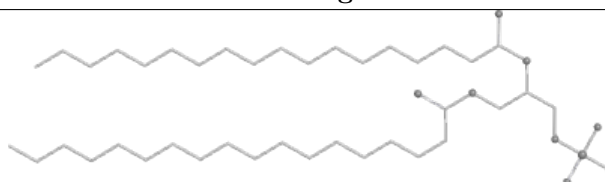
Bond lengths



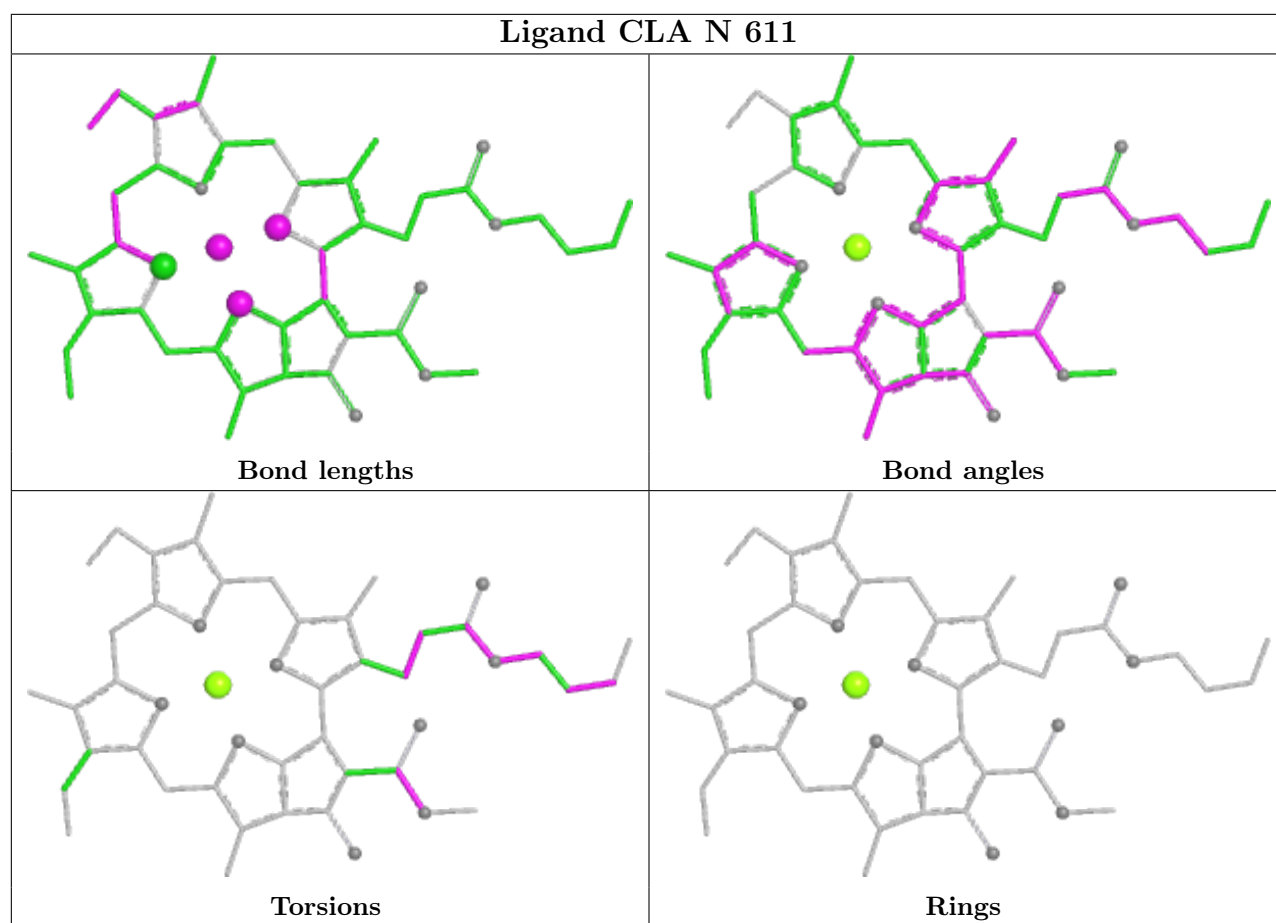
Bond angles

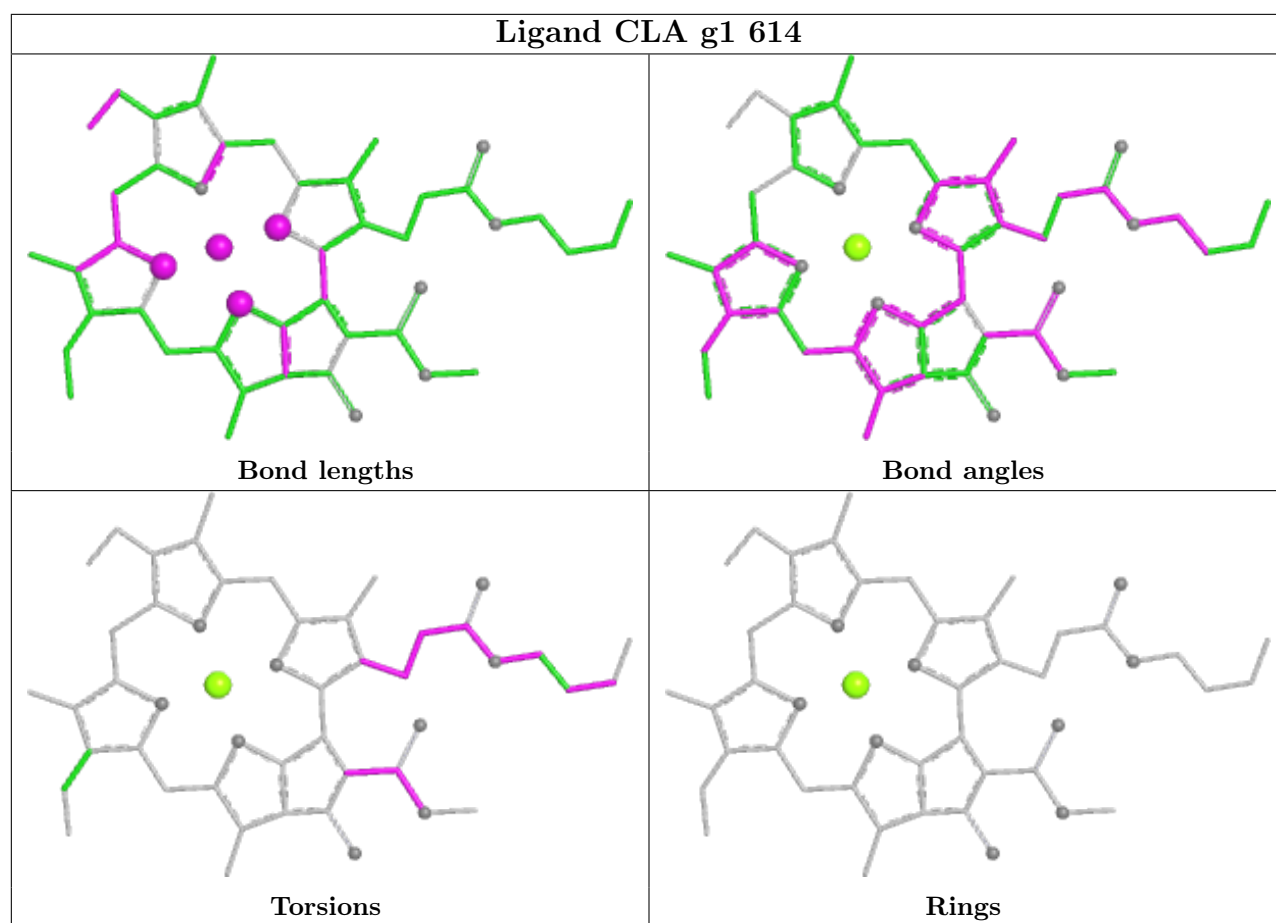


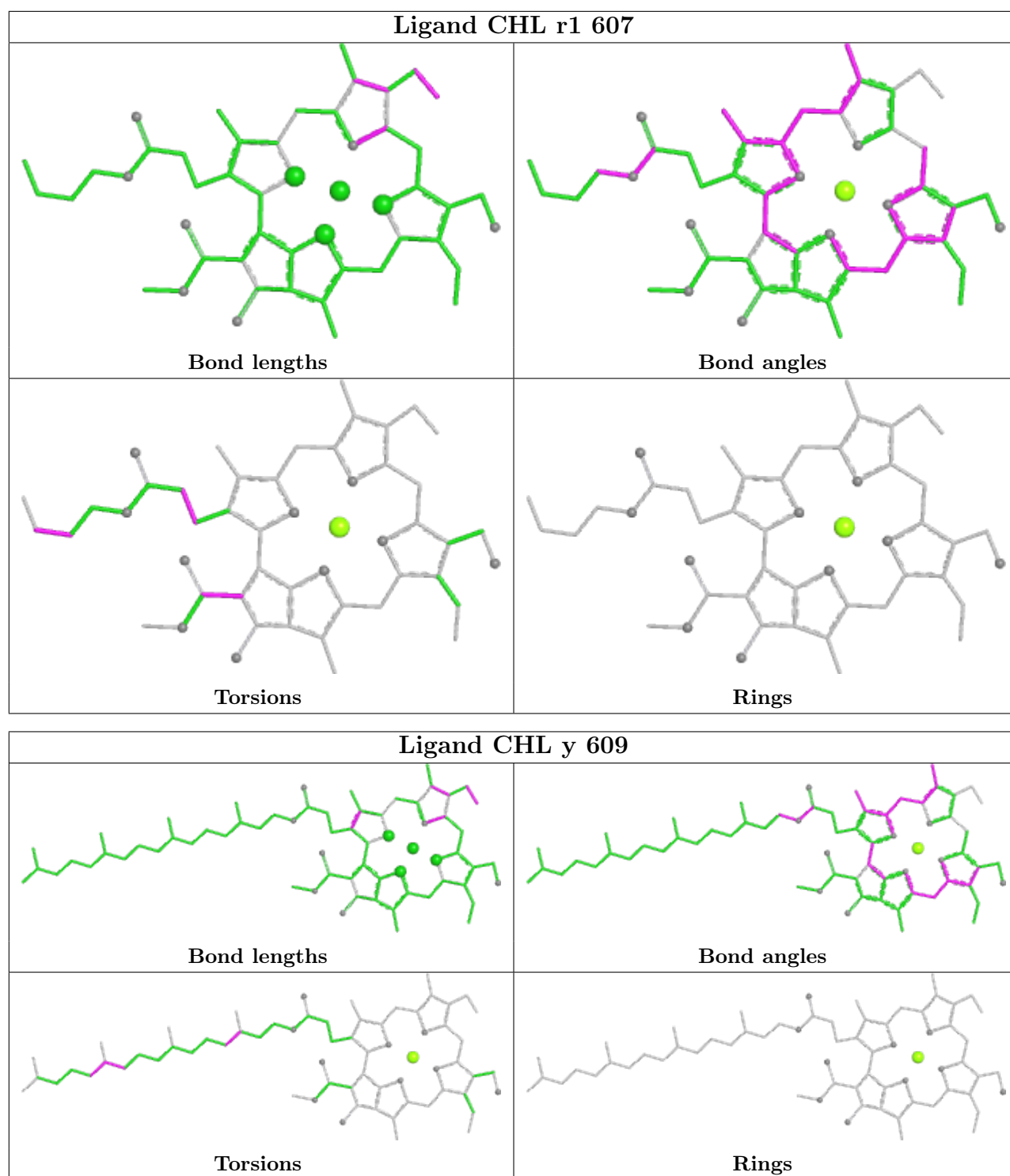
Torsions

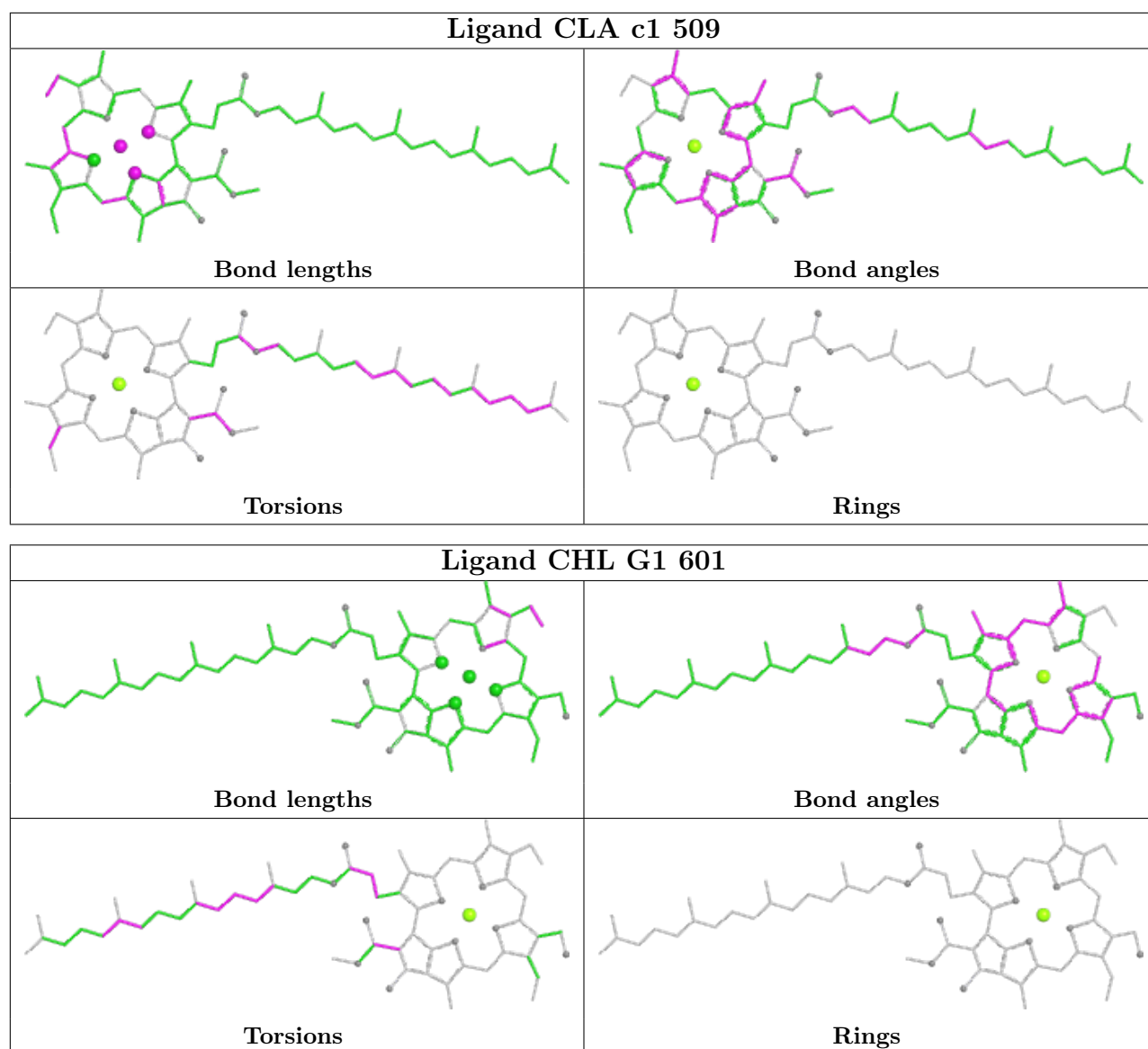


Rings

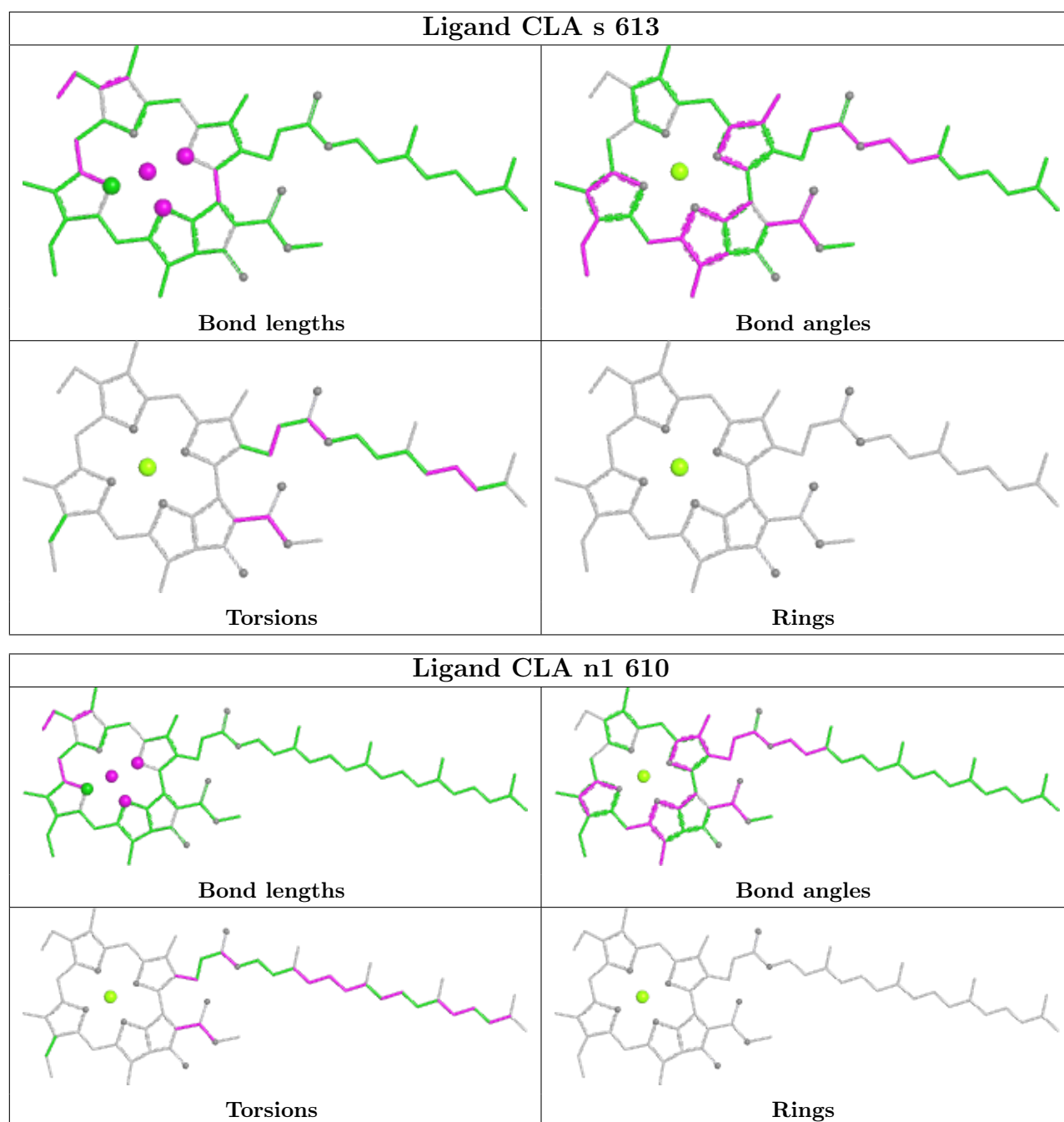












## 5.7 Other polymers [i](#)

There are no such residues in this entry.

## 5.8 Polymer linkage issues [i](#)

The following chains have linkage breaks:

Mol	Chain	Number of breaks
22	r	1
22	r1	1
22	R1	1
22	R	1
20	n1	1
20	n	1
21	G1	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	13.15
1	r1	110:PRO	C	126:GLU	N	13.08
1	R1	110:PRO	C	126:GLU	N	12.94
1	R	110:PRO	C	126:GLU	N	12.16
1	n1	57:PRO	C	58:PRO	N	3.54
1	n	57:PRO	C	58:PRO	N	3.28
1	G1	56:GLU	C	57:PHE	N	1.19

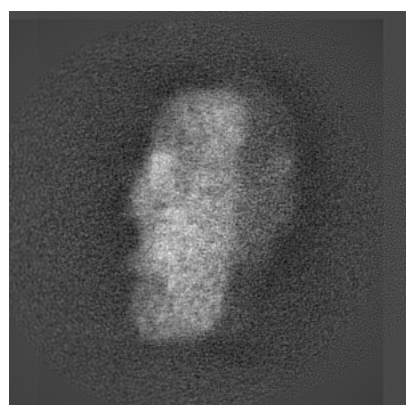
## 6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-13444. These allow visual inspection of the internal detail of the map and identification of artifacts.

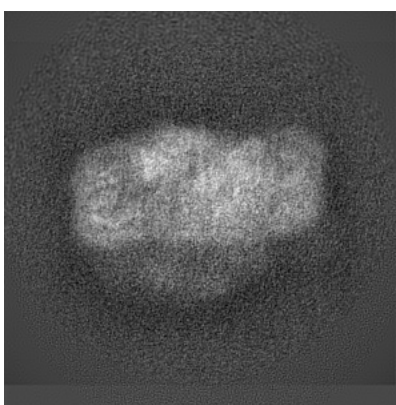
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

### 6.1 Orthogonal projections [i](#)

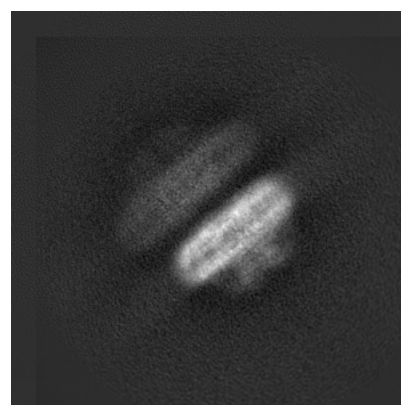
#### 6.1.1 Primary map



X



Y

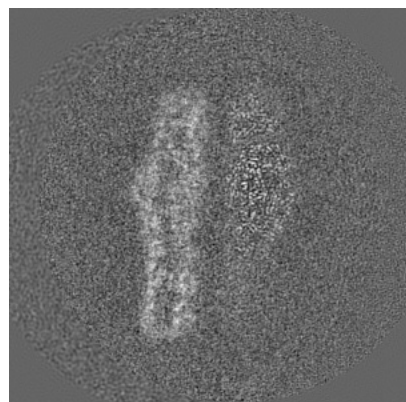


Z

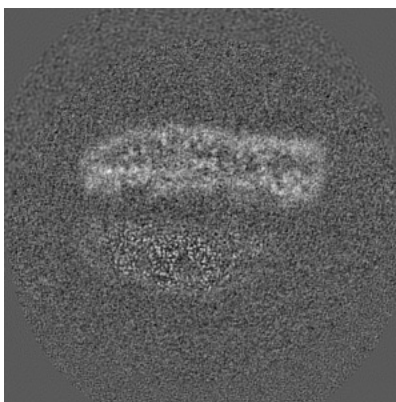
The images above show the map projected in three orthogonal directions.

### 6.2 Central slices [i](#)

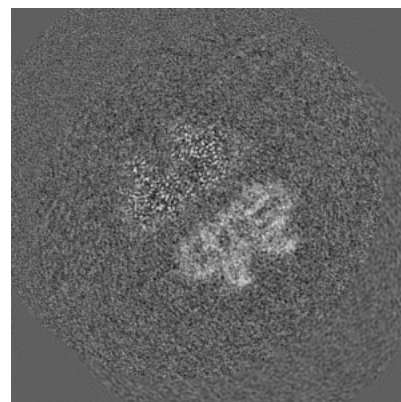
#### 6.2.1 Primary map



X Index: 240



Y Index: 240

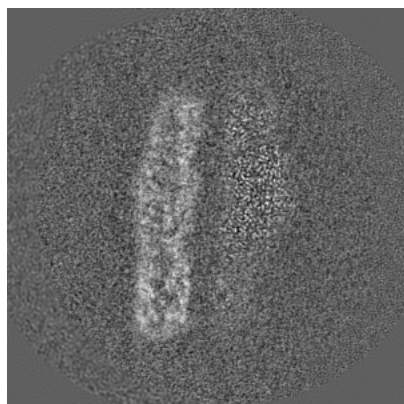


Z Index: 240

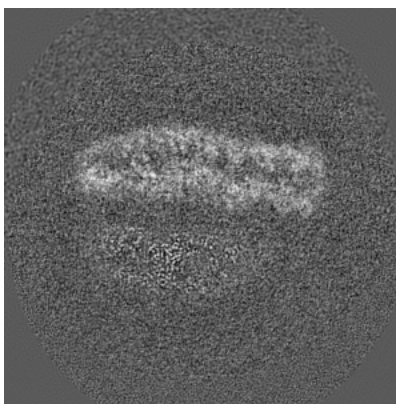
The images above show central slices of the map in three orthogonal directions.

## 6.3 Largest variance slices [i](#)

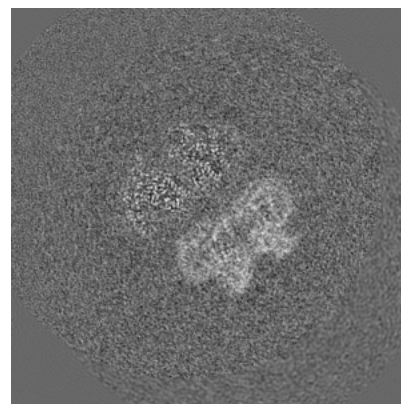
### 6.3.1 Primary map



X Index: 232



Y Index: 233

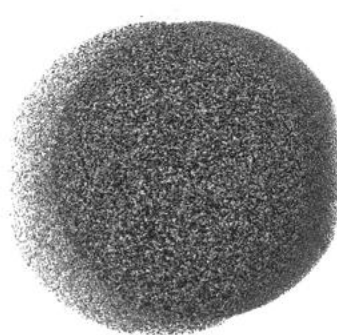


Z Index: 236

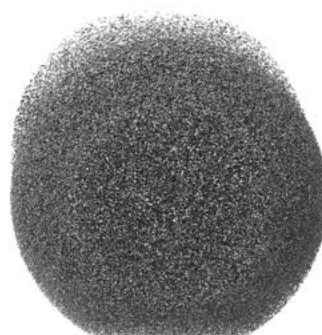
The images above show the largest variance slices of the map in three orthogonal directions.

## 6.4 Orthogonal surface views [i](#)

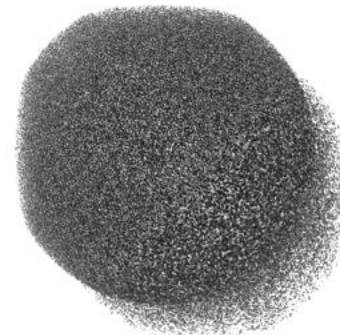
### 6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.013. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

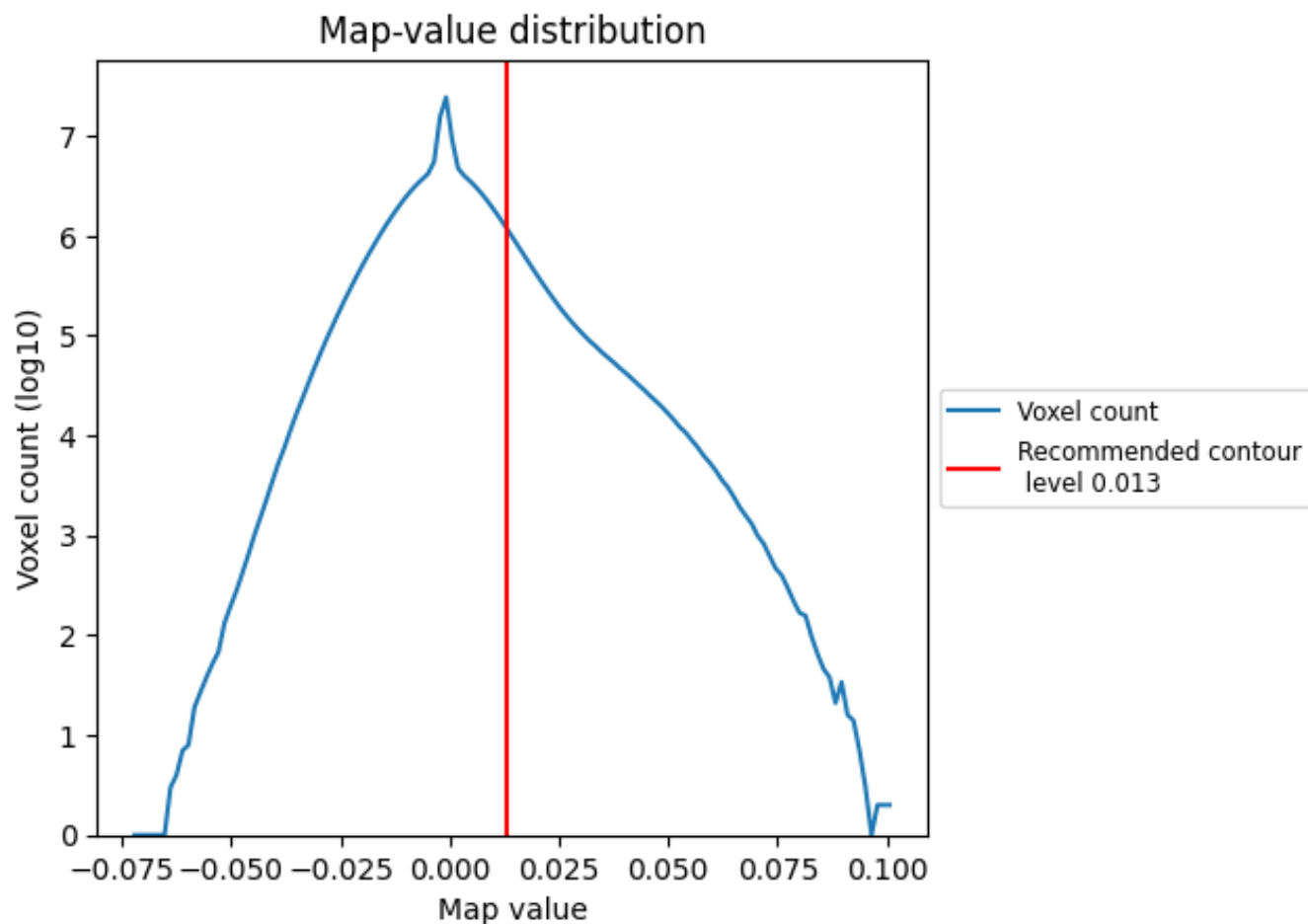
## 6.5 Mask visualisation

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

## 7 Map analysis [i](#)

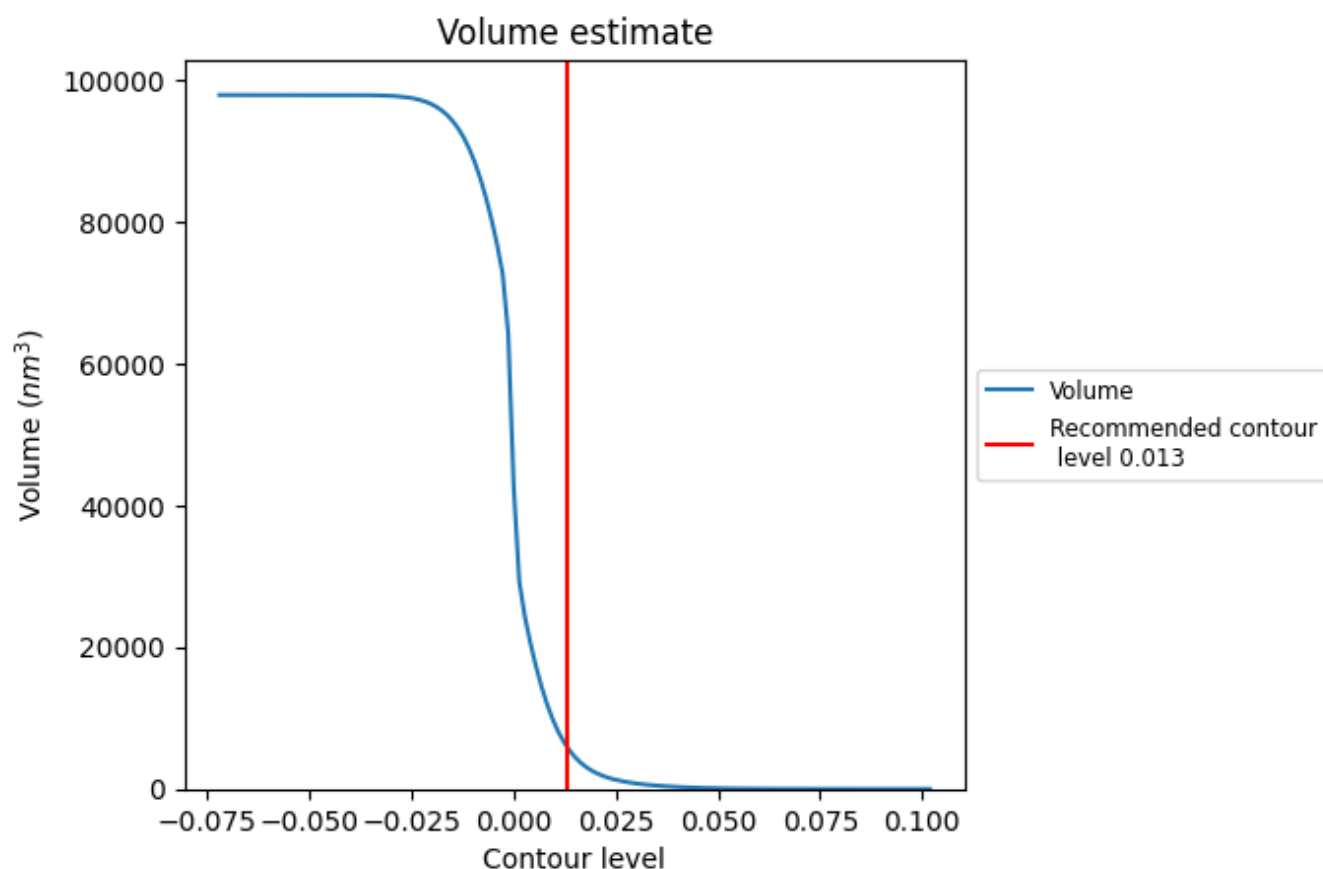
This section contains the results of statistical analysis of the map.

### 7.1 Map-value distribution [i](#)



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.

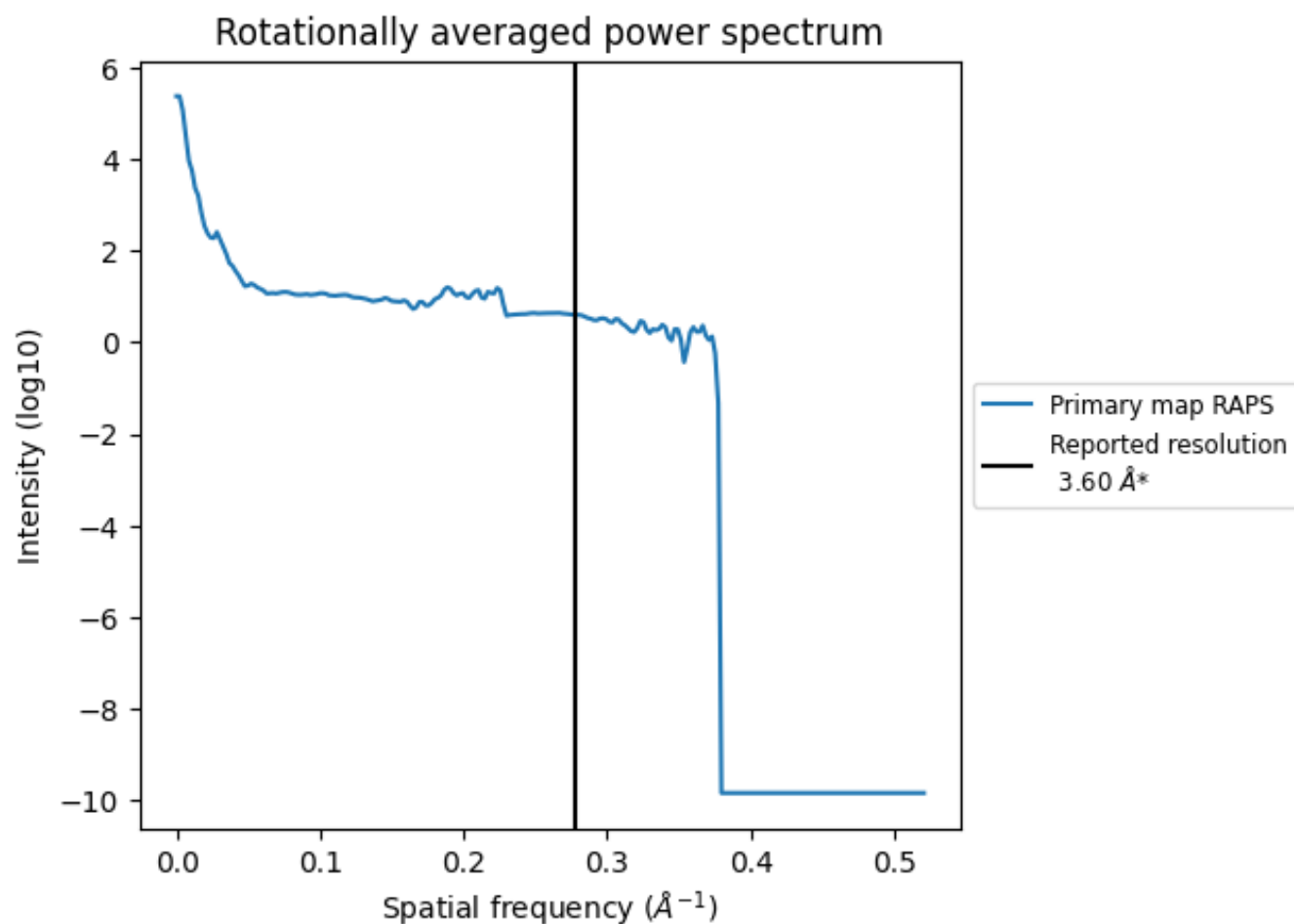
## 7.2 Volume estimate [i](#)



The volume at the recommended contour level is 5989 nm<sup>3</sup>; this corresponds to an approximate mass of 5410 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 ⓘ



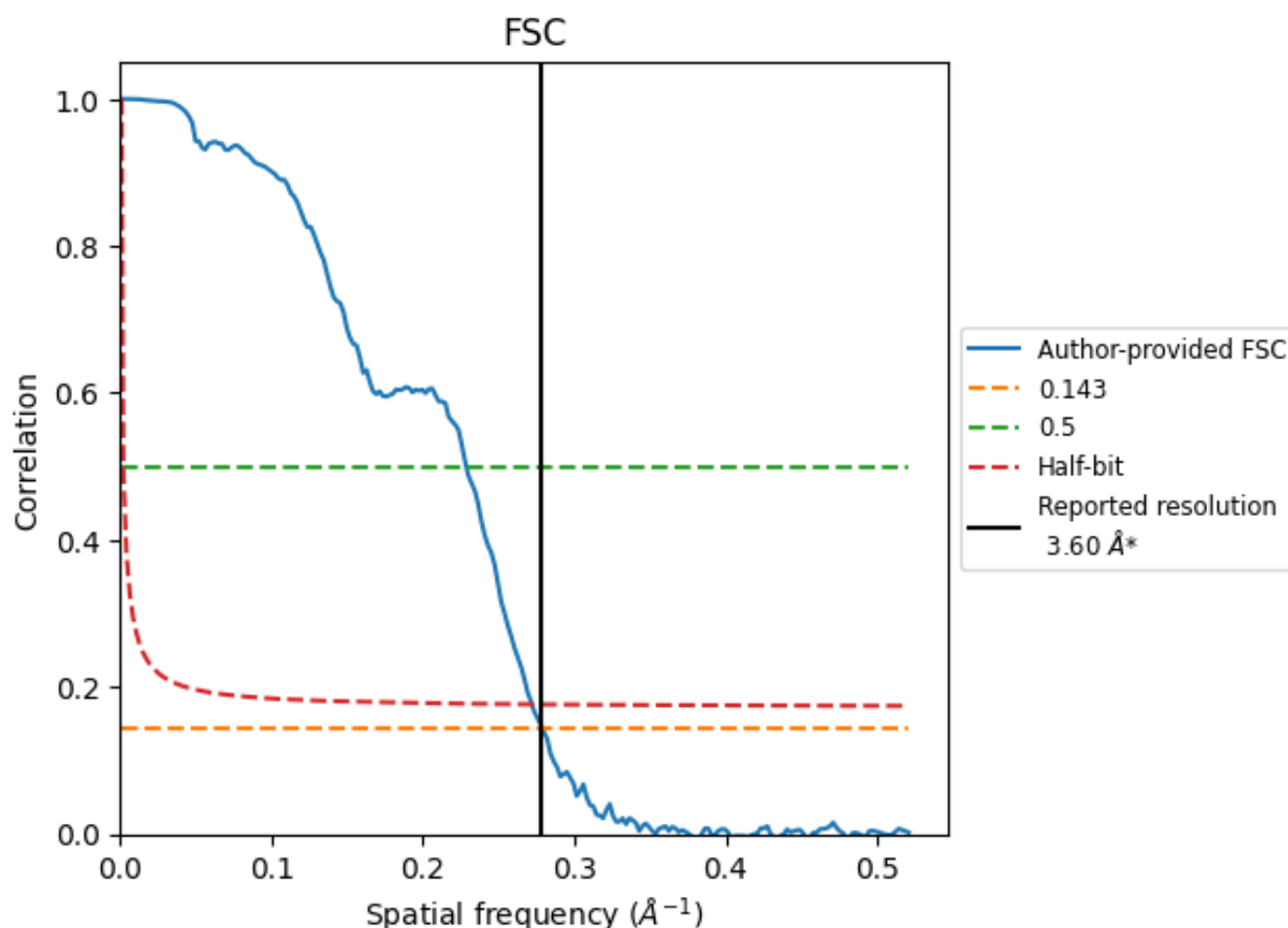
\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>



## 8 Fourier-Shell correlation [i](#)

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 [i](#)



\*Reported resolution corresponds to spatial frequency of 0.278 Å<sup>-1</sup>

## 8.2 Resolution estimates [i](#)

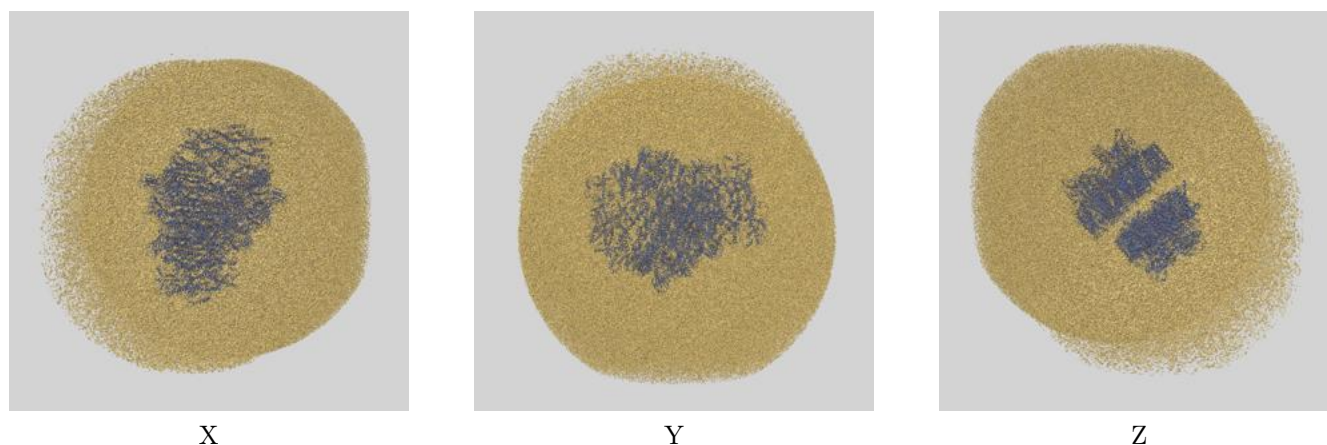
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.60	-	-
Author-provided FSC curve	3.58	4.37	3.68
Unmasked-calculated*	-	-	-

\*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

## 9 Map-model fit [i](#)

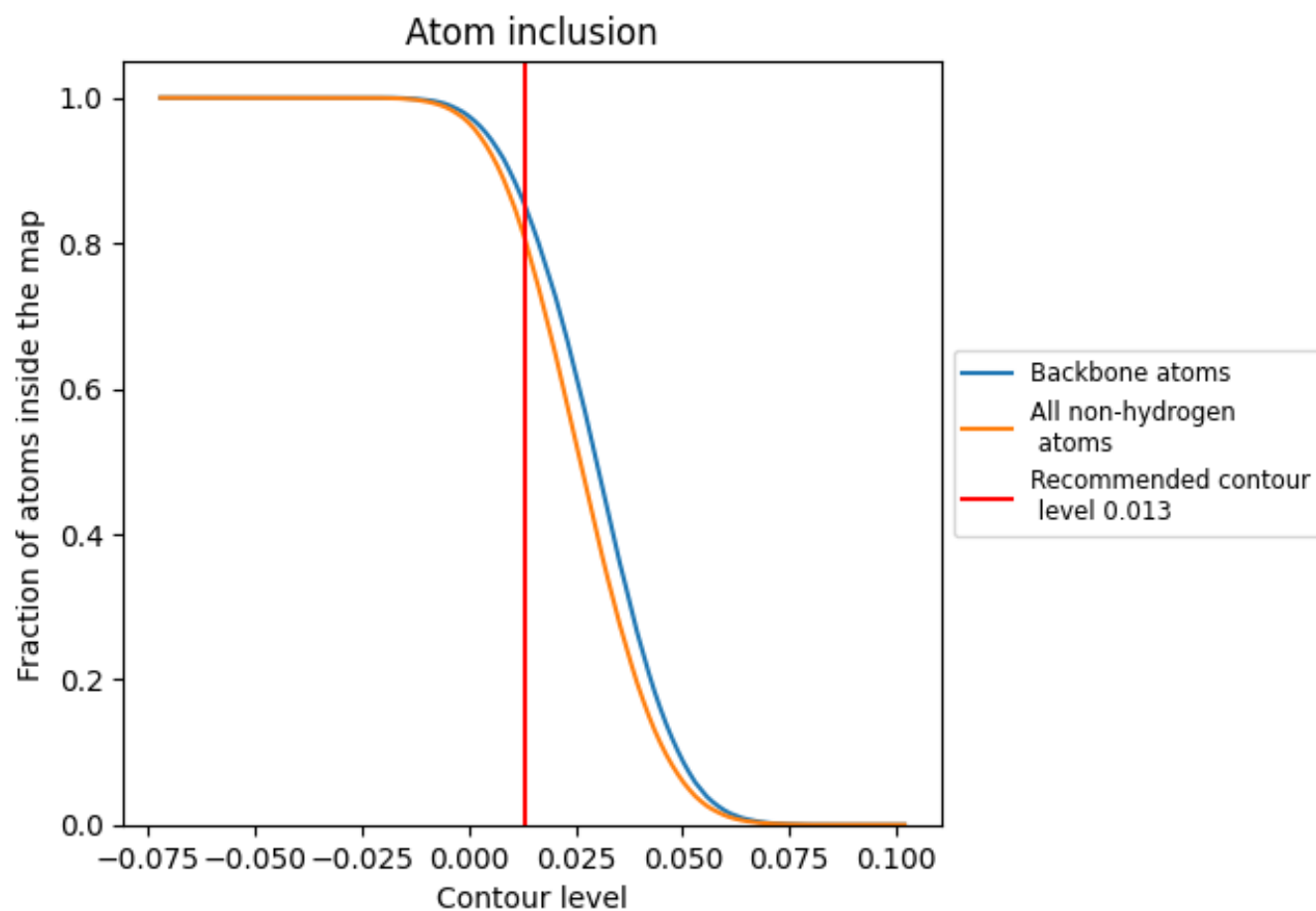
This section contains information regarding the fit between EMDB map EMD-13444 and PDB model 7PIN. Per-residue inclusion information can be found in section [3](#) on page [74](#).

### 9.1 Map-model overlay [i](#)



The images above show the 3D surface view of the map at the recommended contour level 0.013 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 Atom inclusion [i](#)



At the recommended contour level, 85% of all backbone atoms, 81% of all non-hydrogen atoms, are inside the map.