



Full wwPDB EM Validation Report ⓘ

Nov 15, 2022 – 05:25 AM JST

PDB ID : 6KAD
EMDB ID : EMD-9956
Title : Cryo-EM structure of the C2S2M2L2-type PSII-LHCII supercomplex from *Chlamydomonas reinhardtii*
Authors : Sheng, X.; Watanabe, A.; Li, A.J.; Kim, E.; Song, C.; Murata, K.; Song, D.F.; Minagawa, J.; Liu, Z.F.
Deposited on : 2019-06-21
Resolution : 3.40 Å(reported)

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

We welcome your comments at validation@mail.wwpdb.org

A user guide is available at

<https://www.wwpdb.org/validation/2017/EMValidationReportHelp>
with specific help available everywhere you see the ⓘ symbol.

The types of validation reports are described at

<http://www.wwpdb.org/validation/2017/FAQs#types>.

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

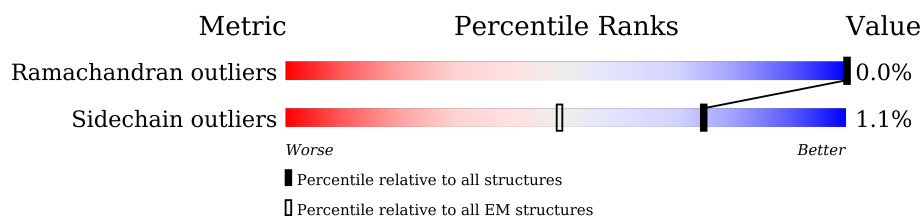
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry (DNA, RNA) : Parkinson et al. (1996)
Validation Pipeline (wwPDB-VP) : 2.31.2

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 3.40 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 ≥ 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	0	256	<div> <div>8%</div> <div>84%</div> <div>16%</div> </div>
1	1	256	<div> <div>•</div> <div>84%</div> <div>15%</div> </div>
1	6	256	<div> <div>11%</div> <div>84%</div> <div>16%</div> </div>
1	7	256	<div> <div>•</div> <div>84%</div> <div>•</div> <div>15%</div> </div>
1	Y	256	<div> <div>•</div> <div>86%</div> <div>14%</div> </div>
1	y	256	<div> <div>•</div> <div>86%</div> <div>14%</div> </div>
2	2	257	<div> <div>19%</div> <div>85%</div> <div>15%</div> </div>
2	3	257	<div> <div>12%</div> <div>84%</div> <div>•</div> <div>15%</div> </div>
2	5	257	<div> <div>48%</div> <div>84%</div> <div>•</div> <div>16%</div> </div>

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Mol	Chain	Length	Quality of chain
2	8	257	
2	9	257	
2	N	257	
2	n	257	
2	p	257	
3	4	249	
3	G	249	
3	g	249	
3	q	249	
4	A	352	
4	a	352	
5	B	508	
5	b	508	
6	C	461	
6	c	461	
7	D	352	
7	d	352	
8	E	82	
8	e	82	
9	F	44	
9	f	44	
10	H	88	
10	h	88	
11	I	37	
11	i	37	

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Mol	Chain	Length	Quality of chain
12	J	42	
12	j	42	
13	K	46	
13	k	46	
14	L	38	
14	l	38	
15	M	34	
15	m	34	
16	O	291	
16	o	291	
17	R	280	
17	r	280	
18	S	289	
18	s	289	
19	T	31	
19	t	31	
20	V	33	
20	v	33	
21	W	115	
21	w	115	
22	X	101	
22	x	101	
23	Z	62	
23	z	62	

The following table lists non-polymeric compounds, carbohydrate monomers and non-standard residues in protein, DNA, RNA chains that are outliers for geometric or electron-density-fit crite-

ria:

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	0	601	X	-	-	-
24	CHL	0	605	X	-	-	-
24	CHL	0	606	X	-	-	-
24	CHL	0	607	X	-	-	-
24	CHL	0	608	X	-	-	-
24	CHL	0	609	X	-	-	-
24	CHL	1	601	X	-	-	-
24	CHL	1	605	X	-	-	-
24	CHL	1	606	X	-	-	-
24	CHL	1	607	X	-	-	-
24	CHL	1	608	X	-	-	-
24	CHL	1	609	X	-	-	-
24	CHL	2	601	X	-	-	-
24	CHL	2	605	X	-	-	-
24	CHL	2	606	X	-	-	-
24	CHL	2	607	X	-	-	-
24	CHL	2	608	X	-	-	-
24	CHL	2	609	X	-	-	-
24	CHL	3	601	X	-	-	-
24	CHL	3	605	X	-	-	-
24	CHL	3	606	X	-	-	-
24	CHL	3	607	X	-	-	-
24	CHL	3	608	X	-	-	-
24	CHL	3	609	X	-	-	-
24	CHL	4	601	X	-	-	-
24	CHL	4	605	X	-	-	-
24	CHL	4	606	X	-	-	-
24	CHL	4	607	X	-	-	-
24	CHL	4	608	X	-	-	-
24	CHL	4	609	X	-	-	-
24	CHL	5	601	X	-	-	-
24	CHL	5	605	X	-	-	-
24	CHL	5	606	X	-	-	-
24	CHL	5	607	X	-	-	-
24	CHL	5	608	X	-	-	-
24	CHL	5	609	X	-	-	-
24	CHL	6	601	X	-	-	-
24	CHL	6	605	X	-	-	-
24	CHL	6	606	X	-	-	-
24	CHL	6	607	X	-	-	-
24	CHL	6	608	X	-	-	-
24	CHL	6	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	7	601	X	-	-	-
24	CHL	7	605	X	-	-	-
24	CHL	7	606	X	-	-	-
24	CHL	7	607	X	-	-	-
24	CHL	7	608	X	-	-	-
24	CHL	7	609	X	-	-	-
24	CHL	8	601	X	-	-	-
24	CHL	8	605	X	-	-	-
24	CHL	8	606	X	-	-	-
24	CHL	8	607	X	-	-	-
24	CHL	8	608	X	-	-	-
24	CHL	8	609	X	-	-	-
24	CHL	9	601	X	-	-	-
24	CHL	9	605	X	-	-	-
24	CHL	9	606	X	-	-	-
24	CHL	9	607	X	-	-	-
24	CHL	9	608	X	-	-	-
24	CHL	9	609	X	-	-	-
24	CHL	G	601	X	-	-	-
24	CHL	G	605	X	-	-	-
24	CHL	G	606	X	-	-	-
24	CHL	G	607	X	-	-	-
24	CHL	G	608	X	-	-	-
24	CHL	G	609	X	-	-	-
24	CHL	N	601	X	-	-	-
24	CHL	N	605	X	-	-	-
24	CHL	N	606	X	-	-	-
24	CHL	N	607	X	-	-	-
24	CHL	N	608	X	-	-	-
24	CHL	N	609	X	-	-	-
24	CHL	R	606	X	-	-	-
24	CHL	R	607	X	-	-	-
24	CHL	R	608	X	-	-	-
24	CHL	S	601	X	-	-	-
24	CHL	S	606	X	-	-	-
24	CHL	S	607	X	-	-	-
24	CHL	S	608	X	-	-	-
24	CHL	Y	601	X	-	-	-
24	CHL	Y	605	X	-	-	-
24	CHL	Y	606	X	-	-	-
24	CHL	Y	607	X	-	-	-
24	CHL	Y	608	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
24	CHL	Y	609	X	-	-	-
24	CHL	g	601	X	-	-	-
24	CHL	g	605	X	-	-	-
24	CHL	g	606	X	-	-	-
24	CHL	g	607	X	-	-	-
24	CHL	g	608	X	-	-	-
24	CHL	g	609	X	-	-	-
24	CHL	n	601	X	-	-	-
24	CHL	n	605	X	-	-	-
24	CHL	n	606	X	-	-	-
24	CHL	n	607	X	-	-	-
24	CHL	n	608	X	-	-	-
24	CHL	n	609	X	-	-	-
24	CHL	p	601	X	-	-	-
24	CHL	p	605	X	-	-	-
24	CHL	p	606	X	-	-	-
24	CHL	p	607	X	-	-	-
24	CHL	p	608	X	-	-	-
24	CHL	p	609	X	-	-	-
24	CHL	q	601	X	-	-	-
24	CHL	q	605	X	-	-	-
24	CHL	q	606	X	-	-	-
24	CHL	q	607	X	-	-	-
24	CHL	q	608	X	-	-	-
24	CHL	q	609	X	-	-	-
24	CHL	r	606	X	-	-	-
24	CHL	r	607	X	-	-	-
24	CHL	r	608	X	-	-	-
24	CHL	s	601	X	-	-	-
24	CHL	s	606	X	-	-	-
24	CHL	s	607	X	-	-	-
24	CHL	s	608	X	-	-	-
24	CHL	y	601	X	-	-	-
24	CHL	y	605	X	-	-	-
24	CHL	y	606	X	-	-	-
24	CHL	y	607	X	-	-	-
24	CHL	y	608	X	-	-	-
24	CHL	y	609	X	-	-	-
25	CLA	0	602	X	-	-	-
25	CLA	0	603	X	-	-	-
25	CLA	0	604	X	-	-	-
25	CLA	0	610	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	0	611	X	-	-	-
25	CLA	0	612	X	-	-	-
25	CLA	0	614	X	-	-	-
25	CLA	1	602	X	-	-	-
25	CLA	1	603	X	-	-	-
25	CLA	1	604	X	-	-	-
25	CLA	1	610	X	-	-	-
25	CLA	1	611	X	-	-	-
25	CLA	1	612	X	-	-	-
25	CLA	1	614	X	-	-	-
25	CLA	2	603	X	-	-	-
25	CLA	2	604	X	-	-	-
25	CLA	2	610	X	-	-	-
25	CLA	2	611	X	-	-	-
25	CLA	2	612	X	-	-	-
25	CLA	2	613	X	-	-	-
25	CLA	3	602	X	-	-	-
25	CLA	3	603	X	-	-	-
25	CLA	3	604	X	-	-	-
25	CLA	3	610	X	-	-	-
25	CLA	3	611	X	-	-	-
25	CLA	3	612	X	-	-	-
25	CLA	3	614	X	-	-	-
25	CLA	4	602	X	-	-	-
25	CLA	4	603	X	-	-	-
25	CLA	4	604	X	-	-	-
25	CLA	4	610	X	-	-	-
25	CLA	4	611	X	-	-	-
25	CLA	4	612	X	-	-	-
25	CLA	4	613	X	-	-	-
25	CLA	4	614	X	-	-	-
25	CLA	5	602	X	-	-	-
25	CLA	5	603	X	-	-	-
25	CLA	5	604	X	-	-	-
25	CLA	5	610	X	-	-	-
25	CLA	5	611	X	-	-	-
25	CLA	5	612	X	-	-	-
25	CLA	5	613	X	-	-	-
25	CLA	6	602	X	-	-	-
25	CLA	6	603	X	-	-	-
25	CLA	6	610	X	-	-	-
25	CLA	6	611	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	6	612	X	-	-	-
25	CLA	6	614	X	-	-	-
25	CLA	7	602	X	-	-	-
25	CLA	7	603	X	-	-	-
25	CLA	7	604	X	-	-	-
25	CLA	7	610	X	-	-	-
25	CLA	7	611	X	-	-	-
25	CLA	7	612	X	-	-	-
25	CLA	7	614	X	-	-	-
25	CLA	8	602	X	-	-	-
25	CLA	8	603	X	-	-	-
25	CLA	8	604	X	-	-	-
25	CLA	8	610	X	-	-	-
25	CLA	8	611	X	-	-	-
25	CLA	8	612	X	-	-	-
25	CLA	8	614	X	-	-	-
25	CLA	9	602	X	-	-	-
25	CLA	9	603	X	-	-	-
25	CLA	9	604	X	-	-	-
25	CLA	9	610	X	-	-	-
25	CLA	9	611	X	-	-	-
25	CLA	9	612	X	-	-	-
25	CLA	9	613	X	-	-	-
25	CLA	A	405	X	-	-	-
25	CLA	A	406	X	-	-	-
25	CLA	A	407	X	-	-	-
25	CLA	A	410	X	-	-	-
25	CLA	B	602	X	-	-	-
25	CLA	B	603	X	-	-	-
25	CLA	B	604	X	-	-	-
25	CLA	B	605	X	-	-	-
25	CLA	B	606	X	-	-	-
25	CLA	B	608	X	-	-	-
25	CLA	B	609	X	-	-	-
25	CLA	B	610	X	-	-	-
25	CLA	B	611	X	-	-	-
25	CLA	B	612	X	-	-	-
25	CLA	B	613	X	-	-	-
25	CLA	B	614	X	-	-	-
25	CLA	B	615	X	-	-	-
25	CLA	B	616	X	-	-	-
25	CLA	B	617	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	C	501	X	-	-	-
25	CLA	C	502	X	-	-	-
25	CLA	C	503	X	-	-	-
25	CLA	C	504	X	-	-	-
25	CLA	C	505	X	-	-	-
25	CLA	C	506	X	-	-	-
25	CLA	C	507	X	-	-	-
25	CLA	C	508	X	-	-	-
25	CLA	C	509	X	-	-	-
25	CLA	C	510	X	-	-	-
25	CLA	C	512	X	-	-	-
25	CLA	C	513	X	-	-	-
25	CLA	D	402	X	-	-	-
25	CLA	D	403	X	-	-	-
25	CLA	G	602	X	-	-	-
25	CLA	G	603	X	-	-	-
25	CLA	G	604	X	-	-	-
25	CLA	G	610	X	-	-	-
25	CLA	G	611	X	-	-	-
25	CLA	G	612	X	-	-	-
25	CLA	G	613	X	-	-	-
25	CLA	G	614	X	-	-	-
25	CLA	N	602	X	-	-	-
25	CLA	N	603	X	-	-	-
25	CLA	N	604	X	-	-	-
25	CLA	N	610	X	-	-	-
25	CLA	N	611	X	-	-	-
25	CLA	N	612	X	-	-	-
25	CLA	N	613	X	-	-	-
25	CLA	N	614	X	-	-	-
25	CLA	R	601	X	-	-	-
25	CLA	R	602	X	-	-	-
25	CLA	R	603	X	-	-	-
25	CLA	R	604	X	-	-	-
25	CLA	R	609	X	-	-	-
25	CLA	R	610	X	-	-	-
25	CLA	R	611	X	-	-	-
25	CLA	R	612	X	-	-	-
25	CLA	S	603	X	-	-	-
25	CLA	S	604	X	-	-	-
25	CLA	S	605	X	-	-	-
25	CLA	S	609	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	S	610	X	-	-	-
25	CLA	S	611	X	-	-	-
25	CLA	S	612	X	-	-	-
25	CLA	S	614	X	-	-	-
25	CLA	Y	602	X	-	-	-
25	CLA	Y	603	X	-	-	-
25	CLA	Y	610	X	-	-	-
25	CLA	Y	611	X	-	-	-
25	CLA	Y	612	X	-	-	-
25	CLA	Y	614	X	-	-	-
25	CLA	a	405	X	-	-	-
25	CLA	a	406	X	-	-	-
25	CLA	a	407	X	-	-	-
25	CLA	a	410	X	-	-	-
25	CLA	b	602	X	-	-	-
25	CLA	b	603	X	-	-	-
25	CLA	b	604	X	-	-	-
25	CLA	b	605	X	-	-	-
25	CLA	b	606	X	-	-	-
25	CLA	b	608	X	-	-	-
25	CLA	b	609	X	-	-	-
25	CLA	b	610	X	-	-	-
25	CLA	b	611	X	-	-	-
25	CLA	b	612	X	-	-	-
25	CLA	b	613	X	-	-	-
25	CLA	b	614	X	-	-	-
25	CLA	b	615	X	-	-	-
25	CLA	b	616	X	-	-	-
25	CLA	b	617	X	-	-	-
25	CLA	c	501	X	-	-	-
25	CLA	c	502	X	-	-	-
25	CLA	c	503	X	-	-	-
25	CLA	c	504	X	-	-	-
25	CLA	c	505	X	-	-	-
25	CLA	c	506	X	-	-	-
25	CLA	c	507	X	-	-	-
25	CLA	c	508	X	-	-	-
25	CLA	c	509	X	-	-	-
25	CLA	c	510	X	-	-	-
25	CLA	c	512	X	-	-	-
25	CLA	c	513	X	-	-	-
25	CLA	d	402	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	d	403	X	-	-	-
25	CLA	g	602	X	-	-	-
25	CLA	g	603	X	-	-	-
25	CLA	g	604	X	-	-	-
25	CLA	g	610	X	-	-	-
25	CLA	g	611	X	-	-	-
25	CLA	g	612	X	-	-	-
25	CLA	g	613	X	-	-	-
25	CLA	g	614	X	-	-	-
25	CLA	n	602	X	-	-	-
25	CLA	n	603	X	-	-	-
25	CLA	n	604	X	-	-	-
25	CLA	n	610	X	-	-	-
25	CLA	n	611	X	-	-	-
25	CLA	n	612	X	-	-	-
25	CLA	n	613	X	-	-	-
25	CLA	n	614	X	-	-	-
25	CLA	p	602	X	-	-	-
25	CLA	p	603	X	-	-	-
25	CLA	p	604	X	-	-	-
25	CLA	p	610	X	-	-	-
25	CLA	p	611	X	-	-	-
25	CLA	p	612	X	-	-	-
25	CLA	p	613	X	-	-	-
25	CLA	q	602	X	-	-	-
25	CLA	q	603	X	-	-	-
25	CLA	q	610	X	-	-	-
25	CLA	q	611	X	-	-	-
25	CLA	q	612	X	-	-	-
25	CLA	q	613	X	-	-	-
25	CLA	q	614	X	-	-	-
25	CLA	r	601	X	-	-	-
25	CLA	r	602	X	-	-	-
25	CLA	r	603	X	-	-	-
25	CLA	r	604	X	-	-	-
25	CLA	r	609	X	-	-	-
25	CLA	r	610	X	-	-	-
25	CLA	r	611	X	-	-	-
25	CLA	r	612	X	-	-	-
25	CLA	s	603	X	-	-	-
25	CLA	s	604	X	-	-	-
25	CLA	s	605	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CLA	s	609	X	-	-	-
25	CLA	s	610	X	-	-	-
25	CLA	s	611	X	-	-	-
25	CLA	s	612	X	-	-	-
25	CLA	s	614	X	-	-	-
25	CLA	y	602	X	-	-	-
25	CLA	y	603	X	-	-	-
25	CLA	y	610	X	-	-	-
25	CLA	y	611	X	-	-	-
25	CLA	y	612	X	-	-	-
25	CLA	y	614	X	-	-	-

2 Entry composition

There are 40 unique types of molecules in this entry. The entry contains 105342 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	217	Total	C	N	O	S	0	0
			1665	1088	268	304	5		
1	6	216	Total	C	N	O	S	0	0
			1656	1083	266	302	5		
1	Y	221	Total	C	N	O	S	0	0
			1693	1104	272	312	5		
1	0	216	Total	C	N	O	S	0	0
			1656	1083	266	302	5		
1	7	217	Total	C	N	O	S	0	0
			1665	1088	268	304	5		
1	y	221	Total	C	N	O	S	0	0
			1693	1104	272	312	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	2	218	Total	C	N	O	S	0	0
			1667	1078	271	313	5		
2	3	218	Total	C	N	O	S	0	0
			1667	1078	271	313	5		
2	5	217	Total	C	N	O	S	0	0
			1661	1075	270	311	5		
2	N	219	Total	C	N	O	S	0	0
			1672	1081	272	314	5		
2	8	218	Total	C	N	O	S	0	0
			1667	1078	271	313	5		
2	9	218	Total	C	N	O	S	0	0
			1667	1078	271	313	5		
2	p	217	Total	C	N	O	S	0	0
			1661	1075	270	311	5		
2	n	219	Total	C	N	O	S	0	0
			1672	1081	272	314	5		

- Molecule 3 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	217	Total	C	N	O	S	0	0
			1656	1076	270	305	5		
3	G	219	Total	C	N	O	S	0	0
			1667	1082	272	308	5		
3	q	217	Total	C	N	O	S	0	0
			1656	1076	270	305	5		
3	g	219	Total	C	N	O	S	0	0
			1667	1082	272	308	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
4	A	336	Total	C	N	O	S	0	0
			2636	1719	434	468	15		
4	a	336	Total	C	N	O	S	0	0
			2636	1719	434	468	15		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
5	B	490	Total	C	N	O	S	0	0
			3836	2509	642	673	12		
5	b	490	Total	C	N	O	S	0	0
			3836	2509	642	673	12		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
6	C	448	Total	C	N	O	S	0	0
			3490	2284	583	606	17		
6	c	448	Total	C	N	O	S	0	0
			3490	2284	583	606	17		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	346	Total	C	N	O	S	0	0
			2755	1816	454	473	12		
7	d	346	Total	C	N	O	S	0	0
			2755	1816	454	473	12		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
8	E	76	Total	C	N	O	0	0
			619	404	102	113		
8	e	76	Total	C	N	O	0	0
			619	404	102	113		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	31	Total	C	N	O	S	0	0
			251	171	42	37	1		
9	f	31	Total	C	N	O	S	0	0
			251	171	42	37	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	68	Total	C	N	O	S	0	0
			519	347	77	93	2		
10	h	68	Total	C	N	O	S	0	0
			519	347	77	93	2		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	35	Total	C	N	O	S	0	0
			283	193	43	45	2		
11	i	35	Total	C	N	O	S	0	0
			283	193	43	45	2		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	J	35	Total	C	N	O	0	0
			255	174	39	42		
12	j	35	Total	C	N	O	0	0
			255	174	39	42		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
13	K	37	Total	C	N	O	0	0
			297	209	43	45		

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Mol	Chain	Residues	Atoms				AltConf	Trace
13	k	37	Total	C	N	O	0	0
			297	209	43	45		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
14	L	37	Total	C	N	O	0	0
			306	205	50	51		
14	l	37	Total	C	N	O	0	0
			306	205	50	51		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
15	M	30	Total	C	N	O	0	0
			230	158	32	40		
15	m	30	Total	C	N	O	0	0
			230	158	32	40		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	230	Total	C	N	O	S	0	0
			1742	1109	278	351	4		
16	o	230	Total	C	N	O	S	0	0
			1742	1109	278	351	4		

- Molecule 17 is a protein called Chlorophyll a-b binding protein CP29.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	R	240	Total	C	N	O	S	0	0
			1826	1156	313	352	5		
17	r	240	Total	C	N	O	S	0	0
			1826	1156	313	352	5		

- Molecule 18 is a protein called Chlorophyll a-b binding protein, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
18	S	252	Total	C	N	O	S	0	0
			1907	1232	312	359	4		
18	s	252	Total	C	N	O	S	0	0
			1907	1232	312	359	4		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
19	T	30	Total	C	N	O	S	0	0
			247	171	36	38	2		
19	t	30	Total	C	N	O	S	0	0
			247	171	36	38	2		

- Molecule 20 is a protein called Photosystem II reaction center protein Ycf12.

Mol	Chain	Residues	Atoms					AltConf	Trace
20	V	33	Total	C	N	O	S	0	0
			232	152	38	41	1		
20	v	33	Total	C	N	O	S	0	0
			232	152	38	41	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
21	W	56	Total	C	N	O	S	0	0
			434	281	70	81	2		
21	w	56	Total	C	N	O	S	0	0
			434	281	70	81	2		

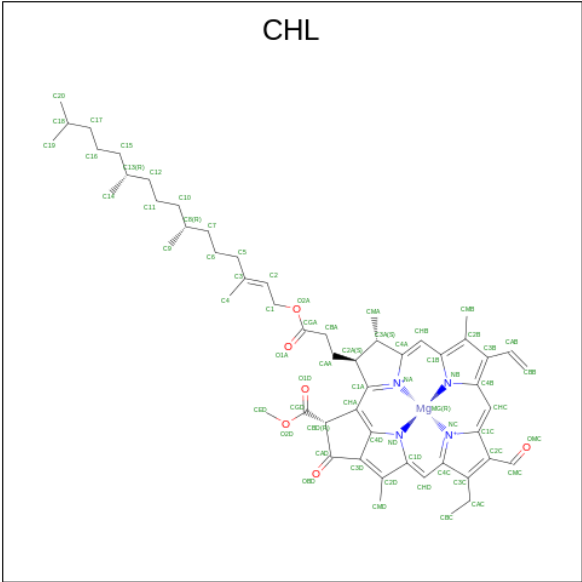
- Molecule 22 is a protein called 4.1 kDa photosystem II subunit.

Mol	Chain	Residues	Atoms				AltConf	Trace
22	X	34	Total	C	N	O	0	0
			233	153	37	43		
22	x	34	Total	C	N	O	0	0
			233	153	37	43		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
23	Z	61	Total	C	N	O	S	0	0
			458	314	68	75	1		
23	z	61	Total	C	N	O	S	0	0
			458	314	68	75	1		

- Molecule 24 is CHLOROPHYLL B (three-letter code: CHL) (formula: $C_{55}H_{70}MgN_4O_6$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
24	1	1	Total	C	Mg	N	O	0
			360	294	6	24	36	
24	1	1	Total	C	Mg	N	O	0
			360	294	6	24	36	
24	1	1	Total	C	Mg	N	O	0
			360	294	6	24	36	
24	1	1	Total	C	Mg	N	O	0
			360	294	6	24	36	
24	1	1	Total	C	Mg	N	O	0
			360	294	6	24	36	
24	1	1	Total	C	Mg	N	O	0
			360	294	6	24	36	
24	2	1	Total	C	Mg	N	O	0
			324	260	6	24	34	
24	2	1	Total	C	Mg	N	O	0
			324	260	6	24	34	
24	2	1	Total	C	Mg	N	O	0
			324	260	6	24	34	
24	2	1	Total	C	Mg	N	O	0
			324	260	6	24	34	
24	2	1	Total	C	Mg	N	O	0
			324	260	6	24	34	
24	3	1	Total	C	Mg	N	O	0
			360	294	6	24	36	
24	3	1	Total	C	Mg	N	O	0
			360	294	6	24	36	

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Mol	Chain	Residues	Atoms					AltConf
24	3	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	3	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	3	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	3	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	4	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	4	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	4	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	4	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	4	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	4	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	5	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	5	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	5	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	5	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	5	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	5	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	6	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	6	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	6	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	6	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	6	1	Total 360	C 294	Mg 6	N 24	O 36	0

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Mol	Chain	Residues	Atoms					AltConf
24	6	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	G	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	G	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	G	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	G	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	G	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	G	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	N	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	N	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	N	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	N	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	N	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	N	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	N	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	R	1	Total 183	C 150	Mg 3	N 12	O 18	0
24	R	1	Total 183	C 150	Mg 3	N 12	O 18	0
24	R	1	Total 183	C 150	Mg 3	N 12	O 18	0
24	S	1	Total 182	C 142	Mg 4	N 16	O 20	0
24	S	1	Total 182	C 142	Mg 4	N 16	O 20	0
24	S	1	Total 182	C 142	Mg 4	N 16	O 20	0
24	S	1	Total 182	C 142	Mg 4	N 16	O 20	0
24	Y	1	Total 360	C 294	Mg 6	N 24	O 36	0

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Mol	Chain	Residues	Atoms					AltConf
24	Y	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	Y	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	Y	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	Y	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	Y	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	0	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	0	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	0	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	0	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	0	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	0	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	0	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	7	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	7	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	7	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	7	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	7	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	7	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	7	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	8	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	8	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	8	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	8	1	Total 360	C 294	Mg 6	N 24	O 36	0

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Mol	Chain	Residues	Atoms					AltConf
24	8	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	8	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	9	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	9	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	9	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	9	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	9	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	9	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	p	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	p	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	p	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	p	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	p	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	p	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	q	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	q	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	q	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	q	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	q	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	q	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	g	1	Total 324	C 260	Mg 6	N 24	O 34	0

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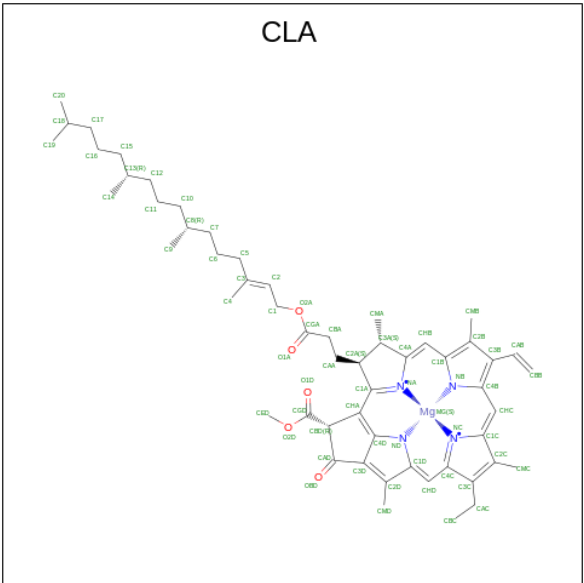
Mol	Chain	Residues	Atoms					AltConf
24	g	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	g	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	g	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	g	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	g	1	Total 324	C 260	Mg 6	N 24	O 34	0
24	n	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	n	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	n	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	n	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	n	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	n	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	n	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	s	1	Total 182	C 142	Mg 4	N 16	O 20	0
24	s	1	Total 182	C 142	Mg 4	N 16	O 20	0
24	s	1	Total 182	C 142	Mg 4	N 16	O 20	0
24	s	1	Total 182	C 142	Mg 4	N 16	O 20	0
24	y	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	y	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	y	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	y	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	y	1	Total 360	C 294	Mg 6	N 24	O 36	0
24	y	1	Total 360	C 294	Mg 6	N 24	O 36	0

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Mol	Chain	Residues	Atoms					AltConf
24	r	1	Total	C	Mg	N	O	0
			183	150	3	12	18	
24	r	1	Total	C	Mg	N	O	0
			183	150	3	12	18	
24	r	1	Total	C	Mg	N	O	0
			183	150	3	12	18	

- Molecule 25 is CHLOROPHYLL A (three-letter code: CLA) (formula: $C_{55}H_{72}MgN_4O_5$) (labeled as "Ligand of Interest" by depositor).



Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total	C	Mg	N	O	0
			509	429	8	32	40	
25	1	1	Total	C	Mg	N	O	0
			509	429	8	32	40	
25	1	1	Total	C	Mg	N	O	0
			509	429	8	32	40	
25	1	1	Total	C	Mg	N	O	0
			509	429	8	32	40	
25	1	1	Total	C	Mg	N	O	0
			509	429	8	32	40	
25	1	1	Total	C	Mg	N	O	0
			509	429	8	32	40	
25	1	1	Total	C	Mg	N	O	0
			509	429	8	32	40	
25	1	1	Total	C	Mg	N	O	0
			509	429	8	32	40	

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Mol	Chain	Residues	Atoms					AltConf
25	2	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	2	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	2	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	2	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	2	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	2	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	2	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	2	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	3	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	3	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	3	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	3	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	3	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	3	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	3	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	3	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	4	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	4	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	4	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	4	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	4	1	Total 446	C 368	Mg 8	N 32	O 38	0

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Mol	Chain	Residues	Atoms					AltConf
25	4	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	4	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	4	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	5	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	5	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	5	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	5	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	5	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	5	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	5	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	5	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	6	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	6	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	6	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	6	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	6	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	6	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	6	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	6	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	A	1	Total 239	C 199	Mg 4	N 16	O 20	0
25	A	1	Total 239	C 199	Mg 4	N 16	O 20	0

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Mol	Chain	Residues	Atoms					AltConf
25	A	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
25	A	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	B	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	

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Mol	Chain	Residues	Atoms					AltConf
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	C	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	D	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
25	D	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
25	G	1	Total	C	Mg	N	O	0
			446	368	8	32	38	
25	G	1	Total	C	Mg	N	O	0
			446	368	8	32	38	
25	G	1	Total	C	Mg	N	O	0
			446	368	8	32	38	
25	G	1	Total	C	Mg	N	O	0
			446	368	8	32	38	
25	G	1	Total	C	Mg	N	O	0
			446	368	8	32	38	
25	G	1	Total	C	Mg	N	O	0
			446	368	8	32	38	
25	G	1	Total	C	Mg	N	O	0
			446	368	8	32	38	
25	N	1	Total	C	Mg	N	O	0
			468	388	8	32	40	

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Mol	Chain	Residues	Atoms					AltConf
25	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	N	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	R	1	Total 563	C 463	Mg 10	N 40	O 50	0
25	R	1	Total 563	C 463	Mg 10	N 40	O 50	0
25	R	1	Total 563	C 463	Mg 10	N 40	O 50	0
25	R	1	Total 563	C 463	Mg 10	N 40	O 50	0
25	R	1	Total 563	C 463	Mg 10	N 40	O 50	0
25	R	1	Total 563	C 463	Mg 10	N 40	O 50	0
25	R	1	Total 563	C 463	Mg 10	N 40	O 50	0
25	R	1	Total 563	C 463	Mg 10	N 40	O 50	0
25	R	1	Total 563	C 463	Mg 10	N 40	O 50	0
25	S	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	S	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	S	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	S	1	Total 471	C 375	Mg 10	N 40	O 46	0

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Mol	Chain	Residues	Atoms					AltConf
25	S	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	S	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	S	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	S	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	S	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	S	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	Y	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	Y	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	Y	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	Y	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	Y	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	Y	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	Y	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	Y	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	0	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	0	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	0	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	0	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	0	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	0	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	0	1	Total 509	C 429	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
25	0	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	7	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	7	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	7	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	7	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	7	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	7	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	7	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	7	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	8	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	8	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	8	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	8	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	8	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	8	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	8	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	8	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	9	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	9	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	9	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	9	1	Total 446	C 368	Mg 8	N 32	O 38	0

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Mol	Chain	Residues	Atoms					AltConf
25	9	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	9	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	9	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	9	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	p	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	p	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	p	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	p	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	p	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	p	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	p	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	p	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	q	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	q	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	q	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	q	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	q	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	q	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	q	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	q	1	Total 446	C 368	Mg 8	N 32	O 38	0
25	a	1	Total 239	C 199	Mg 4	N 16	O 20	0

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Mol	Chain	Residues	Atoms					AltConf
25	a	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
25	a	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
25	a	1	Total	C	Mg	N	O	0
			239	199	4	16	20	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	

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Mol	Chain	Residues	Atoms					AltConf
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
25	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
25	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
25	g	1	Total	C	Mg	N	O	0
			446	368	8	32	38	
25	g	1	Total	C	Mg	N	O	0
			446	368	8	32	38	
25	g	1	Total	C	Mg	N	O	0
			446	368	8	32	38	
25	g	1	Total	C	Mg	N	O	0
			446	368	8	32	38	
25	g	1	Total	C	Mg	N	O	0
			446	368	8	32	38	
25	g	1	Total	C	Mg	N	O	0
			446	368	8	32	38	
25	g	1	Total	C	Mg	N	O	0
			446	368	8	32	38	

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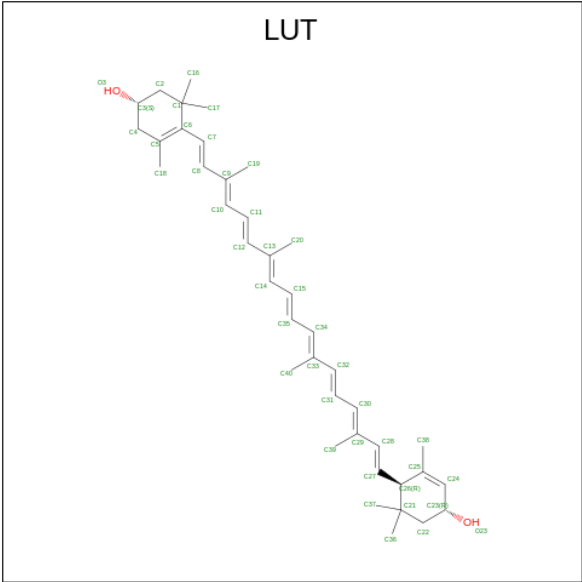
Mol	Chain	Residues	Atoms					AltConf
25	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	n	1	Total 468	C 388	Mg 8	N 32	O 40	0
25	s	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	s	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	s	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	s	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	s	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	s	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	s	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	s	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	s	1	Total 471	C 375	Mg 10	N 40	O 46	0
25	y	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	y	1	Total 509	C 429	Mg 8	N 32	O 40	0
25	y	1	Total 509	C 429	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
25	y	1	Total	C	Mg	N	O	0
			509	429	8	32	40	
25	y	1	Total	C	Mg	N	O	0
			509	429	8	32	40	
25	y	1	Total	C	Mg	N	O	0
			509	429	8	32	40	
25	y	1	Total	C	Mg	N	O	0
			509	429	8	32	40	
25	y	1	Total	C	Mg	N	O	0
			509	429	8	32	40	
25	r	1	Total	C	Mg	N	O	0
			563	463	10	40	50	
25	r	1	Total	C	Mg	N	O	0
			563	463	10	40	50	
25	r	1	Total	C	Mg	N	O	0
			563	463	10	40	50	
25	r	1	Total	C	Mg	N	O	0
			563	463	10	40	50	
25	r	1	Total	C	Mg	N	O	0
			563	463	10	40	50	
25	r	1	Total	C	Mg	N	O	0
			563	463	10	40	50	
25	r	1	Total	C	Mg	N	O	0
			563	463	10	40	50	
25	r	1	Total	C	Mg	N	O	0
			563	463	10	40	50	

- Molecule 26 is (3R,3'R,6S)-4,5-DIDEHYDRO-5,6-DIHYDRO-BETA,BETA-CAROTENE-3,3'-DIOL (three-letter code: LUT) (formula: C₄₀H₅₆O₂).



Mol	Chain	Residues	Atoms			AltConf
26	1	1	Total	C	O	0
			84	80	4	
26	1	1	Total	C	O	0
			84	80	4	
26	2	1	Total	C	O	0
			84	80	4	
26	2	1	Total	C	O	0
			84	80	4	
26	3	1	Total	C	O	0
			84	80	4	
26	3	1	Total	C	O	0
			84	80	4	
26	4	1	Total	C	O	0
			84	80	4	
26	4	1	Total	C	O	0
			84	80	4	
26	5	1	Total	C	O	0
			84	80	4	
26	5	1	Total	C	O	0
			84	80	4	
26	6	1	Total	C	O	0
			84	80	4	
26	6	1	Total	C	O	0
			84	80	4	
26	G	1	Total	C	O	0
			84	80	4	
26	G	1	Total	C	O	0
			84	80	4	

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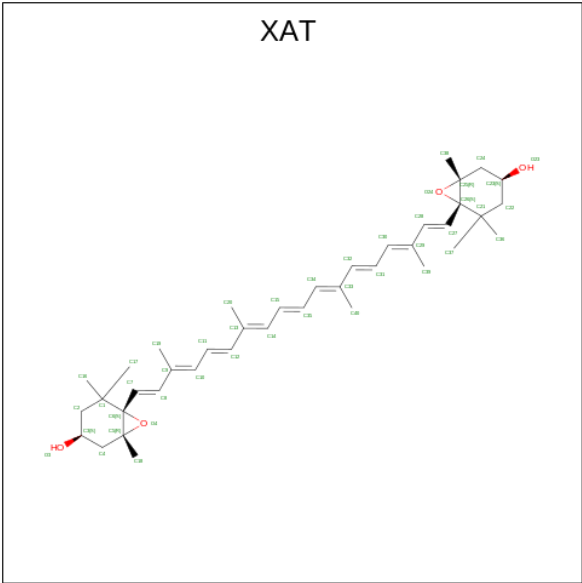
Mol	Chain	Residues	Atoms			AltConf
26	N	1	Total	C	O	0
			84	80	4	
26	N	1	Total	C	O	0
			84	80	4	
26	R	1	Total	C	O	0
			42	40	2	
26	S	1	Total	C	O	0
			84	80	4	
26	S	1	Total	C	O	0
			84	80	4	
26	Y	1	Total	C	O	0
			84	80	4	
26	Y	1	Total	C	O	0
			84	80	4	
26	0	1	Total	C	O	0
			84	80	4	
26	0	1	Total	C	O	0
			84	80	4	
26	7	1	Total	C	O	0
			84	80	4	
26	7	1	Total	C	O	0
			84	80	4	
26	8	1	Total	C	O	0
			84	80	4	
26	8	1	Total	C	O	0
			84	80	4	
26	9	1	Total	C	O	0
			84	80	4	
26	9	1	Total	C	O	0
			84	80	4	
26	p	1	Total	C	O	0
			84	80	4	
26	p	1	Total	C	O	0
			84	80	4	
26	q	1	Total	C	O	0
			84	80	4	
26	q	1	Total	C	O	0
			84	80	4	
26	g	1	Total	C	O	0
			84	80	4	
26	g	1	Total	C	O	0
			84	80	4	

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Mol	Chain	Residues	Atoms			AltConf
26	n	1	Total	C	O	0
			84	80	4	
26	n	1	Total	C	O	0
			84	80	4	
26	s	1	Total	C	O	0
			84	80	4	
26	s	1	Total	C	O	0
			84	80	4	
26	y	1	Total	C	O	0
			84	80	4	
26	y	1	Total	C	O	0
			84	80	4	
26	r	1	Total	C	O	0
			42	40	2	

- Molecule 27 is (3S,5R,6S,3'S,5'R,6'S)-5,6,5',6'-DIEPOXY-5,6,5',6'- TETRAHYDRO-BETA ,BETA-CAROTENE-3,3'-DIOL (three-letter code: XAT) (formula: C₄₀H₅₆O₄).



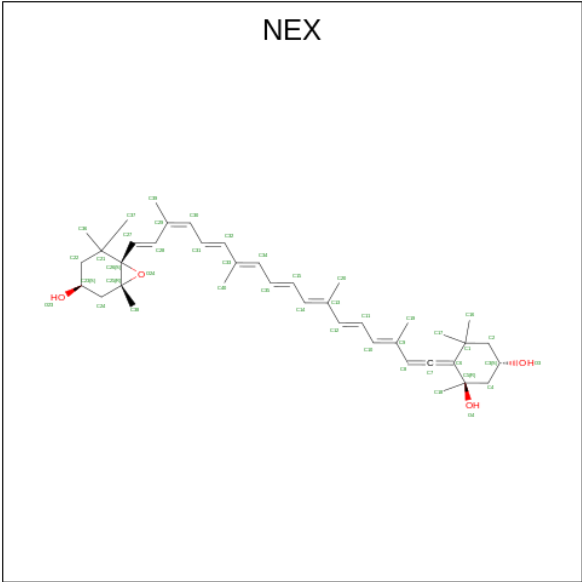
Mol	Chain	Residues	Atoms			AltConf
27	1	1	Total	C	O	0
			44	40	4	
27	2	1	Total	C	O	0
			44	40	4	
27	3	1	Total	C	O	0
			44	40	4	
27	4	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
27	5	1	Total	C	O	0
			44	40	4	
27	6	1	Total	C	O	0
			44	40	4	
27	G	1	Total	C	O	0
			44	40	4	
27	N	1	Total	C	O	0
			44	40	4	
27	R	1	Total	C	O	0
			44	40	4	
27	Y	1	Total	C	O	0
			44	40	4	
27	0	1	Total	C	O	0
			44	40	4	
27	7	1	Total	C	O	0
			44	40	4	
27	8	1	Total	C	O	0
			44	40	4	
27	9	1	Total	C	O	0
			44	40	4	
27	p	1	Total	C	O	0
			44	40	4	
27	q	1	Total	C	O	0
			44	40	4	
27	g	1	Total	C	O	0
			44	40	4	
27	n	1	Total	C	O	0
			44	40	4	
27	y	1	Total	C	O	0
			44	40	4	
27	r	1	Total	C	O	0
			44	40	4	

- Molecule 28 is (1R,3R)-6-[(3E,5E,7E,9E,11E,13E,15E,17E)-18-[(1S,4R,6R)-4-HYDROXY-2,2,6-TRIMETHYL-7-OXABICYCLO[4.1.0]HEPT-1-YL]-3,7,12,16-TETRAMETHYLOCTA DECA-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C₄₀H₅₆O₄).



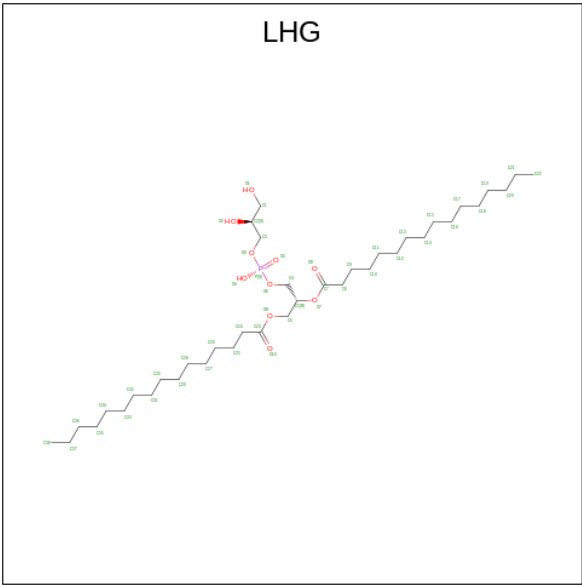
Mol	Chain	Residues	Atoms			AltConf
28	1	1	Total	C	O	0
			44	40	4	
28	2	1	Total	C	O	0
			44	40	4	
28	3	1	Total	C	O	0
			44	40	4	
28	4	1	Total	C	O	0
			44	40	4	
28	5	1	Total	C	O	0
			44	40	4	
28	6	1	Total	C	O	0
			44	40	4	
28	G	1	Total	C	O	0
			44	40	4	
28	N	1	Total	C	O	0
			44	40	4	
28	R	1	Total	C	O	0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

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Mol	Chain	Residues	Atoms			AltConf
28	9	1	Total	C	O	0
			44	40	4	
28	p	1	Total	C	O	0
			44	40	4	
28	q	1	Total	C	O	0
			44	40	4	
28	g	1	Total	C	O	0
			44	40	4	
28	n	1	Total	C	O	0
			44	40	4	
28	s	1	Total	C	O	0
			44	40	4	
28	y	1	Total	C	O	0
			44	40	4	
28	r	1	Total	C	O	0
			44	40	4	

- Molecule 29 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



Mol	Chain	Residues	Atoms				AltConf
29	1	1	Total	C	O	P	0
			49	38	10	1	
29	2	1	Total	C	O	P	0
			49	38	10	1	
29	3	1	Total	C	O	P	0
			49	38	10	1	

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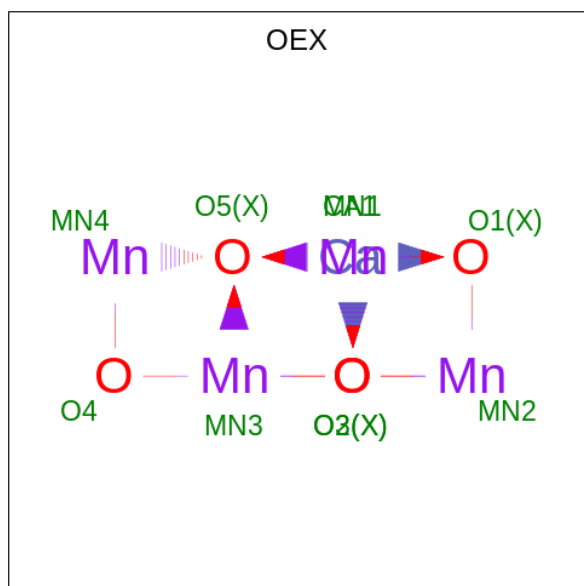
Mol	Chain	Residues	Atoms				AltConf
29	4	1	Total 49	C 38	O 10	P 1	0
29	5	1	Total 49	C 38	O 10	P 1	0
29	6	1	Total 49	C 38	O 10	P 1	0
29	C	1	Total 47	C 36	O 10	P 1	0
29	D	1	Total 132	C 99	O 30	P 3	0
29	D	1	Total 132	C 99	O 30	P 3	0
29	D	1	Total 132	C 99	O 30	P 3	0
29	G	1	Total 49	C 38	O 10	P 1	0
29	L	1	Total 49	C 38	O 10	P 1	0
29	N	1	Total 49	C 38	O 10	P 1	0
29	R	1	Total 38	C 27	O 10	P 1	0
29	S	1	Total 45	C 34	O 10	P 1	0
29	Y	1	Total 49	C 38	O 10	P 1	0
29	0	1	Total 49	C 38	O 10	P 1	0
29	7	1	Total 49	C 38	O 10	P 1	0
29	8	1	Total 49	C 38	O 10	P 1	0
29	9	1	Total 49	C 38	O 10	P 1	0
29	p	1	Total 49	C 38	O 10	P 1	0
29	q	1	Total 49	C 38	O 10	P 1	0
29	c	1	Total 47	C 36	O 10	P 1	0
29	d	1	Total 132	C 99	O 30	P 3	0

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Mol	Chain	Residues	Atoms				AltConf
29	d	1	Total	C	O	P	0
			132	99	30	3	
29	d	1	Total	C	O	P	0
			132	99	30	3	
29	g	1	Total	C	O	P	0
			49	38	10	1	
29	l	1	Total	C	O	P	0
			49	38	10	1	
29	n	1	Total	C	O	P	0
			49	38	10	1	
29	s	1	Total	C	O	P	0
			45	34	10	1	
29	y	1	Total	C	O	P	0
			49	38	10	1	
29	r	1	Total	C	O	P	0
			38	27	10	1	

- Molecule 30 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

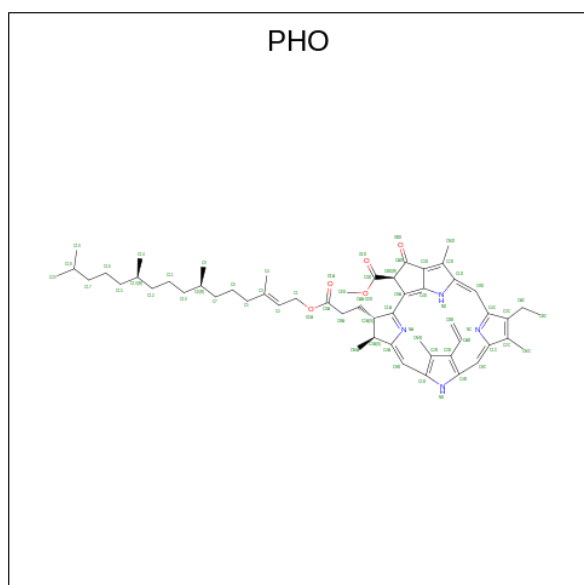
- Molecule 31 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 32 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

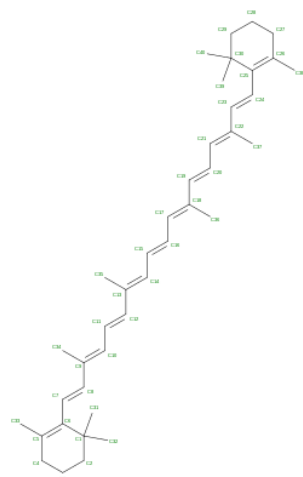
Mol	Chain	Residues	Atoms		AltConf
32	A	1	Total	Cl	0
			1	1	
32	a	1	Total	Cl	0
			1	1	

- Molecule 33 is PHEOPHYTIN A (three-letter code: PHO) (formula: C₅₅H₇₄N₄O₅).



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

- Molecule 34 is BETA-CAROTENE (three-letter code: BCR) (formula: C₄₀H₅₆).

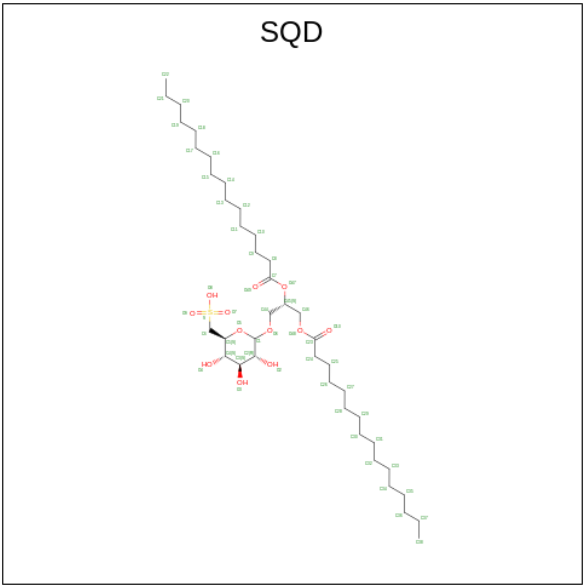


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Mol	Chain	Residues	Atoms		AltConf
34	c	1	Total	C	0
			160	160	
34	c	1	Total	C	0
			160	160	
34	c	1	Total	C	0
			160	160	
34	c	1	Total	C	0
			160	160	
34	d	1	Total	C	0
			40	40	
34	h	1	Total	C	0
			40	40	

- Molecule 35 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: C₄₁H₇₈O₁₂S).



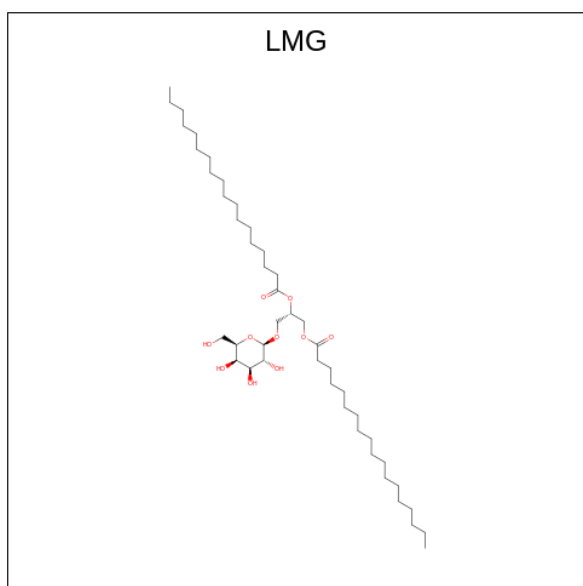
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	O	S	0
			51	38	12	1	
35	B	1	Total	C	O	S	0
			104	78	24	2	
35	B	1	Total	C	O	S	0
			104	78	24	2	
35	D	1	Total	C	O	S	0
			52	39	12	1	
35	a	1	Total	C	O	S	0
			51	38	12	1	

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Mol	Chain	Residues	Atoms				AltConf
35	b	1	Total	C	O	S	0
			104	78	24	2	
35	b	1	Total	C	O	S	0
			104	78	24	2	
35	d	1	Total	C	O	S	0
			52	39	12	1	

- Molecule 36 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



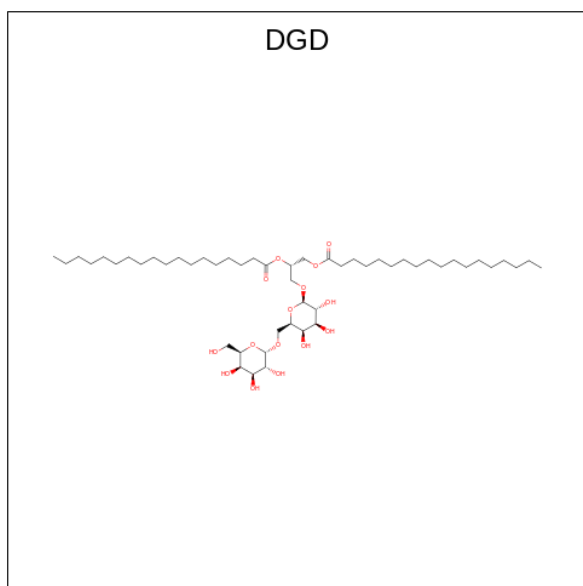
Mol	Chain	Residues	Atoms				AltConf
36	A	1	Total	C	O		0
			48	38	10		
36	B	1	Total	C	O		0
			51	41	10		
36	C	1	Total	C	O		0
			51	41	10		
36	D	1	Total	C	O		0
			92	72	20		
36	D	1	Total	C	O		0
			92	72	20		
36	H	1	Total	C	O		0
			48	38	10		
36	S	1	Total	C	O		0
			52	42	10		
36	a	1	Total	C	O		0
			48	38	10		

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Mol	Chain	Residues	Atoms			AltConf
36	b	1	Total	C	O	0
			51	41	10	
36	c	1	Total	C	O	0
			51	41	10	
36	d	1	Total	C	O	0
			92	72	20	
36	d	1	Total	C	O	0
			92	72	20	
36	h	1	Total	C	O	0
			48	38	10	
36	s	1	Total	C	O	0
			52	42	10	

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



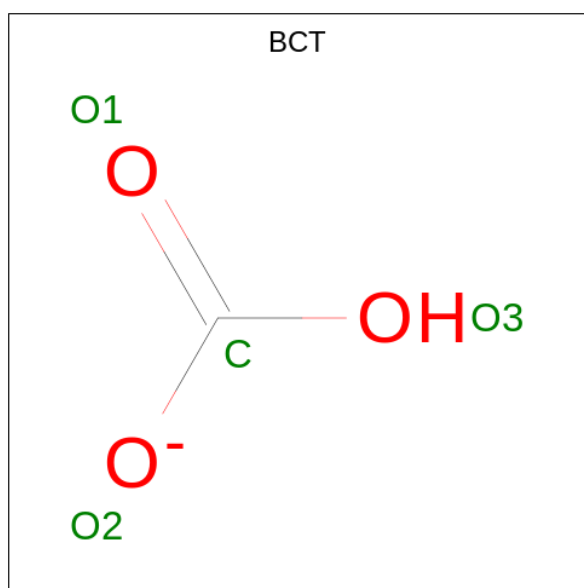
Mol	Chain	Residues	Atoms			AltConf
37	C	1	Total	C	O	0
			308	233	75	
37	C	1	Total	C	O	0
			308	233	75	
37	C	1	Total	C	O	0
			308	233	75	
37	C	1	Total	C	O	0
			308	233	75	
37	C	1	Total	C	O	0
			308	233	75	

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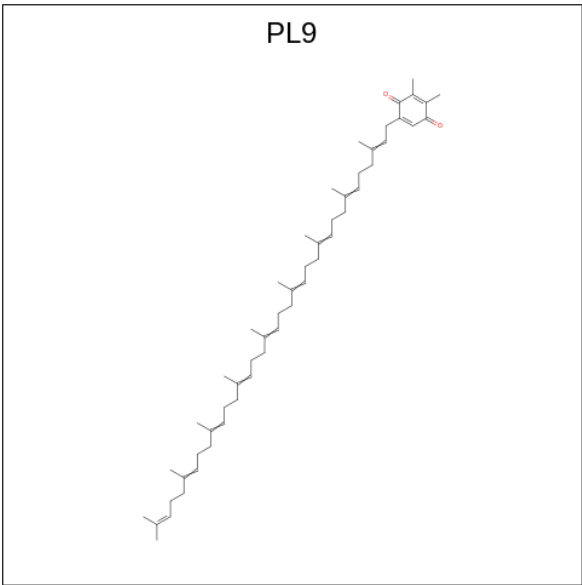
Mol	Chain	Residues	Atoms			AltConf
37	c	1	Total	C	O	0
			308	233	75	
37	c	1	Total	C	O	0
			308	233	75	
37	c	1	Total	C	O	0
			308	233	75	
37	c	1	Total	C	O	0
			308	233	75	
37	c	1	Total	C	O	0
			308	233	75	

- Molecule 38 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



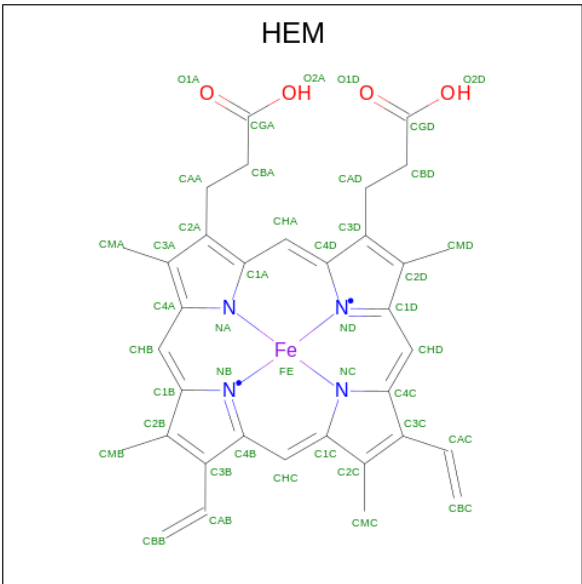
Mol	Chain	Residues	Atoms			AltConf
38	D	1	Total	C	O	0
			4	1	3	
38	d	1	Total	C	O	0
			4	1	3	

- Molecule 39 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
39	D	1	Total	C	O	0
			55	53	2	
39	d	1	Total	C	O	0
			55	53	2	

- Molecule 40 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: $C_{34}H_{32}FeN_4O_4$).



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

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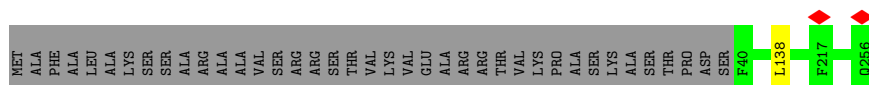
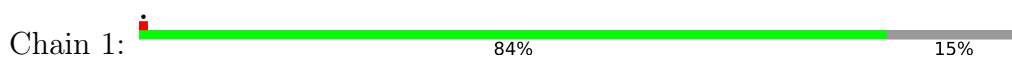
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Mol	Chain	Residues	Atoms					AltConf
			Total	C	Fe	N	O	
40	f	1	43	34	1	4	4	0

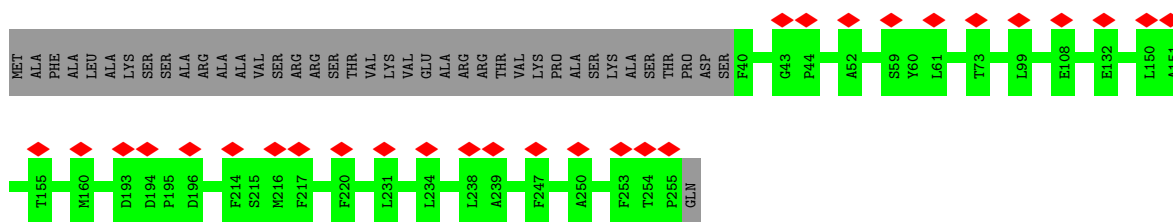
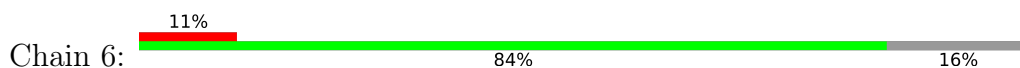
3 Residue-property plots [i](#)

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

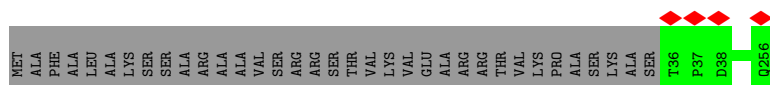
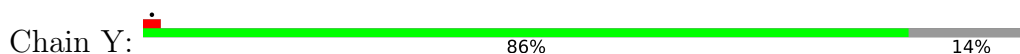
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic



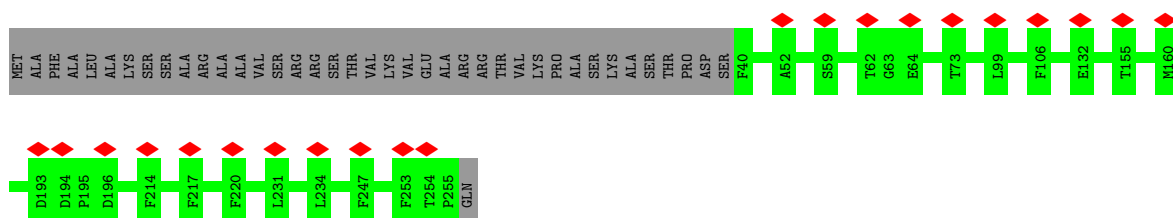
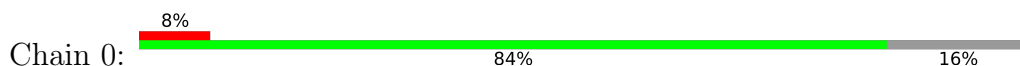
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic




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

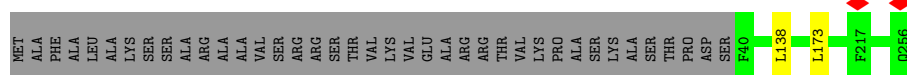


- Molecule 1: Chlorophyll a-b binding protein, chloroplastic




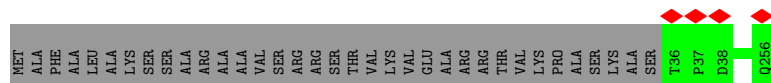
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain 7:  84% 15%




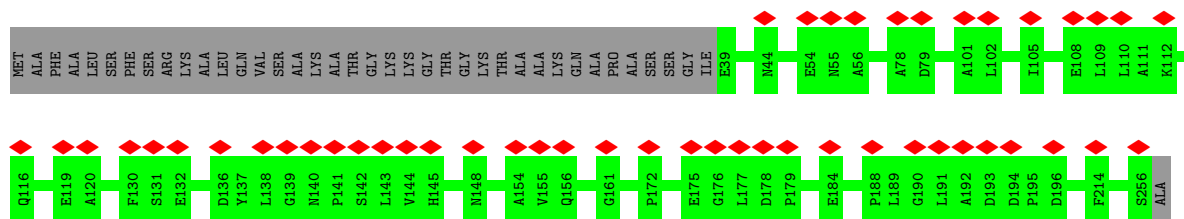
- Molecule 1: Chlorophyll a-b binding protein, chloroplastic

Chain y:  86% 14%




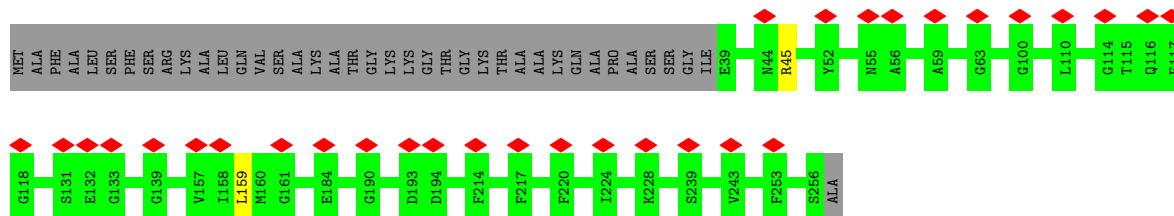
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 2:  19% 85% 15%




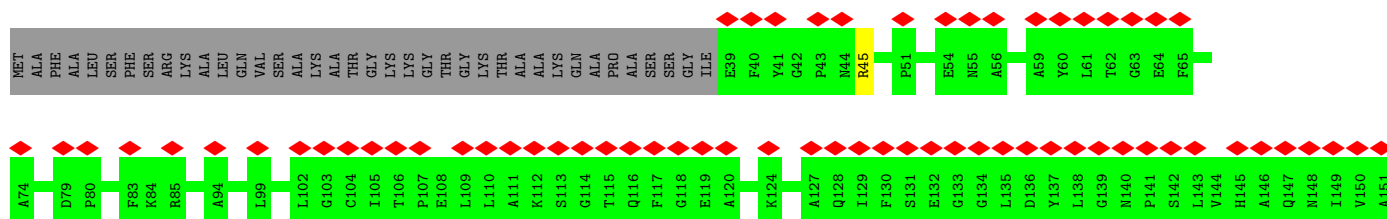
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

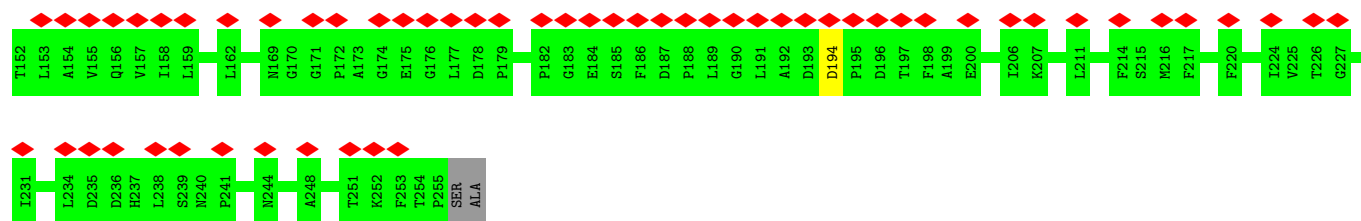
Chain 3:  12% 84% 15%



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

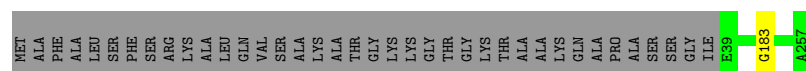
Chain 5:  48% 84% 16%





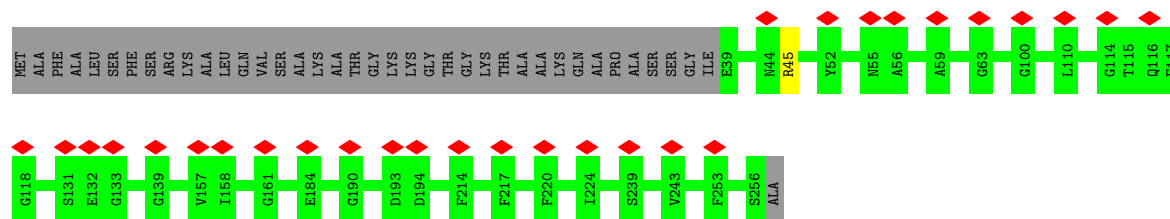
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain N: 85% 15%



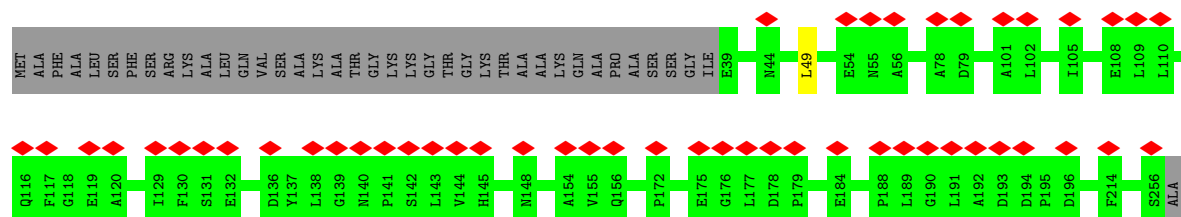
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain 8: 11% 84% 15%



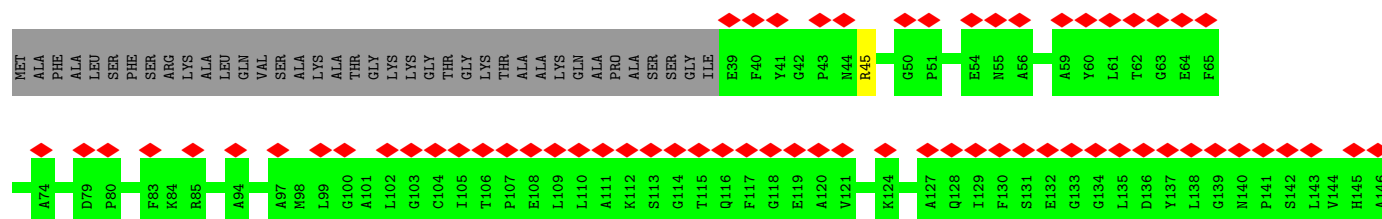
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

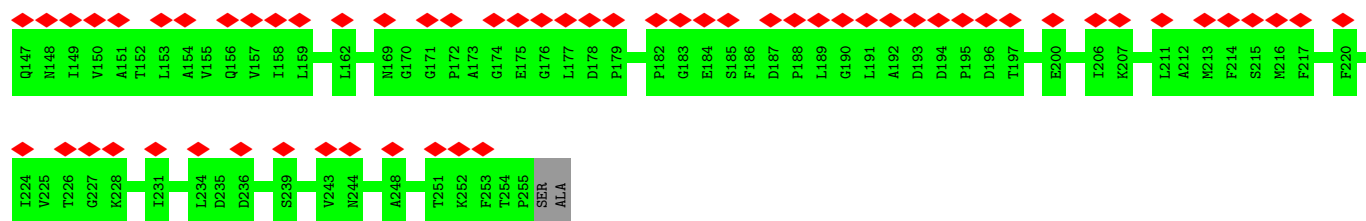
Chain 9: 19% 84% 15%



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

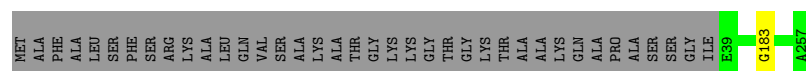
Chain p: 49% 84% 16%





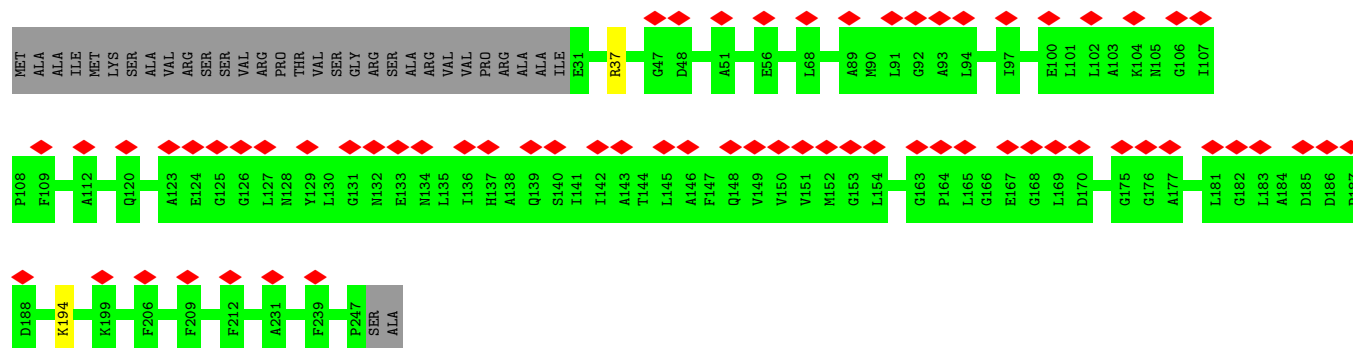
- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

Chain n: 85% 15%



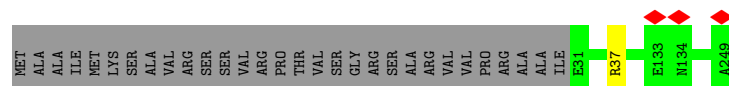
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain 4: 27% 86% 13%



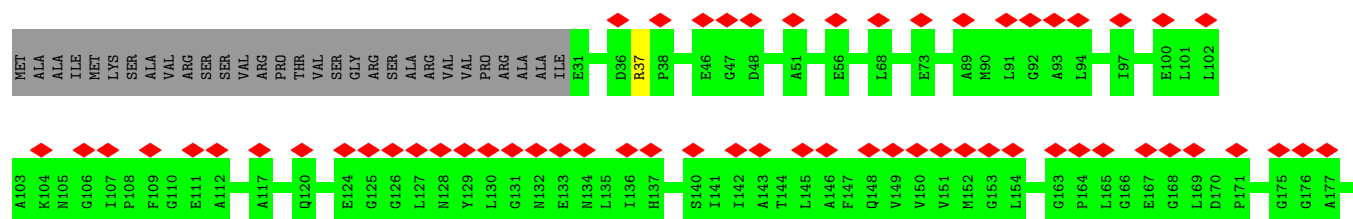
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

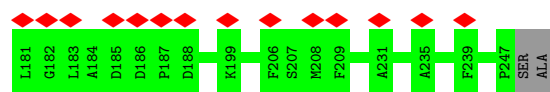
Chain G: 88% 12%



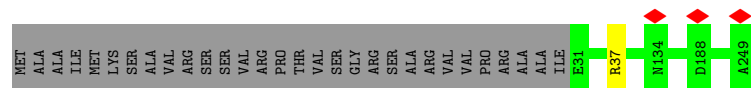
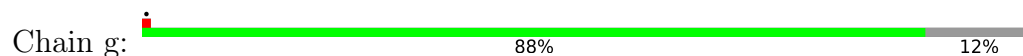
- Molecule 3: Chlorophyll a-b binding protein, chloroplastic

Chain q: 30% 87% 13%

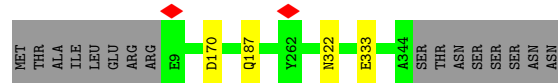




- Molecule 3: Chlorophyll a-b binding protein, chloroplastic



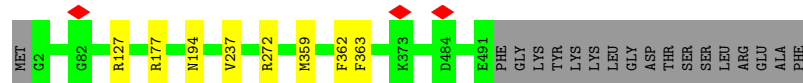
- Molecule 4: Photosystem II protein D1



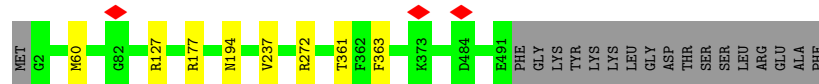
- Molecule 4: Photosystem II protein D1



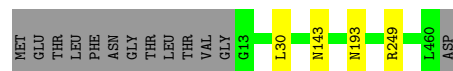
- Molecule 5: Photosystem II CP47 reaction center protein



- Molecule 5: Photosystem II CP47 reaction center protein

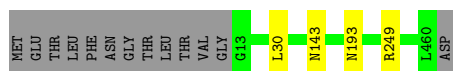


- Molecule 6: Photosystem II CP43 reaction center protein



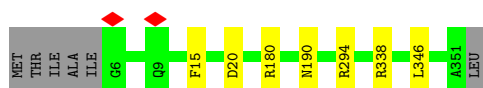
- Molecule 6: Photosystem II CP43 reaction center protein

Chain c:  96%



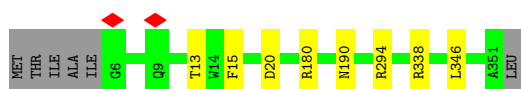
• Molecule 7: Photosystem II D2 protein

Chain D:  96%




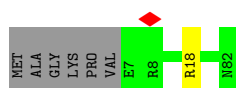
• Molecule 7: Photosystem II D2 protein

Chain d:  96%




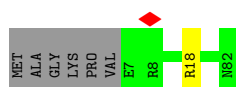
• Molecule 8: Cytochrome b559 subunit alpha

Chain E:  91%



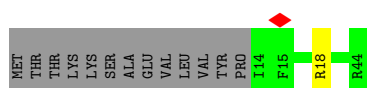
• Molecule 8: Cytochrome b559 subunit alpha

Chain e:  91%



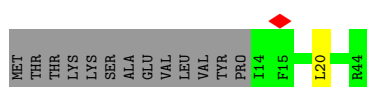
• Molecule 9: Cytochrome b559 subunit beta

Chain F:  68%



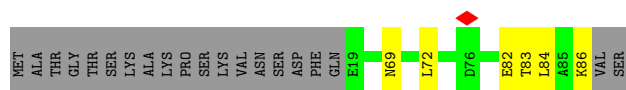
• Molecule 9: Cytochrome b559 subunit beta

Chain f:  68%



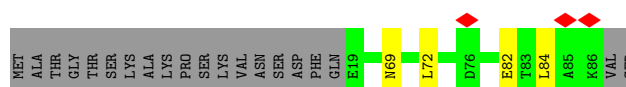
- Molecule 10: Photosystem II reaction center protein H

Chain H:  70% 7% 23%



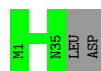
- Molecule 10: Photosystem II reaction center protein H

Chain h:  73% 5% 23%



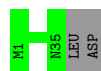
- Molecule 11: Photosystem II reaction center protein I

Chain I:  95% 5%




- Molecule 11: Photosystem II reaction center protein I

Chain i:  95% 5%




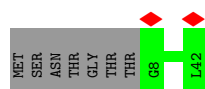
- Molecule 12: Photosystem II reaction center protein J

Chain J:  5% 83% 17%




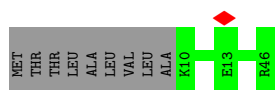
- Molecule 12: Photosystem II reaction center protein J

Chain j:  5% 83% 17%

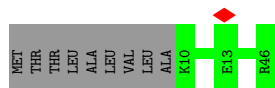
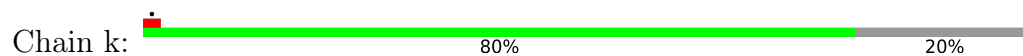


- Molecule 13: Photosystem II reaction center protein K

Chain K:  80% 20%



- Molecule 13: Photosystem II reaction center protein K



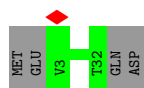
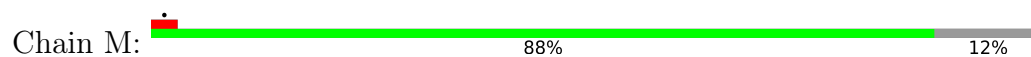
- Molecule 14: Photosystem II reaction center protein L



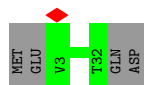
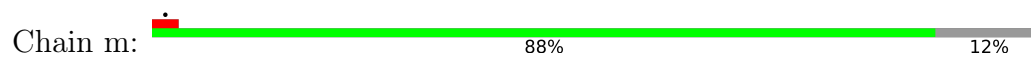
- Molecule 14: Photosystem II reaction center protein L



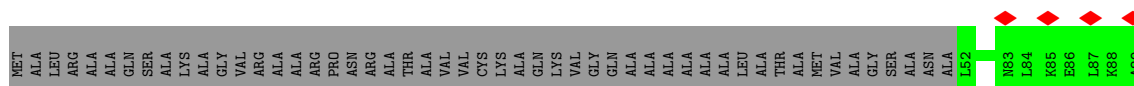
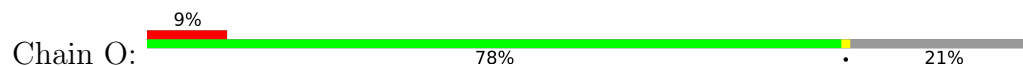
- Molecule 15: Photosystem II reaction center protein M

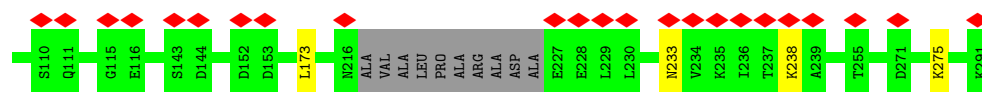


- Molecule 15: Photosystem II reaction center protein M

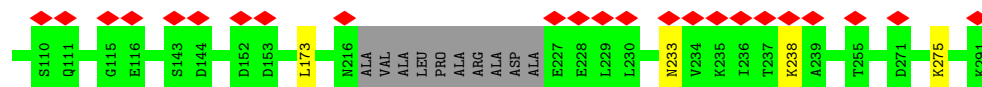
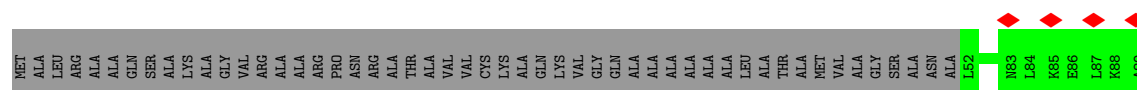
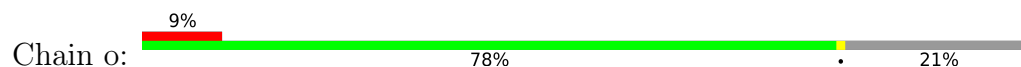


- Molecule 16: Oxygen-evolving enhancer protein 1, chloroplastic

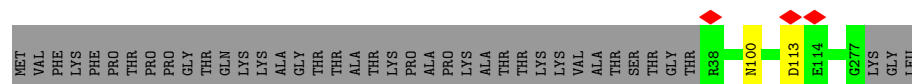
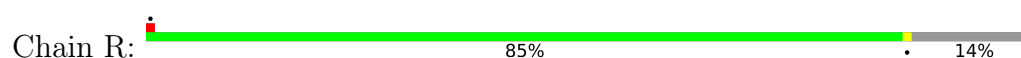




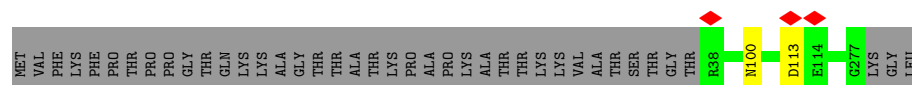
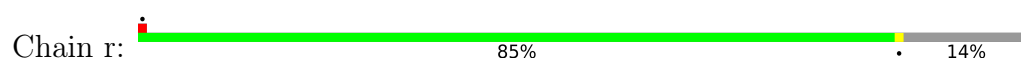
- Molecule 16: Oxygen-evolving enhancer protein 1, chloroplastic



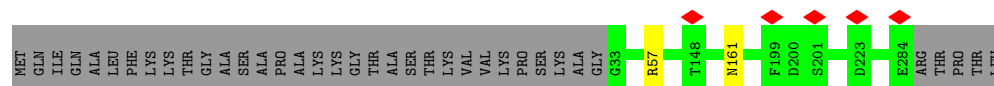
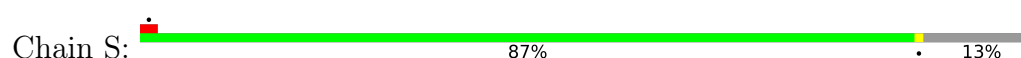
- Molecule 17: Chlorophyll a-b binding protein CP29



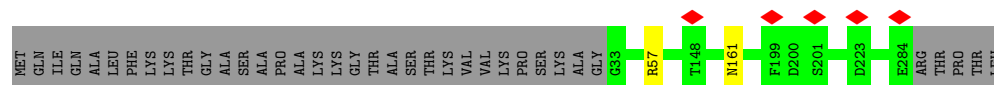
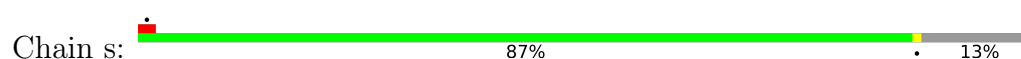
- Molecule 17: Chlorophyll a-b binding protein CP29



- Molecule 18: Chlorophyll a-b binding protein, chloroplastic



- Molecule 18: Chlorophyll a-b binding protein, chloroplastic



- Molecule 19: Photosystem II reaction center protein T





- Molecule 19: Photosystem II reaction center protein T



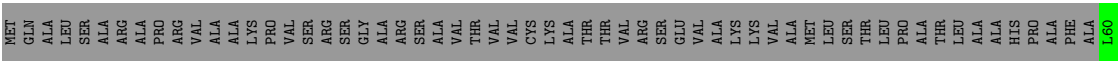
- Molecule 20: Photosystem II reaction center protein Ycf12



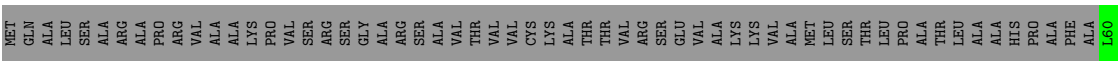
- Molecule 20: Photosystem II reaction center protein Ycf12



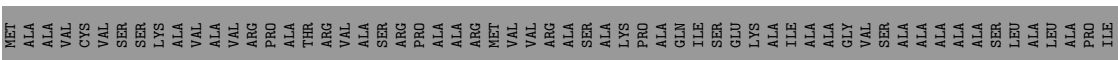
- Molecule 21: Photosystem II reaction center W protein, chloroplastic



- Molecule 21: Photosystem II reaction center W protein, chloroplastic

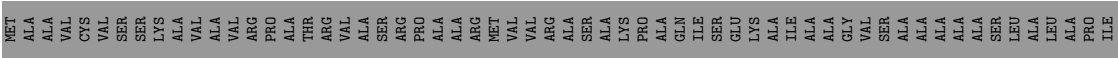


- Molecule 22: 4.1 kDa photosystem II subunit

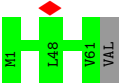




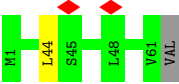
- Molecule 22: 4.1 kDa photosystem II subunit



- Molecule 23: Photosystem II reaction center protein Z



- Molecule 23: Photosystem II reaction center protein Z



4 Experimental information

Property	Value	Source
EM reconstruction method	SINGLE PARTICLE	Depositor
Imposed symmetry	POINT, C2	Depositor
Number of particles used	118423	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TALOS ARCTICA	Depositor
Voltage (kV)	200	Depositor
Electron dose ($e^-/\text{\AA}^2$)	1.31	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	0.082	Depositor
Minimum map value	-0.035	Depositor
Average map value	0.000	Depositor
Map value standard deviation	0.003	Depositor
Recommended contour level	0.012	Depositor
Map size (\AA)	506.88, 506.88, 506.88	wwPDB
Map dimensions	384, 384, 384	wwPDB
Map angles ($^\circ$)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (\AA)	1.32, 1.32, 1.32	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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	0	0.32	0/1708	0.57	0/2322
1	1	0.37	0/1717	0.58	1/2334 (0.0%)
1	6	0.33	0/1708	0.56	0/2322
1	7	0.37	0/1717	0.57	1/2334 (0.0%)
1	Y	0.47	0/1746	0.55	0/2375
1	y	0.47	0/1746	0.56	0/2375
2	2	0.32	0/1715	0.52	0/2334
2	3	0.30	0/1715	0.52	0/2334
2	5	0.29	0/1709	0.54	1/2326 (0.0%)
2	8	0.30	0/1715	0.52	0/2334
2	9	0.32	0/1715	0.56	1/2334 (0.0%)
2	N	0.39	0/1720	0.54	0/2341
2	n	0.39	0/1720	0.53	0/2341
2	p	0.28	0/1709	0.51	0/2326
3	4	0.30	0/1706	0.52	0/2322
3	G	0.38	0/1717	0.54	0/2337
3	g	0.37	0/1717	0.53	0/2337
3	q	0.31	0/1706	0.54	0/2322
4	A	0.52	1/2718 (0.0%)	0.61	2/3706 (0.1%)
4	a	0.52	1/2718 (0.0%)	0.61	2/3706 (0.1%)
5	B	0.46	0/3964	0.56	0/5397
5	b	0.47	0/3964	0.56	1/5397 (0.0%)
6	C	0.46	0/3611	0.55	0/4920
6	c	0.46	0/3611	0.55	0/4920
7	D	0.51	0/2850	0.61	0/3887
7	d	0.51	0/2850	0.61	0/3887
8	E	0.36	0/637	0.54	0/869
8	e	0.36	0/637	0.55	0/869
9	F	0.39	0/258	0.58	0/349
9	f	0.40	0/258	0.60	0/349
10	H	0.45	0/530	0.64	1/725 (0.1%)

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
10	h	0.44	0/530	0.64	1/725 (0.1%)
11	I	0.53	0/291	0.62	0/394
11	i	0.53	0/291	0.62	0/394
12	J	0.38	0/261	0.57	0/356
12	j	0.38	0/261	0.58	0/356
13	K	0.45	0/309	0.66	0/425
13	k	0.45	0/309	0.66	0/425
14	L	0.53	0/314	0.65	0/427
14	l	0.53	0/314	0.65	0/427
15	M	0.45	0/234	0.57	0/321
15	m	0.45	0/234	0.57	0/321
16	O	0.33	0/1771	0.59	1/2386 (0.0%)
16	o	0.33	0/1771	0.58	1/2386 (0.0%)
17	R	0.40	0/1866	0.59	1/2529 (0.0%)
17	r	0.40	0/1866	0.59	1/2529 (0.0%)
18	S	0.37	0/1961	0.54	0/2670
18	s	0.38	0/1961	0.55	0/2670
19	T	0.43	0/254	0.58	0/343
19	t	0.43	0/254	0.59	0/343
20	V	0.31	0/232	0.63	0/317
20	v	0.31	0/232	0.63	0/317
21	W	0.40	0/445	0.60	0/603
21	w	0.40	0/445	0.58	0/603
22	X	0.31	0/235	0.53	0/319
22	x	0.31	0/235	0.53	0/319
23	Z	0.33	0/469	0.58	0/644
23	z	0.33	0/469	0.62	1/644 (0.2%)
All	All	0.41	2/77326 (0.0%)	0.57	16/105224 (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
2	N	0	1
2	n	0	1
All	All	0	2

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
4	a	170	ASP	C-N	5.12	1.42	1.33
4	A	170	ASP	C-N	5.12	1.42	1.33

All (16) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
2	9	49	LEU	CA-CB-CG	7.09	131.60	115.30
5	b	60	MET	CG-SD-CE	-6.59	89.66	100.20
1	7	138	LEU	CA-CB-CG	6.33	129.87	115.30
17	r	113	ASP	CB-CG-OD1	5.98	123.68	118.30
17	R	113	ASP	CB-CG-OD1	5.93	123.64	118.30
4	A	333	GLU	O-C-N	5.93	132.18	122.70
4	a	333	GLU	O-C-N	5.85	132.07	122.70
2	5	194	ASP	CB-CG-OD1	5.64	123.37	118.30
10	h	72	LEU	CA-CB-CG	5.52	128.00	115.30
1	1	138	LEU	CA-CB-CG	5.47	127.89	115.30
16	O	173	LEU	CA-CB-CG	5.41	127.73	115.30
16	o	173	LEU	CA-CB-CG	5.34	127.59	115.30
10	H	72	LEU	CA-CB-CG	5.33	127.56	115.30
4	A	333	GLU	CA-C-N	-5.26	105.62	117.20
23	z	44	LEU	CA-CB-CG	5.26	127.40	115.30
4	a	333	GLU	CA-C-N	-5.21	105.75	117.20

There are no chirality outliers.

All (2) planarity outliers are listed below:

Mol	Chain	Res	Type	Group
2	N	183	GLY	Peptide
2	n	183	GLY	Peptide

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	0	214/256 (84%)	201 (94%)	13 (6%)	0	100	100
1	1	215/256 (84%)	201 (94%)	14 (6%)	0	100	100
1	6	214/256 (84%)	198 (92%)	16 (8%)	0	100	100
1	7	215/256 (84%)	198 (92%)	17 (8%)	0	100	100
1	Y	219/256 (86%)	204 (93%)	15 (7%)	0	100	100
1	y	219/256 (86%)	206 (94%)	13 (6%)	0	100	100
2	2	216/257 (84%)	197 (91%)	19 (9%)	0	100	100
2	3	216/257 (84%)	197 (91%)	19 (9%)	0	100	100
2	5	215/257 (84%)	195 (91%)	20 (9%)	0	100	100
2	8	216/257 (84%)	194 (90%)	22 (10%)	0	100	100
2	9	216/257 (84%)	196 (91%)	20 (9%)	0	100	100
2	N	217/257 (84%)	195 (90%)	22 (10%)	0	100	100
2	n	217/257 (84%)	198 (91%)	19 (9%)	0	100	100
2	p	215/257 (84%)	199 (93%)	16 (7%)	0	100	100
3	4	215/249 (86%)	194 (90%)	21 (10%)	0	100	100
3	G	217/249 (87%)	197 (91%)	20 (9%)	0	100	100
3	g	217/249 (87%)	199 (92%)	18 (8%)	0	100	100
3	q	215/249 (86%)	194 (90%)	21 (10%)	0	100	100
4	A	334/352 (95%)	316 (95%)	18 (5%)	0	100	100
4	a	334/352 (95%)	318 (95%)	16 (5%)	0	100	100
5	B	488/508 (96%)	458 (94%)	30 (6%)	0	100	100
5	b	488/508 (96%)	460 (94%)	28 (6%)	0	100	100
6	C	446/461 (97%)	414 (93%)	32 (7%)	0	100	100
6	c	446/461 (97%)	414 (93%)	32 (7%)	0	100	100
7	D	344/352 (98%)	327 (95%)	17 (5%)	0	100	100
7	d	344/352 (98%)	326 (95%)	18 (5%)	0	100	100
8	E	74/82 (90%)	67 (90%)	7 (10%)	0	100	100
8	e	74/82 (90%)	67 (90%)	7 (10%)	0	100	100
9	F	29/44 (66%)	29 (100%)	0	0	100	100
9	f	29/44 (66%)	28 (97%)	1 (3%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
10	H	66/88 (75%)	60 (91%)	6 (9%)	0	100	100
10	h	66/88 (75%)	62 (94%)	4 (6%)	0	100	100
11	I	33/37 (89%)	33 (100%)	0	0	100	100
11	i	33/37 (89%)	33 (100%)	0	0	100	100
12	J	33/42 (79%)	31 (94%)	2 (6%)	0	100	100
12	j	33/42 (79%)	31 (94%)	2 (6%)	0	100	100
13	K	35/46 (76%)	33 (94%)	2 (6%)	0	100	100
13	k	35/46 (76%)	32 (91%)	3 (9%)	0	100	100
14	L	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
14	l	35/38 (92%)	34 (97%)	1 (3%)	0	100	100
15	M	28/34 (82%)	26 (93%)	2 (7%)	0	100	100
15	m	28/34 (82%)	26 (93%)	2 (7%)	0	100	100
16	O	226/291 (78%)	201 (89%)	25 (11%)	0	100	100
16	o	226/291 (78%)	202 (89%)	24 (11%)	0	100	100
17	R	238/280 (85%)	221 (93%)	16 (7%)	1 (0%)	34	67
17	r	238/280 (85%)	221 (93%)	16 (7%)	1 (0%)	34	67
18	S	250/289 (86%)	224 (90%)	26 (10%)	0	100	100
18	s	250/289 (86%)	223 (89%)	27 (11%)	0	100	100
19	T	28/31 (90%)	28 (100%)	0	0	100	100
19	t	28/31 (90%)	27 (96%)	1 (4%)	0	100	100
20	V	31/33 (94%)	29 (94%)	2 (6%)	0	100	100
20	v	31/33 (94%)	29 (94%)	2 (6%)	0	100	100
21	W	54/115 (47%)	48 (89%)	6 (11%)	0	100	100
21	w	54/115 (47%)	48 (89%)	6 (11%)	0	100	100
22	X	32/101 (32%)	32 (100%)	0	0	100	100
22	x	32/101 (32%)	32 (100%)	0	0	100	100
23	Z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
23	z	59/62 (95%)	58 (98%)	1 (2%)	0	100	100
All	All	9614/11160 (86%)	8903 (93%)	709 (7%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
17	R	100	ASN
17	r	100	ASN

5.3.2 Protein sidechains ⓘ

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	0	165/196 (84%)	165 (100%)	0	100	100
1	1	166/196 (85%)	166 (100%)	0	100	100
1	6	165/196 (84%)	165 (100%)	0	100	100
1	7	166/196 (85%)	165 (99%)	1 (1%)	86	94
1	Y	170/196 (87%)	170 (100%)	0	100	100
1	y	170/196 (87%)	170 (100%)	0	100	100
2	2	169/194 (87%)	169 (100%)	0	100	100
2	3	169/194 (87%)	167 (99%)	2 (1%)	71	85
2	5	168/194 (87%)	167 (99%)	1 (1%)	86	94
2	8	169/194 (87%)	168 (99%)	1 (1%)	86	94
2	9	169/194 (87%)	169 (100%)	0	100	100
2	N	169/194 (87%)	169 (100%)	0	100	100
2	n	169/194 (87%)	169 (100%)	0	100	100
2	p	168/194 (87%)	167 (99%)	1 (1%)	86	94
3	4	163/187 (87%)	161 (99%)	2 (1%)	71	85
3	G	164/187 (88%)	163 (99%)	1 (1%)	86	94
3	g	164/187 (88%)	163 (99%)	1 (1%)	86	94
3	q	163/187 (87%)	162 (99%)	1 (1%)	86	94
4	A	274/289 (95%)	272 (99%)	2 (1%)	84	92
4	a	274/289 (95%)	272 (99%)	2 (1%)	84	92
5	B	392/407 (96%)	384 (98%)	8 (2%)	55	77
5	b	392/407 (96%)	385 (98%)	7 (2%)	59	79

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
6	C	351/362 (97%)	347 (99%)	4 (1%)	73	86
6	c	351/362 (97%)	347 (99%)	4 (1%)	73	86
7	D	276/281 (98%)	269 (98%)	7 (2%)	47	72
7	d	276/281 (98%)	268 (97%)	8 (3%)	42	69
8	E	67/71 (94%)	66 (98%)	1 (2%)	65	82
8	e	67/71 (94%)	66 (98%)	1 (2%)	65	82
9	F	25/37 (68%)	24 (96%)	1 (4%)	31	60
9	f	25/37 (68%)	24 (96%)	1 (4%)	31	60
10	H	58/75 (77%)	53 (91%)	5 (9%)	10	35
10	h	58/75 (77%)	55 (95%)	3 (5%)	23	53
11	I	32/34 (94%)	32 (100%)	0	100	100
11	i	32/34 (94%)	32 (100%)	0	100	100
12	J	26/32 (81%)	26 (100%)	0	100	100
12	j	26/32 (81%)	26 (100%)	0	100	100
13	K	31/38 (82%)	31 (100%)	0	100	100
13	k	31/38 (82%)	31 (100%)	0	100	100
14	L	34/35 (97%)	33 (97%)	1 (3%)	42	69
14	l	34/35 (97%)	33 (97%)	1 (3%)	42	69
15	M	26/30 (87%)	26 (100%)	0	100	100
15	m	26/30 (87%)	26 (100%)	0	100	100
16	O	190/222 (86%)	187 (98%)	3 (2%)	62	81
16	o	190/222 (86%)	187 (98%)	3 (2%)	62	81
17	R	187/218 (86%)	187 (100%)	0	100	100
17	r	187/218 (86%)	187 (100%)	0	100	100
18	S	189/217 (87%)	187 (99%)	2 (1%)	73	86
18	s	189/217 (87%)	187 (99%)	2 (1%)	73	86
19	T	27/28 (96%)	26 (96%)	1 (4%)	34	62
19	t	27/28 (96%)	26 (96%)	1 (4%)	34	62
20	V	27/27 (100%)	26 (96%)	1 (4%)	34	62
20	v	27/27 (100%)	26 (96%)	1 (4%)	34	62
21	W	44/87 (51%)	44 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
21	w	44/87 (51%)	44 (100%)	0	100	100
22	X	24/67 (36%)	24 (100%)	0	100	100
22	x	24/67 (36%)	24 (100%)	0	100	100
23	Z	51/52 (98%)	51 (100%)	0	100	100
23	z	51/52 (98%)	51 (100%)	0	100	100
All	All	7668/8694 (88%)	7587 (99%)	81 (1%)	74	86

All (81) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
2	3	45	ARG
2	3	159	LEU
3	4	37	ARG
3	4	194	LYS
2	5	45	ARG
4	A	187	GLN
4	A	322	ASN
5	B	127	ARG
5	B	177	ARG
5	B	194	ASN
5	B	237	VAL
5	B	272	ARG
5	B	359	MET
5	B	362	PHE
5	B	363	PHE
6	C	30	LEU
6	C	143	ASN
6	C	193	ASN
6	C	249	ARG
7	D	15	PHE
7	D	20	ASP
7	D	180	ARG
7	D	190	ASN
7	D	294	ARG
7	D	338	ARG
7	D	346	LEU
8	E	18	ARG
9	F	18	ARG
3	G	37	ARG
10	H	69	ASN

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Mol	Chain	Res	Type
10	H	82	GLU
10	H	83	THR
10	H	84	LEU
10	H	86	LYS
14	L	5	ASN
16	O	233	ASN
16	O	238	LYS
16	O	275	LYS
18	S	57	ARG
18	S	161	ASN
19	T	24	ARG
20	V	32	ASN
1	7	173	LEU
2	8	45	ARG
2	p	45	ARG
3	q	37	ARG
4	a	187	GLN
4	a	322	ASN
5	b	127	ARG
5	b	177	ARG
5	b	194	ASN
5	b	237	VAL
5	b	272	ARG
5	b	361	THR
5	b	363	PHE
6	c	30	LEU
6	c	143	ASN
6	c	193	ASN
6	c	249	ARG
7	d	13	THR
7	d	15	PHE
7	d	20	ASP
7	d	180	ARG
7	d	190	ASN
7	d	294	ARG
7	d	338	ARG
7	d	346	LEU
8	e	18	ARG
9	f	20	LEU
3	g	37	ARG
10	h	69	ASN
10	h	82	GLU

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Mol	Chain	Res	Type
10	h	84	LEU
14	l	5	ASN
18	s	57	ARG
18	s	161	ASN
19	t	24	ARG
20	v	32	ASN
16	o	233	ASN
16	o	238	LYS
16	o	275	LYS

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (57) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	233	ASN
3	4	120	GLN
1	6	128	GLN
1	6	156	GLN
1	6	240	ASN
4	A	303	ASN
4	A	304	GLN
4	A	322	ASN
5	B	58	GLN
5	B	157	HIS
5	B	194	ASN
6	C	56	ASN
6	C	143	ASN
6	C	193	ASN
6	C	320	GLN
7	D	137	ASN
7	D	190	ASN
8	E	61	GLN
3	G	214	GLN
3	G	225	ASN
14	L	5	ASN
16	O	233	ASN
16	O	266	GLN
17	R	56	ASN
17	R	94	GLN
17	R	119	ASN
18	S	161	ASN
20	V	32	ASN
1	0	233	ASN

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Mol	Chain	Res	Type
1	0	240	ASN
1	7	233	ASN
2	8	55	ASN
2	9	169	ASN
2	p	169	ASN
4	a	303	ASN
4	a	304	GLN
4	a	322	ASN
5	b	58	GLN
5	b	157	HIS
5	b	194	ASN
6	c	56	ASN
6	c	143	ASN
6	c	193	ASN
6	c	320	GLN
7	d	137	ASN
7	d	190	ASN
8	e	61	GLN
3	g	214	GLN
3	g	225	ASN
14	l	5	ASN
2	n	233	ASN
18	s	161	ASN
20	v	32	ASN
17	r	56	ASN
17	r	94	GLN
16	o	233	ASN
16	o	266	GLN

5.3.3 RNA ⓘ

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates ⓘ

There are no monosaccharides in this entry.

5.6 Ligand geometry

Of 560 ligands modelled in this entry, 4 are monoatomic - leaving 556 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
24	CHL	g	608	-	44,52,74	2.22	13 (29%)	46,87,114	3.13	18 (39%)
26	LUT	4	1621	-	42,43,43	0.76	0	51,60,60	1.50	11 (21%)
25	CLA	p	613	2	65,73,73	1.53	7 (10%)	76,113,113	1.31	7 (9%)
24	CHL	y	605	1	46,54,74	2.20	13 (28%)	49,90,114	3.06	20 (40%)
25	CLA	N	614	-	49,57,73	1.71	9 (18%)	55,93,113	1.43	7 (12%)
24	CHL	s	608	-	49,57,74	2.23	15 (30%)	52,93,114	3.06	20 (38%)
24	CHL	8	609	2	66,74,74	1.84	13 (19%)	73,114,114	2.64	22 (30%)
26	LUT	7	1620	-	42,43,43	0.79	1 (2%)	51,60,60	1.58	8 (15%)
24	CHL	3	601	2	66,74,74	1.89	13 (19%)	73,114,114	2.63	22 (30%)
24	CHL	6	608	-	50,58,74	2.15	14 (28%)	52,94,114	3.09	19 (36%)
25	CLA	3	603	-	65,73,73	1.48	10 (15%)	76,113,113	1.40	9 (11%)
25	CLA	7	610	1	65,73,73	1.46	8 (12%)	76,113,113	1.32	8 (10%)
25	CLA	5	612	2	45,53,73	1.82	9 (20%)	52,89,113	1.56	8 (15%)
25	CLA	B	610	-	65,73,73	1.44	10 (15%)	76,113,113	1.41	6 (7%)
25	CLA	n	614	-	49,57,73	1.70	9 (18%)	55,93,113	1.43	7 (12%)
25	CLA	N	612	2	45,53,73	1.81	10 (22%)	52,89,113	1.55	7 (13%)
25	CLA	6	611	29	65,73,73	1.47	6 (9%)	76,113,113	1.36	8 (10%)
25	CLA	S	611	29	49,57,73	1.65	10 (20%)	55,93,113	1.47	6 (10%)
25	CLA	8	603	-	65,73,73	1.47	10 (15%)	76,113,113	1.41	9 (11%)
25	CLA	c	506	-	65,73,73	1.52	10 (15%)	76,113,113	1.42	7 (9%)
25	CLA	D	402	-	65,73,73	1.53	10 (15%)	76,113,113	1.42	9 (11%)
25	CLA	y	602	1	65,73,73	1.42	8 (12%)	76,113,113	1.37	7 (9%)
28	NEX	q	1623	-	38,46,46	0.91	2 (5%)	50,70,70	2.34	17 (34%)
24	CHL	y	601	1	66,74,74	1.87	14 (21%)	73,114,114	2.76	24 (32%)
25	CLA	B	602	-	65,73,73	1.47	10 (15%)	76,113,113	1.21	5 (6%)
25	CLA	r	609	17	58,66,73	1.60	10 (17%)	67,104,113	1.44	6 (8%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	q	612	3	43,51,73	1.82	8 (18%)	49,86,113	1.62	9 (18%)
24	CHL	1	609	1	66,74,74	1.84	15 (22%)	73,114,114	2.65	21 (28%)
26	LUT	5	1620	-	42,43,43	0.76	0	51,60,60	1.83	13 (25%)
25	CLA	R	612	-	49,57,73	1.65	9 (18%)	55,93,113	1.54	8 (14%)
37	DGD	c	519	-	63,63,67	0.81	2 (3%)	77,77,81	1.15	6 (7%)
34	BCR	B	620	-	41,41,41	0.84	1 (2%)	56,56,56	1.87	19 (33%)
24	CHL	1	607	-	66,74,74	1.89	14 (21%)	73,114,114	2.58	25 (34%)
25	CLA	4	603	-	65,73,73	1.45	8 (12%)	76,113,113	1.48	9 (11%)
24	CHL	5	606	-	46,54,74	2.35	16 (34%)	49,90,114	2.95	18 (36%)
29	LHG	G	2630	25	48,48,48	0.89	2 (4%)	51,54,54	1.12	4 (7%)
25	CLA	c	511	6	65,73,73	1.45	10 (15%)	76,113,113	1.52	9 (11%)
25	CLA	6	602	1	65,73,73	1.49	8 (12%)	76,113,113	1.25	6 (7%)
25	CLA	C	503	-	65,73,73	1.45	11 (16%)	76,113,113	1.40	7 (9%)
24	CHL	6	601	1	66,74,74	1.88	13 (19%)	73,114,114	2.68	25 (34%)
25	CLA	B	606	-	65,73,73	1.46	9 (13%)	76,113,113	1.19	7 (9%)
25	CLA	p	611	29	49,57,73	1.72	6 (12%)	55,93,113	1.46	6 (10%)
24	CHL	q	606	-	50,58,74	2.34	16 (32%)	52,94,114	2.82	17 (32%)
25	CLA	a	406	-	65,73,73	1.42	11 (16%)	76,113,113	1.37	8 (10%)
25	CLA	7	612	1	65,73,73	1.49	10 (15%)	76,113,113	1.33	8 (10%)
25	CLA	B	612	-	65,73,73	1.48	10 (15%)	76,113,113	1.45	8 (10%)
25	CLA	g	614	-	49,57,73	1.70	9 (18%)	55,93,113	1.33	8 (14%)
26	LUT	g	1621	-	42,43,43	0.80	1 (2%)	51,60,60	1.62	7 (13%)
25	CLA	G	610	3	65,73,73	1.44	9 (13%)	76,113,113	1.33	9 (11%)
25	CLA	Y	613	1	65,73,73	1.51	11 (16%)	76,113,113	1.28	7 (9%)
25	CLA	A	410	-	60,68,73	1.51	11 (18%)	70,107,113	1.50	9 (12%)
24	CHL	q	609	3	66,74,74	2.13	17 (25%)	73,114,114	2.68	21 (28%)
24	CHL	p	601	2	66,74,74	1.90	14 (21%)	73,114,114	2.70	23 (31%)
40	HEM	f	101	8,9	41,50,50	1.48	3 (7%)	45,82,82	1.30	3 (6%)
25	CLA	n	613	2	65,73,73	1.51	10 (15%)	76,113,113	1.44	7 (9%)
25	CLA	5	614	-	49,57,73	1.75	6 (12%)	55,93,113	1.43	8 (14%)
24	CHL	2	601	2	66,74,74	1.88	14 (21%)	73,114,114	2.57	23 (31%)
25	CLA	Y	614	-	54,62,73	1.60	9 (16%)	62,99,113	1.38	8 (12%)
24	CHL	7	605	1	46,54,74	2.30	14 (30%)	49,90,114	3.06	18 (36%)
25	CLA	r	610	17	65,73,73	1.47	9 (13%)	76,113,113	1.39	8 (10%)
33	PHO	a	408	-	51,69,69	1.13	8 (15%)	47,99,99	1.28	9 (19%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	8	605	2	66,74,74	2.02	15 (22%)	73,114,114	2.61	21 (28%)
24	CHL	y	609	1	66,74,74	1.84	13 (19%)	73,114,114	2.76	24 (32%)
25	CLA	4	611	29	45,53,73	1.76	8 (17%)	52,89,113	1.50	6 (11%)
35	SQD	b	623	-	49,50,54	1.20	4 (8%)	58,61,65	1.36	6 (10%)
28	NEX	R	623	-	38,46,46	0.99	2 (5%)	50,70,70	2.39	15 (30%)
25	CLA	n	603	-	65,73,73	1.46	12 (18%)	76,113,113	1.43	8 (10%)
26	LUT	y	1620	-	42,43,43	0.93	1 (2%)	51,60,60	1.64	17 (33%)
25	CLA	y	610	1	65,73,73	1.41	8 (12%)	76,113,113	1.33	8 (10%)
24	CHL	p	605	2	66,74,74	2.04	15 (22%)	73,114,114	2.70	23 (31%)
25	CLA	B	616	-	65,73,73	1.51	11 (16%)	76,113,113	1.51	14 (18%)
24	CHL	9	607	-	50,58,74	2.23	15 (30%)	52,94,114	2.97	19 (36%)
25	CLA	B	614	-	65,73,73	1.43	10 (15%)	76,113,113	1.45	7 (9%)
24	CHL	3	608	-	50,58,74	2.16	13 (26%)	52,94,114	2.99	20 (38%)
24	CHL	q	605	3	48,56,74	2.34	15 (31%)	51,92,114	3.12	20 (39%)
27	XAT	q	1622	-	39,47,47	0.89	0	54,74,74	2.58	17 (31%)
24	CHL	1	605	1	46,54,74	2.30	14 (30%)	49,90,114	3.06	18 (36%)
24	CHL	0	607	-	66,74,74	1.85	13 (19%)	73,114,114	2.66	18 (24%)
25	CLA	0	610	1	65,73,73	1.48	9 (13%)	76,113,113	1.23	8 (10%)
25	CLA	p	604	-	65,73,73	1.51	7 (10%)	76,113,113	1.26	8 (10%)
25	CLA	s	612	18	45,53,73	1.81	11 (24%)	52,89,113	1.63	9 (17%)
24	CHL	N	608	-	50,58,74	2.05	14 (28%)	52,94,114	3.13	18 (34%)
29	LHG	2	2630	25	48,48,48	0.93	2 (4%)	51,54,54	1.06	2 (3%)
37	DGD	C	520	-	60,60,67	0.85	2 (3%)	74,74,81	0.99	4 (5%)
24	CHL	s	607	-	43,51,74	2.33	13 (30%)	45,86,114	2.99	18 (40%)
25	CLA	p	602	2	65,73,73	1.53	7 (10%)	76,113,113	1.29	7 (9%)
26	LUT	6	1620	-	42,43,43	0.77	0	51,60,60	1.70	13 (25%)
25	CLA	Y	603	-	65,73,73	1.46	11 (16%)	76,113,113	1.51	9 (11%)
25	CLA	b	608	-	65,73,73	1.48	11 (16%)	76,113,113	1.38	7 (9%)
25	CLA	N	603	-	65,73,73	1.46	12 (18%)	76,113,113	1.44	8 (10%)
24	CHL	r	607	-	56,64,74	1.97	12 (21%)	61,102,114	2.87	20 (32%)
25	CLA	A	405	-	65,73,73	1.49	10 (15%)	76,113,113	1.46	7 (9%)
29	LHG	L	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.12	4 (7%)
25	CLA	9	611	29	45,53,73	1.77	9 (20%)	52,89,113	1.47	7 (13%)
26	LUT	8	1621	-	42,43,43	0.79	0	51,60,60	1.56	10 (19%)
24	CHL	R	607	-	56,64,74	1.98	13 (23%)	61,102,114	2.87	20 (32%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
34	BCR	c	514	-	41,41,41	0.78	0	56,56,56	1.57	10 (17%)
25	CLA	4	602	3	65,73,73	1.50	7 (10%)	76,113,113	1.29	7 (9%)
27	XAT	2	1622	-	39,47,47	0.90	0	54,74,74	2.68	19 (35%)
36	LMG	h	102	-	48,48,55	0.93	2 (4%)	56,56,63	1.22	5 (8%)
24	CHL	1	608	-	50,58,74	2.08	14 (28%)	52,94,114	3.17	19 (36%)
25	CLA	A	406	-	65,73,73	1.43	11 (16%)	76,113,113	1.37	8 (10%)
25	CLA	c	513	-	65,73,73	1.46	10 (15%)	76,113,113	1.37	8 (10%)
36	LMG	s	2631	-	52,52,55	0.92	2 (3%)	60,60,63	1.11	4 (6%)
36	LMG	H	102	-	48,48,55	0.93	2 (4%)	56,56,63	1.26	5 (8%)
25	CLA	b	607	-	65,73,73	1.49	9 (13%)	76,113,113	1.44	10 (13%)
25	CLA	6	613	1	65,73,73	1.50	6 (9%)	76,113,113	1.37	7 (9%)
25	CLA	a	405	-	65,73,73	1.49	10 (15%)	76,113,113	1.47	7 (9%)
24	CHL	7	609	1	66,74,74	1.84	14 (21%)	73,114,114	2.67	19 (26%)
25	CLA	r	602	17	60,68,73	1.53	9 (15%)	70,107,113	1.41	8 (11%)
35	SQD	D	413	-	51,52,54	1.18	4 (7%)	60,63,65	1.20	6 (10%)
25	CLA	4	604	-	49,57,73	1.75	9 (18%)	55,93,113	1.38	7 (12%)
27	XAT	p	1622	-	39,47,47	0.91	0	54,74,74	2.56	17 (31%)
25	CLA	G	611	29	45,53,73	1.78	9 (20%)	52,89,113	1.58	8 (15%)
29	LHG	8	2630	25	48,48,48	0.93	2 (4%)	51,54,54	0.98	2 (3%)
26	LUT	1	1621	-	42,43,43	0.82	0	51,60,60	1.71	16 (31%)
25	CLA	p	610	2	65,73,73	1.51	7 (10%)	76,113,113	1.26	7 (9%)
25	CLA	2	611	29	45,53,73	1.78	9 (20%)	52,89,113	1.48	7 (13%)
25	CLA	5	602	2	65,73,73	1.52	7 (10%)	76,113,113	1.29	7 (9%)
25	CLA	7	603	-	65,73,73	1.53	11 (16%)	76,113,113	1.34	7 (9%)
25	CLA	B	603	-	65,73,73	1.42	11 (16%)	76,113,113	1.42	9 (11%)
24	CHL	0	605	1	46,54,74	2.29	16 (34%)	49,90,114	3.06	21 (42%)
24	CHL	G	601	3	66,74,74	1.82	11 (16%)	73,114,114	2.78	27 (36%)
24	CHL	3	609	2	66,74,74	1.82	12 (18%)	73,114,114	2.65	22 (30%)
25	CLA	r	604	-	48,56,73	1.74	9 (18%)	55,92,113	1.55	7 (12%)
34	BCR	c	517	-	41,41,41	0.83	2 (4%)	56,56,56	1.82	12 (21%)
36	LMG	d	412	-	46,46,55	0.94	2 (4%)	54,54,63	1.09	4 (7%)
24	CHL	n	608	-	50,58,74	2.03	13 (26%)	52,94,114	3.12	17 (32%)
25	CLA	q	602	3	65,73,73	1.50	7 (10%)	76,113,113	1.31	7 (9%)
24	CHL	0	609	1	66,74,74	1.95	16 (24%)	73,114,114	2.61	21 (28%)
25	CLA	a	407	-	49,57,73	1.64	11 (22%)	55,93,113	1.52	6 (10%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	q	608	-	44,52,74	2.40	14 (31%)	46,87,114	3.21	16 (34%)
24	CHL	y	606	-	66,74,74	1.82	14 (21%)	73,114,114	2.73	20 (27%)
25	CLA	8	610	2	65,73,73	1.50	7 (10%)	76,113,113	1.25	7 (9%)
25	CLA	B	617	-	65,73,73	1.40	9 (13%)	76,113,113	1.47	9 (11%)
24	CHL	7	608	-	50,58,74	2.05	14 (28%)	52,94,114	3.16	17 (32%)
36	LMG	d	411	-	46,46,55	0.97	2 (4%)	54,54,63	1.13	3 (5%)
25	CLA	S	613	18	49,57,73	1.74	11 (22%)	55,93,113	1.46	7 (12%)
24	CHL	Y	601	1	66,74,74	1.86	15 (22%)	73,114,114	2.71	25 (34%)
26	LUT	G	1620	-	42,43,43	0.78	0	51,60,60	1.48	6 (11%)
27	XAT	N	1622	-	39,47,47	1.04	3 (7%)	54,74,74	2.85	21 (38%)
30	OEX	A	401	4,6	0,15,15	-	-	-	-	-
26	LUT	y	1621	-	42,43,43	0.89	1 (2%)	51,60,60	1.67	14 (27%)
24	CHL	G	606	-	50,58,74	2.13	14 (28%)	52,94,114	3.10	22 (42%)
24	CHL	9	609	2	66,74,74	1.99	15 (22%)	73,114,114	2.66	20 (27%)
25	CLA	8	602	2	65,73,73	1.49	7 (10%)	76,113,113	1.31	6 (7%)
25	CLA	p	612	2	45,53,73	1.81	7 (15%)	52,89,113	1.56	8 (15%)
25	CLA	G	604	-	49,57,73	1.69	10 (20%)	55,93,113	1.48	8 (14%)
25	CLA	n	610	2	65,73,73	1.46	9 (13%)	76,113,113	1.23	8 (10%)
24	CHL	S	607	-	43,51,74	2.33	13 (30%)	45,86,114	2.98	19 (42%)
28	NEX	S	1623	-	38,46,46	0.93	2 (5%)	50,70,70	2.46	16 (32%)
24	CHL	9	601	2	66,74,74	1.91	14 (21%)	73,114,114	2.55	24 (32%)
28	NEX	7	1623	-	38,46,46	1.03	2 (5%)	50,70,70	2.38	20 (40%)
25	CLA	0	614	-	54,62,73	1.65	5 (9%)	62,99,113	1.48	7 (11%)
25	CLA	2	613	2	65,73,73	1.49	8 (12%)	76,113,113	1.35	7 (9%)
29	LHG	r	2630	25	37,37,48	1.04	2 (5%)	40,43,54	1.19	3 (7%)
24	CHL	2	609	2	66,74,74	1.94	14 (21%)	73,114,114	2.70	19 (26%)
24	CHL	1	606	-	66,74,74	1.90	14 (21%)	73,114,114	2.61	20 (27%)
34	BCR	C	516	-	41,41,41	0.76	0	56,56,56	1.70	11 (19%)
25	CLA	G	612	3	43,51,73	1.80	10 (23%)	49,86,113	1.47	7 (14%)
25	CLA	g	613	3	65,73,73	1.48	10 (15%)	76,113,113	1.33	6 (7%)
24	CHL	4	605	3	48,56,74	2.36	16 (33%)	51,92,114	3.06	21 (41%)
25	CLA	c	510	-	65,73,73	1.44	8 (12%)	76,113,113	1.49	8 (10%)
36	LMG	D	412	-	46,46,55	0.95	2 (4%)	54,54,63	1.08	4 (7%)
25	CLA	4	614	-	49,57,73	1.70	8 (16%)	55,93,113	1.41	7 (12%)
26	LUT	7	1621	-	42,43,43	0.77	0	51,60,60	1.60	11 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
28	NEX	2	1623	-	38,46,46	0.93	2 (5%)	50,70,70	2.35	13 (26%)
25	CLA	b	613	-	65,73,73	1.43	9 (13%)	76,113,113	1.60	8 (10%)
24	CHL	g	607	-	50,58,74	2.12	13 (26%)	52,94,114	3.14	23 (44%)
24	CHL	p	606	-	46,54,74	2.41	15 (32%)	49,90,114	2.85	18 (36%)
25	CLA	y	611	29	65,73,73	1.49	10 (15%)	76,113,113	1.32	6 (7%)
25	CLA	8	612	2	45,53,73	1.79	7 (15%)	52,89,113	1.62	8 (15%)
24	CHL	6	605	1	46,54,74	2.32	16 (34%)	49,90,114	3.00	21 (42%)
24	CHL	N	607	-	66,74,74	1.82	14 (21%)	73,114,114	2.84	25 (34%)
25	CLA	y	603	-	65,73,73	1.46	11 (16%)	76,113,113	1.50	9 (11%)
26	LUT	p	1621	-	42,43,43	0.73	0	51,60,60	1.55	9 (17%)
34	BCR	c	515	-	41,41,41	0.91	2 (4%)	56,56,56	1.74	11 (19%)
29	LHG	y	2630	25	48,48,48	0.89	2 (4%)	51,54,54	1.18	5 (9%)
29	LHG	d	408	-	43,43,48	0.98	2 (4%)	46,49,54	1.02	3 (6%)
25	CLA	b	609	-	65,73,73	1.44	11 (16%)	76,113,113	1.43	7 (9%)
24	CHL	6	609	1	66,74,74	1.89	14 (21%)	73,114,114	2.61	22 (30%)
24	CHL	4	606	-	50,58,74	2.30	16 (32%)	52,94,114	2.86	19 (36%)
26	LUT	Y	1620	-	42,43,43	0.93	1 (2%)	51,60,60	1.64	16 (31%)
25	CLA	c	502	-	65,73,73	1.52	12 (18%)	76,113,113	1.69	10 (13%)
25	CLA	1	612	1	65,73,73	1.47	10 (15%)	76,113,113	1.33	8 (10%)
34	BCR	C	515	-	41,41,41	0.92	2 (4%)	56,56,56	1.73	11 (19%)
25	CLA	6	603	-	65,73,73	1.46	9 (13%)	76,113,113	1.42	7 (9%)
25	CLA	c	512	-	65,73,73	1.50	10 (15%)	76,113,113	1.44	7 (9%)
25	CLA	C	502	-	65,73,73	1.51	12 (18%)	76,113,113	1.68	11 (14%)
24	CHL	N	605	2	66,74,74	1.87	12 (18%)	73,114,114	2.63	23 (31%)
25	CLA	r	613	17	60,68,73	1.53	10 (16%)	70,107,113	1.43	8 (11%)
38	BCT	d	401	31	2,3,3	1.32	0	2,3,3	4.16	2 (100%)
24	CHL	q	607	-	50,58,74	2.30	16 (32%)	52,94,114	2.93	18 (34%)
25	CLA	B	608	-	65,73,73	1.47	11 (16%)	76,113,113	1.36	7 (9%)
24	CHL	7	607	-	66,74,74	1.89	14 (21%)	73,114,114	2.62	25 (34%)
37	DGD	c	523	-	67,67,67	0.81	2 (2%)	81,81,81	1.03	3 (3%)
27	XAT	r	622	-	39,47,47	0.99	2 (5%)	54,74,74	2.48	17 (31%)
25	CLA	b	605	-	65,73,73	1.49	10 (15%)	76,113,113	1.46	11 (14%)
25	CLA	C	507	-	65,73,73	1.41	11 (16%)	76,113,113	1.45	11 (14%)
34	BCR	b	618	-	41,41,41	0.79	0	56,56,56	1.90	13 (23%)
34	BCR	d	404	-	41,41,41	0.80	1 (2%)	56,56,56	2.02	14 (25%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	g	601	3	66,74,74	1.82	12 (18%)	73,114,114	2.77	29 (39%)
26	LUT	r	620	-	42,43,43	0.84	1 (2%)	51,60,60	1.76	13 (25%)
25	CLA	2	603	-	65,73,73	1.50	8 (12%)	76,113,113	1.37	9 (11%)
25	CLA	9	602	2	65,73,73	1.44	8 (12%)	76,113,113	1.39	9 (11%)
24	CHL	R	608	-	61,69,74	1.93	13 (21%)	67,108,114	2.82	23 (34%)
35	SQD	B	623	-	49,50,54	1.20	4 (8%)	58,61,65	1.36	6 (10%)
27	XAT	7	1622	-	39,47,47	0.94	0	54,74,74	4.18	22 (40%)
26	LUT	R	620	-	42,43,43	0.84	1 (2%)	51,60,60	1.76	13 (25%)
24	CHL	5	601	2	66,74,74	1.90	13 (19%)	73,114,114	2.71	23 (31%)
25	CLA	0	602	1	65,73,73	1.49	8 (12%)	76,113,113	1.26	6 (7%)
25	CLA	q	613	3	65,73,73	1.46	7 (10%)	76,113,113	1.47	6 (7%)
25	CLA	b	610	-	65,73,73	1.44	10 (15%)	76,113,113	1.40	6 (7%)
28	NEX	N	1623	-	38,46,46	0.99	2 (5%)	50,70,70	2.36	14 (28%)
25	CLA	9	613	2	65,73,73	1.48	7 (10%)	76,113,113	1.35	7 (9%)
28	NEX	r	623	-	38,46,46	1.04	3 (7%)	50,70,70	2.40	16 (32%)
25	CLA	p	603	-	65,73,73	1.51	7 (10%)	76,113,113	1.36	7 (9%)
24	CHL	0	608	-	50,58,74	2.16	14 (28%)	52,94,114	3.07	18 (34%)
25	CLA	0	604	-	65,73,73	1.50	9 (13%)	76,113,113	1.25	7 (9%)
34	BCR	B	619	-	41,41,41	0.78	1 (2%)	56,56,56	1.97	17 (30%)
26	LUT	g	1620	-	42,43,43	0.78	0	51,60,60	1.47	6 (11%)
25	CLA	b	602	-	65,73,73	1.48	10 (15%)	76,113,113	1.21	5 (6%)
24	CHL	5	608	-	50,58,74	2.14	14 (28%)	52,94,114	3.12	17 (32%)
29	LHG	3	2630	25	48,48,48	0.92	2 (4%)	51,54,54	0.99	2 (3%)
28	NEX	9	1623	-	38,46,46	0.95	2 (5%)	50,70,70	2.33	12 (24%)
24	CHL	S	601	18	46,54,74	2.32	14 (30%)	49,90,114	3.10	22 (44%)
24	CHL	Y	605	1	46,54,74	2.20	13 (28%)	49,90,114	3.05	20 (40%)
25	CLA	g	604	-	49,57,73	1.69	8 (16%)	55,93,113	1.48	8 (14%)
26	LUT	9	1621	-	42,43,43	0.77	0	51,60,60	1.74	13 (25%)
25	CLA	q	614	-	49,57,73	1.68	7 (14%)	55,93,113	1.41	6 (10%)
24	CHL	n	605	2	66,74,74	1.86	12 (18%)	73,114,114	2.64	26 (35%)
27	XAT	0	1622	-	39,47,47	0.94	2 (5%)	54,74,74	4.20	22 (40%)
26	LUT	6	1621	-	42,43,43	0.80	0	51,60,60	1.61	9 (17%)
27	XAT	9	1622	-	39,47,47	0.91	0	54,74,74	2.65	19 (35%)
24	CHL	2	606	-	50,58,74	2.23	15 (30%)	52,94,114	2.94	19 (36%)
25	CLA	R	613	17	60,68,73	1.53	10 (16%)	70,107,113	1.43	8 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
29	LHG	p	2630	25	48,48,48	0.95	2 (4%)	51,54,54	1.04	3 (5%)
24	CHL	n	609	2	66,74,74	1.88	14 (21%)	73,114,114	2.66	25 (34%)
24	CHL	N	609	2	66,74,74	1.86	14 (21%)	73,114,114	2.68	24 (32%)
30	OEX	a	401	4,6	0,15,15	-	-	-		
25	CLA	1	611	29	65,73,73	1.48	9 (13%)	76,113,113	1.31	6 (7%)
25	CLA	B	615	-	65,73,73	1.47	12 (18%)	76,113,113	1.29	6 (7%)
25	CLA	y	604	-	65,73,73	1.53	11 (16%)	76,113,113	1.36	7 (9%)
29	LHG	6	2630	25	48,48,48	0.93	2 (4%)	51,54,54	0.96	2 (3%)
25	CLA	c	503	-	65,73,73	1.45	11 (16%)	76,113,113	1.40	8 (10%)
24	CHL	3	605	2	66,74,74	2.02	15 (22%)	73,114,114	2.60	21 (28%)
29	LHG	4	2630	25	48,48,48	0.93	2 (4%)	51,54,54	1.10	4 (7%)
34	BCR	A	411	-	41,41,41	0.82	0	56,56,56	1.70	12 (21%)
26	LUT	0	1621	-	42,43,43	0.79	0	51,60,60	1.61	10 (19%)
25	CLA	G	602	3	65,73,73	1.43	9 (13%)	76,113,113	1.40	8 (10%)
28	NEX	1	1623	-	38,46,46	0.96	2 (5%)	50,70,70	2.45	17 (34%)
25	CLA	7	604	-	65,73,73	1.51	11 (16%)	76,113,113	1.31	9 (11%)
35	SQD	a	412	-	50,51,54	1.22	4 (8%)	59,62,65	3.79	9 (15%)
25	CLA	q	610	3	65,73,73	1.49	8 (12%)	76,113,113	1.26	8 (10%)
26	LUT	s	1621	-	42,43,43	0.82	0	51,60,60	1.80	14 (27%)
25	CLA	C	511	6	65,73,73	1.44	11 (16%)	76,113,113	1.53	10 (13%)
27	XAT	y	1622	-	39,47,47	0.96	2 (5%)	54,74,74	4.30	23 (42%)
26	LUT	q	1621	-	42,43,43	0.74	0	51,60,60	1.60	10 (19%)
25	CLA	3	613	2	65,73,73	1.48	7 (10%)	76,113,113	1.49	8 (10%)
25	CLA	D	403	-	65,73,73	1.46	11 (16%)	76,113,113	1.32	8 (10%)
26	LUT	S	1621	-	42,43,43	0.81	0	51,60,60	1.79	14 (27%)
34	BCR	D	404	-	41,41,41	0.80	1 (2%)	56,56,56	2.02	14 (25%)
28	NEX	s	1623	-	38,46,46	1.03	3 (7%)	50,70,70	2.55	18 (36%)
35	SQD	d	413	-	51,52,54	1.18	4 (7%)	60,63,65	1.20	6 (10%)
24	CHL	g	609	3	66,74,74	1.90	15 (22%)	73,114,114	2.61	20 (27%)
25	CLA	r	611	29	49,57,73	1.69	11 (22%)	55,93,113	1.48	6 (10%)
25	CLA	S	610	18	49,57,73	1.70	10 (20%)	55,93,113	1.37	8 (14%)
25	CLA	G	614	-	49,57,73	1.67	9 (18%)	55,93,113	1.33	8 (14%)
24	CHL	7	601	1	66,74,74	1.88	12 (18%)	73,114,114	2.83	25 (34%)
24	CHL	Y	609	1	66,74,74	1.84	14 (21%)	73,114,114	2.76	24 (32%)
27	XAT	6	1622	-	39,47,47	0.92	2 (5%)	54,74,74	4.25	21 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	S	602	18	49,57,73	1.71	9 (18%)	55,93,113	1.57	7 (12%)
25	CLA	2	604	-	49,57,73	1.71	6 (12%)	55,93,113	1.48	8 (14%)
25	CLA	Y	611	29	65,73,73	1.49	10 (15%)	76,113,113	1.33	6 (7%)
24	CHL	5	607	-	66,74,74	1.90	14 (21%)	73,114,114	2.61	21 (28%)
25	CLA	s	611	29	49,57,73	1.66	10 (20%)	55,93,113	1.47	6 (10%)
25	CLA	8	604	-	65,73,73	1.49	7 (10%)	76,113,113	1.40	7 (9%)
28	NEX	5	1623	-	38,46,46	0.90	1 (2%)	50,70,70	2.54	15 (30%)
25	CLA	b	614	-	65,73,73	1.43	9 (13%)	76,113,113	1.44	7 (9%)
25	CLA	2	610	2	65,73,73	1.48	7 (10%)	76,113,113	1.31	7 (9%)
25	CLA	c	504	-	65,73,73	1.50	10 (15%)	76,113,113	1.30	7 (9%)
28	NEX	3	1623	-	38,46,46	0.91	1 (2%)	50,70,70	2.35	13 (26%)
37	DGD	c	524	-	67,67,67	0.83	3 (4%)	81,81,81	1.00	5 (6%)
26	LUT	3	1621	-	42,43,43	0.77	0	51,60,60	1.56	11 (21%)
29	LHG	l	101	-	48,48,48	0.91	2 (4%)	51,54,54	1.13	4 (7%)
28	NEX	y	1623	-	38,46,46	0.99	2 (5%)	50,70,70	2.44	17 (34%)
33	PHO	A	408	-	51,69,69	1.14	8 (15%)	47,99,99	1.28	9 (19%)
25	CLA	c	501	-	65,73,73	1.47	11 (16%)	76,113,113	1.33	8 (10%)
27	XAT	8	1622	-	39,47,47	0.92	0	54,74,74	2.62	19 (35%)
29	LHG	s	2630	25	44,44,48	0.95	2 (4%)	47,50,54	1.12	3 (6%)
24	CHL	6	606	-	66,74,74	1.92	15 (22%)	73,114,114	2.64	21 (28%)
25	CLA	1	613	1	65,73,73	1.44	8 (12%)	76,113,113	1.48	7 (9%)
29	LHG	C	2630	-	46,46,48	0.93	2 (4%)	49,52,54	1.02	3 (6%)
25	CLA	d	403	-	65,73,73	1.46	11 (16%)	76,113,113	1.32	8 (10%)
36	LMG	A	413	-	48,48,55	0.93	2 (4%)	56,56,63	1.15	4 (7%)
25	CLA	r	601	17	49,57,73	1.68	10 (20%)	55,93,113	1.74	10 (18%)
25	CLA	N	602	2	65,73,73	1.47	10 (15%)	76,113,113	1.29	8 (10%)
24	CHL	Y	606	-	66,74,74	1.82	16 (24%)	73,114,114	2.72	20 (27%)
25	CLA	b	604	-	65,73,73	1.50	10 (15%)	76,113,113	1.27	7 (9%)
24	CHL	Y	608	-	50,58,74	2.06	14 (28%)	52,94,114	3.23	19 (36%)
27	XAT	4	1622	-	39,47,47	0.89	0	54,74,74	2.60	16 (29%)
25	CLA	R	601	17	49,57,73	1.68	10 (20%)	55,93,113	1.72	10 (18%)
25	CLA	C	505	-	65,73,73	1.45	9 (13%)	76,113,113	1.39	8 (10%)
25	CLA	c	508	-	65,73,73	1.50	10 (15%)	76,113,113	1.46	8 (10%)
28	NEX	6	1623	-	38,46,46	0.98	1 (2%)	50,70,70	2.32	12 (24%)
24	CHL	8	606	-	46,54,74	2.42	15 (32%)	49,90,114	2.99	19 (38%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	XAT	1	1622	-	39,47,47	0.94	2 (5%)	54,74,74	4.22	24 (44%)
25	CLA	5	613	2	65,73,73	1.51	7 (10%)	76,113,113	1.47	7 (9%)
25	CLA	1	610	1	65,73,73	1.45	8 (12%)	76,113,113	1.32	8 (10%)
25	CLA	R	602	17	60,68,73	1.53	9 (15%)	70,107,113	1.41	8 (11%)
25	CLA	y	612	1	65,73,73	1.50	11 (16%)	76,113,113	1.38	9 (11%)
25	CLA	2	612	2	43,51,73	1.81	9 (20%)	49,86,113	1.59	7 (14%)
24	CHL	9	605	2	48,56,74	2.34	16 (33%)	51,92,114	2.98	21 (41%)
28	NEX	p	1623	-	38,46,46	0.88	1 (2%)	50,70,70	2.39	16 (32%)
26	LUT	n	1621	-	42,43,43	0.85	1 (2%)	51,60,60	1.60	9 (17%)
25	CLA	1	602	1	65,73,73	1.48	7 (10%)	76,113,113	1.28	6 (7%)
25	CLA	C	513	-	65,73,73	1.44	10 (15%)	76,113,113	1.35	8 (10%)
25	CLA	g	612	3	43,51,73	1.79	10 (23%)	49,86,113	1.47	7 (14%)
24	CHL	2	605	2	48,56,74	2.34	16 (33%)	51,92,114	2.98	21 (41%)
36	LMG	D	411	-	46,46,55	0.97	2 (4%)	54,54,63	1.12	3 (5%)
26	LUT	N	1621	-	42,43,43	0.86	1 (2%)	51,60,60	1.58	9 (17%)
24	CHL	S	608	-	49,57,74	2.22	15 (30%)	52,93,114	3.05	20 (38%)
25	CLA	3	610	2	65,73,73	1.50	7 (10%)	76,113,113	1.25	7 (9%)
24	CHL	q	601	3	66,74,74	1.93	14 (21%)	73,114,114	2.67	25 (34%)
24	CHL	G	608	-	44,52,74	2.24	13 (29%)	46,87,114	3.10	18 (39%)
25	CLA	7	602	1	65,73,73	1.48	9 (13%)	76,113,113	1.29	8 (10%)
25	CLA	1	604	-	65,73,73	1.50	11 (16%)	76,113,113	1.20	7 (9%)
25	CLA	r	612	-	49,57,73	1.67	9 (18%)	55,93,113	1.56	8 (14%)
26	LUT	2	1620	-	42,43,43	0.77	0	51,60,60	1.55	10 (19%)
26	LUT	8	1620	-	42,43,43	0.72	0	51,60,60	1.62	12 (23%)
24	CHL	5	605	2	66,74,74	2.00	16 (24%)	73,114,114	2.78	25 (34%)
25	CLA	s	613	18	49,57,73	1.74	11 (22%)	55,93,113	1.46	7 (12%)
27	XAT	3	1622	-	39,47,47	0.92	0	54,74,74	2.60	20 (37%)
29	LHG	S	2630	25	44,44,48	0.94	2 (4%)	47,50,54	1.12	3 (6%)
25	CLA	y	614	-	54,62,73	1.60	9 (16%)	62,99,113	1.39	8 (12%)
27	XAT	n	1622	-	39,47,47	1.05	3 (7%)	54,74,74	2.82	22 (40%)
25	CLA	7	613	1	65,73,73	1.45	9 (13%)	76,113,113	1.49	8 (10%)
25	CLA	s	605	18	50,58,73	1.70	8 (16%)	58,95,113	1.37	7 (12%)
25	CLA	C	512	-	65,73,73	1.50	10 (15%)	76,113,113	1.42	7 (9%)
25	CLA	B	605	-	65,73,73	1.50	10 (15%)	76,113,113	1.46	11 (14%)
34	BCR	B	618	-	41,41,41	0.79	0	56,56,56	1.90	13 (23%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	LUT	p	1620	-	42,43,43	0.75	0	51,60,60	1.76	9 (17%)
25	CLA	R	609	17	58,66,73	1.60	10 (17%)	67,104,113	1.44	6 (8%)
25	CLA	9	614	-	49,57,73	1.73	8 (16%)	55,93,113	1.37	7 (12%)
25	CLA	b	617	-	65,73,73	1.40	9 (13%)	76,113,113	1.47	9 (11%)
25	CLA	N	611	29	49,57,73	1.67	10 (20%)	55,93,113	1.46	6 (10%)
25	CLA	C	506	-	65,73,73	1.51	10 (15%)	76,113,113	1.42	7 (9%)
25	CLA	s	609	18	41,49,73	1.85	7 (17%)	47,84,113	1.53	9 (19%)
24	CHL	p	608	-	50,58,74	2.15	15 (30%)	52,94,114	3.12	17 (32%)
36	LMG	B	622	-	51,51,55	0.87	2 (3%)	59,59,63	1.11	3 (5%)
25	CLA	6	610	1	65,73,73	1.47	9 (13%)	76,113,113	1.22	8 (10%)
24	CHL	5	609	2	66,74,74	1.96	14 (21%)	73,114,114	2.65	20 (27%)
25	CLA	2	614	-	49,57,73	1.72	8 (16%)	55,93,113	1.37	7 (12%)
29	LHG	D	408	-	43,43,48	0.98	2 (4%)	46,49,54	1.02	3 (6%)
25	CLA	R	604	-	48,56,73	1.73	9 (18%)	55,92,113	1.55	7 (12%)
25	CLA	R	616	17	65,73,73	1.50	9 (13%)	76,113,113	1.29	9 (11%)
25	CLA	3	612	2	45,53,73	1.79	7 (15%)	52,89,113	1.64	8 (15%)
39	PL9	D	405	-	55,55,55	2.03	13 (23%)	68,69,69	1.54	11 (16%)
26	LUT	Y	1621	-	42,43,43	0.89	1 (2%)	51,60,60	1.66	14 (27%)
25	CLA	B	609	-	65,73,73	1.44	11 (16%)	76,113,113	1.43	7 (9%)
25	CLA	R	610	17	65,73,73	1.47	9 (13%)	76,113,113	1.40	8 (10%)
25	CLA	q	603	-	65,73,73	1.47	8 (12%)	76,113,113	1.41	8 (10%)
29	LHG	N	2630	25	48,48,48	0.91	2 (4%)	51,54,54	1.10	3 (5%)
36	LMG	a	413	-	48,48,55	0.94	2 (4%)	56,56,63	1.15	4 (7%)
25	CLA	n	612	2	45,53,73	1.82	10 (22%)	52,89,113	1.54	9 (17%)
24	CHL	Y	607	-	66,74,74	1.84	14 (21%)	73,114,114	2.89	24 (32%)
24	CHL	8	601	2	66,74,74	1.90	12 (18%)	73,114,114	2.65	21 (28%)
24	CHL	4	608	-	44,52,74	2.31	14 (31%)	46,87,114	3.22	17 (36%)
29	LHG	q	2630	25	48,48,48	0.93	2 (4%)	51,54,54	1.13	4 (7%)
25	CLA	p	614	-	49,57,73	1.76	6 (12%)	55,93,113	1.41	8 (14%)
25	CLA	8	614	-	49,57,73	1.72	5 (10%)	55,93,113	1.33	8 (14%)
24	CHL	n	607	-	66,74,74	1.83	13 (19%)	73,114,114	2.82	25 (34%)
24	CHL	9	606	-	50,58,74	2.24	15 (30%)	52,94,114	2.91	20 (38%)
28	NEX	4	1623	-	38,46,46	0.91	2 (5%)	50,70,70	2.36	18 (36%)
25	CLA	b	615	-	65,73,73	1.46	11 (16%)	76,113,113	1.29	6 (7%)
28	NEX	n	1623	-	38,46,46	0.93	2 (5%)	50,70,70	2.37	15 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	S	603	-	42,50,73	1.82	9 (21%)	48,85,113	1.65	8 (16%)
25	CLA	g	611	29	45,53,73	1.78	9 (20%)	52,89,113	1.57	8 (15%)
25	CLA	7	611	29	65,73,73	1.47	9 (13%)	76,113,113	1.32	6 (7%)
27	XAT	5	1622	-	39,47,47	0.90	0	54,74,74	2.65	18 (33%)
27	XAT	Y	1622	-	39,47,47	0.97	2 (5%)	54,74,74	4.30	23 (42%)
35	SQD	b	621	-	53,54,54	1.17	4 (7%)	62,65,65	1.14	4 (6%)
25	CLA	C	504	-	65,73,73	1.50	11 (16%)	76,113,113	1.31	7 (9%)
24	CHL	y	607	-	66,74,74	1.84	14 (21%)	73,114,114	2.88	24 (32%)
34	BCR	a	411	-	41,41,41	0.82	0	56,56,56	1.71	12 (21%)
25	CLA	C	510	-	65,73,73	1.43	8 (12%)	76,113,113	1.48	8 (10%)
34	BCR	b	620	-	41,41,41	0.83	1 (2%)	56,56,56	1.87	19 (33%)
37	DGD	C	524	-	67,67,67	0.83	3 (4%)	81,81,81	1.00	5 (6%)
24	CHL	1	601	1	66,74,74	1.89	12 (18%)	73,114,114	2.82	25 (34%)
24	CHL	4	607	-	50,58,74	2.27	15 (30%)	52,94,114	3.00	19 (36%)
25	CLA	1	614	-	54,62,73	1.64	8 (14%)	62,99,113	1.35	6 (9%)
25	CLA	6	612	1	65,73,73	1.50	9 (13%)	76,113,113	1.29	9 (11%)
29	LHG	g	2630	25	48,48,48	0.89	2 (4%)	51,54,54	1.12	4 (7%)
29	LHG	7	2630	25	48,48,48	0.92	2 (4%)	51,54,54	1.11	4 (7%)
25	CLA	3	602	2	65,73,73	1.49	6 (9%)	76,113,113	1.30	6 (7%)
24	CHL	r	606	-	66,74,74	1.80	14 (21%)	73,114,114	2.76	23 (31%)
25	CLA	4	612	3	43,51,73	1.83	8 (18%)	49,86,113	1.63	10 (20%)
25	CLA	S	609	18	41,49,73	1.85	8 (19%)	47,84,113	1.53	9 (19%)
24	CHL	R	606	-	66,74,74	1.80	13 (19%)	73,114,114	2.76	23 (31%)
40	HEM	F	101	8,9	41,50,50	1.46	3 (7%)	45,82,82	1.24	4 (8%)
25	CLA	n	611	29	49,57,73	1.66	10 (20%)	55,93,113	1.48	6 (10%)
24	CHL	0	606	-	66,74,74	1.95	15 (22%)	73,114,114	2.62	21 (28%)
24	CHL	6	607	-	66,74,74	1.88	15 (22%)	73,114,114	2.60	19 (26%)
34	BCR	H	101	-	41,41,41	0.81	0	56,56,56	2.03	16 (28%)
25	CLA	Y	612	1	65,73,73	1.50	11 (16%)	76,113,113	1.37	9 (11%)
25	CLA	s	610	18	49,57,73	1.69	10 (20%)	55,93,113	1.37	8 (14%)
25	CLA	N	613	2	65,73,73	1.51	10 (15%)	76,113,113	1.44	8 (10%)
24	CHL	9	608	-	44,52,74	2.22	15 (34%)	46,87,114	3.21	17 (36%)
24	CHL	s	606	-	44,52,74	2.17	14 (31%)	46,87,114	3.29	20 (43%)
25	CLA	C	508	-	65,73,73	1.50	10 (15%)	76,113,113	1.46	8 (10%)
25	CLA	g	610	3	65,73,73	1.44	9 (13%)	76,113,113	1.33	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	DGD	C	519	-	63,63,67	0.81	2 (3%)	77,77,81	1.15	6 (7%)
28	NEX	Y	1623	-	38,46,46	1.04	3 (7%)	50,70,70	2.39	16 (32%)
24	CHL	p	607	-	66,74,74	1.94	15 (22%)	73,114,114	2.56	22 (30%)
25	CLA	G	613	3	65,73,73	1.48	10 (15%)	76,113,113	1.33	6 (7%)
25	CLA	d	402	-	65,73,73	1.53	11 (16%)	76,113,113	1.43	7 (9%)
36	LMG	c	521	-	51,51,55	0.87	2 (3%)	59,59,63	1.08	4 (6%)
24	CHL	8	607	-	66,74,74	1.88	14 (21%)	73,114,114	2.77	23 (31%)
34	BCR	b	619	-	41,41,41	0.78	1 (2%)	56,56,56	1.98	16 (28%)
25	CLA	S	614	-	48,56,73	1.67	7 (14%)	55,92,113	1.47	8 (14%)
25	CLA	1	603	-	65,73,73	1.52	11 (16%)	76,113,113	1.35	7 (9%)
25	CLA	2	602	2	65,73,73	1.45	8 (12%)	76,113,113	1.35	7 (9%)
38	BCT	D	401	31	2,3,3	1.32	0	2,3,3	4.16	2 (100%)
24	CHL	3	606	-	46,54,74	2.42	15 (32%)	49,90,114	2.99	18 (36%)
24	CHL	G	607	-	50,58,74	2.11	13 (26%)	52,94,114	3.14	22 (42%)
28	NEX	G	1623	-	38,46,46	0.93	2 (5%)	50,70,70	2.42	19 (38%)
25	CLA	b	611	-	65,73,73	1.51	11 (16%)	76,113,113	1.54	8 (10%)
24	CHL	2	608	-	44,52,74	2.20	17 (38%)	46,87,114	3.25	19 (41%)
24	CHL	8	608	-	50,58,74	2.15	14 (28%)	52,94,114	3.01	21 (40%)
25	CLA	r	603	-	60,68,73	1.52	11 (18%)	70,107,113	1.53	7 (10%)
33	PHO	a	409	-	51,69,69	1.08	6 (11%)	47,99,99	1.37	7 (14%)
29	LHG	D	410	-	38,38,48	1.04	2 (5%)	41,44,54	1.22	2 (4%)
24	CHL	0	601	1	66,74,74	1.90	14 (21%)	73,114,114	2.62	21 (28%)
37	DGD	c	518	-	56,56,67	0.88	2 (3%)	70,70,81	1.12	6 (8%)
25	CLA	8	611	29	49,57,73	1.71	7 (14%)	55,93,113	1.44	8 (14%)
25	CLA	R	603	-	60,68,73	1.51	11 (18%)	70,107,113	1.53	7 (10%)
25	CLA	5	604	-	65,73,73	1.49	7 (10%)	76,113,113	1.28	8 (10%)
24	CHL	s	601	18	46,54,74	2.32	14 (30%)	49,90,114	3.11	21 (42%)
39	PL9	d	405	-	55,55,55	2.03	13 (23%)	68,69,69	1.55	10 (14%)
29	LHG	d	410	-	38,38,48	1.04	2 (5%)	41,44,54	1.22	2 (4%)
26	LUT	5	1621	-	42,43,43	0.74	0	51,60,60	1.58	11 (21%)
25	CLA	q	604	-	49,57,73	1.73	9 (18%)	55,93,113	1.49	8 (14%)
29	LHG	1	2630	25	48,48,48	0.91	2 (4%)	51,54,54	1.10	5 (9%)
25	CLA	s	602	18	49,57,73	1.70	9 (18%)	55,93,113	1.56	7 (12%)
34	BCR	h	101	-	41,41,41	0.81	0	56,56,56	2.03	17 (30%)
25	CLA	C	509	-	65,73,73	1.40	11 (16%)	76,113,113	1.55	10 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	G	605	3	48,56,74	2.27	15 (31%)	51,92,114	3.07	20 (39%)
29	LHG	9	2630	25	48,48,48	0.92	2 (4%)	51,54,54	1.07	2 (3%)
27	XAT	R	622	-	39,47,47	0.99	2 (5%)	54,74,74	2.47	16 (29%)
25	CLA	s	604	-	49,57,73	1.66	7 (14%)	55,93,113	1.50	8 (14%)
25	CLA	6	604	-	65,73,73	1.55	9 (13%)	76,113,113	1.29	6 (7%)
25	CLA	S	604	-	49,57,73	1.67	8 (16%)	55,93,113	1.50	8 (14%)
29	LHG	0	2630	25	48,48,48	0.93	2 (4%)	51,54,54	0.96	2 (3%)
36	LMG	C	521	-	51,51,55	0.87	2 (3%)	59,59,63	1.08	4 (6%)
24	CHL	G	609	3	66,74,74	1.92	15 (22%)	73,114,114	2.61	21 (28%)
24	CHL	3	607	-	66,74,74	1.88	14 (21%)	73,114,114	2.78	22 (30%)
26	LUT	q	1620	-	42,43,43	0.72	0	51,60,60	1.57	13 (25%)
25	CLA	5	611	29	49,57,73	1.72	7 (14%)	55,93,113	1.39	6 (10%)
26	LUT	2	1621	-	42,43,43	0.76	0	51,60,60	1.78	11 (21%)
25	CLA	B	607	-	65,73,73	1.50	9 (13%)	76,113,113	1.43	10 (13%)
35	SQD	A	412	-	50,51,54	1.22	4 (8%)	59,62,65	3.78	9 (15%)
26	LUT	9	1620	-	42,43,43	0.77	0	51,60,60	1.61	13 (25%)
25	CLA	7	614	-	54,62,73	1.66	8 (14%)	62,99,113	1.37	7 (11%)
25	CLA	9	610	2	65,73,73	1.48	7 (10%)	76,113,113	1.28	8 (10%)
24	CHL	n	606	-	46,54,74	2.18	13 (28%)	49,90,114	3.24	19 (38%)
29	LHG	R	2630	25	37,37,48	1.04	2 (5%)	40,43,54	1.19	3 (7%)
28	NEX	g	1623	-	38,46,46	0.95	2 (5%)	50,70,70	2.41	21 (42%)
25	CLA	q	611	29	45,53,73	1.75	8 (17%)	52,89,113	1.54	6 (11%)
25	CLA	N	604	-	65,73,73	1.52	10 (15%)	76,113,113	1.33	6 (7%)
24	CHL	y	608	-	50,58,74	2.06	14 (28%)	52,94,114	3.24	19 (36%)
29	LHG	5	2630	25	48,48,48	0.94	2 (4%)	51,54,54	1.06	3 (5%)
25	CLA	R	611	29	49,57,73	1.68	11 (22%)	55,93,113	1.47	6 (10%)
26	LUT	s	1620	-	42,43,43	0.79	0	51,60,60	1.56	11 (21%)
37	DGD	c	520	-	60,60,67	0.86	2 (3%)	74,74,81	0.98	4 (5%)
25	CLA	C	501	-	65,73,73	1.47	11 (16%)	76,113,113	1.33	8 (10%)
25	CLA	b	606	-	65,73,73	1.46	9 (13%)	76,113,113	1.20	7 (9%)
24	CHL	S	606	-	44,52,74	2.18	14 (31%)	46,87,114	3.30	20 (43%)
25	CLA	5	603	-	65,73,73	1.51	7 (10%)	76,113,113	1.35	7 (9%)
33	PHO	A	409	-	51,69,69	1.08	6 (11%)	47,99,99	1.37	8 (17%)
25	CLA	S	605	18	50,58,73	1.70	9 (18%)	58,95,113	1.37	8 (13%)
34	BCR	C	517	-	41,41,41	0.83	2 (4%)	56,56,56	1.82	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
24	CHL	r	608	-	61,69,74	1.93	15 (24%)	67,108,114	2.81	23 (34%)
24	CHL	4	609	3	66,74,74	2.10	17 (25%)	73,114,114	2.58	19 (26%)
37	DGD	C	523	-	67,67,67	0.82	2 (2%)	81,81,81	1.02	4 (4%)
24	CHL	g	606	-	50,58,74	2.13	14 (28%)	52,94,114	3.11	22 (42%)
24	CHL	4	601	3	66,74,74	1.95	15 (22%)	73,114,114	2.58	23 (31%)
24	CHL	n	601	2	66,74,74	1.83	11 (16%)	73,114,114	2.78	28 (38%)
25	CLA	9	612	2	43,51,73	1.83	8 (18%)	49,86,113	1.58	8 (16%)
25	CLA	3	611	29	49,57,73	1.73	7 (14%)	55,93,113	1.44	9 (16%)
25	CLA	Y	602	1	65,73,73	1.42	8 (12%)	76,113,113	1.37	7 (9%)
26	LUT	S	1620	-	42,43,43	0.79	0	51,60,60	1.55	11 (21%)
25	CLA	a	410	-	60,68,73	1.52	11 (18%)	70,107,113	1.50	9 (12%)
24	CHL	N	606	-	46,54,74	2.17	13 (28%)	49,90,114	3.21	19 (38%)
26	LUT	0	1620	-	42,43,43	0.76	0	51,60,60	1.59	11 (21%)
25	CLA	n	602	2	65,73,73	1.47	10 (15%)	76,113,113	1.29	8 (10%)
25	CLA	g	603	-	65,73,73	1.48	10 (15%)	76,113,113	1.36	8 (10%)
25	CLA	b	616	-	65,73,73	1.49	11 (16%)	76,113,113	1.52	14 (18%)
25	CLA	Y	604	-	65,73,73	1.54	11 (16%)	76,113,113	1.37	7 (9%)
25	CLA	3	604	-	65,73,73	1.50	7 (10%)	76,113,113	1.41	7 (9%)
25	CLA	n	604	-	65,73,73	1.52	10 (15%)	76,113,113	1.33	6 (7%)
25	CLA	b	603	-	65,73,73	1.42	11 (16%)	76,113,113	1.42	9 (11%)
24	CHL	2	607	-	50,58,74	2.25	16 (32%)	52,94,114	2.94	20 (38%)
34	BCR	C	514	-	41,41,41	0.78	0	56,56,56	1.57	10 (17%)
25	CLA	r	616	17	65,73,73	1.51	9 (13%)	76,113,113	1.29	8 (10%)
25	CLA	b	612	-	65,73,73	1.48	10 (15%)	76,113,113	1.45	8 (10%)
24	CHL	p	609	2	66,74,74	1.94	14 (21%)	73,114,114	2.67	21 (28%)
35	SQD	B	621	-	53,54,54	1.17	4 (7%)	62,65,65	1.13	4 (6%)
25	CLA	c	505	-	65,73,73	1.45	9 (13%)	76,113,113	1.40	9 (11%)
24	CHL	N	601	2	66,74,74	1.84	11 (16%)	73,114,114	2.76	26 (35%)
36	LMG	S	2631	-	52,52,55	0.92	2 (3%)	60,60,63	1.10	4 (6%)
25	CLA	0	613	1	65,73,73	1.47	8 (12%)	76,113,113	1.33	9 (11%)
24	CHL	g	605	3	48,56,74	2.27	15 (31%)	51,92,114	3.09	21 (41%)
25	CLA	y	613	1	65,73,73	1.52	11 (16%)	76,113,113	1.29	7 (9%)
27	XAT	g	1622	-	39,47,47	0.97	1 (2%)	54,74,74	2.54	19 (35%)
25	CLA	0	612	1	65,73,73	1.50	9 (13%)	76,113,113	1.31	8 (10%)
24	CHL	7	606	-	66,74,74	1.90	14 (21%)	73,114,114	2.59	22 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	B	613	-	65,73,73	1.42	9 (13%)	76,113,113	1.60	8 (10%)
25	CLA	B	604	-	65,73,73	1.50	10 (15%)	76,113,113	1.27	7 (9%)
25	CLA	c	509	-	65,73,73	1.41	11 (16%)	76,113,113	1.55	10 (13%)
25	CLA	s	614	-	48,56,73	1.68	7 (14%)	55,92,113	1.47	8 (14%)
28	NEX	0	1623	-	38,46,46	0.97	1 (2%)	50,70,70	2.38	12 (24%)
25	CLA	6	614	-	54,62,73	1.66	5 (9%)	62,99,113	1.47	7 (11%)
25	CLA	9	603	-	65,73,73	1.50	9 (13%)	76,113,113	1.36	9 (11%)
26	LUT	3	1620	-	42,43,43	0.73	0	51,60,60	1.67	12 (23%)
26	LUT	4	1620	-	42,43,43	0.74	0	51,60,60	1.61	15 (29%)
26	LUT	n	1620	-	42,43,43	0.78	0	51,60,60	1.53	10 (19%)
29	LHG	d	409	-	48,48,48	0.91	2 (4%)	51,54,54	0.96	2 (3%)
25	CLA	4	610	3	65,73,73	1.49	8 (12%)	76,113,113	1.30	7 (9%)
27	XAT	G	1622	-	39,47,47	0.97	1 (2%)	54,74,74	2.54	20 (37%)
29	LHG	c	2630	-	46,46,48	0.93	2 (4%)	49,52,54	1.04	3 (6%)
26	LUT	1	1620	-	42,43,43	0.79	1 (2%)	51,60,60	1.58	9 (17%)
29	LHG	D	409	-	48,48,48	0.91	2 (4%)	51,54,54	0.96	2 (3%)
36	LMG	b	622	-	51,51,55	0.87	2 (3%)	59,59,63	1.11	3 (5%)
25	CLA	G	603	-	65,73,73	1.48	11 (16%)	76,113,113	1.36	8 (10%)
25	CLA	8	613	2	65,73,73	1.49	7 (10%)	76,113,113	1.48	8 (10%)
34	BCR	c	516	-	41,41,41	0.76	0	56,56,56	1.70	11 (19%)
37	DGD	C	518	-	56,56,67	0.89	2 (3%)	70,70,81	1.12	6 (8%)
25	CLA	9	604	-	49,57,73	1.70	8 (16%)	55,93,113	1.48	7 (12%)
29	LHG	Y	2630	25	48,48,48	0.88	2 (4%)	51,54,54	1.21	5 (9%)
28	NEX	8	1623	-	38,46,46	0.87	1 (2%)	50,70,70	2.31	12 (24%)
25	CLA	4	613	3	65,73,73	1.47	7 (10%)	76,113,113	1.37	6 (7%)
25	CLA	0	611	29	65,73,73	1.46	6 (9%)	76,113,113	1.38	8 (10%)
29	LHG	n	2630	25	48,48,48	0.92	2 (4%)	51,54,54	1.10	3 (5%)
25	CLA	5	610	2	65,73,73	1.51	7 (10%)	76,113,113	1.21	7 (9%)
25	CLA	Y	610	1	65,73,73	1.43	8 (12%)	76,113,113	1.32	8 (10%)
25	CLA	3	614	-	49,57,73	1.72	6 (12%)	55,93,113	1.34	8 (14%)
25	CLA	c	507	-	65,73,73	1.40	11 (16%)	76,113,113	1.45	12 (15%)
26	LUT	N	1620	-	42,43,43	0.77	0	51,60,60	1.49	8 (15%)
25	CLA	B	611	-	65,73,73	1.51	11 (16%)	76,113,113	1.55	9 (11%)
25	CLA	N	610	2	65,73,73	1.46	9 (13%)	76,113,113	1.25	8 (10%)
25	CLA	S	612	18	45,53,73	1.83	11 (24%)	52,89,113	1.63	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CLA	0	603	-	65,73,73	1.46	9 (13%)	76,113,113	1.44	8 (10%)
25	CLA	g	602	3	65,73,73	1.43	8 (12%)	76,113,113	1.38	8 (10%)
26	LUT	G	1621	-	42,43,43	0.78	0	51,60,60	1.65	11 (21%)
25	CLA	s	603	-	42,50,73	1.81	9 (21%)	48,85,113	1.64	7 (14%)
25	CLA	A	407	-	49,57,73	1.65	11 (22%)	55,93,113	1.52	6 (10%)

In the following table, the Chirals column lists the number of chiral outliers, the number of chiral centers analysed, the number of these observed in the model and the number defined in the Chemical Component Dictionary. Similar counts are reported in the Torsion and Rings columns. '-' means no outliers of that kind were identified.

Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	g	608	-	3/3/15/26	3/13/111/137	-
26	LUT	4	1621	-	-	7/29/67/67	0/2/2/2
25	CLA	p	613	2	1/1/15/20	11/37/115/115	-
24	CHL	y	605	1	3/3/16/26	6/15/113/137	-
25	CLA	N	614	-	1/1/11/20	6/18/96/115	-
24	CHL	s	608	-	3/3/16/26	11/19/117/137	-
24	CHL	8	609	2	3/3/20/26	20/39/137/137	-
26	LUT	7	1620	-	-	2/29/67/67	0/2/2/2
24	CHL	3	601	2	3/3/20/26	24/39/137/137	-
24	CHL	6	608	-	3/3/16/26	8/20/118/137	-
25	CLA	3	603	-	1/1/15/20	13/37/115/115	-
25	CLA	7	610	1	1/1/15/20	15/37/115/115	-
25	CLA	5	612	2	1/1/11/20	6/13/91/115	-
25	CLA	B	610	-	1/1/15/20	8/37/115/115	-
25	CLA	n	614	-	1/1/11/20	6/18/96/115	-
25	CLA	N	612	2	1/1/11/20	6/13/91/115	-
25	CLA	6	611	29	1/1/15/20	12/37/115/115	-
25	CLA	S	611	29	1/1/11/20	6/18/96/115	-
25	CLA	8	603	-	1/1/15/20	14/37/115/115	-
25	CLA	c	506	-	1/1/15/20	20/37/115/115	-
25	CLA	D	402	-	1/1/15/20	14/37/115/115	-
25	CLA	y	602	1	1/1/15/20	12/37/115/115	-
28	NEX	q	1623	-	-	3/27/83/83	0/3/3/3
24	CHL	y	601	1	3/3/20/26	14/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	B	602	-	1/1/15/20	17/37/115/115	-
25	CLA	r	609	17	1/1/13/20	6/29/107/115	-
25	CLA	q	612	3	1/1/10/20	7/11/89/115	-
24	CHL	1	609	1	3/3/20/26	17/39/137/137	-
26	LUT	5	1620	-	-	4/29/67/67	0/2/2/2
25	CLA	R	612	-	1/1/11/20	8/18/96/115	-
37	DGD	c	519	-	-	20/51/91/95	0/2/2/2
34	BCR	B	620	-	-	4/29/63/63	0/2/2/2
24	CHL	1	607	-	3/3/20/26	19/39/137/137	-
25	CLA	4	603	-	1/1/15/20	18/37/115/115	-
24	CHL	5	606	-	3/3/16/26	4/15/113/137	-
29	LHG	G	2630	25	-	12/53/53/53	-
25	CLA	c	511	6	-	14/37/115/115	-
25	CLA	6	602	1	1/1/15/20	12/37/115/115	-
25	CLA	C	503	-	1/1/15/20	10/37/115/115	-
24	CHL	6	601	1	3/3/20/26	10/39/137/137	-
25	CLA	B	606	-	1/1/15/20	12/37/115/115	-
25	CLA	p	611	29	1/1/11/20	6/18/96/115	-
24	CHL	q	606	-	3/3/16/26	5/20/118/137	-
25	CLA	a	406	-	1/1/15/20	3/37/115/115	-
25	CLA	7	612	1	1/1/15/20	13/37/115/115	-
25	CLA	B	612	-	1/1/15/20	9/37/115/115	-
25	CLA	g	614	-	1/1/11/20	9/18/96/115	-
26	LUT	g	1621	-	-	2/29/67/67	0/2/2/2
25	CLA	G	610	3	1/1/15/20	10/37/115/115	-
25	CLA	Y	613	1	-	9/37/115/115	-
25	CLA	A	410	-	1/1/14/20	6/31/109/115	-
24	CHL	q	609	3	3/3/20/26	20/39/137/137	-
24	CHL	p	601	2	3/3/20/26	16/39/137/137	-
40	HEM	f	101	8,9	-	3/12/54/54	-
25	CLA	n	613	2	1/1/15/20	14/37/115/115	-
25	CLA	5	614	-	-	8/18/96/115	-
24	CHL	2	601	2	3/3/20/26	24/39/137/137	-
25	CLA	Y	614	-	1/1/12/20	10/24/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	7	605	1	3/3/16/26	8/15/113/137	-
25	CLA	r	610	17	1/1/15/20	14/37/115/115	-
33	PHO	a	408	-	-	10/37/103/103	0/5/6/6
24	CHL	8	605	2	3/3/20/26	15/39/137/137	-
24	CHL	y	609	1	3/3/20/26	17/39/137/137	-
25	CLA	4	611	29	1/1/11/20	7/13/91/115	-
35	SQD	b	623	-	-	14/45/65/69	0/1/1/1
28	NEX	R	623	-	-	2/27/83/83	0/3/3/3
25	CLA	n	603	-	1/1/15/20	7/37/115/115	-
26	LUT	y	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	y	610	1	1/1/15/20	11/37/115/115	-
24	CHL	p	605	2	3/3/20/26	17/39/137/137	-
25	CLA	B	616	-	1/1/15/20	10/37/115/115	-
24	CHL	9	607	-	3/3/16/26	11/20/118/137	-
25	CLA	B	614	-	1/1/15/20	10/37/115/115	-
24	CHL	3	608	-	3/3/16/26	11/20/118/137	-
24	CHL	q	605	3	3/3/16/26	8/18/116/137	-
27	XAT	q	1622	-	-	3/31/93/93	0/4/4/4
24	CHL	1	605	1	3/3/16/26	8/15/113/137	-
24	CHL	0	607	-	3/3/20/26	24/39/137/137	-
25	CLA	0	610	1	1/1/15/20	6/37/115/115	-
25	CLA	p	604	-	1/1/15/20	15/37/115/115	-
25	CLA	s	612	18	1/1/11/20	4/13/91/115	-
24	CHL	N	608	-	3/3/16/26	6/20/118/137	-
29	LHG	2	2630	25	-	22/53/53/53	-
37	DGD	C	520	-	-	10/48/88/95	0/2/2/2
24	CHL	s	607	-	3/3/15/26	4/12/110/137	-
25	CLA	p	602	2	1/1/15/20	12/37/115/115	-
26	LUT	6	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	Y	603	-	1/1/15/20	14/37/115/115	-
25	CLA	b	608	-	1/1/15/20	18/37/115/115	-
25	CLA	N	603	-	1/1/15/20	6/37/115/115	-
24	CHL	r	607	-	3/3/18/26	17/27/125/137	-
25	CLA	A	405	-	1/1/15/20	11/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	LHG	L	101	-	-	17/53/53/53	-
25	CLA	9	611	29	1/1/11/20	8/13/91/115	-
26	LUT	8	1621	-	-	0/29/67/67	0/2/2/2
24	CHL	R	607	-	3/3/18/26	17/27/125/137	-
34	BCR	c	514	-	-	4/29/63/63	0/2/2/2
25	CLA	4	602	3	1/1/15/20	10/37/115/115	-
27	XAT	2	1622	-	-	2/31/93/93	0/4/4/4
36	LMG	h	102	-	-	14/43/63/70	0/1/1/1
24	CHL	1	608	-	3/3/16/26	9/20/118/137	-
25	CLA	A	406	-	1/1/15/20	3/37/115/115	-
25	CLA	c	513	-	1/1/15/20	18/37/115/115	-
36	LMG	s	2631	-	-	10/47/67/70	0/1/1/1
36	LMG	H	102	-	-	15/43/63/70	0/1/1/1
25	CLA	b	607	-	-	15/37/115/115	-
25	CLA	6	613	1	-	20/37/115/115	-
25	CLA	a	405	-	1/1/15/20	11/37/115/115	-
24	CHL	7	609	1	3/3/20/26	17/39/137/137	-
25	CLA	r	602	17	1/1/14/20	6/31/109/115	-
35	SQD	D	413	-	-	10/47/67/69	0/1/1/1
25	CLA	4	604	-	1/1/11/20	13/18/96/115	-
27	XAT	p	1622	-	-	0/31/93/93	0/4/4/4
25	CLA	G	611	29	1/1/11/20	6/13/91/115	-
29	LHG	8	2630	25	-	10/53/53/53	-
26	LUT	1	1621	-	-	3/29/67/67	0/2/2/2
25	CLA	p	610	2	1/1/15/20	9/37/115/115	-
25	CLA	2	611	29	1/1/11/20	8/13/91/115	-
25	CLA	5	602	2	1/1/15/20	16/37/115/115	-
25	CLA	7	603	-	1/1/15/20	15/37/115/115	-
25	CLA	B	603	-	1/1/15/20	13/37/115/115	-
24	CHL	0	605	1	3/3/16/26	7/15/113/137	-
24	CHL	G	601	3	3/3/20/26	18/39/137/137	-
24	CHL	3	609	2	3/3/20/26	18/39/137/137	-
25	CLA	r	604	-	1/1/11/20	8/17/95/115	-
34	BCR	c	517	-	-	0/29/63/63	0/2/2/2
36	LMG	d	412	-	-	5/41/61/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
24	CHL	n	608	-	3/3/16/26	12/20/118/137	-
25	CLA	q	602	3	1/1/15/20	15/37/115/115	-
24	CHL	0	609	1	3/3/20/26	19/39/137/137	-
25	CLA	a	407	-	1/1/11/20	6/18/96/115	-
24	CHL	q	608	-	3/3/15/26	6/13/111/137	-
24	CHL	y	606	-	3/3/20/26	21/39/137/137	-
25	CLA	8	610	2	1/1/15/20	9/37/115/115	-
25	CLA	B	617	-	1/1/15/20	10/37/115/115	-
24	CHL	7	608	-	3/3/16/26	12/20/118/137	-
36	LMG	d	411	-	-	8/41/61/70	0/1/1/1
25	CLA	S	613	18	-	9/18/96/115	-
24	CHL	Y	601	1	3/3/20/26	13/39/137/137	-
26	LUT	G	1620	-	-	3/29/67/67	0/2/2/2
27	XAT	N	1622	-	-	0/31/93/93	0/4/4/4
26	LUT	y	1621	-	-	4/29/67/67	0/2/2/2
24	CHL	G	606	-	3/3/16/26	5/20/118/137	-
24	CHL	9	609	2	3/3/20/26	19/39/137/137	-
25	CLA	8	602	2	1/1/15/20	11/37/115/115	-
25	CLA	p	612	2	1/1/11/20	4/13/91/115	-
25	CLA	G	604	-	1/1/11/20	7/18/96/115	-
25	CLA	n	610	2	1/1/15/20	6/37/115/115	-
24	CHL	S	607	-	3/3/15/26	4/12/110/137	-
28	NEX	S	1623	-	-	4/27/83/83	0/3/3/3
24	CHL	9	601	2	3/3/20/26	21/39/137/137	-
28	NEX	7	1623	-	-	4/27/83/83	0/3/3/3
25	CLA	0	614	-	1/1/12/20	9/24/102/115	-
25	CLA	2	613	2	1/1/15/20	8/37/115/115	-
29	LHG	r	2630	25	-	16/42/42/53	-
24	CHL	2	609	2	3/3/20/26	20/39/137/137	-
24	CHL	1	606	-	3/3/20/26	19/39/137/137	-
34	BCR	C	516	-	-	9/29/63/63	0/2/2/2
25	CLA	G	612	3	1/1/10/20	4/11/89/115	-
25	CLA	g	613	3	1/1/15/20	13/37/115/115	-
24	CHL	4	605	3	3/3/16/26	12/18/116/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	c	510	-	1/1/15/20	10/37/115/115	-
36	LMG	D	412	-	-	5/41/61/70	0/1/1/1
25	CLA	4	614	-	1/1/11/20	8/18/96/115	-
26	LUT	7	1621	-	-	3/29/67/67	0/2/2/2
28	NEX	2	1623	-	-	4/27/83/83	0/3/3/3
25	CLA	b	613	-	1/1/15/20	14/37/115/115	-
24	CHL	g	607	-	3/3/16/26	10/20/118/137	-
24	CHL	p	606	-	3/3/16/26	5/15/113/137	-
25	CLA	y	611	29	1/1/15/20	8/37/115/115	-
25	CLA	8	612	2	1/1/11/20	7/13/91/115	-
24	CHL	6	605	1	3/3/16/26	5/15/113/137	-
24	CHL	N	607	-	3/3/20/26	14/39/137/137	-
25	CLA	y	603	-	1/1/15/20	15/37/115/115	-
26	LUT	p	1621	-	-	4/29/67/67	0/2/2/2
34	BCR	c	515	-	-	4/29/63/63	0/2/2/2
29	LHG	y	2630	25	-	24/53/53/53	-
29	LHG	d	408	-	-	10/48/48/53	-
25	CLA	b	609	-	1/1/15/20	12/37/115/115	-
24	CHL	6	609	1	3/3/20/26	19/39/137/137	-
24	CHL	4	606	-	3/3/16/26	8/20/118/137	-
26	LUT	Y	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	c	502	-	1/1/15/20	17/37/115/115	-
25	CLA	1	612	1	1/1/15/20	15/37/115/115	-
34	BCR	C	515	-	-	4/29/63/63	0/2/2/2
25	CLA	6	603	-	1/1/15/20	10/37/115/115	-
25	CLA	c	512	-	1/1/15/20	13/37/115/115	-
25	CLA	C	502	-	1/1/15/20	18/37/115/115	-
24	CHL	N	605	2	3/3/20/26	23/39/137/137	-
25	CLA	r	613	17	-	15/31/109/115	-
24	CHL	q	607	-	3/3/16/26	13/20/118/137	-
25	CLA	B	608	-	1/1/15/20	16/37/115/115	-
24	CHL	7	607	-	3/3/20/26	19/39/137/137	-
37	DGD	c	523	-	-	12/55/95/95	0/2/2/2
27	XAT	r	622	-	-	0/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	b	605	-	1/1/15/20	15/37/115/115	-
25	CLA	C	507	-	1/1/15/20	11/37/115/115	-
34	BCR	b	618	-	-	5/29/63/63	0/2/2/2
34	BCR	d	404	-	-	4/29/63/63	0/2/2/2
24	CHL	g	601	3	3/3/20/26	19/39/137/137	-
26	LUT	r	620	-	-	2/29/67/67	0/2/2/2
25	CLA	2	603	-	1/1/15/20	20/37/115/115	-
25	CLA	9	602	2	1/1/15/20	16/37/115/115	-
24	CHL	R	608	-	3/3/19/26	15/33/131/137	-
35	SQD	B	623	-	-	11/45/65/69	0/1/1/1
27	XAT	7	1622	-	-	2/31/93/93	0/4/4/4
26	LUT	R	620	-	-	2/29/67/67	0/2/2/2
24	CHL	5	601	2	3/3/20/26	18/39/137/137	-
25	CLA	0	602	1	1/1/15/20	11/37/115/115	-
25	CLA	q	613	3	1/1/15/20	16/37/115/115	-
25	CLA	b	610	-	1/1/15/20	8/37/115/115	-
28	NEX	N	1623	-	-	2/27/83/83	0/3/3/3
25	CLA	9	613	2	1/1/15/20	8/37/115/115	-
28	NEX	r	623	-	-	2/27/83/83	0/3/3/3
25	CLA	p	603	-	1/1/15/20	14/37/115/115	-
24	CHL	0	608	-	3/3/16/26	6/20/118/137	-
25	CLA	0	604	-	1/1/15/20	17/37/115/115	-
34	BCR	B	619	-	-	0/29/63/63	0/2/2/2
26	LUT	g	1620	-	-	3/29/67/67	0/2/2/2
25	CLA	b	602	-	1/1/15/20	17/37/115/115	-
24	CHL	5	608	-	3/3/16/26	11/20/118/137	-
29	LHG	3	2630	25	-	12/53/53/53	-
28	NEX	9	1623	-	-	4/27/83/83	0/3/3/3
24	CHL	S	601	18	3/3/16/26	9/15/113/137	-
24	CHL	Y	605	1	3/3/16/26	6/15/113/137	-
25	CLA	g	604	-	1/1/11/20	8/18/96/115	-
26	LUT	9	1621	-	-	3/29/67/67	0/2/2/2
25	CLA	q	614	-	1/1/11/20	8/18/96/115	-
24	CHL	n	605	2	3/3/20/26	20/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	XAT	0	1622	-	-	2/31/93/93	0/4/4/4
26	LUT	6	1621	-	-	3/29/67/67	0/2/2/2
27	XAT	9	1622	-	-	2/31/93/93	0/4/4/4
24	CHL	2	606	-	3/3/16/26	9/20/118/137	-
25	CLA	R	613	17	-	15/31/109/115	-
29	LHG	p	2630	25	-	12/53/53/53	-
24	CHL	n	609	2	3/3/20/26	20/39/137/137	-
24	CHL	N	609	2	3/3/20/26	19/39/137/137	-
25	CLA	1	611	29	1/1/15/20	8/37/115/115	-
25	CLA	B	615	-	1/1/15/20	15/37/115/115	-
25	CLA	y	604	-	-	18/37/115/115	-
29	LHG	6	2630	25	-	19/53/53/53	-
25	CLA	c	503	-	1/1/15/20	14/37/115/115	-
24	CHL	3	605	2	3/3/20/26	17/39/137/137	-
29	LHG	4	2630	25	-	19/53/53/53	-
34	BCR	A	411	-	-	2/29/63/63	0/2/2/2
26	LUT	0	1621	-	-	3/29/67/67	0/2/2/2
25	CLA	G	602	3	1/1/15/20	11/37/115/115	-
28	NEX	1	1623	-	-	4/27/83/83	0/3/3/3
25	CLA	7	604	-	1/1/15/20	17/37/115/115	-
35	SQD	a	412	-	-	18/46/66/69	0/1/1/1
25	CLA	q	610	3	1/1/15/20	9/37/115/115	-
26	LUT	s	1621	-	-	0/29/67/67	0/2/2/2
25	CLA	C	511	6	-	14/37/115/115	-
27	XAT	y	1622	-	-	0/31/93/93	0/4/4/4
26	LUT	q	1621	-	-	5/29/67/67	0/2/2/2
25	CLA	3	613	2	-	15/37/115/115	-
25	CLA	D	403	-	1/1/15/20	12/37/115/115	-
26	LUT	S	1621	-	-	0/29/67/67	0/2/2/2
34	BCR	D	404	-	-	4/29/63/63	0/2/2/2
28	NEX	s	1623	-	-	4/27/83/83	0/3/3/3
35	SQD	d	413	-	-	9/47/67/69	0/1/1/1
24	CHL	g	609	3	3/3/20/26	15/39/137/137	-
25	CLA	r	611	29	1/1/11/20	10/18/96/115	-
25	CLA	S	610	18	1/1/11/20	9/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	G	614	-	1/1/11/20	9/18/96/115	-
24	CHL	7	601	1	3/3/20/26	16/39/137/137	-
24	CHL	Y	609	1	3/3/20/26	17/39/137/137	-
27	XAT	6	1622	-	-	2/31/93/93	0/4/4/4
25	CLA	S	602	18	-	10/18/96/115	-
25	CLA	2	604	-	1/1/11/20	9/18/96/115	-
25	CLA	Y	611	29	1/1/15/20	8/37/115/115	-
24	CHL	5	607	-	3/3/20/26	19/39/137/137	-
25	CLA	s	611	29	1/1/11/20	6/18/96/115	-
25	CLA	8	604	-	1/1/15/20	10/37/115/115	-
28	NEX	5	1623	-	-	4/27/83/83	0/3/3/3
25	CLA	b	614	-	1/1/15/20	10/37/115/115	-
25	CLA	2	610	2	1/1/15/20	4/37/115/115	-
25	CLA	c	504	-	1/1/15/20	15/37/115/115	-
28	NEX	3	1623	-	-	5/27/83/83	0/3/3/3
37	DGD	c	524	-	-	9/55/95/95	0/2/2/2
26	LUT	3	1621	-	-	0/29/67/67	0/2/2/2
29	LHG	l	101	-	-	18/53/53/53	-
28	NEX	y	1623	-	-	5/27/83/83	0/3/3/3
33	PHO	A	408	-	-	10/37/103/103	0/5/6/6
25	CLA	c	501	-	1/1/15/20	14/37/115/115	-
27	XAT	8	1622	-	-	1/31/93/93	0/4/4/4
29	LHG	s	2630	25	-	18/49/49/53	-
24	CHL	6	606	-	3/3/20/26	22/39/137/137	-
25	CLA	1	613	1	-	14/37/115/115	-
29	LHG	C	2630	-	-	19/51/51/53	-
25	CLA	d	403	-	1/1/15/20	12/37/115/115	-
36	LMG	A	413	-	-	12/43/63/70	0/1/1/1
25	CLA	r	601	17	1/1/11/20	8/18/96/115	-
25	CLA	N	602	2	1/1/15/20	6/37/115/115	-
24	CHL	Y	606	-	3/3/20/26	21/39/137/137	-
25	CLA	b	604	-	1/1/15/20	11/37/115/115	-
24	CHL	Y	608	-	3/3/16/26	4/20/118/137	-
27	XAT	4	1622	-	-	2/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	R	601	17	1/1/11/20	8/18/96/115	-
25	CLA	C	505	-	1/1/15/20	18/37/115/115	-
25	CLA	c	508	-	1/1/15/20	13/37/115/115	-
28	NEX	6	1623	-	-	3/27/83/83	0/3/3/3
24	CHL	8	606	-	3/3/16/26	8/15/113/137	-
27	XAT	1	1622	-	-	2/31/93/93	0/4/4/4
25	CLA	5	613	2	1/1/15/20	12/37/115/115	-
25	CLA	1	610	1	1/1/15/20	14/37/115/115	-
25	CLA	R	602	17	1/1/14/20	6/31/109/115	-
25	CLA	y	612	1	1/1/15/20	15/37/115/115	-
25	CLA	2	612	2	1/1/10/20	4/11/89/115	-
24	CHL	9	605	2	3/3/16/26	6/18/116/137	-
28	NEX	p	1623	-	-	4/27/83/83	0/3/3/3
26	LUT	n	1621	-	-	5/29/67/67	0/2/2/2
25	CLA	1	602	1	1/1/15/20	11/37/115/115	-
25	CLA	C	513	-	1/1/15/20	17/37/115/115	-
25	CLA	g	612	3	1/1/10/20	4/11/89/115	-
24	CHL	2	605	2	3/3/16/26	6/18/116/137	-
36	LMG	D	411	-	-	8/41/61/70	0/1/1/1
26	LUT	N	1621	-	-	5/29/67/67	0/2/2/2
24	CHL	S	608	-	3/3/16/26	11/19/117/137	-
25	CLA	3	610	2	1/1/15/20	6/37/115/115	-
24	CHL	q	601	3	3/3/20/26	19/39/137/137	-
24	CHL	G	608	-	3/3/15/26	6/13/111/137	-
25	CLA	7	602	1	1/1/15/20	13/37/115/115	-
25	CLA	1	604	-	1/1/15/20	15/37/115/115	-
25	CLA	r	612	-	1/1/11/20	8/18/96/115	-
26	LUT	2	1620	-	-	2/29/67/67	0/2/2/2
26	LUT	8	1620	-	-	4/29/67/67	0/2/2/2
24	CHL	5	605	2	3/3/20/26	20/39/137/137	-
25	CLA	s	613	18	-	9/18/96/115	-
27	XAT	3	1622	-	-	1/31/93/93	0/4/4/4
29	LHG	S	2630	25	-	16/49/49/53	-
25	CLA	y	614	-	1/1/12/20	10/24/102/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
27	XAT	n	1622	-	-	2/31/93/93	0/4/4/4
25	CLA	7	613	1	-	15/37/115/115	-
25	CLA	s	605	18	1/1/12/20	8/19/97/115	-
25	CLA	C	512	-	1/1/15/20	15/37/115/115	-
25	CLA	B	605	-	1/1/15/20	15/37/115/115	-
34	BCR	B	618	-	-	5/29/63/63	0/2/2/2
26	LUT	p	1620	-	-	6/29/67/67	0/2/2/2
25	CLA	R	609	17	1/1/13/20	6/29/107/115	-
25	CLA	9	614	-	-	8/18/96/115	-
25	CLA	b	617	-	1/1/15/20	11/37/115/115	-
25	CLA	N	611	29	1/1/11/20	9/18/96/115	-
25	CLA	C	506	-	1/1/15/20	20/37/115/115	-
25	CLA	s	609	18	1/1/10/20	4/8/86/115	-
24	CHL	p	608	-	3/3/16/26	13/20/118/137	-
36	LMG	B	622	-	-	9/46/66/70	0/1/1/1
25	CLA	6	610	1	1/1/15/20	6/37/115/115	-
24	CHL	5	609	2	3/3/20/26	19/39/137/137	-
25	CLA	2	614	-	-	7/18/96/115	-
29	LHG	D	408	-	-	10/48/48/53	-
25	CLA	R	604	-	1/1/11/20	8/17/95/115	-
25	CLA	R	616	17	-	22/37/115/115	-
25	CLA	3	612	2	1/1/11/20	8/13/91/115	-
39	PL9	D	405	-	-	14/53/73/73	0/1/1/1
26	LUT	Y	1621	-	-	4/29/67/67	0/2/2/2
25	CLA	B	609	-	1/1/15/20	12/37/115/115	-
25	CLA	R	610	17	1/1/15/20	14/37/115/115	-
25	CLA	q	603	-	1/1/15/20	17/37/115/115	-
29	LHG	N	2630	25	-	15/53/53/53	-
36	LMG	a	413	-	-	12/43/63/70	0/1/1/1
25	CLA	n	612	2	1/1/11/20	6/13/91/115	-
24	CHL	Y	607	-	3/3/20/26	21/39/137/137	-
24	CHL	8	601	2	3/3/20/26	24/39/137/137	-
24	CHL	4	608	-	3/3/15/26	4/13/111/137	-
29	LHG	q	2630	25	-	17/53/53/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	p	614	-	-	7/18/96/115	-
25	CLA	8	614	-	1/1/11/20	8/18/96/115	-
24	CHL	n	607	-	3/3/20/26	14/39/137/137	-
24	CHL	9	606	-	3/3/16/26	10/20/118/137	-
28	NEX	4	1623	-	-	3/27/83/83	0/3/3/3
25	CLA	b	615	-	1/1/15/20	14/37/115/115	-
28	NEX	n	1623	-	-	2/27/83/83	0/3/3/3
25	CLA	S	603	-	1/1/10/20	5/10/88/115	-
25	CLA	g	611	29	1/1/11/20	6/13/91/115	-
25	CLA	7	611	29	1/1/15/20	8/37/115/115	-
27	XAT	5	1622	-	-	0/31/93/93	0/4/4/4
27	XAT	Y	1622	-	-	0/31/93/93	0/4/4/4
35	SQD	b	621	-	-	17/49/69/69	0/1/1/1
25	CLA	C	504	-	1/1/15/20	15/37/115/115	-
24	CHL	y	607	-	3/3/20/26	18/39/137/137	-
34	BCR	a	411	-	-	2/29/63/63	0/2/2/2
25	CLA	C	510	-	1/1/15/20	10/37/115/115	-
34	BCR	b	620	-	-	4/29/63/63	0/2/2/2
37	DGD	C	524	-	-	9/55/95/95	0/2/2/2
24	CHL	1	601	1	3/3/20/26	14/39/137/137	-
24	CHL	4	607	-	3/3/16/26	13/20/118/137	-
25	CLA	1	614	-	1/1/12/20	13/24/102/115	-
25	CLA	6	612	1	1/1/15/20	11/37/115/115	-
29	LHG	g	2630	25	-	12/53/53/53	-
29	LHG	7	2630	25	-	18/53/53/53	-
25	CLA	3	602	2	1/1/15/20	11/37/115/115	-
24	CHL	r	606	-	3/3/20/26	22/39/137/137	-
25	CLA	4	612	3	1/1/10/20	7/11/89/115	-
25	CLA	S	609	18	1/1/10/20	4/8/86/115	-
24	CHL	R	606	-	3/3/20/26	22/39/137/137	-
40	HEM	F	101	8,9	-	4/12/54/54	-
25	CLA	n	611	29	1/1/11/20	9/18/96/115	-
24	CHL	0	606	-	3/3/20/26	21/39/137/137	-
24	CHL	6	607	-	3/3/20/26	25/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
34	BCR	H	101	-	-	5/29/63/63	0/2/2/2
25	CLA	Y	612	1	1/1/15/20	15/37/115/115	-
25	CLA	s	610	18	1/1/11/20	9/18/96/115	-
25	CLA	N	613	2	1/1/15/20	14/37/115/115	-
24	CHL	9	608	-	3/3/15/26	4/13/111/137	-
24	CHL	s	606	-	3/3/15/26	10/13/111/137	-
25	CLA	C	508	-	1/1/15/20	15/37/115/115	-
25	CLA	g	610	3	1/1/15/20	10/37/115/115	-
37	DGD	C	519	-	-	20/51/91/95	0/2/2/2
28	NEX	Y	1623	-	-	5/27/83/83	0/3/3/3
24	CHL	p	607	-	3/3/20/26	22/39/137/137	-
25	CLA	G	613	3	1/1/15/20	14/37/115/115	-
25	CLA	d	402	-	1/1/15/20	14/37/115/115	-
36	LMG	c	521	-	-	10/46/66/70	0/1/1/1
24	CHL	8	607	-	3/3/20/26	24/39/137/137	-
34	BCR	b	619	-	-	0/29/63/63	0/2/2/2
25	CLA	S	614	-	1/1/11/20	7/17/95/115	-
25	CLA	1	603	-	1/1/15/20	17/37/115/115	-
25	CLA	2	602	2	-	12/37/115/115	-
24	CHL	3	606	-	3/3/16/26	8/15/113/137	-
24	CHL	G	607	-	3/3/16/26	7/20/118/137	-
28	NEX	G	1623	-	-	3/27/83/83	0/3/3/3
25	CLA	b	611	-	1/1/15/20	8/37/115/115	-
24	CHL	2	608	-	3/3/15/26	5/13/111/137	-
24	CHL	8	608	-	3/3/16/26	11/20/118/137	-
25	CLA	r	603	-	1/1/14/20	10/31/109/115	-
33	PHO	a	409	-	-	9/37/103/103	0/5/6/6
29	LHG	D	410	-	-	10/43/43/53	-
24	CHL	0	601	1	3/3/20/26	11/39/137/137	-
37	DGD	c	518	-	-	7/44/84/95	0/2/2/2
25	CLA	8	611	29	1/1/11/20	8/18/96/115	-
25	CLA	R	603	-	1/1/14/20	10/31/109/115	-
25	CLA	5	604	-	1/1/15/20	16/37/115/115	-
24	CHL	s	601	18	3/3/16/26	9/15/113/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
39	PL9	d	405	-	-	14/53/73/73	0/1/1/1
29	LHG	d	410	-	-	12/43/43/53	-
26	LUT	5	1621	-	-	2/29/67/67	0/2/2/2
25	CLA	q	604	-	-	12/18/96/115	-
29	LHG	1	2630	25	-	16/53/53/53	-
25	CLA	s	602	18	-	7/18/96/115	-
34	BCR	h	101	-	-	5/29/63/63	0/2/2/2
25	CLA	C	509	-	1/1/15/20	4/37/115/115	-
24	CHL	G	605	3	3/3/16/26	10/18/116/137	-
29	LHG	9	2630	25	-	20/53/53/53	-
27	XAT	R	622	-	-	0/31/93/93	0/4/4/4
25	CLA	s	604	-	1/1/11/20	10/18/96/115	-
25	CLA	6	604	-	-	18/37/115/115	-
25	CLA	S	604	-	1/1/11/20	10/18/96/115	-
29	LHG	0	2630	25	-	18/53/53/53	-
36	LMG	C	521	-	-	10/46/66/70	0/1/1/1
24	CHL	G	609	3	3/3/20/26	14/39/137/137	-
24	CHL	3	607	-	3/3/20/26	24/39/137/137	-
26	LUT	q	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	5	611	29	1/1/11/20	11/18/96/115	-
26	LUT	2	1621	-	-	6/29/67/67	0/2/2/2
25	CLA	B	607	-	-	15/37/115/115	-
35	SQD	A	412	-	-	18/46/66/69	0/1/1/1
26	LUT	9	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	7	614	-	1/1/12/20	13/24/102/115	-
25	CLA	9	610	2	1/1/15/20	4/37/115/115	-
24	CHL	n	606	-	3/3/16/26	9/15/113/137	-
29	LHG	R	2630	25	-	16/42/42/53	-
28	NEX	g	1623	-	-	3/27/83/83	0/3/3/3
25	CLA	q	611	29	1/1/11/20	7/13/91/115	-
25	CLA	N	604	-	1/1/15/20	9/37/115/115	-
24	CHL	y	608	-	3/3/16/26	4/20/118/137	-
29	LHG	5	2630	25	-	13/53/53/53	-
25	CLA	R	611	29	1/1/11/20	9/18/96/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	LUT	s	1620	-	-	2/29/67/67	0/2/2/2
37	DGD	c	520	-	-	10/48/88/95	0/2/2/2
25	CLA	C	501	-	1/1/15/20	14/37/115/115	-
25	CLA	b	606	-	1/1/15/20	12/37/115/115	-
24	CHL	S	606	-	3/3/15/26	10/13/111/137	-
25	CLA	5	603	-	1/1/15/20	13/37/115/115	-
33	PHO	A	409	-	-	9/37/103/103	0/5/6/6
25	CLA	S	605	18	1/1/12/20	9/19/97/115	-
34	BCR	C	517	-	-	0/29/63/63	0/2/2/2
24	CHL	r	608	-	3/3/19/26	15/33/131/137	-
24	CHL	4	609	3	3/3/20/26	18/39/137/137	-
37	DGD	C	523	-	-	12/55/95/95	0/2/2/2
24	CHL	g	606	-	3/3/16/26	5/20/118/137	-
24	CHL	4	601	3	3/3/20/26	18/39/137/137	-
24	CHL	n	601	2	3/3/20/26	8/39/137/137	-
25	CLA	9	612	2	1/1/10/20	4/11/89/115	-
25	CLA	3	611	29	1/1/11/20	8/18/96/115	-
25	CLA	Y	602	1	1/1/15/20	12/37/115/115	-
26	LUT	S	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	a	410	-	1/1/14/20	6/31/109/115	-
24	CHL	N	606	-	3/3/16/26	9/15/113/137	-
26	LUT	0	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	n	602	2	1/1/15/20	6/37/115/115	-
25	CLA	g	603	-	1/1/15/20	7/37/115/115	-
25	CLA	b	616	-	1/1/15/20	10/37/115/115	-
25	CLA	Y	604	-	-	18/37/115/115	-
25	CLA	3	604	-	1/1/15/20	8/37/115/115	-
25	CLA	n	604	-	1/1/15/20	9/37/115/115	-
25	CLA	b	603	-	1/1/15/20	13/37/115/115	-
24	CHL	2	607	-	3/3/16/26	10/20/118/137	-
34	BCR	C	514	-	-	4/29/63/63	0/2/2/2
25	CLA	r	616	17	-	22/37/115/115	-
25	CLA	b	612	-	1/1/15/20	9/37/115/115	-
24	CHL	p	609	2	3/3/20/26	19/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
35	SQD	B	621	-	-	17/49/69/69	0/1/1/1
25	CLA	c	505	-	1/1/15/20	18/37/115/115	-
24	CHL	N	601	2	3/3/20/26	8/39/137/137	-
36	LMG	S	2631	-	-	12/47/67/70	0/1/1/1
25	CLA	0	613	1	-	16/37/115/115	-
24	CHL	g	605	3	3/3/16/26	9/18/116/137	-
25	CLA	y	613	1	-	9/37/115/115	-
27	XAT	g	1622	-	-	0/31/93/93	0/4/4/4
25	CLA	0	612	1	1/1/15/20	11/37/115/115	-
24	CHL	7	606	-	3/3/20/26	20/39/137/137	-
25	CLA	B	613	-	1/1/15/20	14/37/115/115	-
25	CLA	B	604	-	1/1/15/20	11/37/115/115	-
25	CLA	c	509	-	1/1/15/20	5/37/115/115	-
25	CLA	s	614	-	1/1/11/20	7/17/95/115	-
28	NEX	0	1623	-	-	5/27/83/83	0/3/3/3
25	CLA	6	614	-	1/1/12/20	9/24/102/115	-
25	CLA	9	603	-	1/1/15/20	21/37/115/115	-
26	LUT	3	1620	-	-	6/29/67/67	0/2/2/2
26	LUT	4	1620	-	-	6/29/67/67	0/2/2/2
26	LUT	n	1620	-	-	2/29/67/67	0/2/2/2
29	LHG	d	409	-	-	12/53/53/53	-
25	CLA	4	610	3	1/1/15/20	12/37/115/115	-
27	XAT	G	1622	-	-	0/31/93/93	0/4/4/4
29	LHG	c	2630	-	-	15/51/51/53	-
26	LUT	1	1620	-	-	2/29/67/67	0/2/2/2
29	LHG	D	409	-	-	12/53/53/53	-
36	LMG	b	622	-	-	8/46/66/70	0/1/1/1
25	CLA	G	603	-	1/1/15/20	7/37/115/115	-
25	CLA	8	613	2	-	15/37/115/115	-
34	BCR	c	516	-	-	8/29/63/63	0/2/2/2
37	DGD	C	518	-	-	7/44/84/95	0/2/2/2
25	CLA	9	604	-	1/1/11/20	8/18/96/115	-
29	LHG	Y	2630	25	-	23/53/53/53	-
28	NEX	8	1623	-	-	3/27/83/83	0/3/3/3

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CLA	4	613	3	1/1/15/20	17/37/115/115	-
25	CLA	0	611	29	1/1/15/20	7/37/115/115	-
29	LHG	n	2630	25	-	15/53/53/53	-
25	CLA	5	610	2	1/1/15/20	8/37/115/115	-
25	CLA	Y	610	1	1/1/15/20	11/37/115/115	-
25	CLA	3	614	-	1/1/11/20	8/18/96/115	-
25	CLA	c	507	-	1/1/15/20	12/37/115/115	-
26	LUT	N	1620	-	-	2/29/67/67	0/2/2/2
25	CLA	B	611	-	1/1/15/20	8/37/115/115	-
25	CLA	N	610	2	1/1/15/20	6/37/115/115	-
25	CLA	S	612	18	1/1/11/20	4/13/91/115	-
25	CLA	0	603	-	1/1/15/20	11/37/115/115	-
25	CLA	g	602	3	1/1/15/20	11/37/115/115	-
26	LUT	G	1621	-	-	2/29/67/67	0/2/2/2
25	CLA	s	603	-	1/1/10/20	5/10/88/115	-
25	CLA	A	407	-	1/1/11/20	6/18/96/115	-

All (4330) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	614	CLA	C4B-NB	7.88	1.42	1.35
25	p	602	CLA	C4B-NB	7.84	1.42	1.35
25	0	614	CLA	C4B-NB	7.80	1.42	1.35
25	p	614	CLA	C4B-NB	7.80	1.42	1.35
25	4	612	CLA	C4B-NB	7.79	1.42	1.35
25	p	613	CLA	C4B-NB	7.75	1.42	1.35
25	5	614	CLA	C4B-NB	7.75	1.42	1.35
25	6	604	CLA	C4B-NB	7.73	1.42	1.35
25	5	602	CLA	C4B-NB	7.72	1.42	1.35
25	s	609	CLA	C4B-NB	7.67	1.42	1.35
25	q	612	CLA	C4B-NB	7.67	1.42	1.35
25	p	611	CLA	C4B-NB	7.66	1.42	1.35
25	3	614	CLA	C4B-NB	7.65	1.42	1.35
25	3	604	CLA	C4B-NB	7.65	1.42	1.35
25	5	610	CLA	C4B-NB	7.64	1.42	1.35
25	4	604	CLA	C4B-NB	7.63	1.42	1.35
25	p	610	CLA	C4B-NB	7.63	1.42	1.35
25	S	609	CLA	C4B-NB	7.62	1.42	1.35
25	p	603	CLA	C4B-NB	7.62	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	9	612	CLA	C4B-NB	7.60	1.42	1.35
25	5	603	CLA	C4B-NB	7.58	1.42	1.35
25	8	610	CLA	C4B-NB	7.58	1.42	1.35
25	8	614	CLA	C4B-NB	7.58	1.42	1.35
25	p	604	CLA	C4B-NB	7.57	1.42	1.35
25	5	611	CLA	C4B-NB	7.57	1.42	1.35
25	5	613	CLA	C4B-NB	7.57	1.42	1.35
25	3	611	CLA	C4B-NB	7.57	1.42	1.35
25	9	614	CLA	C4B-NB	7.54	1.41	1.35
25	s	605	CLA	C4B-NB	7.54	1.41	1.35
25	7	614	CLA	C4B-NB	7.54	1.41	1.35
25	q	604	CLA	C4B-NB	7.53	1.41	1.35
25	S	605	CLA	C4B-NB	7.52	1.41	1.35
25	p	612	CLA	C4B-NB	7.51	1.41	1.35
25	3	613	CLA	C4B-NB	7.49	1.41	1.35
25	2	614	CLA	C4B-NB	7.49	1.41	1.35
25	5	612	CLA	C4B-NB	7.48	1.41	1.35
25	8	613	CLA	C4B-NB	7.47	1.41	1.35
25	8	604	CLA	C4B-NB	7.47	1.41	1.35
25	3	610	CLA	C4B-NB	7.47	1.41	1.35
25	6	613	CLA	C4B-NB	7.47	1.41	1.35
25	2	613	CLA	C4B-NB	7.46	1.41	1.35
25	2	612	CLA	C4B-NB	7.46	1.41	1.35
25	q	602	CLA	C4B-NB	7.45	1.41	1.35
25	7	602	CLA	C4B-NB	7.44	1.41	1.35
25	0	604	CLA	C4B-NB	7.43	1.41	1.35
25	9	613	CLA	C4B-NB	7.42	1.41	1.35
25	8	611	CLA	C4B-NB	7.41	1.41	1.35
25	r	616	CLA	C4B-NB	7.40	1.41	1.35
25	4	602	CLA	C4B-NB	7.40	1.41	1.35
25	1	614	CLA	C4B-NB	7.39	1.41	1.35
25	2	603	CLA	C4B-NB	7.39	1.41	1.35
25	8	612	CLA	C4B-NB	7.39	1.41	1.35
25	9	603	CLA	C4B-NB	7.38	1.41	1.35
25	1	602	CLA	C4B-NB	7.37	1.41	1.35
25	n	612	CLA	C4B-NB	7.36	1.41	1.35
25	3	602	CLA	C4B-NB	7.35	1.41	1.35
25	0	612	CLA	C4B-NB	7.35	1.41	1.35
25	3	612	CLA	C4B-NB	7.34	1.41	1.35
25	6	612	CLA	C4B-NB	7.33	1.41	1.35
25	2	604	CLA	C4B-NB	7.33	1.41	1.35
25	R	616	CLA	C4B-NB	7.33	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	9	604	CLA	C4B-NB	7.33	1.41	1.35
25	0	610	CLA	C4B-NB	7.33	1.41	1.35
25	8	602	CLA	C4B-NB	7.32	1.41	1.35
25	5	604	CLA	C4B-NB	7.32	1.41	1.35
25	R	604	CLA	C4B-NB	7.30	1.41	1.35
25	r	611	CLA	C4B-NB	7.29	1.41	1.35
25	2	610	CLA	C4B-NB	7.29	1.41	1.35
25	6	610	CLA	C4B-NB	7.29	1.41	1.35
25	N	612	CLA	C4B-NB	7.29	1.41	1.35
25	q	613	CLA	C4B-NB	7.29	1.41	1.35
25	r	604	CLA	C4B-NB	7.28	1.41	1.35
25	n	613	CLA	C4B-NB	7.28	1.41	1.35
25	S	612	CLA	C4B-NB	7.27	1.41	1.35
25	c	506	CLA	C4B-NB	7.25	1.41	1.35
25	q	603	CLA	C4B-NB	7.24	1.41	1.35
25	4	614	CLA	C4B-NB	7.22	1.41	1.35
25	R	611	CLA	C4B-NB	7.22	1.41	1.35
25	7	603	CLA	C4B-NB	7.22	1.41	1.35
25	9	610	CLA	C4B-NB	7.22	1.41	1.35
25	N	613	CLA	C4B-NB	7.21	1.41	1.35
25	2	611	CLA	C4B-NB	7.21	1.41	1.35
25	6	602	CLA	C4B-NB	7.21	1.41	1.35
25	C	506	CLA	C4B-NB	7.20	1.41	1.35
25	r	609	CLA	C4B-NB	7.20	1.41	1.35
25	0	613	CLA	C4B-NB	7.19	1.41	1.35
25	7	612	CLA	C4B-NB	7.18	1.41	1.35
25	4	613	CLA	C4B-NB	7.18	1.41	1.35
25	q	614	CLA	C4B-NB	7.18	1.41	1.35
25	R	609	CLA	C4B-NB	7.16	1.41	1.35
25	0	602	CLA	C4B-NB	7.16	1.41	1.35
25	S	613	CLA	C4B-NB	7.15	1.41	1.35
25	s	613	CLA	C4B-NB	7.15	1.41	1.35
25	1	603	CLA	C4B-NB	7.15	1.41	1.35
25	Y	604	CLA	C4B-NB	7.15	1.41	1.35
25	N	614	CLA	C4B-NB	7.14	1.41	1.35
25	9	611	CLA	C4B-NB	7.14	1.41	1.35
25	4	610	CLA	C4B-NB	7.13	1.41	1.35
25	s	612	CLA	C4B-NB	7.13	1.41	1.35
25	B	607	CLA	C4B-NB	7.12	1.41	1.35
25	4	611	CLA	C4B-NB	7.12	1.41	1.35
25	n	604	CLA	C4B-NB	7.12	1.41	1.35
25	4	603	CLA	C4B-NB	7.11	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	l	611	CLA	C4B-NB	7.10	1.41	1.35
25	n	614	CLA	C4B-NB	7.08	1.41	1.35
25	y	604	CLA	C4B-NB	7.07	1.41	1.35
25	S	602	CLA	C4B-NB	7.06	1.41	1.35
25	7	611	CLA	C4B-NB	7.06	1.41	1.35
25	b	607	CLA	C4B-NB	7.06	1.41	1.35
25	q	610	CLA	C4B-NB	7.06	1.41	1.35
25	6	611	CLA	C4B-NB	7.05	1.41	1.35
25	B	605	CLA	C4B-NB	7.04	1.41	1.35
25	l	612	CLA	C4B-NB	7.03	1.41	1.35
25	N	604	CLA	C4B-NB	7.03	1.41	1.35
25	R	602	CLA	C4B-NB	7.01	1.41	1.35
25	6	603	CLA	C4B-NB	7.01	1.41	1.35
25	g	614	CLA	C4B-NB	7.01	1.41	1.35
25	3	603	CLA	C4B-NB	7.00	1.41	1.35
25	g	611	CLA	C4B-NB	7.00	1.41	1.35
25	s	602	CLA	C4B-NB	7.00	1.41	1.35
25	y	613	CLA	C4B-NB	7.00	1.41	1.35
25	g	604	CLA	C4B-NB	7.00	1.41	1.35
25	G	604	CLA	C4B-NB	6.99	1.41	1.35
25	C	504	CLA	C4B-NB	6.99	1.41	1.35
25	c	504	CLA	C4B-NB	6.99	1.41	1.35
25	r	602	CLA	C4B-NB	6.98	1.41	1.35
25	r	612	CLA	C4B-NB	6.98	1.41	1.35
25	0	603	CLA	C4B-NB	6.97	1.41	1.35
25	G	612	CLA	C4B-NB	6.97	1.41	1.35
25	g	612	CLA	C4B-NB	6.97	1.41	1.35
25	b	605	CLA	C4B-NB	6.96	1.41	1.35
25	S	603	CLA	C4B-NB	6.96	1.41	1.35
25	0	611	CLA	C4B-NB	6.95	1.41	1.35
25	G	611	CLA	C4B-NB	6.94	1.41	1.35
25	2	602	CLA	C4B-NB	6.93	1.41	1.35
25	G	613	CLA	C4B-NB	6.93	1.41	1.35
25	8	603	CLA	C4B-NB	6.93	1.41	1.35
25	s	603	CLA	C4B-NB	6.93	1.41	1.35
25	N	610	CLA	C4B-NB	6.92	1.41	1.35
25	7	613	CLA	C4B-NB	6.92	1.41	1.35
25	r	613	CLA	C4B-NB	6.92	1.41	1.35
25	q	611	CLA	C4B-NB	6.92	1.41	1.35
25	s	614	CLA	C4B-NB	6.92	1.41	1.35
25	d	402	CLA	C4B-NB	6.90	1.41	1.35
25	R	613	CLA	C4B-NB	6.90	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	612	CLA	C4B-NB	6.89	1.41	1.35
25	Y	613	CLA	C4B-NB	6.89	1.41	1.35
25	S	604	CLA	C4B-NB	6.89	1.41	1.35
25	r	610	CLA	C4B-NB	6.89	1.41	1.35
25	g	603	CLA	C4B-NB	6.89	1.41	1.35
25	R	610	CLA	C4B-NB	6.87	1.41	1.35
25	7	610	CLA	C4B-NB	6.87	1.41	1.35
25	n	610	CLA	C4B-NB	6.86	1.41	1.35
25	1	613	CLA	C4B-NB	6.86	1.41	1.35
25	D	402	CLA	C4B-NB	6.85	1.41	1.35
25	G	603	CLA	C4B-NB	6.85	1.41	1.35
25	7	604	CLA	C4B-NB	6.84	1.41	1.35
25	Y	611	CLA	C4B-NB	6.83	1.41	1.35
25	G	614	CLA	C4B-NB	6.83	1.41	1.35
25	S	614	CLA	C4B-NB	6.82	1.41	1.35
25	g	613	CLA	C4B-NB	6.82	1.41	1.35
39	d	405	PL9	C7-C3	-6.82	1.44	1.51
25	N	611	CLA	C4B-NB	6.81	1.41	1.35
25	1	610	CLA	C4B-NB	6.79	1.41	1.35
25	s	604	CLA	C4B-NB	6.79	1.41	1.35
25	B	616	CLA	C4B-NB	6.78	1.41	1.35
25	y	611	CLA	C4B-NB	6.77	1.41	1.35
25	Y	612	CLA	C4B-NB	6.77	1.41	1.35
25	b	608	CLA	C4B-NB	6.77	1.41	1.35
25	S	610	CLA	C4B-NB	6.77	1.41	1.35
25	s	611	CLA	C4B-NB	6.76	1.41	1.35
25	c	512	CLA	C4B-NB	6.75	1.41	1.35
25	N	602	CLA	C4B-NB	6.74	1.41	1.35
25	R	601	CLA	C4B-NB	6.71	1.41	1.35
25	B	608	CLA	C4B-NB	6.71	1.41	1.35
39	D	405	PL9	C7-C3	-6.71	1.44	1.51
25	S	611	CLA	C4B-NB	6.71	1.41	1.35
25	n	611	CLA	C4B-NB	6.70	1.41	1.35
25	c	508	CLA	C4B-NB	6.69	1.41	1.35
25	y	612	CLA	C4B-NB	6.67	1.41	1.35
25	n	602	CLA	C4B-NB	6.66	1.41	1.35
25	r	601	CLA	C4B-NB	6.66	1.41	1.35
25	s	610	CLA	C4B-NB	6.66	1.41	1.35
25	C	508	CLA	C4B-NB	6.66	1.41	1.35
25	b	602	CLA	C4B-NB	6.65	1.41	1.35
25	c	513	CLA	C4B-NB	6.65	1.41	1.35
25	D	403	CLA	C4B-NB	6.63	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	604	CLA	C4B-NB	6.62	1.41	1.35
25	C	512	CLA	C4B-NB	6.62	1.41	1.35
25	9	602	CLA	C4B-NB	6.61	1.41	1.35
25	b	616	CLA	C4B-NB	6.61	1.41	1.35
25	C	513	CLA	C4B-NB	6.60	1.41	1.35
25	a	410	CLA	C4B-NB	6.59	1.41	1.35
25	A	407	CLA	C4B-NB	6.57	1.41	1.35
25	B	602	CLA	C4B-NB	6.57	1.41	1.35
25	Y	614	CLA	C4B-NB	6.57	1.41	1.35
25	y	614	CLA	C4B-NB	6.56	1.41	1.35
25	d	403	CLA	C4B-NB	6.56	1.41	1.35
25	a	407	CLA	C4B-NB	6.53	1.41	1.35
25	B	609	CLA	C4B-NB	6.51	1.41	1.35
25	b	609	CLA	C4B-NB	6.51	1.41	1.35
25	B	615	CLA	C4B-NB	6.49	1.41	1.35
25	c	501	CLA	C4B-NB	6.49	1.41	1.35
25	A	410	CLA	C4B-NB	6.49	1.41	1.35
25	G	610	CLA	C4B-NB	6.48	1.41	1.35
25	g	610	CLA	C4B-NB	6.48	1.41	1.35
25	g	602	CLA	C4B-NB	6.46	1.41	1.35
25	B	606	CLA	C4B-NB	6.42	1.40	1.35
25	b	606	CLA	C4B-NB	6.42	1.40	1.35
25	C	505	CLA	C4B-NB	6.42	1.40	1.35
25	Y	610	CLA	C4B-NB	6.41	1.40	1.35
25	c	510	CLA	C4B-NB	6.40	1.40	1.35
25	c	505	CLA	C4B-NB	6.40	1.40	1.35
25	r	603	CLA	C4B-NB	6.40	1.40	1.35
25	C	501	CLA	C4B-NB	6.39	1.40	1.35
25	C	503	CLA	C4B-NB	6.39	1.40	1.35
25	c	511	CLA	C4B-NB	6.37	1.40	1.35
25	A	405	CLA	C4B-NB	6.37	1.40	1.35
25	C	510	CLA	C4B-NB	6.37	1.40	1.35
25	b	615	CLA	C4B-NB	6.37	1.40	1.35
25	R	603	CLA	C4B-NB	6.37	1.40	1.35
25	a	405	CLA	C4B-NB	6.36	1.40	1.35
25	n	603	CLA	C4B-NB	6.36	1.40	1.35
25	B	611	CLA	C4B-NB	6.34	1.40	1.35
25	G	602	CLA	C4B-NB	6.34	1.40	1.35
25	b	611	CLA	C4B-NB	6.34	1.40	1.35
25	y	603	CLA	C4B-NB	6.34	1.40	1.35
25	N	603	CLA	C4B-NB	6.33	1.40	1.35
25	c	503	CLA	C4B-NB	6.32	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	610	CLA	C4B-NB	6.31	1.40	1.35
25	Y	603	CLA	C4B-NB	6.29	1.40	1.35
25	y	610	CLA	C4B-NB	6.27	1.40	1.35
25	C	511	CLA	C4B-NB	6.25	1.40	1.35
25	B	610	CLA	C4B-NB	6.23	1.40	1.35
25	y	602	CLA	C4B-NB	6.22	1.40	1.35
25	B	614	CLA	C4B-NB	6.21	1.40	1.35
25	b	612	CLA	C4B-NB	6.18	1.40	1.35
25	B	604	CLA	C4B-NB	6.18	1.40	1.35
25	Y	602	CLA	C4B-NB	6.17	1.40	1.35
25	B	612	CLA	C4B-NB	6.14	1.40	1.35
25	b	604	CLA	C4B-NB	6.13	1.40	1.35
25	b	614	CLA	C4B-NB	6.13	1.40	1.35
39	D	405	PL9	C3-C4	-6.12	1.39	1.49
25	B	613	CLA	C4B-NB	6.09	1.40	1.35
25	b	613	CLA	C4B-NB	6.09	1.40	1.35
25	b	603	CLA	C4B-NB	6.05	1.40	1.35
25	B	603	CLA	C4B-NB	6.04	1.40	1.35
39	d	405	PL9	C3-C4	-6.03	1.39	1.49
25	C	507	CLA	C4B-NB	5.91	1.40	1.35
24	G	609	CHL	C3D-C4D	-5.77	1.31	1.44
25	a	406	CLA	C4B-NB	5.77	1.40	1.35
25	c	507	CLA	C4B-NB	5.77	1.40	1.35
25	A	406	CLA	C4B-NB	5.77	1.40	1.35
24	G	601	CHL	C3D-C4D	-5.77	1.31	1.44
24	g	609	CHL	C3D-C4D	-5.76	1.31	1.44
24	g	601	CHL	C3D-C4D	-5.73	1.31	1.44
24	y	609	CHL	C3D-C4D	-5.67	1.31	1.44
24	y	601	CHL	C3D-C4D	-5.67	1.31	1.44
24	Y	601	CHL	C3D-C4D	-5.67	1.31	1.44
25	B	617	CLA	C4B-NB	5.65	1.40	1.35
25	b	617	CLA	C4B-NB	5.65	1.40	1.35
24	Y	609	CHL	C3D-C4D	-5.63	1.31	1.44
24	q	606	CHL	CHC-C1C	5.62	1.49	1.35
25	c	502	CLA	C4B-NB	5.57	1.40	1.35
25	C	509	CLA	C4B-NB	5.56	1.40	1.35
24	R	608	CHL	C3D-C4D	-5.55	1.31	1.44
24	r	608	CHL	C3D-C4D	-5.55	1.31	1.44
25	c	509	CLA	C4B-NB	5.55	1.40	1.35
24	4	606	CHL	CHC-C1C	5.51	1.49	1.35
24	q	608	CHL	C3B-C2B	5.50	1.48	1.40
25	C	502	CLA	C4B-NB	5.49	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	605	CHL	C3B-C2B	5.48	1.48	1.40
24	Y	608	CHL	C3D-C4D	-5.46	1.31	1.44
24	4	609	CHL	CHC-C1C	5.45	1.48	1.35
24	N	607	CHL	C3D-C4D	-5.44	1.31	1.44
24	q	609	CHL	CHC-C1C	5.43	1.48	1.35
24	y	608	CHL	C3D-C4D	-5.43	1.31	1.44
24	9	605	CHL	C3B-C2B	5.43	1.47	1.40
24	q	609	CHL	C3B-C2B	5.42	1.47	1.40
24	N	609	CHL	C3D-C4D	-5.42	1.31	1.44
24	n	607	CHL	C3D-C4D	-5.42	1.32	1.44
24	p	605	CHL	C3B-C2B	5.41	1.47	1.40
24	4	605	CHL	C3B-C2B	5.40	1.47	1.40
24	N	601	CHL	C3D-C4D	-5.39	1.32	1.44
24	r	606	CHL	C3D-C4D	-5.38	1.32	1.44
24	n	609	CHL	C3D-C4D	-5.37	1.32	1.44
24	n	601	CHL	C3D-C4D	-5.36	1.32	1.44
24	1	606	CHL	C3D-C4D	-5.36	1.32	1.44
24	R	606	CHL	C3D-C4D	-5.35	1.32	1.44
24	7	601	CHL	C3D-C4D	-5.34	1.32	1.44
24	1	601	CHL	C3D-C4D	-5.34	1.32	1.44
24	7	606	CHL	C3D-C4D	-5.33	1.32	1.44
24	9	605	CHL	O2D-CGD	5.31	1.46	1.33
24	R	607	CHL	C3D-C4D	-5.31	1.32	1.44
24	q	605	CHL	O2D-CGD	5.30	1.46	1.33
24	y	607	CHL	C3D-C4D	-5.30	1.32	1.44
24	q	605	CHL	C3B-C2B	5.30	1.47	1.40
24	5	605	CHL	O2D-CGD	5.29	1.46	1.33
24	2	605	CHL	O2D-CGD	5.29	1.46	1.33
24	1	609	CHL	C3D-C4D	-5.28	1.32	1.44
24	3	606	CHL	CHC-C1C	5.28	1.48	1.35
24	Y	607	CHL	C3D-C4D	-5.28	1.32	1.44
24	4	609	CHL	C3D-C4D	-5.27	1.32	1.44
24	y	606	CHL	C3D-C4D	-5.27	1.32	1.44
24	q	608	CHL	CHC-C1C	5.26	1.48	1.35
24	G	606	CHL	C3D-C4D	-5.26	1.32	1.44
24	p	605	CHL	O2D-CGD	5.26	1.46	1.33
24	4	608	CHL	C3B-C2B	5.26	1.47	1.40
24	4	605	CHL	O2D-CGD	5.26	1.46	1.33
24	7	609	CHL	C3D-C4D	-5.25	1.32	1.44
24	Y	606	CHL	C3D-C4D	-5.25	1.32	1.44
24	g	606	CHL	C3D-C4D	-5.25	1.32	1.44
24	r	607	CHL	C3D-C4D	-5.25	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	p	606	CHL	O2D-CGD	5.24	1.46	1.33
24	4	609	CHL	C3B-C2B	5.24	1.47	1.40
24	n	606	CHL	C3D-C4D	-5.24	1.32	1.44
24	N	605	CHL	C3D-C4D	-5.24	1.32	1.44
24	3	606	CHL	C3D-C4D	-5.24	1.32	1.44
24	8	606	CHL	C3D-C4D	-5.23	1.32	1.44
24	n	605	CHL	C3D-C4D	-5.23	1.32	1.44
24	s	601	CHL	C3D-C4D	-5.23	1.32	1.44
24	5	606	CHL	C3B-C2B	5.22	1.47	1.40
24	5	605	CHL	C3B-C2B	5.22	1.47	1.40
24	3	605	CHL	O2D-CGD	5.22	1.45	1.33
24	3	605	CHL	CHC-C1C	5.22	1.48	1.35
24	S	601	CHL	CHC-C1C	5.22	1.48	1.35
24	N	606	CHL	C3D-C4D	-5.21	1.32	1.44
24	q	601	CHL	C3D-C4D	-5.21	1.32	1.44
24	8	605	CHL	O2D-CGD	5.21	1.45	1.33
24	N	608	CHL	C3D-C4D	-5.21	1.32	1.44
24	8	605	CHL	C3B-C2B	5.20	1.47	1.40
24	8	605	CHL	CHC-C1C	5.20	1.48	1.35
24	2	601	CHL	C3D-C4D	-5.20	1.32	1.44
24	S	601	CHL	C3D-C4D	-5.20	1.32	1.44
24	s	601	CHL	CHC-C1C	5.19	1.48	1.35
24	8	606	CHL	CHC-C1C	5.19	1.48	1.35
24	6	601	CHL	O2D-CGD	5.19	1.45	1.33
24	p	608	CHL	O2D-CGD	5.19	1.45	1.33
24	5	606	CHL	O2D-CGD	5.18	1.45	1.33
24	q	606	CHL	O2D-CGD	5.18	1.45	1.33
24	q	609	CHL	C3D-C4D	-5.18	1.32	1.44
24	4	608	CHL	CHC-C1C	5.17	1.48	1.35
39	d	405	PL9	C6-C1	-5.17	1.39	1.48
24	4	607	CHL	CHC-C1C	5.17	1.48	1.35
24	7	605	CHL	C3D-C4D	-5.17	1.32	1.44
24	4	606	CHL	O2D-CGD	5.16	1.45	1.33
24	0	606	CHL	C3D-C4D	-5.16	1.32	1.44
24	6	608	CHL	C3D-C4D	-5.16	1.32	1.44
24	q	607	CHL	CHC-C1C	5.16	1.48	1.35
24	s	607	CHL	C3D-C4D	-5.15	1.32	1.44
24	9	606	CHL	O2D-CGD	5.15	1.45	1.33
24	p	601	CHL	O2D-CGD	5.15	1.45	1.33
24	1	605	CHL	C3D-C4D	-5.14	1.32	1.44
24	5	608	CHL	O2D-CGD	5.14	1.45	1.33
24	p	606	CHL	C3B-C2B	5.14	1.47	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	608	CHL	C3D-C4D	-5.14	1.32	1.44
24	5	605	CHL	CHC-C1C	5.14	1.48	1.35
24	8	606	CHL	O2D-CGD	5.14	1.45	1.33
24	s	608	CHL	C3D-C4D	-5.14	1.32	1.44
24	n	608	CHL	C3D-C4D	-5.13	1.32	1.44
24	2	606	CHL	O2D-CGD	5.13	1.45	1.33
24	0	605	CHL	O2D-CGD	5.13	1.45	1.33
24	p	607	CHL	O2D-CGD	5.13	1.45	1.33
24	3	605	CHL	C3B-C2B	5.13	1.47	1.40
24	G	605	CHL	O2D-CGD	5.12	1.45	1.33
24	g	605	CHL	O2D-CGD	5.12	1.45	1.33
24	0	601	CHL	O2D-CGD	5.12	1.45	1.33
24	9	601	CHL	C3D-C4D	-5.12	1.32	1.44
24	0	608	CHL	C3D-C4D	-5.12	1.32	1.44
24	q	607	CHL	O2D-CGD	5.12	1.45	1.33
24	3	606	CHL	O2D-CGD	5.11	1.45	1.33
39	D	405	PL9	C6-C1	-5.11	1.39	1.48
24	5	601	CHL	O2D-CGD	5.11	1.45	1.33
24	S	607	CHL	C3D-C4D	-5.11	1.32	1.44
24	s	601	CHL	O2D-CGD	5.11	1.45	1.33
24	S	601	CHL	O2D-CGD	5.11	1.45	1.33
24	p	605	CHL	CHC-C1C	5.11	1.48	1.35
24	6	605	CHL	O2D-CGD	5.10	1.45	1.33
24	4	607	CHL	O2D-CGD	5.10	1.45	1.33
24	9	605	CHL	CHC-C1C	5.10	1.48	1.35
24	q	607	CHL	C3B-C2B	5.10	1.47	1.40
24	2	605	CHL	CHC-C1C	5.10	1.48	1.35
24	6	605	CHL	C3B-C2B	5.10	1.47	1.40
24	9	607	CHL	O2D-CGD	5.09	1.45	1.33
24	5	606	CHL	CHC-C1C	5.09	1.48	1.35
24	2	607	CHL	O2D-CGD	5.09	1.45	1.33
24	5	609	CHL	O2D-CGD	5.09	1.45	1.33
24	5	607	CHL	O2D-CGD	5.09	1.45	1.33
24	S	606	CHL	C3D-C4D	-5.08	1.32	1.44
24	9	608	CHL	O2D-CGD	5.07	1.45	1.33
24	4	605	CHL	CHC-C1C	5.07	1.48	1.35
24	p	609	CHL	O2D-CGD	5.07	1.45	1.33
24	4	601	CHL	C3D-C4D	-5.06	1.32	1.44
24	g	608	CHL	C3D-C4D	-5.06	1.32	1.44
24	p	606	CHL	CHC-C1C	5.06	1.47	1.35
24	S	607	CHL	C3B-C2B	5.05	1.47	1.40
24	0	609	CHL	CHC-C1C	5.05	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	606	CHL	C3D-C4D	-5.05	1.32	1.44
24	0	605	CHL	C3B-C2B	5.04	1.47	1.40
24	q	609	CHL	C2C-C3C	5.04	1.47	1.36
24	G	608	CHL	C3D-C4D	-5.04	1.32	1.44
24	g	607	CHL	C3D-C4D	-5.04	1.32	1.44
24	7	608	CHL	C3D-C4D	-5.04	1.32	1.44
24	p	606	CHL	C3D-C4D	-5.03	1.32	1.44
24	s	607	CHL	C3B-C2B	5.03	1.47	1.40
24	3	608	CHL	O2D-CGD	5.03	1.45	1.33
24	0	608	CHL	O2D-CGD	5.03	1.45	1.33
24	s	606	CHL	C3D-C4D	-5.02	1.32	1.44
24	9	608	CHL	CHC-C1C	5.02	1.47	1.35
24	4	607	CHL	C3B-C2B	5.02	1.47	1.40
24	q	609	CHL	O2D-CGD	5.02	1.45	1.33
24	1	607	CHL	O2D-CGD	5.02	1.45	1.33
24	q	606	CHL	C3B-C2B	5.02	1.47	1.40
24	8	601	CHL	C3D-C4D	-5.01	1.32	1.44
24	4	609	CHL	O2D-CGD	5.01	1.45	1.33
24	3	601	CHL	C3D-C4D	-5.01	1.32	1.44
24	9	609	CHL	C2C-C3C	5.01	1.47	1.36
24	5	609	CHL	C3B-C2B	5.01	1.47	1.40
24	g	605	CHL	C3B-C2B	5.01	1.47	1.40
24	8	608	CHL	O2D-CGD	5.01	1.45	1.33
24	Y	605	CHL	C3D-C4D	-5.00	1.32	1.44
24	y	605	CHL	C3D-C4D	-5.00	1.32	1.44
24	G	605	CHL	C3B-C2B	5.00	1.47	1.40
24	2	607	CHL	CHC-C1C	5.00	1.47	1.35
24	1	606	CHL	O2D-CGD	5.00	1.45	1.33
24	3	607	CHL	CHC-C1C	5.00	1.47	1.35
24	7	607	CHL	O2D-CGD	4.99	1.45	1.33
24	6	608	CHL	O2D-CGD	4.99	1.45	1.33
24	6	605	CHL	CHC-C1C	4.99	1.47	1.35
24	5	609	CHL	C3D-C4D	-4.99	1.32	1.44
24	q	605	CHL	CHC-C1C	4.99	1.47	1.35
24	0	605	CHL	CHC-C1C	4.98	1.47	1.35
24	q	601	CHL	O2D-CGD	4.98	1.45	1.33
24	q	608	CHL	O2D-CGD	4.98	1.45	1.33
24	3	607	CHL	O2D-CGD	4.98	1.45	1.33
24	0	609	CHL	O2D-CGD	4.98	1.45	1.33
24	6	609	CHL	O2D-CGD	4.98	1.45	1.33
24	1	608	CHL	C3D-C4D	-4.98	1.32	1.44
24	s	606	CHL	O2D-CGD	4.98	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	606	CHL	C3D-C4D	-4.98	1.32	1.44
24	q	609	CHL	CHD-C1D	4.98	1.48	1.38
24	G	607	CHL	C3D-C4D	-4.98	1.32	1.44
24	2	608	CHL	CHC-C1C	4.97	1.47	1.35
24	7	606	CHL	O2D-CGD	4.97	1.45	1.33
24	6	609	CHL	C3D-C4D	-4.97	1.33	1.44
24	8	607	CHL	CHC-C1C	4.97	1.47	1.35
24	1	607	CHL	C3D-C4D	-4.97	1.33	1.44
24	7	607	CHL	C3D-C4D	-4.97	1.33	1.44
24	2	607	CHL	C3B-C2B	4.97	1.47	1.40
24	3	609	CHL	O2D-CGD	4.97	1.45	1.33
24	4	606	CHL	C3B-C2B	4.96	1.47	1.40
24	3	609	CHL	C3D-C4D	-4.96	1.33	1.44
24	S	606	CHL	O2D-CGD	4.96	1.45	1.33
24	9	607	CHL	CHC-C1C	4.96	1.47	1.35
24	p	607	CHL	CHC-C1C	4.95	1.47	1.35
24	3	601	CHL	O2D-CGD	4.95	1.45	1.33
24	5	606	CHL	C3D-C4D	-4.95	1.33	1.44
24	p	609	CHL	C3D-C4D	-4.95	1.33	1.44
24	8	609	CHL	O2D-CGD	4.95	1.45	1.33
24	7	607	CHL	CHC-C1C	4.95	1.47	1.35
24	n	606	CHL	O2D-CGD	4.95	1.45	1.33
24	0	601	CHL	CHC-C1C	4.94	1.47	1.35
24	G	609	CHL	O2D-CGD	4.94	1.45	1.33
24	G	606	CHL	O2D-CGD	4.94	1.45	1.33
24	9	606	CHL	C3D-C4D	-4.94	1.33	1.44
24	2	608	CHL	O2D-CGD	4.94	1.45	1.33
24	0	609	CHL	C3D-C4D	-4.94	1.33	1.44
24	4	608	CHL	O2D-CGD	4.94	1.45	1.33
24	5	608	CHL	CHC-C1C	4.94	1.47	1.35
24	4	601	CHL	O2D-CGD	4.93	1.45	1.33
24	g	606	CHL	O2D-CGD	4.93	1.45	1.33
24	9	609	CHL	C3D-C4D	-4.93	1.33	1.44
24	p	609	CHL	C3B-C2B	4.93	1.47	1.40
24	8	607	CHL	O2D-CGD	4.93	1.45	1.33
24	3	608	CHL	CHC-C1C	4.93	1.47	1.35
24	6	601	CHL	C3D-C4D	-4.92	1.33	1.44
24	3	606	CHL	C3B-C2B	4.92	1.47	1.40
24	4	601	CHL	CHC-C1C	4.92	1.47	1.35
24	2	606	CHL	CHC-C1C	4.92	1.47	1.35
24	4	601	CHL	C3B-C2B	4.92	1.47	1.40
24	8	609	CHL	C3D-C4D	-4.92	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	608	CHL	CHC-C1C	4.92	1.47	1.35
24	S	607	CHL	CHC-C1C	4.92	1.47	1.35
24	n	607	CHL	CHC-C1C	4.92	1.47	1.35
24	s	607	CHL	CHC-C1C	4.92	1.47	1.35
35	A	412	SQD	O8-S	4.91	1.65	1.47
24	N	606	CHL	O2D-CGD	4.91	1.45	1.33
24	8	601	CHL	O2D-CGD	4.91	1.45	1.33
24	6	607	CHL	C3D-C4D	-4.91	1.33	1.44
24	1	607	CHL	CHC-C1C	4.91	1.47	1.35
24	4	609	CHL	C2C-C3C	4.91	1.47	1.36
24	s	608	CHL	CHC-C1C	4.90	1.47	1.35
24	2	609	CHL	O2D-CGD	4.90	1.45	1.33
24	y	601	CHL	CHC-C1C	4.90	1.47	1.35
24	Y	601	CHL	CHC-C1C	4.90	1.47	1.35
24	Y	607	CHL	CHC-C1C	4.90	1.47	1.35
24	7	605	CHL	O2D-CGD	4.90	1.45	1.33
24	g	608	CHL	O2D-CGD	4.90	1.45	1.33
24	p	605	CHL	C3D-C4D	-4.90	1.33	1.44
24	0	606	CHL	C3B-C2B	4.90	1.47	1.40
24	g	609	CHL	O2D-CGD	4.90	1.45	1.33
24	s	607	CHL	O2D-CGD	4.90	1.45	1.33
24	8	608	CHL	CHC-C1C	4.89	1.47	1.35
24	y	607	CHL	CHC-C1C	4.89	1.47	1.35
24	G	608	CHL	O2D-CGD	4.89	1.45	1.33
24	S	607	CHL	O2D-CGD	4.89	1.45	1.33
24	9	609	CHL	O2D-CGD	4.89	1.45	1.33
35	a	412	SQD	O8-S	4.89	1.64	1.47
24	5	607	CHL	CHC-C1C	4.89	1.47	1.35
24	1	605	CHL	CHC-C1C	4.88	1.47	1.35
24	4	607	CHL	C3D-C4D	-4.88	1.33	1.44
24	1	605	CHL	O2D-CGD	4.88	1.45	1.33
24	1	608	CHL	O2D-CGD	4.88	1.45	1.33
24	7	608	CHL	O2D-CGD	4.88	1.45	1.33
24	N	607	CHL	CHC-C1C	4.87	1.47	1.35
24	9	606	CHL	CHC-C1C	4.87	1.47	1.35
24	2	609	CHL	C2C-C3C	4.87	1.47	1.36
24	S	608	CHL	O2D-CGD	4.87	1.45	1.33
24	s	608	CHL	O2D-CGD	4.87	1.45	1.33
24	q	601	CHL	CHC-C1C	4.87	1.47	1.35
24	2	609	CHL	C3D-C4D	-4.87	1.33	1.44
24	q	608	CHL	C2C-C3C	4.86	1.47	1.36
24	2	601	CHL	O2D-CGD	4.86	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	605	CHL	O2D-CGD	4.86	1.45	1.33
24	y	605	CHL	O2D-CGD	4.86	1.45	1.33
24	4	608	CHL	C3D-C4D	-4.86	1.33	1.44
24	7	605	CHL	CHC-C1C	4.86	1.47	1.35
24	0	601	CHL	C3D-C4D	-4.85	1.33	1.44
24	5	605	CHL	C2C-C3C	4.85	1.47	1.36
24	p	608	CHL	CHC-C1C	4.85	1.47	1.35
24	8	608	CHL	C3D-C4D	-4.85	1.33	1.44
24	6	608	CHL	CHC-C1C	4.85	1.47	1.35
24	5	601	CHL	C3D-C4D	-4.85	1.33	1.44
24	4	606	CHL	C3D-C4D	-4.84	1.33	1.44
24	p	605	CHL	CHD-C1D	4.84	1.47	1.38
24	7	609	CHL	O2D-CGD	4.84	1.45	1.33
24	y	609	CHL	O2D-CGD	4.84	1.45	1.33
24	N	607	CHL	O2D-CGD	4.84	1.45	1.33
24	9	607	CHL	C3B-C2B	4.84	1.47	1.40
24	s	601	CHL	C3B-C2B	4.84	1.47	1.40
24	8	605	CHL	C2C-C3C	4.84	1.47	1.36
24	q	607	CHL	C3D-C4D	-4.84	1.33	1.44
24	0	608	CHL	CHC-C1C	4.84	1.47	1.35
24	2	608	CHL	C3D-C4D	-4.84	1.33	1.44
24	9	601	CHL	O2D-CGD	4.83	1.45	1.33
24	G	608	CHL	CHC-C1C	4.83	1.47	1.35
24	Y	605	CHL	CHC-C1C	4.83	1.47	1.35
24	9	606	CHL	C3B-C2B	4.82	1.47	1.40
24	4	609	CHL	CHD-C1D	4.82	1.47	1.38
24	y	605	CHL	CHC-C1C	4.82	1.47	1.35
24	0	606	CHL	O2D-CGD	4.82	1.45	1.33
24	2	607	CHL	C3D-C4D	-4.82	1.33	1.44
24	8	607	CHL	C3D-C4D	-4.82	1.33	1.44
24	9	607	CHL	C3D-C4D	-4.81	1.33	1.44
24	3	605	CHL	C2C-C3C	4.81	1.47	1.36
24	3	608	CHL	C3D-C4D	-4.81	1.33	1.44
24	5	607	CHL	C3D-C4D	-4.81	1.33	1.44
24	9	609	CHL	CHC-C1C	4.81	1.47	1.35
24	q	606	CHL	C3D-C4D	-4.81	1.33	1.44
24	7	605	CHL	C3B-C2B	4.80	1.47	1.40
24	0	607	CHL	O2D-CGD	4.80	1.44	1.33
24	6	606	CHL	C3B-C2B	4.80	1.47	1.40
24	8	606	CHL	C3B-C2B	4.80	1.47	1.40
24	p	607	CHL	C3D-C4D	-4.79	1.33	1.44
24	0	607	CHL	C3D-C4D	-4.79	1.33	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	607	CHL	O2D-CGD	4.79	1.44	1.33
24	q	605	CHL	C3D-C4D	-4.79	1.33	1.44
24	S	601	CHL	C3B-C2B	4.79	1.47	1.40
24	g	606	CHL	CHC-C1C	4.79	1.47	1.35
24	9	608	CHL	C3D-C4D	-4.79	1.33	1.44
24	1	605	CHL	C3B-C2B	4.79	1.47	1.40
24	R	606	CHL	O2D-CGD	4.79	1.44	1.33
24	0	606	CHL	CHC-C1C	4.79	1.47	1.35
24	6	601	CHL	CHC-C1C	4.79	1.47	1.35
24	Y	607	CHL	O2D-CGD	4.79	1.44	1.33
24	r	606	CHL	O2D-CGD	4.78	1.44	1.33
24	g	608	CHL	CHC-C1C	4.78	1.47	1.35
24	p	601	CHL	CHC-C1C	4.78	1.47	1.35
24	4	605	CHL	C3D-C4D	-4.78	1.33	1.44
24	5	605	CHL	C3D-C4D	-4.78	1.33	1.44
24	7	601	CHL	O2D-CGD	4.78	1.44	1.33
24	8	605	CHL	C3D-C4D	-4.77	1.33	1.44
24	7	607	CHL	C3B-C2B	4.77	1.47	1.40
24	p	606	CHL	CHD-C1D	4.77	1.47	1.38
24	y	607	CHL	O2D-CGD	4.77	1.44	1.33
24	6	606	CHL	CHC-C1C	4.77	1.47	1.35
24	3	607	CHL	C3D-C4D	-4.77	1.33	1.44
24	p	601	CHL	C3D-C4D	-4.77	1.33	1.44
24	g	605	CHL	CHC-C1C	4.77	1.47	1.35
24	5	601	CHL	CHC-C1C	4.77	1.47	1.35
24	g	607	CHL	O2D-CGD	4.77	1.44	1.33
24	3	606	CHL	CHD-C1D	4.77	1.47	1.38
24	5	609	CHL	C2C-C3C	4.76	1.47	1.36
24	p	605	CHL	C2C-C3C	4.76	1.47	1.36
24	G	607	CHL	O2D-CGD	4.76	1.44	1.33
24	6	607	CHL	CHC-C1C	4.76	1.47	1.35
24	6	606	CHL	O2D-CGD	4.76	1.44	1.33
24	6	607	CHL	O2D-CGD	4.76	1.44	1.33
24	q	608	CHL	C3D-C4D	-4.76	1.33	1.44
24	1	601	CHL	O2D-CGD	4.76	1.44	1.33
24	p	609	CHL	C2C-C3C	4.76	1.46	1.36
24	N	605	CHL	O2D-CGD	4.76	1.44	1.33
24	8	606	CHL	CHD-C1D	4.75	1.47	1.38
24	8	601	CHL	CHC-C1C	4.75	1.47	1.35
24	G	606	CHL	CHC-C1C	4.75	1.47	1.35
24	1	608	CHL	C3B-C2B	4.74	1.46	1.40
24	2	607	CHL	C2C-C3C	4.74	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	607	CHL	C3B-C2B	4.74	1.46	1.40
24	6	609	CHL	CHC-C1C	4.74	1.47	1.35
24	Y	606	CHL	O2D-CGD	4.74	1.44	1.33
24	y	606	CHL	O2D-CGD	4.74	1.44	1.33
24	n	606	CHL	CHC-C1C	4.74	1.47	1.35
24	G	605	CHL	CHC-C1C	4.73	1.47	1.35
24	1	606	CHL	CHC-C1C	4.73	1.47	1.35
24	1	607	CHL	C3B-C2B	4.73	1.46	1.40
24	2	606	CHL	C3B-C2B	4.73	1.46	1.40
24	2	609	CHL	CHC-C1C	4.73	1.47	1.35
24	3	605	CHL	C3D-C4D	-4.73	1.33	1.44
24	G	607	CHL	CHC-C1C	4.73	1.47	1.35
24	9	608	CHL	C3B-C2B	4.72	1.46	1.40
24	p	607	CHL	C3B-C2B	4.72	1.46	1.40
24	0	607	CHL	C3B-C2B	4.72	1.46	1.40
24	9	609	CHL	C3B-C2B	4.72	1.46	1.40
24	9	609	CHL	CHD-C1D	4.72	1.47	1.38
24	1	601	CHL	CHC-C1C	4.71	1.47	1.35
24	q	605	CHL	CHD-C1D	4.71	1.47	1.38
24	g	607	CHL	CHC-C1C	4.71	1.47	1.35
24	G	605	CHL	C3D-C4D	-4.71	1.33	1.44
24	9	606	CHL	C2C-C3C	4.71	1.46	1.36
24	6	605	CHL	C3D-C4D	-4.71	1.33	1.44
24	n	601	CHL	O2D-CGD	4.71	1.44	1.33
24	q	606	CHL	CHD-C1D	4.71	1.47	1.38
24	0	605	CHL	C3D-C4D	-4.70	1.33	1.44
24	1	609	CHL	O2D-CGD	4.70	1.44	1.33
24	N	605	CHL	CHC-C1C	4.70	1.47	1.35
24	0	609	CHL	C3B-C2B	4.70	1.46	1.40
24	Y	609	CHL	O2D-CGD	4.70	1.44	1.33
24	q	606	CHL	C2C-C3C	4.70	1.46	1.36
24	8	606	CHL	C2C-C3C	4.69	1.46	1.36
24	n	605	CHL	O2D-CGD	4.69	1.44	1.33
24	7	601	CHL	CHC-C1C	4.69	1.47	1.35
24	2	605	CHL	CHD-C1D	4.68	1.47	1.38
24	N	601	CHL	O2D-CGD	4.68	1.44	1.33
24	R	607	CHL	CHC-C1C	4.68	1.47	1.35
24	g	605	CHL	C3D-C4D	-4.67	1.33	1.44
24	n	608	CHL	O2D-CGD	4.67	1.44	1.33
24	N	608	CHL	O2D-CGD	4.67	1.44	1.33
24	N	606	CHL	CHC-C1C	4.67	1.46	1.35
24	2	609	CHL	C3B-C2B	4.66	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	605	CHL	CHC-C1C	4.66	1.46	1.35
24	p	607	CHL	C2C-C3C	4.66	1.46	1.36
24	3	606	CHL	C2C-C3C	4.66	1.46	1.36
24	3	601	CHL	CHC-C1C	4.66	1.46	1.35
24	9	605	CHL	CHD-C1D	4.65	1.47	1.38
24	s	606	CHL	CHC-C1C	4.65	1.46	1.35
24	Y	606	CHL	CHC-C1C	4.65	1.46	1.35
24	2	606	CHL	C2C-C3C	4.65	1.46	1.36
24	9	605	CHL	C2C-C3C	4.65	1.46	1.36
24	n	609	CHL	O2D-CGD	4.65	1.44	1.33
24	0	607	CHL	CHC-C1C	4.65	1.46	1.35
24	4	605	CHL	CHD-C1D	4.65	1.47	1.38
24	9	607	CHL	C2C-C3C	4.65	1.46	1.36
24	9	601	CHL	C2C-C3C	4.64	1.46	1.36
24	y	606	CHL	CHC-C1C	4.64	1.46	1.35
24	r	607	CHL	CHC-C1C	4.64	1.46	1.35
24	R	608	CHL	CHC-C1C	4.64	1.46	1.35
24	p	606	CHL	C2C-C3C	4.64	1.46	1.36
24	q	605	CHL	C2C-C3C	4.64	1.46	1.36
24	g	605	CHL	C2C-C3C	4.64	1.46	1.36
24	7	609	CHL	CHC-C1C	4.64	1.46	1.35
24	q	607	CHL	CHD-C1D	4.63	1.47	1.38
24	r	608	CHL	CHC-C1C	4.63	1.46	1.35
24	p	608	CHL	C3D-C4D	-4.63	1.33	1.44
24	1	608	CHL	CHC-C1C	4.63	1.46	1.35
24	G	605	CHL	C2C-C3C	4.63	1.46	1.36
24	6	605	CHL	C2C-C3C	4.62	1.46	1.36
24	G	601	CHL	CHC-C1C	4.62	1.46	1.35
24	5	609	CHL	CHD-C1D	4.62	1.47	1.38
24	p	601	CHL	C3B-C2B	4.62	1.46	1.40
24	S	608	CHL	C2C-C3C	4.62	1.46	1.36
24	q	601	CHL	C3B-C2B	4.62	1.46	1.40
24	s	608	CHL	C2C-C3C	4.61	1.46	1.36
24	7	608	CHL	CHC-C1C	4.61	1.46	1.35
24	R	606	CHL	CHC-C1C	4.61	1.46	1.35
24	S	606	CHL	CHC-C1C	4.61	1.46	1.35
24	9	608	CHL	C2C-C3C	4.61	1.46	1.36
24	5	608	CHL	C3D-C4D	-4.61	1.33	1.44
24	N	609	CHL	O2D-CGD	4.61	1.44	1.33
24	8	601	CHL	C3B-C2B	4.60	1.46	1.40
24	n	601	CHL	CHC-C1C	4.60	1.46	1.35
24	4	606	CHL	C2C-C3C	4.60	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	9	601	CHL	CHC-C1C	4.60	1.46	1.35
35	B	621	SQD	O8-S	4.60	1.63	1.47
24	4	601	CHL	C2C-C3C	4.60	1.46	1.36
24	N	601	CHL	CHC-C1C	4.60	1.46	1.35
24	g	601	CHL	CHC-C1C	4.59	1.46	1.35
24	2	608	CHL	C3B-C2B	4.59	1.46	1.40
24	2	605	CHL	C2C-C3C	4.59	1.46	1.36
24	5	607	CHL	C2C-C3C	4.59	1.46	1.36
24	r	606	CHL	CHC-C1C	4.59	1.46	1.35
24	9	601	CHL	CHD-C1D	4.59	1.47	1.38
24	4	605	CHL	C2C-C3C	4.59	1.46	1.36
24	0	605	CHL	C2C-C3C	4.59	1.46	1.36
24	5	609	CHL	CHC-C1C	4.59	1.46	1.35
24	y	608	CHL	O2D-CGD	4.58	1.44	1.33
35	b	623	SQD	O8-S	4.58	1.63	1.47
24	2	609	CHL	CHD-C1D	4.58	1.47	1.38
24	6	608	CHL	C3B-C2B	4.58	1.46	1.40
24	3	605	CHL	CHD-C1D	4.58	1.47	1.38
24	8	605	CHL	CHD-C1D	4.57	1.47	1.38
35	B	623	SQD	O8-S	4.57	1.63	1.47
35	b	621	SQD	O8-S	4.57	1.63	1.47
24	Y	608	CHL	O2D-CGD	4.57	1.44	1.33
24	0	609	CHL	C2C-C3C	4.57	1.46	1.36
24	3	601	CHL	C3B-C2B	4.57	1.46	1.40
24	2	605	CHL	C3D-C4D	-4.57	1.33	1.44
24	p	609	CHL	CHD-C1D	4.57	1.47	1.38
24	p	608	CHL	C2C-C3C	4.57	1.46	1.36
24	1	609	CHL	CHC-C1C	4.56	1.46	1.35
24	p	608	CHL	C3B-C2B	4.56	1.46	1.40
24	s	608	CHL	C3B-C2B	4.56	1.46	1.40
24	2	601	CHL	C2C-C3C	4.56	1.46	1.36
24	9	605	CHL	C3D-C4D	-4.56	1.33	1.44
24	r	607	CHL	O2D-CGD	4.56	1.44	1.33
24	7	606	CHL	CHC-C1C	4.55	1.46	1.35
24	2	608	CHL	C2C-C3C	4.55	1.46	1.36
24	4	608	CHL	C2C-C3C	4.55	1.46	1.36
24	s	607	CHL	C2C-C3C	4.55	1.46	1.36
24	q	607	CHL	C2C-C3C	4.55	1.46	1.36
24	2	601	CHL	CHC-C1C	4.54	1.46	1.35
24	0	601	CHL	C3B-C2B	4.54	1.46	1.40
24	y	608	CHL	CHC-C1C	4.54	1.46	1.35
24	S	608	CHL	C3B-C2B	4.54	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	606	CHL	CHD-C1D	4.54	1.47	1.38
24	R	607	CHL	O2D-CGD	4.53	1.44	1.33
24	G	608	CHL	C3B-C2B	4.53	1.46	1.40
24	6	601	CHL	C2C-C3C	4.53	1.46	1.36
24	6	606	CHL	C2C-C3C	4.53	1.46	1.36
24	q	601	CHL	C2C-C3C	4.52	1.46	1.36
24	Y	601	CHL	O2D-CGD	4.52	1.44	1.33
24	8	608	CHL	C3B-C2B	4.52	1.46	1.40
24	0	606	CHL	C2C-C3C	4.52	1.46	1.36
24	5	601	CHL	C3B-C2B	4.52	1.46	1.40
24	3	608	CHL	C3B-C2B	4.52	1.46	1.40
24	y	601	CHL	O2D-CGD	4.52	1.44	1.33
24	5	606	CHL	C2C-C3C	4.51	1.46	1.36
35	D	413	SQD	O8-S	4.51	1.63	1.47
24	8	609	CHL	C2C-C3C	4.51	1.46	1.36
24	8	609	CHL	CHC-C1C	4.51	1.46	1.35
24	3	609	CHL	C2C-C3C	4.51	1.46	1.36
24	S	607	CHL	C2C-C3C	4.51	1.46	1.36
24	Y	608	CHL	CHC-C1C	4.51	1.46	1.35
35	d	413	SQD	O8-S	4.50	1.63	1.47
24	7	606	CHL	C3B-C2B	4.50	1.46	1.40
24	1	609	CHL	O2A-CGA	4.50	1.46	1.33
24	N	608	CHL	CHC-C1C	4.50	1.46	1.35
24	1	606	CHL	O2A-CGA	4.50	1.46	1.33
24	5	605	CHL	O2A-CGA	4.50	1.46	1.33
24	8	601	CHL	O2A-CGA	4.50	1.46	1.33
24	1	605	CHL	C2C-C3C	4.50	1.46	1.36
24	8	606	CHL	O2A-CGA	4.50	1.45	1.30
24	s	601	CHL	O2A-CGA	4.50	1.45	1.30
24	6	609	CHL	C3B-C2B	4.49	1.46	1.40
24	7	605	CHL	C2C-C3C	4.49	1.46	1.36
24	7	609	CHL	O2A-CGA	4.49	1.46	1.33
24	y	607	CHL	O2A-CGA	4.49	1.46	1.33
24	4	607	CHL	CHD-C1D	4.49	1.47	1.38
24	p	601	CHL	O2A-CGA	4.49	1.46	1.33
24	0	601	CHL	C2C-C3C	4.49	1.46	1.36
24	g	601	CHL	O2D-CGD	4.48	1.44	1.33
24	8	607	CHL	O2A-CGA	4.48	1.46	1.33
24	G	601	CHL	O2D-CGD	4.48	1.44	1.33
24	8	601	CHL	C2C-C3C	4.48	1.46	1.36
24	5	608	CHL	C2C-C3C	4.47	1.46	1.36
24	G	609	CHL	CHC-C1C	4.47	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	608	CHL	C3B-C2B	4.47	1.46	1.40
24	S	601	CHL	O2A-CGA	4.47	1.45	1.30
24	3	606	CHL	O2A-CGA	4.47	1.45	1.30
24	1	606	CHL	C3B-C2B	4.47	1.46	1.40
24	3	601	CHL	O2A-CGA	4.47	1.46	1.33
24	7	605	CHL	O2A-CGA	4.47	1.45	1.30
24	1	605	CHL	O2A-CGA	4.47	1.45	1.30
24	p	609	CHL	CHC-C1C	4.46	1.46	1.35
24	n	608	CHL	CHC-C1C	4.46	1.46	1.35
24	r	608	CHL	O2D-CGD	4.46	1.44	1.33
24	7	606	CHL	O2A-CGA	4.46	1.46	1.33
24	6	607	CHL	C3B-C2B	4.46	1.46	1.40
24	5	606	CHL	O2A-CGA	4.46	1.45	1.30
24	G	605	CHL	CHD-C1D	4.46	1.47	1.38
24	R	608	CHL	O2D-CGD	4.46	1.44	1.33
24	3	608	CHL	C2C-C3C	4.45	1.46	1.36
24	q	609	CHL	O2A-CGA	4.45	1.46	1.33
24	3	607	CHL	O2A-CGA	4.45	1.46	1.33
24	Y	605	CHL	O2A-CGA	4.44	1.45	1.30
24	g	609	CHL	CHC-C1C	4.44	1.46	1.35
24	n	606	CHL	O2A-CGA	4.44	1.45	1.30
24	Y	607	CHL	O2A-CGA	4.43	1.46	1.33
24	S	601	CHL	C2C-C3C	4.43	1.46	1.36
24	p	605	CHL	O2A-CGA	4.43	1.46	1.33
24	0	605	CHL	O2A-CGA	4.43	1.45	1.30
24	5	605	CHL	CHD-C1D	4.43	1.47	1.38
24	N	606	CHL	O2A-CGA	4.43	1.45	1.30
24	0	608	CHL	C3B-C2B	4.43	1.46	1.40
24	5	606	CHL	CHD-C1D	4.43	1.47	1.38
24	2	607	CHL	CHD-C1D	4.43	1.47	1.38
24	6	605	CHL	CHD-C1D	4.42	1.47	1.38
24	y	601	CHL	O2A-CGA	4.42	1.46	1.33
24	y	609	CHL	O2A-CGA	4.42	1.46	1.33
24	Y	609	CHL	O2A-CGA	4.42	1.46	1.33
24	4	607	CHL	C2C-C3C	4.42	1.46	1.36
24	q	608	CHL	CHD-C1D	4.42	1.47	1.38
24	y	605	CHL	O2A-CGA	4.42	1.45	1.30
24	n	609	CHL	CHC-C1C	4.42	1.46	1.35
24	9	607	CHL	CHD-C1D	4.42	1.47	1.38
24	6	608	CHL	C2C-C3C	4.42	1.46	1.36
24	3	609	CHL	O2A-CGA	4.42	1.46	1.33
24	1	608	CHL	O2A-CGA	4.42	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	g	605	CHL	CHD-C1D	4.42	1.47	1.38
24	8	607	CHL	C3B-C2B	4.42	1.46	1.40
24	G	607	CHL	C3B-C2B	4.41	1.46	1.40
24	8	608	CHL	C2C-C3C	4.41	1.46	1.36
24	s	601	CHL	CHD-C1D	4.41	1.47	1.38
24	7	608	CHL	C3B-C2B	4.41	1.46	1.40
24	7	605	CHL	CHD-C1D	4.41	1.46	1.38
24	3	609	CHL	CHC-C1C	4.40	1.46	1.35
24	0	608	CHL	C2C-C3C	4.40	1.46	1.36
24	Y	609	CHL	C2C-C3C	4.40	1.46	1.36
24	3	607	CHL	C3B-C2B	4.40	1.46	1.40
24	p	606	CHL	O2A-CGA	4.40	1.45	1.30
24	6	605	CHL	O2A-CGA	4.40	1.45	1.30
24	S	607	CHL	CHD-C1D	4.40	1.46	1.38
24	4	601	CHL	O2A-CGA	4.39	1.46	1.33
24	y	609	CHL	C2C-C3C	4.38	1.46	1.36
24	6	609	CHL	C2C-C3C	4.38	1.46	1.36
24	s	607	CHL	CHD-C1D	4.38	1.46	1.38
24	3	607	CHL	C2C-C3C	4.38	1.46	1.36
24	0	606	CHL	O2A-CGA	4.37	1.46	1.33
24	6	601	CHL	C3B-C2B	4.37	1.46	1.40
24	S	608	CHL	O2A-CGA	4.37	1.46	1.33
24	G	608	CHL	C2C-C3C	4.37	1.46	1.36
24	7	608	CHL	O2A-CGA	4.37	1.46	1.33
24	5	601	CHL	O2A-CGA	4.37	1.46	1.33
24	5	601	CHL	C2C-C3C	4.37	1.46	1.36
24	s	601	CHL	C2C-C3C	4.37	1.46	1.36
24	S	601	CHL	CHD-C1D	4.37	1.46	1.38
24	G	609	CHL	O2A-CGA	4.36	1.46	1.33
24	g	609	CHL	O2A-CGA	4.36	1.46	1.33
24	g	607	CHL	C3B-C2B	4.36	1.46	1.40
24	p	609	CHL	O2A-CGA	4.35	1.46	1.33
24	6	606	CHL	O2A-CGA	4.35	1.46	1.33
24	q	606	CHL	O2A-CGA	4.35	1.46	1.33
24	2	606	CHL	CHD-C1D	4.34	1.46	1.38
24	s	608	CHL	O2A-CGA	4.34	1.46	1.33
24	4	605	CHL	O2A-CGA	4.34	1.46	1.33
24	q	601	CHL	O2A-CGA	4.34	1.46	1.33
24	5	609	CHL	O2A-CGA	4.34	1.46	1.33
24	q	605	CHL	O2A-CGA	4.34	1.46	1.33
24	5	601	CHL	CHD-C1D	4.34	1.46	1.38
24	G	606	CHL	O2A-CGA	4.33	1.46	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	8	607	CHL	C2C-C3C	4.33	1.46	1.36
24	G	605	CHL	O2A-CGA	4.33	1.46	1.33
24	4	608	CHL	CHD-C1D	4.33	1.46	1.38
24	4	609	CHL	O2A-CGA	4.33	1.46	1.33
24	g	606	CHL	O2A-CGA	4.33	1.46	1.33
24	8	609	CHL	O2A-CGA	4.32	1.46	1.33
24	g	607	CHL	O2A-CGA	4.32	1.46	1.33
24	g	608	CHL	C2C-C3C	4.32	1.46	1.36
24	1	605	CHL	CHD-C1D	4.32	1.46	1.38
24	N	609	CHL	CHC-C1C	4.32	1.46	1.35
24	N	605	CHL	C2C-C3C	4.32	1.46	1.36
24	g	608	CHL	C3B-C2B	4.32	1.46	1.40
24	3	601	CHL	C2C-C3C	4.31	1.46	1.36
24	7	601	CHL	CHD-C1D	4.31	1.46	1.38
24	q	607	CHL	O2A-CGA	4.31	1.45	1.33
24	g	605	CHL	O2A-CGA	4.31	1.45	1.33
24	9	606	CHL	CHD-C1D	4.31	1.46	1.38
24	n	608	CHL	O2A-CGA	4.31	1.45	1.33
24	q	609	CHL	CHD-C4C	4.30	1.49	1.39
24	7	601	CHL	C3B-C2B	4.30	1.46	1.40
24	y	606	CHL	O2A-CGA	4.30	1.45	1.33
24	g	606	CHL	C3B-C2B	4.29	1.46	1.40
24	6	607	CHL	O2A-CGA	4.29	1.45	1.33
29	p	2630	LHG	O8-C23	4.29	1.45	1.33
24	2	606	CHL	O2A-CGA	4.28	1.45	1.33
24	G	607	CHL	O2A-CGA	4.28	1.45	1.33
24	1	601	CHL	CHD-C1D	4.28	1.46	1.38
24	4	607	CHL	O2A-CGA	4.28	1.45	1.33
24	Y	606	CHL	O2A-CGA	4.28	1.45	1.33
29	0	2630	LHG	O8-C23	4.28	1.45	1.33
24	p	607	CHL	CHD-C1D	4.28	1.46	1.38
24	4	606	CHL	O2A-CGA	4.28	1.45	1.33
24	3	605	CHL	O2A-CGA	4.27	1.45	1.33
24	0	606	CHL	CHD-C1D	4.27	1.46	1.38
24	1	607	CHL	O2A-CGA	4.27	1.45	1.33
24	3	606	CHL	CHD-C4C	4.27	1.49	1.39
24	G	606	CHL	C3B-C2B	4.27	1.46	1.40
24	1	601	CHL	C3B-C2B	4.26	1.46	1.40
36	S	2631	LMG	O8-C28	4.26	1.45	1.33
37	c	524	DGD	O1G-C1A	4.26	1.45	1.33
24	1	601	CHL	O2A-CGA	4.26	1.45	1.33
24	2	609	CHL	O2A-CGA	4.26	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	9	601	CHL	O2A-CGA	4.26	1.45	1.33
24	y	605	CHL	C2C-C3C	4.26	1.45	1.36
24	8	605	CHL	O2A-CGA	4.26	1.45	1.33
24	7	607	CHL	O2A-CGA	4.25	1.45	1.33
24	p	601	CHL	C2C-C3C	4.25	1.45	1.36
24	n	601	CHL	O2A-CGA	4.25	1.45	1.33
29	5	2630	LHG	O7-C7	4.25	1.46	1.34
24	2	601	CHL	CHD-C1D	4.25	1.46	1.38
24	9	605	CHL	O2A-CGA	4.24	1.45	1.33
24	7	609	CHL	C3B-C2B	4.24	1.46	1.40
24	2	605	CHL	O2A-CGA	4.24	1.45	1.33
24	N	608	CHL	O2A-CGA	4.24	1.45	1.33
24	9	601	CHL	C3B-C2B	4.24	1.46	1.40
24	1	609	CHL	C3B-C2B	4.24	1.46	1.40
36	s	2631	LMG	O8-C28	4.24	1.45	1.33
24	Y	605	CHL	C2C-C3C	4.24	1.45	1.36
24	Y	609	CHL	CHC-C1C	4.23	1.45	1.35
24	n	605	CHL	C2C-C3C	4.23	1.45	1.36
24	n	605	CHL	CHD-C1D	4.23	1.46	1.38
29	N	2630	LHG	O8-C23	4.23	1.45	1.33
24	8	606	CHL	CHD-C4C	4.23	1.48	1.39
24	4	601	CHL	CHD-C1D	4.23	1.46	1.38
24	8	608	CHL	O2A-CGA	4.23	1.45	1.33
24	q	601	CHL	CHD-C1D	4.23	1.46	1.38
24	0	608	CHL	O2A-CGA	4.23	1.45	1.33
24	8	608	CHL	CHD-C1D	4.23	1.46	1.38
29	6	2630	LHG	O8-C23	4.23	1.45	1.33
24	N	601	CHL	O2A-CGA	4.23	1.45	1.33
24	6	608	CHL	O2A-CGA	4.23	1.45	1.33
24	y	609	CHL	CHC-C1C	4.22	1.45	1.35
24	0	607	CHL	O2A-CGA	4.22	1.45	1.33
37	C	524	DGD	O1G-C1A	4.22	1.45	1.33
24	8	609	CHL	C3B-C2B	4.22	1.46	1.40
24	6	607	CHL	CHD-C1D	4.22	1.46	1.38
24	G	608	CHL	CHD-C1D	4.22	1.46	1.38
24	0	609	CHL	CHD-C1D	4.22	1.46	1.38
29	8	2630	LHG	O8-C23	4.22	1.45	1.33
24	s	606	CHL	C2C-C3C	4.21	1.45	1.36
29	n	2630	LHG	O8-C23	4.21	1.45	1.33
24	9	606	CHL	O2A-CGA	4.21	1.45	1.33
24	S	606	CHL	C3B-C2B	4.21	1.46	1.40
24	s	606	CHL	C3B-C2B	4.20	1.46	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	608	CHL	CHD-C1D	4.20	1.46	1.38
24	3	608	CHL	O2A-CGA	4.20	1.45	1.33
24	N	605	CHL	CHD-C1D	4.20	1.46	1.38
29	2	2630	LHG	O8-C23	4.20	1.45	1.33
24	Y	601	CHL	O2A-CGA	4.20	1.45	1.33
24	S	606	CHL	C2C-C3C	4.19	1.45	1.36
37	C	523	DGD	O2G-C1B	4.19	1.46	1.34
36	a	413	LMG	O7-C10	4.19	1.46	1.34
24	5	607	CHL	O2A-CGA	4.19	1.45	1.33
24	9	609	CHL	O2A-CGA	4.19	1.45	1.33
36	S	2631	LMG	O7-C10	4.19	1.46	1.34
24	9	608	CHL	CHD-C1D	4.19	1.46	1.38
24	G	609	CHL	CHD-C1D	4.19	1.46	1.38
24	N	609	CHL	O2A-CGA	4.19	1.45	1.33
24	0	609	CHL	O2A-CGA	4.19	1.45	1.33
29	5	2630	LHG	O8-C23	4.18	1.45	1.33
24	r	608	CHL	C2C-C3C	4.18	1.45	1.36
36	D	411	LMG	O8-C28	4.18	1.45	1.33
29	3	2630	LHG	O8-C23	4.18	1.45	1.33
24	7	601	CHL	O2A-CGA	4.18	1.45	1.33
24	6	609	CHL	O2A-CGA	4.18	1.45	1.33
24	2	607	CHL	O2A-CGA	4.18	1.45	1.33
35	A	412	SQD	O48-C23	4.18	1.45	1.33
24	3	608	CHL	CHD-C1D	4.18	1.46	1.38
24	9	607	CHL	O2A-CGA	4.18	1.45	1.33
36	d	411	LMG	O7-C10	4.18	1.46	1.34
29	9	2630	LHG	O8-C23	4.17	1.45	1.33
24	1	607	CHL	CHD-C1D	4.17	1.46	1.38
24	p	607	CHL	O2A-CGA	4.17	1.45	1.33
36	s	2631	LMG	O7-C10	4.17	1.46	1.34
35	a	412	SQD	O48-C23	4.17	1.45	1.33
24	n	609	CHL	O2A-CGA	4.17	1.45	1.33
36	A	413	LMG	O7-C10	4.17	1.46	1.34
29	q	2630	LHG	O7-C7	4.16	1.46	1.34
37	c	523	DGD	O2G-C1B	4.16	1.46	1.34
29	4	2630	LHG	O7-C7	4.16	1.46	1.34
29	d	409	LHG	O8-C23	4.16	1.45	1.33
24	2	601	CHL	C3B-C2B	4.16	1.46	1.40
29	D	409	LHG	O8-C23	4.16	1.45	1.33
29	7	2630	LHG	O8-C23	4.16	1.45	1.33
24	1	606	CHL	CHD-C1D	4.15	1.46	1.38
24	p	601	CHL	CHD-C1D	4.15	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	q	606	CHL	CHD-C4C	4.15	1.48	1.39
24	R	608	CHL	C2C-C3C	4.15	1.45	1.36
24	R	607	CHL	C3B-C2B	4.15	1.46	1.40
24	r	607	CHL	C3B-C2B	4.15	1.46	1.40
24	p	608	CHL	O2A-CGA	4.15	1.45	1.33
24	0	608	CHL	CHD-C1D	4.15	1.46	1.38
36	d	411	LMG	O8-C28	4.15	1.45	1.33
24	0	605	CHL	CHD-C1D	4.15	1.46	1.38
29	l	101	LHG	O8-C23	4.15	1.45	1.33
24	R	606	CHL	O2A-CGA	4.15	1.45	1.33
24	N	608	CHL	C3B-C2B	4.15	1.46	1.40
24	1	601	CHL	C2C-C3C	4.15	1.45	1.36
24	p	608	CHL	CHD-C1D	4.14	1.46	1.38
29	L	101	LHG	O8-C23	4.14	1.45	1.33
24	g	609	CHL	CHD-C1D	4.14	1.46	1.38
24	5	608	CHL	O2A-CGA	4.14	1.45	1.33
36	D	411	LMG	O7-C10	4.14	1.46	1.34
24	3	601	CHL	CHD-C1D	4.14	1.46	1.38
24	7	606	CHL	CHD-C1D	4.14	1.46	1.38
24	7	601	CHL	C2C-C3C	4.14	1.45	1.36
37	C	518	DGD	O1G-C1A	4.14	1.45	1.33
24	S	606	CHL	CHD-C1D	4.13	1.46	1.38
29	1	2630	LHG	O8-C23	4.13	1.45	1.33
29	C	2630	LHG	O8-C23	4.13	1.45	1.33
29	q	2630	LHG	O8-C23	4.12	1.45	1.33
24	2	601	CHL	O2A-CGA	4.12	1.45	1.33
24	s	606	CHL	CHD-C1D	4.12	1.46	1.38
29	D	410	LHG	O8-C23	4.12	1.45	1.33
24	y	608	CHL	O2A-CGA	4.12	1.45	1.33
35	B	623	SQD	O48-C23	4.12	1.45	1.33
24	6	607	CHL	C2C-C3C	4.12	1.45	1.36
24	r	606	CHL	O2A-CGA	4.11	1.45	1.33
29	d	410	LHG	O8-C23	4.11	1.45	1.33
24	0	607	CHL	C2C-C3C	4.11	1.45	1.36
35	B	623	SQD	O47-C7	4.11	1.45	1.34
24	g	608	CHL	CHD-C1D	4.11	1.46	1.38
24	Y	608	CHL	C3B-C2B	4.11	1.46	1.40
24	n	609	CHL	CHD-C1D	4.11	1.46	1.38
37	c	518	DGD	O1G-C1A	4.11	1.45	1.33
24	n	608	CHL	C3B-C2B	4.11	1.46	1.40
24	p	606	CHL	CHD-C4C	4.10	1.48	1.39
29	p	2630	LHG	O7-C7	4.10	1.45	1.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	D	412	LMG	O8-C28	4.10	1.45	1.33
25	R	609	CLA	C4D-ND	-4.10	1.32	1.37
25	r	609	CLA	C4D-ND	-4.10	1.32	1.37
24	6	601	CHL	O2A-CGA	4.10	1.45	1.33
24	4	609	CHL	CHD-C4C	4.10	1.48	1.39
35	b	621	SQD	O47-C7	4.10	1.45	1.34
36	d	412	LMG	O8-C28	4.10	1.45	1.33
35	b	623	SQD	O48-C23	4.09	1.45	1.33
24	y	606	CHL	C2C-C3C	4.09	1.45	1.36
25	A	406	CLA	C4D-ND	-4.09	1.32	1.37
25	a	406	CLA	C4D-ND	-4.09	1.32	1.37
35	B	621	SQD	O47-C7	4.09	1.45	1.34
29	d	408	LHG	O8-C23	4.09	1.45	1.33
29	D	408	LHG	O8-C23	4.09	1.45	1.33
24	6	608	CHL	CHD-C1D	4.09	1.46	1.38
35	b	623	SQD	O47-C7	4.09	1.45	1.34
35	b	621	SQD	O48-C23	4.08	1.45	1.33
24	Y	608	CHL	O2A-CGA	4.08	1.45	1.33
24	n	607	CHL	O2A-CGA	4.08	1.45	1.33
29	c	2630	LHG	O8-C23	4.08	1.45	1.33
24	8	601	CHL	CHD-C1D	4.08	1.46	1.38
24	G	609	CHL	C3B-C2B	4.08	1.46	1.40
24	5	608	CHL	CHD-C1D	4.08	1.46	1.38
24	s	608	CHL	CHD-C1D	4.08	1.46	1.38
29	9	2630	LHG	O7-C7	4.08	1.45	1.34
24	Y	608	CHL	C2C-C3C	4.08	1.45	1.36
24	Y	607	CHL	C2C-C3C	4.07	1.45	1.36
35	B	621	SQD	O48-C23	4.07	1.45	1.33
24	7	607	CHL	C2C-C3C	4.07	1.45	1.36
24	Y	605	CHL	CHD-C1D	4.07	1.46	1.38
24	y	605	CHL	CHD-C1D	4.07	1.46	1.38
25	g	613	CLA	C4D-ND	-4.07	1.32	1.37
29	4	2630	LHG	O8-C23	4.07	1.45	1.33
24	y	607	CHL	C2C-C3C	4.07	1.45	1.36
24	y	608	CHL	C2C-C3C	4.07	1.45	1.36
35	a	412	SQD	O47-C7	4.06	1.45	1.34
24	3	609	CHL	C3B-C2B	4.06	1.46	1.40
24	y	608	CHL	C3B-C2B	4.06	1.46	1.40
24	9	605	CHL	CHD-C4C	4.06	1.48	1.39
24	6	606	CHL	CHD-C1D	4.06	1.46	1.38
24	7	607	CHL	CHD-C1D	4.06	1.46	1.38
24	R	608	CHL	O2A-CGA	4.05	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
35	d	413	SQD	O48-C23	4.05	1.45	1.33
29	2	2630	LHG	O7-C7	4.05	1.45	1.34
24	q	607	CHL	CHD-C4C	4.05	1.48	1.39
24	r	608	CHL	O2A-CGA	4.05	1.45	1.33
37	C	520	DGD	O1G-C1A	4.05	1.45	1.33
37	c	520	DGD	O1G-C1A	4.05	1.45	1.33
24	g	607	CHL	C2C-C3C	4.05	1.45	1.36
24	Y	606	CHL	C2C-C3C	4.05	1.45	1.36
24	1	601	CHL	CHD-C4C	4.05	1.48	1.39
24	2	605	CHL	CHD-C4C	4.05	1.48	1.39
35	A	412	SQD	O47-C7	4.04	1.45	1.34
35	D	413	SQD	O48-C23	4.04	1.45	1.33
24	g	601	CHL	O2A-CGA	4.04	1.45	1.33
29	d	410	LHG	O7-C7	4.04	1.45	1.34
24	g	607	CHL	CHD-C1D	4.04	1.46	1.38
29	D	410	LHG	O7-C7	4.03	1.45	1.34
25	G	613	CLA	C4D-ND	-4.03	1.32	1.37
24	N	609	CHL	CHD-C1D	4.03	1.46	1.38
24	S	608	CHL	CHD-C1D	4.03	1.46	1.38
36	D	412	LMG	O7-C10	4.03	1.45	1.34
40	F	101	HEM	C3C-C2C	-4.03	1.34	1.40
24	0	601	CHL	O2A-CGA	4.03	1.45	1.33
29	s	2630	LHG	O7-C7	4.03	1.45	1.34
24	G	607	CHL	C2C-C3C	4.03	1.45	1.36
24	G	601	CHL	O2A-CGA	4.03	1.45	1.33
24	N	601	CHL	C2C-C3C	4.02	1.45	1.36
36	d	412	LMG	O7-C10	4.02	1.45	1.34
24	4	607	CHL	CHD-C4C	4.01	1.48	1.39
29	d	408	LHG	O7-C7	4.01	1.45	1.34
24	4	605	CHL	CHD-C4C	4.01	1.48	1.39
24	6	609	CHL	CHD-C1D	4.01	1.46	1.38
24	N	601	CHL	C3B-C2B	4.01	1.45	1.40
24	g	606	CHL	CHD-C1D	4.01	1.46	1.38
24	N	605	CHL	C3B-C2B	4.01	1.45	1.40
24	1	606	CHL	C2C-C3C	4.01	1.45	1.36
24	n	609	CHL	C2C-C3C	4.00	1.45	1.36
24	r	607	CHL	O2A-CGA	4.00	1.45	1.33
24	7	601	CHL	CHD-C4C	4.00	1.48	1.39
24	p	605	CHL	CHD-C4C	4.00	1.48	1.39
29	R	2630	LHG	O7-C7	4.00	1.45	1.34
36	h	102	LMG	O8-C28	4.00	1.45	1.33
24	7	606	CHL	C2C-C3C	4.00	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	R	607	CHL	O2A-CGA	4.00	1.45	1.33
24	G	606	CHL	CHD-C1D	4.00	1.46	1.38
36	C	521	LMG	O8-C28	4.00	1.45	1.33
29	S	2630	LHG	O7-C7	4.00	1.45	1.34
24	G	607	CHL	CHD-C1D	4.00	1.46	1.38
36	H	102	LMG	O8-C28	3.99	1.45	1.33
35	D	413	SQD	O47-C7	3.99	1.45	1.34
24	0	607	CHL	CHD-C1D	3.99	1.46	1.38
29	r	2630	LHG	O8-C23	3.99	1.45	1.33
24	n	605	CHL	C3B-C2B	3.99	1.45	1.40
29	D	408	LHG	O7-C7	3.99	1.45	1.34
24	g	609	CHL	C3B-C2B	3.98	1.45	1.40
35	d	413	SQD	O47-C7	3.98	1.45	1.34
25	5	612	CLA	C1D-ND	3.98	1.42	1.37
29	R	2630	LHG	O8-C23	3.98	1.45	1.33
36	c	521	LMG	O8-C28	3.98	1.45	1.33
40	f	101	HEM	C3C-C2C	-3.98	1.34	1.40
29	r	2630	LHG	O7-C7	3.98	1.45	1.34
37	c	520	DGD	O2G-C1B	3.98	1.45	1.34
24	7	609	CHL	C2C-C3C	3.97	1.45	1.36
29	s	2630	LHG	O8-C23	3.97	1.45	1.33
36	h	102	LMG	O7-C10	3.97	1.45	1.34
24	g	609	CHL	C2C-C3C	3.97	1.45	1.36
36	H	102	LMG	O7-C10	3.97	1.45	1.34
36	b	622	LMG	O8-C28	3.97	1.44	1.33
24	N	608	CHL	C2C-C3C	3.97	1.45	1.36
25	B	612	CLA	C4D-ND	-3.97	1.32	1.37
25	b	612	CLA	C4D-ND	-3.97	1.32	1.37
24	N	607	CHL	O2A-CGA	3.97	1.44	1.33
24	q	605	CHL	CHD-C4C	3.96	1.48	1.39
29	8	2630	LHG	O7-C7	3.96	1.45	1.34
24	1	609	CHL	C2C-C3C	3.96	1.45	1.36
24	g	606	CHL	C2C-C3C	3.96	1.45	1.36
24	4	606	CHL	CHD-C4C	3.96	1.48	1.39
25	C	504	CLA	C4D-ND	-3.96	1.32	1.37
29	0	2630	LHG	O7-C7	3.96	1.45	1.34
24	1	607	CHL	C2C-C3C	3.96	1.45	1.36
24	y	601	CHL	CHD-C1D	3.95	1.46	1.38
24	9	609	CHL	CHD-C4C	3.95	1.48	1.39
36	b	622	LMG	O7-C10	3.95	1.45	1.34
24	1	608	CHL	C2C-C3C	3.95	1.45	1.36
24	G	609	CHL	C2C-C3C	3.95	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	508	CLA	C4D-ND	-3.95	1.32	1.37
29	y	2630	LHG	O8-C23	3.95	1.44	1.33
24	n	608	CHL	C2C-C3C	3.95	1.45	1.36
24	n	606	CHL	C2C-C3C	3.94	1.45	1.36
36	B	622	LMG	O8-C28	3.94	1.44	1.33
24	6	601	CHL	CHD-C1D	3.94	1.46	1.38
37	C	520	DGD	O2G-C1B	3.94	1.45	1.34
24	G	606	CHL	C2C-C3C	3.94	1.45	1.36
36	B	622	LMG	O7-C10	3.94	1.45	1.34
29	3	2630	LHG	O7-C7	3.94	1.45	1.34
24	7	608	CHL	C2C-C3C	3.94	1.45	1.36
29	S	2630	LHG	O8-C23	3.93	1.44	1.33
25	C	502	CLA	C4D-ND	-3.93	1.32	1.37
29	g	2630	LHG	O7-C7	3.92	1.45	1.34
25	b	604	CLA	C4D-ND	-3.92	1.32	1.37
25	b	616	CLA	C4D-ND	-3.92	1.32	1.37
40	f	101	HEM	C3C-CAC	3.92	1.55	1.47
37	C	518	DGD	O2G-C1B	3.92	1.45	1.34
29	7	2630	LHG	O7-C7	3.92	1.45	1.34
24	0	601	CHL	CHD-C1D	3.92	1.46	1.38
24	n	605	CHL	O2A-CGA	3.92	1.44	1.33
24	s	601	CHL	CHD-C4C	3.92	1.48	1.39
25	c	502	CLA	C4D-ND	-3.92	1.32	1.37
29	G	2630	LHG	O7-C7	3.91	1.45	1.34
24	N	606	CHL	C2C-C3C	3.91	1.45	1.36
24	G	605	CHL	CHD-C4C	3.91	1.48	1.39
24	3	605	CHL	CHD-C4C	3.91	1.48	1.39
24	n	607	CHL	C2C-C3C	3.91	1.45	1.36
29	1	2630	LHG	O7-C7	3.91	1.45	1.34
24	G	601	CHL	CHD-C1D	3.91	1.46	1.38
25	c	508	CLA	C4D-ND	-3.91	1.32	1.37
24	5	607	CHL	CHD-C1D	3.90	1.46	1.38
24	g	601	CHL	CHD-C1D	3.90	1.46	1.38
29	6	2630	LHG	O7-C7	3.90	1.45	1.34
25	c	504	CLA	C4D-ND	-3.90	1.32	1.37
24	Y	601	CHL	CHD-C1D	3.89	1.45	1.38
29	n	2630	LHG	O7-C7	3.89	1.45	1.34
24	S	601	CHL	CHD-C4C	3.89	1.48	1.39
29	Y	2630	LHG	O8-C23	3.89	1.44	1.33
37	c	518	DGD	O2G-C1B	3.89	1.45	1.34
29	N	2630	LHG	O7-C7	3.89	1.45	1.34
25	0	611	CLA	C1D-ND	3.89	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	605	CHL	C3B-C2B	3.89	1.45	1.40
25	B	604	CLA	C4D-ND	-3.88	1.32	1.37
24	N	609	CHL	C3B-C2B	3.88	1.45	1.40
25	B	616	CLA	C4D-ND	-3.88	1.32	1.37
24	g	605	CHL	CHD-C4C	3.88	1.48	1.39
24	5	609	CHL	CHD-C4C	3.88	1.48	1.39
24	5	606	CHL	CHD-C4C	3.87	1.48	1.39
24	8	605	CHL	CHD-C4C	3.87	1.48	1.39
25	R	601	CLA	C1D-ND	3.87	1.42	1.37
36	a	413	LMG	O8-C28	3.87	1.44	1.33
36	A	413	LMG	O8-C28	3.87	1.44	1.33
24	4	608	CHL	CHD-C4C	3.87	1.48	1.39
25	d	402	CLA	C4D-ND	-3.87	1.32	1.37
25	d	403	CLA	C4D-ND	-3.87	1.32	1.37
24	y	605	CHL	C3B-C2B	3.87	1.45	1.40
25	r	601	CLA	C1D-ND	3.87	1.42	1.37
25	p	612	CLA	C1D-ND	3.87	1.42	1.37
24	N	601	CHL	CHD-C1D	3.86	1.45	1.38
24	2	607	CHL	CHD-C4C	3.86	1.48	1.39
24	N	605	CHL	O2A-CGA	3.86	1.44	1.33
25	D	403	CLA	C4D-ND	-3.86	1.32	1.37
25	B	609	CLA	C4D-ND	-3.86	1.32	1.37
24	N	607	CHL	C2C-C3C	3.86	1.45	1.36
24	5	605	CHL	CHD-C4C	3.86	1.48	1.39
24	R	607	CHL	C2C-C3C	3.86	1.45	1.36
29	C	2630	LHG	O7-C7	3.85	1.45	1.34
24	5	601	CHL	CHD-C4C	3.85	1.48	1.39
24	2	609	CHL	CHD-C4C	3.85	1.48	1.39
37	C	519	DGD	O1G-C1A	3.85	1.44	1.33
25	4	610	CLA	C1D-ND	3.85	1.42	1.37
24	q	608	CHL	CHD-C4C	3.85	1.48	1.39
24	n	601	CHL	CHD-C1D	3.84	1.45	1.38
25	q	610	CLA	C1D-ND	3.84	1.42	1.37
24	r	607	CHL	C2C-C3C	3.84	1.45	1.36
24	9	607	CHL	CHD-C4C	3.84	1.48	1.39
36	C	521	LMG	O7-C10	3.84	1.45	1.34
36	c	521	LMG	O7-C10	3.84	1.45	1.34
24	2	606	CHL	CHD-C4C	3.84	1.48	1.39
25	D	402	CLA	C4D-ND	-3.84	1.32	1.37
24	g	601	CHL	C3B-C2B	3.84	1.45	1.40
25	b	609	CLA	C4D-ND	-3.83	1.32	1.37
24	n	601	CHL	C3B-C2B	3.83	1.45	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
37	c	519	DGD	O1G-C1A	3.83	1.44	1.33
24	n	601	CHL	C2C-C3C	3.83	1.45	1.36
24	9	601	CHL	CHD-C4C	3.83	1.48	1.39
37	c	519	DGD	O2G-C1B	3.82	1.45	1.34
24	3	601	CHL	CHD-C4C	3.82	1.48	1.39
25	5	610	CLA	C1D-ND	3.82	1.42	1.37
25	5	614	CLA	C1D-ND	3.82	1.42	1.37
40	F	101	HEM	C3C-CAC	3.82	1.55	1.47
25	p	604	CLA	C1D-ND	3.82	1.42	1.37
25	3	612	CLA	C1D-ND	3.82	1.42	1.37
29	c	2630	LHG	O7-C7	3.82	1.45	1.34
24	6	605	CHL	CHD-C4C	3.82	1.47	1.39
25	B	615	CLA	C4D-ND	-3.81	1.32	1.37
37	C	519	DGD	O2G-C1B	3.81	1.45	1.34
24	q	601	CHL	CHD-C4C	3.81	1.47	1.39
25	C	503	CLA	C4D-ND	-3.81	1.32	1.37
24	n	609	CHL	C3B-C2B	3.81	1.45	1.40
24	N	609	CHL	C2C-C3C	3.81	1.44	1.36
37	C	523	DGD	O1G-C1A	3.81	1.44	1.33
37	c	523	DGD	O1G-C1A	3.81	1.44	1.33
29	L	101	LHG	O7-C7	3.81	1.45	1.34
24	G	601	CHL	C2C-C3C	3.80	1.44	1.36
25	6	611	CLA	C1D-ND	3.80	1.42	1.37
24	p	601	CHL	CHD-C4C	3.80	1.47	1.39
25	c	503	CLA	C4D-ND	-3.80	1.32	1.37
24	p	607	CHL	CHD-C4C	3.80	1.47	1.39
25	A	405	CLA	C4D-ND	-3.80	1.32	1.37
25	6	614	CLA	C1D-ND	3.79	1.42	1.37
24	8	609	CHL	CHD-C1D	3.79	1.45	1.38
25	s	613	CLA	C4D-ND	-3.79	1.32	1.37
24	p	601	CHL	OBD-CAD	3.79	1.29	1.22
25	p	613	CLA	C1D-ND	3.79	1.42	1.37
24	G	601	CHL	C3B-C2B	3.79	1.45	1.40
24	4	608	CHL	OBD-CAD	3.79	1.29	1.22
29	G	2630	LHG	O8-C23	3.79	1.44	1.33
24	9	606	CHL	CHD-C4C	3.79	1.47	1.39
24	2	601	CHL	CHD-C4C	3.78	1.47	1.39
25	c	512	CLA	C4D-ND	-3.78	1.32	1.37
25	b	614	CLA	C4D-ND	-3.78	1.32	1.37
25	y	603	CLA	C4D-ND	-3.78	1.32	1.37
24	6	601	CHL	CHD-C4C	3.78	1.47	1.39
25	C	512	CLA	C4D-ND	-3.77	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	607	CHL	CHD-C4C	3.77	1.47	1.39
25	C	502	CLA	C3B-C2B	-3.77	1.35	1.40
25	c	506	CLA	C4D-ND	-3.77	1.32	1.37
25	b	615	CLA	C4D-ND	-3.77	1.32	1.37
29	g	2630	LHG	O8-C23	3.77	1.44	1.33
25	Y	614	CLA	C4D-ND	-3.76	1.32	1.37
24	p	609	CHL	CHD-C4C	3.76	1.47	1.39
25	0	613	CLA	C1D-ND	3.76	1.42	1.37
24	g	601	CHL	C2C-C3C	3.76	1.44	1.36
29	l	101	LHG	O7-C7	3.76	1.44	1.34
25	8	614	CLA	C1D-ND	3.76	1.42	1.37
25	C	506	CLA	C4D-ND	-3.76	1.32	1.37
25	p	614	CLA	C1D-ND	3.76	1.42	1.37
24	q	608	CHL	OBD-CAD	3.76	1.29	1.22
25	B	606	CLA	C4D-ND	-3.75	1.32	1.37
25	b	606	CLA	C4D-ND	-3.75	1.32	1.37
25	c	513	CLA	C4D-ND	-3.75	1.32	1.37
24	1	609	CHL	CHD-C1D	3.75	1.45	1.38
24	8	601	CHL	CHD-C4C	3.75	1.47	1.39
24	3	609	CHL	CHD-C1D	3.75	1.45	1.38
25	7	614	CLA	C1D-ND	3.75	1.42	1.37
25	a	405	CLA	C4D-ND	-3.75	1.32	1.37
25	y	613	CLA	C4D-ND	-3.75	1.32	1.37
24	S	608	CHL	CHD-C4C	3.75	1.47	1.39
25	B	614	CLA	C4D-ND	-3.74	1.32	1.37
24	9	605	CHL	OBD-CAD	3.74	1.28	1.22
25	0	614	CLA	C1D-ND	3.74	1.42	1.37
25	4	602	CLA	C1D-ND	3.74	1.42	1.37
29	D	409	LHG	O7-C7	3.74	1.44	1.34
25	q	602	CLA	C1D-ND	3.74	1.42	1.37
24	R	606	CHL	C3B-C2B	3.73	1.45	1.40
25	c	502	CLA	C3B-C2B	-3.73	1.35	1.40
24	q	605	CHL	OBD-CAD	3.73	1.28	1.22
24	r	606	CHL	CHD-C1D	3.73	1.45	1.38
25	A	410	CLA	C4D-ND	-3.73	1.32	1.37
25	a	410	CLA	C4D-ND	-3.73	1.32	1.37
24	s	608	CHL	CHD-C4C	3.73	1.47	1.39
25	A	407	CLA	C4D-ND	-3.73	1.32	1.37
25	Y	603	CLA	C4D-ND	-3.73	1.32	1.37
24	0	606	CHL	CHD-C4C	3.73	1.47	1.39
25	c	507	CLA	C4D-ND	-3.73	1.32	1.37
25	6	613	CLA	C1D-ND	3.73	1.42	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	608	CHL	OBD-CAD	3.73	1.28	1.22
24	y	601	CHL	C2C-C3C	3.73	1.44	1.36
25	B	611	CLA	C4D-ND	-3.73	1.32	1.37
24	2	605	CHL	OBD-CAD	3.72	1.28	1.22
25	S	613	CLA	C4D-ND	-3.72	1.32	1.37
24	R	606	CHL	CHD-C1D	3.72	1.45	1.38
24	p	605	CHL	OBD-CAD	3.72	1.28	1.22
25	B	603	CLA	C4D-ND	-3.72	1.32	1.37
25	Y	613	CLA	C4D-ND	-3.72	1.32	1.37
29	d	409	LHG	O7-C7	3.72	1.44	1.34
25	6	602	CLA	C1D-ND	3.71	1.42	1.37
24	6	606	CHL	OBD-CAD	3.71	1.28	1.22
25	b	603	CLA	C4D-ND	-3.71	1.32	1.37
24	r	606	CHL	C3B-C2B	3.71	1.45	1.40
25	r	602	CLA	C4D-ND	-3.71	1.32	1.37
24	2	607	CHL	OBD-CAD	3.71	1.28	1.22
24	n	605	CHL	CHD-C4C	3.71	1.47	1.39
25	C	507	CLA	C4D-ND	-3.71	1.32	1.37
24	N	605	CHL	CHD-C4C	3.71	1.47	1.39
24	s	607	CHL	CHD-C4C	3.71	1.47	1.39
25	y	614	CLA	C4D-ND	-3.70	1.32	1.37
29	y	2630	LHG	O7-C7	3.70	1.44	1.34
25	5	613	CLA	C1D-ND	3.70	1.42	1.37
24	R	608	CHL	CHD-C1D	3.70	1.45	1.38
24	0	605	CHL	CHD-C4C	3.70	1.47	1.39
24	0	608	CHL	CHD-C4C	3.70	1.47	1.39
24	9	608	CHL	CHD-C4C	3.70	1.47	1.39
24	4	601	CHL	CHD-C4C	3.70	1.47	1.39
24	5	605	CHL	OBD-CAD	3.70	1.28	1.22
25	R	602	CLA	C4D-ND	-3.70	1.32	1.37
25	b	617	CLA	C4D-ND	-3.69	1.32	1.37
24	9	607	CHL	OBD-CAD	3.69	1.28	1.22
24	0	607	CHL	OBD-CAD	3.69	1.28	1.22
24	2	608	CHL	CHD-C4C	3.69	1.47	1.39
25	3	611	CLA	C1D-ND	3.69	1.42	1.37
25	Y	611	CLA	C4D-ND	-3.69	1.32	1.37
24	y	607	CHL	CHD-C1D	3.69	1.45	1.38
25	C	501	CLA	C4D-ND	-3.68	1.32	1.37
25	6	604	CLA	C1D-ND	3.68	1.42	1.37
25	1	614	CLA	C1D-ND	3.68	1.42	1.37
24	g	605	CHL	OBD-CAD	3.68	1.28	1.22
25	b	611	CLA	C4D-ND	-3.68	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	603	CLA	C4D-ND	-3.68	1.32	1.37
25	5	604	CLA	C1D-ND	3.68	1.42	1.37
25	C	513	CLA	C4D-ND	-3.68	1.32	1.37
25	s	602	CLA	C4D-ND	-3.68	1.32	1.37
24	8	607	CHL	CHD-C1D	3.68	1.45	1.38
24	S	607	CHL	CHD-C4C	3.68	1.47	1.39
24	Y	601	CHL	C2C-C3C	3.67	1.44	1.36
25	a	407	CLA	C4D-ND	-3.67	1.32	1.37
24	p	608	CHL	CHD-C4C	3.67	1.47	1.39
24	q	607	CHL	OBD-CAD	3.67	1.28	1.22
25	c	501	CLA	C4D-ND	-3.67	1.32	1.37
25	9	610	CLA	C1D-ND	3.67	1.42	1.37
24	5	601	CHL	OBD-CAD	3.67	1.28	1.22
25	8	612	CLA	C1D-ND	3.67	1.42	1.37
25	y	611	CLA	C4D-ND	-3.67	1.32	1.37
24	r	608	CHL	CHD-C1D	3.66	1.45	1.38
24	p	607	CHL	OBD-CAD	3.66	1.28	1.22
25	9	612	CLA	C1D-ND	3.66	1.42	1.37
25	B	617	CLA	C4D-ND	-3.66	1.32	1.37
25	3	604	CLA	C4D-ND	-3.66	1.32	1.37
25	0	602	CLA	C1D-ND	3.66	1.42	1.37
25	p	603	CLA	C1D-ND	3.66	1.42	1.37
24	g	608	CHL	OBD-CAD	3.65	1.28	1.22
24	0	606	CHL	OBD-CAD	3.65	1.28	1.22
25	g	602	CLA	C4D-ND	-3.65	1.32	1.37
25	2	604	CLA	C1D-ND	3.65	1.42	1.37
25	5	603	CLA	C1D-ND	3.65	1.42	1.37
25	R	610	CLA	C4D-ND	-3.65	1.32	1.37
24	G	605	CHL	OBD-CAD	3.65	1.28	1.22
25	4	614	CLA	C1D-ND	3.65	1.42	1.37
24	G	608	CHL	CHD-C4C	3.65	1.47	1.39
24	Y	607	CHL	CHD-C1D	3.65	1.45	1.38
24	Y	606	CHL	CHD-C1D	3.65	1.45	1.38
29	Y	2630	LHG	O7-C7	3.64	1.44	1.34
25	n	603	CLA	C4D-ND	-3.64	1.32	1.37
24	g	609	CHL	CHD-C4C	3.64	1.47	1.39
25	c	502	CLA	CMB-C2B	-3.64	1.44	1.51
24	G	609	CHL	CHD-C4C	3.64	1.47	1.39
24	5	608	CHL	CHD-C4C	3.64	1.47	1.39
25	G	611	CLA	C1D-ND	3.64	1.42	1.37
24	4	605	CHL	OBD-CAD	3.64	1.28	1.22
25	c	505	CLA	C4D-ND	-3.64	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	601	CHL	CHD-C4C	3.64	1.47	1.39
25	q	612	CLA	C1D-ND	3.64	1.42	1.37
24	6	605	CHL	OBD-CAD	3.64	1.28	1.22
25	N	613	CLA	C4D-ND	-3.64	1.32	1.37
24	N	606	CHL	CHD-C1D	3.64	1.45	1.38
25	3	614	CLA	C1D-ND	3.64	1.42	1.37
25	g	610	CLA	C4D-ND	-3.63	1.32	1.37
25	9	604	CLA	C1D-ND	3.63	1.42	1.37
25	8	610	CLA	C1D-ND	3.63	1.42	1.37
24	0	601	CHL	CHD-C4C	3.63	1.47	1.39
24	6	606	CHL	CHD-C4C	3.63	1.47	1.39
24	8	608	CHL	CHD-C4C	3.63	1.47	1.39
25	q	604	CLA	C1D-ND	3.62	1.42	1.37
25	C	505	CLA	C4D-ND	-3.62	1.32	1.37
25	n	602	CLA	C4D-ND	-3.62	1.32	1.37
25	c	509	CLA	C4D-ND	-3.62	1.32	1.37
24	3	608	CHL	CHD-C4C	3.62	1.47	1.39
25	g	611	CLA	C1D-ND	3.62	1.42	1.37
24	N	607	CHL	C3B-C2B	3.62	1.45	1.40
25	b	608	CLA	C4D-ND	-3.62	1.32	1.37
24	g	606	CHL	CHD-C4C	3.62	1.47	1.39
24	y	601	CHL	CHD-C4C	3.62	1.47	1.39
24	3	607	CHL	OBD-CAD	3.61	1.28	1.22
25	S	602	CLA	C4D-ND	-3.61	1.32	1.37
37	C	524	DGD	O2G-C1B	3.61	1.44	1.34
24	4	609	CHL	OBD-CAD	3.61	1.28	1.22
25	7	603	CLA	C4D-ND	-3.61	1.32	1.37
25	4	604	CLA	C1D-ND	3.61	1.42	1.37
25	C	502	CLA	CMB-C2B	-3.61	1.44	1.51
25	n	604	CLA	C4D-ND	-3.61	1.32	1.37
25	C	509	CLA	C4D-ND	-3.61	1.32	1.37
25	3	613	CLA	C1D-ND	3.61	1.42	1.37
24	r	608	CHL	C3B-C2B	3.61	1.45	1.40
25	y	612	CLA	C4D-ND	-3.61	1.32	1.37
25	G	610	CLA	C4D-ND	-3.61	1.32	1.37
25	R	613	CLA	C4D-ND	-3.61	1.32	1.37
25	r	613	CLA	C4D-ND	-3.61	1.32	1.37
25	3	610	CLA	C1D-ND	3.61	1.42	1.37
25	s	610	CLA	C4D-ND	-3.60	1.32	1.37
24	n	607	CHL	C3B-C2B	3.60	1.45	1.40
25	g	603	CLA	C4D-ND	-3.60	1.32	1.37
24	7	607	CHL	CHD-C4C	3.60	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	602	CLA	C4D-ND	-3.60	1.32	1.37
25	r	610	CLA	C4D-ND	-3.60	1.32	1.37
24	n	606	CHL	CHD-C1D	3.60	1.45	1.38
25	B	608	CLA	C4D-ND	-3.60	1.32	1.37
24	R	608	CHL	C3B-C2B	3.60	1.45	1.40
25	n	613	CLA	C4D-ND	-3.60	1.32	1.37
24	3	607	CHL	CHD-C1D	3.60	1.45	1.38
25	8	611	CLA	C1D-ND	3.60	1.42	1.37
24	n	609	CHL	CHD-C4C	3.60	1.47	1.39
24	q	606	CHL	OBD-CAD	3.60	1.28	1.22
25	8	613	CLA	C1D-ND	3.60	1.42	1.37
25	2	610	CLA	C1D-ND	3.60	1.42	1.37
24	N	608	CHL	CHD-C1D	3.60	1.45	1.38
24	y	606	CHL	CHD-C1D	3.59	1.45	1.38
25	4	612	CLA	C1D-ND	3.59	1.42	1.37
25	N	611	CLA	C4D-ND	-3.59	1.32	1.37
24	8	607	CHL	OBD-CAD	3.59	1.28	1.22
24	3	601	CHL	OBD-CAD	3.59	1.28	1.22
24	y	609	CHL	C3B-C2B	3.59	1.45	1.40
24	7	609	CHL	CHD-C1D	3.59	1.45	1.38
24	g	608	CHL	CHD-C4C	3.59	1.47	1.39
24	G	606	CHL	CHD-C4C	3.59	1.47	1.39
24	Y	609	CHL	C3B-C2B	3.58	1.45	1.40
25	R	603	CLA	C4D-ND	-3.58	1.32	1.37
25	S	610	CLA	C4D-ND	-3.58	1.32	1.37
37	c	524	DGD	O2G-C1B	3.58	1.44	1.34
25	b	607	CLA	C4D-ND	-3.58	1.32	1.37
24	7	608	CHL	CHD-C1D	3.58	1.45	1.38
25	N	602	CLA	C4D-ND	-3.58	1.32	1.37
24	8	605	CHL	OBD-CAD	3.58	1.28	1.22
24	0	609	CHL	CHD-C4C	3.58	1.47	1.39
24	4	607	CHL	OBD-CAD	3.58	1.28	1.22
25	q	614	CLA	C1D-ND	3.58	1.42	1.37
25	N	604	CLA	C4D-ND	-3.57	1.32	1.37
25	B	613	CLA	C4D-ND	-3.57	1.32	1.37
25	G	611	CLA	C4D-ND	-3.57	1.32	1.37
25	b	613	CLA	C4D-ND	-3.57	1.32	1.37
24	5	607	CHL	OBD-CAD	3.57	1.28	1.22
25	p	610	CLA	C1D-ND	3.57	1.42	1.37
24	0	607	CHL	CHD-C4C	3.57	1.47	1.39
25	4	613	CLA	C1D-ND	3.57	1.42	1.37
24	S	606	CHL	CHD-C4C	3.57	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	p	602	CLA	C1D-ND	3.57	1.42	1.37
24	4	606	CHL	OBD-CAD	3.57	1.28	1.22
24	9	609	CHL	OBD-CAD	3.57	1.28	1.22
25	y	604	CLA	CMB-C2B	-3.57	1.44	1.51
25	r	603	CLA	C4D-ND	-3.57	1.32	1.37
24	2	609	CHL	OBD-CAD	3.57	1.28	1.22
24	7	605	CHL	CHD-C4C	3.56	1.47	1.39
24	2	606	CHL	OBD-CAD	3.56	1.28	1.22
24	9	606	CHL	OBD-CAD	3.56	1.28	1.22
24	0	605	CHL	OBD-CAD	3.56	1.28	1.22
24	3	605	CHL	OBD-CAD	3.56	1.28	1.22
24	1	607	CHL	CHD-C4C	3.56	1.47	1.39
24	6	609	CHL	CHD-C4C	3.56	1.47	1.39
25	G	604	CLA	C4D-ND	-3.56	1.32	1.37
25	S	611	CLA	C4D-ND	-3.56	1.32	1.37
25	7	613	CLA	C1D-ND	3.56	1.42	1.37
25	B	610	CLA	C4D-ND	-3.56	1.32	1.37
25	Y	604	CLA	C3B-C2B	-3.56	1.35	1.40
25	5	602	CLA	C1D-ND	3.56	1.42	1.37
24	r	607	CHL	CHD-C1D	3.55	1.45	1.38
24	s	606	CHL	CHD-C4C	3.55	1.47	1.39
24	3	608	CHL	OBD-CAD	3.55	1.28	1.22
25	b	610	CLA	C4D-ND	-3.55	1.32	1.37
24	y	605	CHL	CHD-C4C	3.55	1.47	1.39
25	1	603	CLA	C4D-ND	-3.55	1.32	1.37
25	G	603	CLA	C4D-ND	-3.55	1.32	1.37
25	s	611	CLA	C4D-ND	-3.55	1.32	1.37
24	8	606	CHL	OBD-CAD	3.54	1.28	1.22
24	n	608	CHL	CHD-C1D	3.54	1.45	1.38
25	Y	604	CLA	CMB-C2B	-3.54	1.44	1.51
24	1	608	CHL	CHD-C1D	3.54	1.45	1.38
25	Y	612	CLA	C4D-ND	-3.54	1.32	1.37
25	9	602	CLA	C4D-ND	-3.54	1.32	1.37
24	7	606	CHL	CHD-C4C	3.54	1.47	1.39
24	5	607	CHL	CHD-C4C	3.54	1.47	1.39
25	2	612	CLA	C1D-ND	3.54	1.42	1.37
25	n	611	CLA	C4D-ND	-3.54	1.32	1.37
24	8	601	CHL	OBD-CAD	3.54	1.28	1.22
25	1	611	CLA	C4D-ND	-3.53	1.32	1.37
25	8	604	CLA	C4D-ND	-3.53	1.32	1.37
25	c	510	CLA	C4D-ND	-3.53	1.32	1.37
25	9	613	CLA	C4D-ND	-3.53	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	G	601	CHL	CHD-C4C	3.53	1.47	1.39
24	Y	605	CHL	CHD-C4C	3.53	1.47	1.39
24	0	601	CHL	OBD-CAD	3.53	1.28	1.22
25	n	614	CLA	C1D-ND	3.53	1.42	1.37
25	2	613	CLA	C4D-ND	-3.52	1.32	1.37
25	S	603	CLA	C1D-ND	3.52	1.42	1.37
24	6	608	CHL	CHD-C4C	3.52	1.47	1.39
25	S	614	CLA	C4D-ND	-3.52	1.32	1.37
25	n	614	CLA	C4D-ND	-3.52	1.32	1.37
25	S	609	CLA	C1D-ND	3.52	1.42	1.37
25	s	609	CLA	C1D-ND	3.52	1.42	1.37
24	1	605	CHL	CHD-C4C	3.52	1.47	1.39
25	g	604	CLA	C4D-ND	-3.52	1.32	1.37
25	r	603	CLA	C1D-ND	3.52	1.42	1.37
25	8	604	CLA	C1D-ND	3.52	1.42	1.37
24	n	606	CHL	C3B-C2B	3.52	1.45	1.40
24	0	609	CHL	OBD-CAD	3.52	1.28	1.22
24	8	609	CHL	OBD-CAD	3.52	1.28	1.22
24	q	609	CHL	MG-NA	-3.52	1.97	2.06
24	p	608	CHL	OBD-CAD	3.52	1.28	1.22
24	R	607	CHL	CHD-C1D	3.51	1.45	1.38
24	1	606	CHL	CHD-C4C	3.51	1.47	1.39
25	q	603	CLA	C1D-ND	3.51	1.42	1.37
25	B	607	CLA	C4D-ND	-3.51	1.32	1.37
24	g	601	CHL	CHD-C4C	3.51	1.47	1.39
24	n	607	CHL	CHD-C1D	3.51	1.45	1.38
25	s	614	CLA	C4D-ND	-3.51	1.32	1.37
25	7	611	CLA	C4D-ND	-3.51	1.32	1.37
25	y	604	CLA	C3B-C2B	-3.51	1.35	1.40
25	S	604	CLA	C4D-ND	-3.50	1.32	1.37
24	p	609	CHL	OBD-CAD	3.50	1.28	1.22
25	9	614	CLA	C1D-ND	3.50	1.42	1.37
24	3	606	CHL	OBD-CAD	3.50	1.28	1.22
24	4	601	CHL	OBD-CAD	3.50	1.28	1.22
25	p	611	CLA	C1D-ND	3.50	1.42	1.37
24	6	609	CHL	OBD-CAD	3.50	1.28	1.22
25	2	614	CLA	C1D-ND	3.50	1.42	1.37
25	R	603	CLA	C1D-ND	3.49	1.42	1.37
24	4	609	CHL	MG-NA	-3.49	1.98	2.06
24	7	607	CHL	OBD-CAD	3.49	1.28	1.22
25	q	613	CLA	C1D-ND	3.49	1.42	1.37
25	g	612	CLA	C4D-ND	-3.49	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	s	604	CLA	C4D-ND	-3.49	1.32	1.37
24	1	607	CHL	OBD-CAD	3.49	1.28	1.22
25	b	605	CLA	C4D-ND	-3.49	1.32	1.37
24	5	609	CHL	OBD-CAD	3.49	1.28	1.22
25	B	605	CLA	C4D-ND	-3.48	1.32	1.37
24	5	608	CHL	OBD-CAD	3.48	1.28	1.22
24	y	607	CHL	C3B-C2B	3.48	1.45	1.40
24	8	608	CHL	OBD-CAD	3.48	1.28	1.22
24	Y	607	CHL	C3B-C2B	3.48	1.45	1.40
24	S	607	CHL	OBD-CAD	3.48	1.28	1.22
25	2	602	CLA	C4D-ND	-3.48	1.32	1.37
25	7	610	CLA	C4D-ND	-3.48	1.32	1.37
25	1	610	CLA	C4D-ND	-3.48	1.32	1.37
25	N	614	CLA	C4D-ND	-3.48	1.32	1.37
24	N	601	CHL	CHD-C4C	3.48	1.47	1.39
24	s	606	CHL	OBD-CAD	3.48	1.28	1.22
25	y	610	CLA	C4D-ND	-3.47	1.32	1.37
25	S	612	CLA	C4D-ND	-3.46	1.32	1.37
25	c	511	CLA	C4D-ND	-3.46	1.32	1.37
24	1	609	CHL	CHD-C4C	3.46	1.47	1.39
25	S	614	CLA	C1D-ND	3.46	1.42	1.37
24	N	607	CHL	CHD-C1D	3.46	1.45	1.38
24	n	601	CHL	CHD-C4C	3.46	1.47	1.39
24	1	601	CHL	OBD-CAD	3.46	1.28	1.22
25	C	511	CLA	C4D-ND	-3.46	1.32	1.37
25	g	614	CLA	C4D-ND	-3.46	1.32	1.37
24	s	607	CHL	OBD-CAD	3.46	1.28	1.22
25	s	603	CLA	C1D-ND	3.45	1.42	1.37
25	6	612	CLA	C1D-ND	3.45	1.42	1.37
25	S	605	CLA	C4D-ND	-3.45	1.32	1.37
24	7	601	CHL	OBD-CAD	3.45	1.28	1.22
25	C	510	CLA	C4D-ND	-3.45	1.32	1.37
25	G	612	CLA	C4D-ND	-3.45	1.33	1.37
25	Y	602	CLA	C4D-ND	-3.45	1.33	1.37
24	7	605	CHL	OBD-CAD	3.45	1.28	1.22
24	R	606	CHL	CHD-C4C	3.45	1.47	1.39
25	3	604	CLA	C1D-ND	3.45	1.42	1.37
25	q	611	CLA	C1D-ND	3.45	1.42	1.37
25	g	611	CLA	C4D-ND	-3.44	1.33	1.37
25	N	614	CLA	C1D-ND	3.44	1.42	1.37
25	0	612	CLA	C1D-ND	3.44	1.42	1.37
25	y	602	CLA	C4D-ND	-3.44	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	606	CHL	OBD-CAD	3.44	1.28	1.22
25	5	611	CLA	C4D-ND	-3.44	1.33	1.37
24	N	606	CHL	OBD-CAD	3.44	1.28	1.22
24	1	605	CHL	OBD-CAD	3.44	1.28	1.22
25	Y	610	CLA	C4D-ND	-3.43	1.33	1.37
24	N	606	CHL	C3B-C2B	3.43	1.45	1.40
25	8	603	CLA	C1D-ND	3.43	1.42	1.37
24	y	606	CHL	C3B-C2B	3.43	1.45	1.40
24	g	607	CHL	CHD-C4C	3.43	1.47	1.39
25	s	605	CLA	C4D-ND	-3.42	1.33	1.37
25	s	614	CLA	C1D-ND	3.42	1.42	1.37
24	S	608	CHL	OBD-CAD	3.42	1.28	1.22
24	3	609	CHL	OBD-CAD	3.42	1.28	1.22
24	6	607	CHL	OBD-CAD	3.42	1.28	1.22
24	s	608	CHL	OBD-CAD	3.42	1.28	1.22
25	1	613	CLA	C1D-ND	3.42	1.42	1.37
24	Y	606	CHL	C3B-C2B	3.41	1.45	1.40
24	7	609	CHL	CHD-C4C	3.41	1.47	1.39
25	s	612	CLA	C4D-ND	-3.41	1.33	1.37
25	1	604	CLA	C4D-ND	-3.41	1.33	1.37
25	1	604	CLA	C1D-ND	3.41	1.42	1.37
24	1	608	CHL	OBD-CAD	3.41	1.28	1.22
25	G	614	CLA	C4D-ND	-3.41	1.33	1.37
25	3	602	CLA	C4D-ND	-3.41	1.33	1.37
24	N	609	CHL	CHD-C4C	3.40	1.47	1.39
24	r	606	CHL	CHD-C4C	3.40	1.47	1.39
25	b	602	CLA	C4D-ND	-3.40	1.33	1.37
25	r	611	CLA	C4D-ND	-3.40	1.33	1.37
25	R	611	CLA	C4D-ND	-3.39	1.33	1.37
24	6	601	CHL	OBD-CAD	3.39	1.28	1.22
25	c	511	CLA	C1D-ND	3.39	1.42	1.37
25	n	604	CLA	CMB-C2B	-3.39	1.44	1.51
25	C	511	CLA	C1D-ND	3.39	1.41	1.37
24	1	606	CHL	OBD-CAD	3.39	1.28	1.22
25	N	604	CLA	CMB-C2B	-3.38	1.44	1.51
25	1	603	CLA	C1D-ND	3.38	1.41	1.37
25	3	603	CLA	C1D-ND	3.38	1.41	1.37
24	n	606	CHL	OBD-CAD	3.38	1.28	1.22
24	g	607	CHL	OBD-CAD	3.38	1.28	1.22
25	S	602	CLA	C1D-ND	3.38	1.41	1.37
25	R	613	CLA	C1D-ND	3.38	1.41	1.37
25	2	611	CLA	C4D-ND	-3.38	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	604	CLA	C4D-ND	-3.38	1.33	1.37
25	r	604	CLA	C4D-ND	-3.38	1.33	1.37
25	C	503	CLA	C1D-ND	3.37	1.41	1.37
24	G	607	CHL	OBD-CAD	3.37	1.28	1.22
25	5	611	CLA	C1D-ND	3.37	1.41	1.37
25	4	611	CLA	C1D-ND	3.37	1.41	1.37
25	9	603	CLA	C4D-ND	-3.37	1.33	1.37
25	9	602	CLA	C1D-ND	3.37	1.41	1.37
25	B	602	CLA	C4D-ND	-3.37	1.33	1.37
25	8	602	CLA	C4D-ND	-3.37	1.33	1.37
25	n	610	CLA	C1D-ND	3.37	1.41	1.37
25	7	603	CLA	C1D-ND	3.37	1.41	1.37
25	3	603	CLA	C4D-ND	-3.37	1.33	1.37
25	g	604	CLA	C1D-ND	3.37	1.41	1.37
24	Y	608	CHL	CHD-C1D	3.37	1.44	1.38
24	y	608	CHL	CHD-C1D	3.37	1.44	1.38
25	N	604	CLA	C1D-ND	3.36	1.41	1.37
25	b	604	CLA	C3B-C2B	-3.36	1.35	1.40
24	N	605	CHL	OBD-CAD	3.36	1.28	1.22
24	8	607	CHL	CHD-C4C	3.36	1.46	1.39
25	b	608	CLA	C1D-ND	3.36	1.41	1.37
24	n	605	CHL	OBD-CAD	3.36	1.28	1.22
25	n	612	CLA	C1D-ND	3.35	1.41	1.37
24	N	608	CHL	CHD-C4C	3.35	1.46	1.39
24	G	607	CHL	CHD-C4C	3.35	1.46	1.39
25	8	603	CLA	C4D-ND	-3.35	1.33	1.37
25	4	602	CLA	C4D-ND	-3.35	1.33	1.37
25	2	611	CLA	C1D-ND	3.35	1.41	1.37
25	B	608	CLA	C1D-ND	3.34	1.41	1.37
25	N	610	CLA	C1D-ND	3.34	1.41	1.37
25	N	613	CLA	C1D-ND	3.34	1.41	1.37
25	r	616	CLA	C1D-ND	3.34	1.41	1.37
25	g	610	CLA	C1D-ND	3.34	1.41	1.37
25	0	604	CLA	C4D-ND	-3.34	1.33	1.37
25	s	602	CLA	C1D-ND	3.34	1.41	1.37
25	Y	604	CLA	C4D-ND	-3.34	1.33	1.37
25	p	611	CLA	C4D-ND	-3.34	1.33	1.37
25	c	503	CLA	C1D-ND	3.34	1.41	1.37
25	4	603	CLA	C1D-ND	3.34	1.41	1.37
25	R	616	CLA	C1D-ND	3.34	1.41	1.37
25	B	604	CLA	C3B-C2B	-3.33	1.35	1.40
25	S	603	CLA	C4D-ND	-3.33	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	502	CLA	C1D-ND	3.33	1.41	1.37
25	9	603	CLA	C1D-ND	3.33	1.41	1.37
25	R	604	CLA	C4D-ND	-3.33	1.33	1.37
24	q	609	CHL	OBD-CAD	3.33	1.28	1.22
25	n	604	CLA	C1D-ND	3.33	1.41	1.37
24	7	606	CHL	OBD-CAD	3.33	1.28	1.22
25	G	610	CLA	C1D-ND	3.33	1.41	1.37
25	6	604	CLA	C4D-ND	-3.32	1.33	1.37
25	6	611	CLA	C4D-ND	-3.32	1.33	1.37
25	1	613	CLA	C4D-ND	-3.32	1.33	1.37
24	n	608	CHL	CHD-C4C	3.32	1.46	1.39
24	R	608	CHL	CHD-C4C	3.32	1.46	1.39
24	r	608	CHL	CHD-C4C	3.32	1.46	1.39
25	n	613	CLA	C1D-ND	3.32	1.41	1.37
25	N	612	CLA	C1D-ND	3.32	1.41	1.37
25	7	612	CLA	C1D-ND	3.31	1.41	1.37
25	1	602	CLA	C4D-ND	-3.31	1.33	1.37
25	0	611	CLA	C4D-ND	-3.31	1.33	1.37
25	S	612	CLA	C1D-ND	3.31	1.41	1.37
25	9	611	CLA	C1D-ND	3.31	1.41	1.37
25	r	613	CLA	C1D-ND	3.31	1.41	1.37
24	9	608	CHL	OBD-CAD	3.31	1.28	1.22
25	1	611	CLA	C1D-ND	3.30	1.41	1.37
25	2	603	CLA	C1D-ND	3.30	1.41	1.37
25	2	610	CLA	C4D-ND	-3.30	1.33	1.37
25	y	604	CLA	C4D-ND	-3.30	1.33	1.37
25	9	613	CLA	C1D-ND	3.30	1.41	1.37
24	g	601	CHL	OBD-CAD	3.30	1.28	1.22
25	C	502	CLA	C1D-ND	3.30	1.41	1.37
25	1	612	CLA	C1D-ND	3.30	1.41	1.37
24	3	607	CHL	CHD-C4C	3.30	1.46	1.39
24	G	601	CHL	OBD-CAD	3.29	1.28	1.22
25	2	603	CLA	C4D-ND	-3.29	1.33	1.37
24	N	601	CHL	OBD-CAD	3.29	1.28	1.22
25	5	613	CLA	C4D-ND	-3.29	1.33	1.37
25	7	612	CLA	C4D-ND	-3.29	1.33	1.37
25	r	601	CLA	C4D-ND	-3.29	1.33	1.37
24	p	605	CHL	C1D-C2D	3.29	1.51	1.45
24	Y	605	CHL	OBD-CAD	3.29	1.28	1.22
24	y	605	CHL	OBD-CAD	3.29	1.28	1.22
25	7	610	CLA	C1D-ND	3.29	1.41	1.37
25	b	602	CLA	C1D-ND	3.29	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	q	609	CHL	C1D-C2D	3.28	1.51	1.45
25	s	603	CLA	C4D-ND	-3.28	1.33	1.37
25	C	508	CLA	CMC-C2C	-3.27	1.43	1.50
25	G	604	CLA	C1D-ND	3.27	1.41	1.37
24	n	601	CHL	OBD-CAD	3.27	1.28	1.22
25	r	612	CLA	C4D-ND	-3.27	1.33	1.37
24	R	608	CHL	OBD-CAD	3.27	1.28	1.22
24	7	608	CHL	OBD-CAD	3.27	1.28	1.22
25	7	611	CLA	C1D-ND	3.27	1.41	1.37
25	4	613	CLA	C4D-ND	-3.27	1.33	1.37
25	1	604	CLA	C3B-C2B	-3.27	1.35	1.40
25	4	611	CLA	C4D-ND	-3.27	1.33	1.37
25	7	602	CLA	C4D-ND	-3.27	1.33	1.37
24	q	608	CHL	MG-NA	-3.27	1.98	2.06
25	n	612	CLA	C4D-ND	-3.27	1.33	1.37
24	q	601	CHL	OBD-CAD	3.26	1.28	1.22
25	G	614	CLA	C1D-ND	3.26	1.41	1.37
25	9	614	CLA	C4D-ND	-3.26	1.33	1.37
25	q	613	CLA	C4D-ND	-3.26	1.33	1.37
25	2	614	CLA	C4D-ND	-3.26	1.33	1.37
25	s	612	CLA	C1D-ND	3.26	1.41	1.37
25	2	613	CLA	C1D-ND	3.25	1.41	1.37
25	R	601	CLA	C4D-ND	-3.25	1.33	1.37
25	7	604	CLA	C1D-ND	3.25	1.41	1.37
25	6	613	CLA	C4D-ND	-3.25	1.33	1.37
25	N	612	CLA	C4D-ND	-3.25	1.33	1.37
25	0	604	CLA	C1D-ND	3.25	1.41	1.37
24	r	608	CHL	OBD-CAD	3.25	1.28	1.22
24	5	606	CHL	OBD-CAD	3.24	1.28	1.22
25	1	612	CLA	C4D-ND	-3.24	1.33	1.37
25	B	602	CLA	C1D-ND	3.24	1.41	1.37
25	q	611	CLA	C4D-ND	-3.24	1.33	1.37
24	y	609	CHL	CHD-C1D	3.24	1.44	1.38
25	B	612	CLA	CMC-C2C	-3.24	1.43	1.50
25	b	612	CLA	CMC-C2C	-3.24	1.43	1.50
25	9	611	CLA	C4D-ND	-3.24	1.33	1.37
25	7	613	CLA	C4D-ND	-3.23	1.33	1.37
24	Y	609	CHL	CHD-C1D	3.23	1.44	1.38
24	3	606	CHL	MG-NA	-3.23	1.98	2.06
25	g	614	CLA	C1D-ND	3.23	1.41	1.37
25	c	509	CLA	C1D-ND	3.23	1.41	1.37
25	c	508	CLA	CMC-C2C	-3.23	1.44	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	p	606	CHL	OBD-CAD	3.23	1.28	1.22
25	8	611	CLA	C4D-ND	-3.23	1.33	1.37
28	7	1623	NEX	C7-C8	-3.23	1.26	1.32
25	p	613	CLA	C4D-ND	-3.22	1.33	1.37
25	4	604	CLA	C4D-ND	-3.22	1.33	1.37
25	R	602	CLA	C1D-ND	3.22	1.41	1.37
25	b	617	CLA	C1D-ND	3.22	1.41	1.37
24	N	606	CHL	CHD-C4C	3.22	1.46	1.39
24	G	609	CHL	MG-NA	-3.21	1.98	2.06
24	n	607	CHL	CHD-C4C	3.21	1.46	1.39
25	6	603	CLA	C4D-ND	-3.21	1.33	1.37
25	R	612	CLA	C4D-ND	-3.21	1.33	1.37
25	0	602	CLA	C4D-ND	-3.21	1.33	1.37
24	s	601	CHL	OBD-CAD	3.21	1.28	1.22
24	Y	607	CHL	CHD-C4C	3.21	1.46	1.39
24	n	606	CHL	CHD-C4C	3.20	1.46	1.39
25	4	610	CLA	C4D-ND	-3.20	1.33	1.37
25	q	602	CLA	C4D-ND	-3.20	1.33	1.37
24	N	607	CHL	CHD-C4C	3.20	1.46	1.39
24	R	607	CHL	CHD-C4C	3.20	1.46	1.39
25	9	604	CLA	C4D-ND	-3.19	1.33	1.37
25	R	616	CLA	C4D-ND	-3.19	1.33	1.37
25	Y	614	CLA	C1D-ND	3.19	1.41	1.37
25	1	610	CLA	C1D-ND	3.19	1.41	1.37
24	8	606	CHL	MG-NA	-3.19	1.98	2.06
25	S	604	CLA	C1D-ND	3.19	1.41	1.37
25	s	604	CLA	C1D-ND	3.19	1.41	1.37
25	3	611	CLA	C4D-ND	-3.19	1.33	1.37
25	0	610	CLA	C1D-ND	3.19	1.41	1.37
25	r	604	CLA	C1D-ND	3.19	1.41	1.37
25	C	509	CLA	C1D-ND	3.19	1.41	1.37
25	r	602	CLA	C1D-ND	3.19	1.41	1.37
25	6	602	CLA	C4D-ND	-3.18	1.33	1.37
25	8	613	CLA	C4D-ND	-3.18	1.33	1.37
24	r	607	CHL	CHD-C4C	3.18	1.46	1.39
25	B	617	CLA	C1D-ND	3.18	1.41	1.37
25	r	616	CLA	C4D-ND	-3.18	1.33	1.37
25	3	602	CLA	C1D-ND	3.18	1.41	1.37
24	S	601	CHL	OBD-CAD	3.18	1.28	1.22
25	0	610	CLA	C4D-ND	-3.18	1.33	1.37
24	Y	601	CHL	OBD-CAD	3.18	1.28	1.22
25	0	603	CLA	C4D-ND	-3.18	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	9	610	CLA	C4D-ND	-3.18	1.33	1.37
25	8	602	CLA	C1D-ND	3.17	1.41	1.37
25	2	604	CLA	C4D-ND	-3.17	1.33	1.37
25	n	610	CLA	C4D-ND	-3.17	1.33	1.37
33	A	408	PHO	CAC-C3C	-3.17	1.46	1.52
33	a	408	PHO	CAC-C3C	-3.17	1.46	1.52
24	2	608	CHL	OBD-CAD	3.17	1.27	1.22
35	b	621	SQD	C6-S	-3.16	1.65	1.77
25	p	610	CLA	C4D-ND	-3.16	1.33	1.37
25	6	603	CLA	C1D-ND	3.16	1.41	1.37
28	s	1623	NEX	C7-C8	-3.16	1.26	1.32
25	n	611	CLA	C1D-ND	3.16	1.41	1.37
24	y	607	CHL	CHD-C4C	3.16	1.46	1.39
24	n	608	CHL	OBD-CAD	3.16	1.27	1.22
24	N	608	CHL	OBD-CAD	3.16	1.27	1.22
24	y	601	CHL	OBD-CAD	3.16	1.27	1.22
35	B	621	SQD	C6-S	-3.15	1.65	1.77
25	s	613	CLA	C1D-ND	3.15	1.41	1.37
24	8	609	CHL	CHD-C4C	3.15	1.46	1.39
24	9	609	CHL	C1D-C2D	3.15	1.51	1.45
24	g	609	CHL	MG-NA	-3.15	1.98	2.06
25	S	605	CLA	C1D-ND	3.15	1.41	1.37
24	q	605	CHL	C1D-C2D	3.15	1.51	1.45
25	3	613	CLA	C4D-ND	-3.15	1.33	1.37
24	R	606	CHL	C2C-C3C	3.15	1.43	1.36
24	0	608	CHL	OBD-CAD	3.15	1.27	1.22
25	R	612	CLA	C1D-ND	3.15	1.41	1.37
25	r	612	CLA	C1D-ND	3.15	1.41	1.37
24	y	601	CHL	C3B-C2B	3.15	1.44	1.40
25	s	611	CLA	C1D-ND	3.15	1.41	1.37
24	s	607	CHL	MG-NA	-3.15	1.98	2.06
24	S	607	CHL	MG-NA	-3.14	1.98	2.06
25	B	611	CLA	C3B-C2B	-3.14	1.36	1.40
25	0	603	CLA	C1D-ND	3.14	1.41	1.37
24	1	609	CHL	OBD-CAD	3.14	1.27	1.22
25	3	610	CLA	C4D-ND	-3.14	1.33	1.37
24	Y	601	CHL	C3B-C2B	3.14	1.44	1.40
25	8	612	CLA	C4D-ND	-3.14	1.33	1.37
25	q	610	CLA	C4D-ND	-3.14	1.33	1.37
25	N	611	CLA	C1D-ND	3.14	1.41	1.37
25	R	604	CLA	C1D-ND	3.13	1.41	1.37
24	y	606	CHL	CHD-C4C	3.13	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	y	608	CHL	OBD-CAD	3.13	1.27	1.22
25	r	610	CLA	C1D-ND	3.13	1.41	1.37
24	q	607	CHL	MG-NA	-3.13	1.98	2.06
25	C	512	CLA	C1D-ND	3.13	1.41	1.37
35	d	413	SQD	C6-S	-3.13	1.65	1.77
25	s	605	CLA	C1D-ND	3.13	1.41	1.37
25	y	614	CLA	C1D-ND	3.13	1.41	1.37
24	5	605	CHL	C1D-C2D	3.13	1.51	1.45
25	S	611	CLA	C1D-ND	3.13	1.41	1.37
25	b	611	CLA	C3B-C2B	-3.13	1.36	1.40
24	r	606	CHL	C2C-C3C	3.13	1.43	1.36
24	7	609	CHL	OBD-CAD	3.13	1.27	1.22
24	Y	606	CHL	CHD-C4C	3.12	1.46	1.39
25	0	614	CLA	C4D-ND	-3.12	1.33	1.37
25	8	610	CLA	C4D-ND	-3.12	1.33	1.37
25	r	604	CLA	CMB-C2B	-3.12	1.45	1.51
25	3	612	CLA	C4D-ND	-3.12	1.33	1.37
24	Y	608	CHL	CHD-C4C	3.12	1.46	1.39
25	6	610	CLA	C4D-ND	-3.12	1.33	1.37
25	p	603	CLA	C4D-ND	-3.12	1.33	1.37
25	S	613	CLA	C1D-ND	3.12	1.41	1.37
24	Y	608	CHL	OBD-CAD	3.12	1.27	1.22
24	4	607	CHL	MG-NA	-3.11	1.98	2.06
24	2	601	CHL	OBD-CAD	3.11	1.27	1.22
25	N	610	CLA	C4D-ND	-3.11	1.33	1.37
24	y	608	CHL	CHD-C4C	3.11	1.46	1.39
25	5	602	CLA	C4D-ND	-3.11	1.33	1.37
25	q	604	CLA	C4D-ND	-3.11	1.33	1.37
25	7	614	CLA	C4D-ND	-3.11	1.33	1.37
35	D	413	SQD	C6-S	-3.11	1.65	1.77
25	R	604	CLA	CMB-C2B	-3.10	1.45	1.51
25	b	613	CLA	C1D-ND	3.10	1.41	1.37
25	6	610	CLA	C1D-ND	3.10	1.41	1.37
24	4	605	CHL	C1D-C2D	3.10	1.51	1.45
25	6	614	CLA	C4D-ND	-3.10	1.33	1.37
24	8	605	CHL	MG-NA	-3.10	1.98	2.06
24	3	609	CHL	CHD-C4C	3.10	1.46	1.39
25	4	603	CLA	C4D-ND	-3.10	1.33	1.37
25	g	613	CLA	C1D-ND	3.09	1.41	1.37
25	p	604	CLA	C4D-ND	-3.09	1.33	1.37
24	n	609	CHL	MG-NA	-3.09	1.98	2.06
25	B	616	CLA	C1D-ND	3.09	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	N	605	CHL	MG-NA	-3.09	1.98	2.06
25	7	604	CLA	CMB-C2B	-3.09	1.45	1.51
25	5	603	CLA	C4D-ND	-3.09	1.33	1.37
25	Y	610	CLA	C1D-ND	3.09	1.41	1.37
24	G	606	CHL	OBD-CAD	3.09	1.27	1.22
24	2	609	CHL	C1D-C2D	3.08	1.51	1.45
24	7	608	CHL	CHD-C4C	3.08	1.46	1.39
24	Y	609	CHL	CHD-C4C	3.08	1.46	1.39
25	q	614	CLA	C4D-ND	-3.08	1.33	1.37
25	S	610	CLA	C1D-ND	3.08	1.41	1.37
25	B	604	CLA	CMB-C2B	-3.08	1.45	1.51
25	1	614	CLA	C4D-ND	-3.08	1.33	1.37
24	9	601	CHL	OBD-CAD	3.08	1.27	1.22
25	5	610	CLA	C4D-ND	-3.08	1.33	1.37
24	1	608	CHL	CHD-C4C	3.08	1.46	1.39
25	R	609	CLA	C1D-ND	3.07	1.41	1.37
25	r	609	CLA	C1D-ND	3.07	1.41	1.37
25	6	612	CLA	C4D-ND	-3.07	1.33	1.37
24	3	605	CHL	MG-NA	-3.07	1.99	2.06
25	4	614	CLA	C4D-ND	-3.07	1.33	1.37
24	n	607	CHL	OBD-CAD	3.07	1.27	1.22
25	S	612	CLA	C3B-C2B	-3.06	1.36	1.40
25	R	610	CLA	C1D-ND	3.06	1.41	1.37
24	y	607	CHL	OBD-CAD	3.06	1.27	1.22
25	b	604	CLA	CMB-C2B	-3.06	1.45	1.51
24	N	607	CHL	OBD-CAD	3.06	1.27	1.22
39	d	405	PL9	C53-C6	-3.06	1.44	1.50
39	D	405	PL9	C53-C6	-3.06	1.44	1.50
28	N	1623	NEX	C7-C8	-3.05	1.26	1.32
24	Y	607	CHL	OBD-CAD	3.05	1.27	1.22
25	s	610	CLA	C1D-ND	3.05	1.41	1.37
24	N	609	CHL	MG-NA	-3.05	1.99	2.06
25	b	611	CLA	C1D-ND	3.05	1.41	1.37
25	d	403	CLA	C1D-ND	3.05	1.41	1.37
25	B	607	CLA	C1D-ND	3.05	1.41	1.37
24	0	601	CHL	MG-NA	-3.04	1.99	2.06
25	c	506	CLA	CMB-C2B	-3.04	1.45	1.51
25	c	512	CLA	C1D-ND	3.04	1.41	1.37
25	G	613	CLA	C1D-ND	3.04	1.41	1.37
24	y	609	CHL	CHD-C4C	3.04	1.46	1.39
25	B	613	CLA	C1D-ND	3.04	1.41	1.37
25	5	611	CLA	CHC-C1C	3.04	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	n	605	CHL	MG-NA	-3.04	1.99	2.06
25	B	611	CLA	C1D-ND	3.04	1.41	1.37
25	7	604	CLA	C3B-C2B	-3.04	1.36	1.40
25	0	612	CLA	C4D-ND	-3.03	1.33	1.37
39	D	405	PL9	C41-C39	-3.03	1.45	1.51
24	R	607	CHL	MG-NA	-3.03	1.99	2.06
24	1	607	CHL	MG-NA	-3.03	1.99	2.06
25	1	604	CLA	CMB-C2B	-3.02	1.45	1.51
39	d	405	PL9	C41-C39	-3.02	1.45	1.51
25	s	612	CLA	C3B-C2B	-3.02	1.36	1.40
25	y	610	CLA	C1D-ND	3.02	1.41	1.37
24	4	609	CHL	C3D-C2D	3.02	1.47	1.39
24	r	607	CHL	MG-NA	-3.02	1.99	2.06
25	p	602	CLA	CHC-C1C	3.02	1.42	1.35
25	1	602	CLA	C1D-ND	3.02	1.41	1.37
25	5	602	CLA	CHC-C1C	3.01	1.42	1.35
25	q	603	CLA	C4D-ND	-3.01	1.33	1.37
25	8	614	CLA	C4D-ND	-3.01	1.33	1.37
24	g	606	CHL	OBD-CAD	3.01	1.27	1.22
25	Y	611	CLA	C3B-C2B	-3.01	1.36	1.40
24	3	605	CHL	C1D-C2D	3.01	1.51	1.45
25	y	602	CLA	C1D-ND	3.01	1.41	1.37
25	y	612	CLA	C3B-C2B	-3.01	1.36	1.40
25	c	507	CLA	C1D-ND	3.00	1.41	1.37
24	8	605	CHL	C1D-C2D	3.00	1.51	1.45
28	4	1623	NEX	C7-C8	-3.00	1.27	1.32
25	6	614	CLA	CHC-C1C	3.00	1.42	1.35
25	C	507	CLA	C1D-ND	3.00	1.41	1.37
25	B	605	CLA	CMB-C2B	-3.00	1.45	1.51
25	b	616	CLA	C1D-ND	3.00	1.41	1.37
25	p	602	CLA	C4D-ND	-2.99	1.33	1.37
24	1	601	CHL	C1D-C2D	2.99	1.51	1.45
24	5	609	CHL	C1D-C2D	2.99	1.51	1.45
24	G	609	CHL	OBD-CAD	2.99	1.27	1.22
24	R	608	CHL	MG-NA	-2.99	1.99	2.06
25	G	602	CLA	C1D-ND	2.99	1.41	1.37
25	Y	602	CLA	C1D-ND	2.99	1.41	1.37
24	q	609	CHL	C3D-C2D	2.99	1.47	1.39
24	p	609	CHL	C1D-C2D	2.99	1.51	1.45
25	R	611	CLA	C1D-ND	2.98	1.41	1.37
24	4	609	CHL	C1D-C2D	2.98	1.51	1.45
25	B	610	CLA	CMB-C2B	-2.98	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	b	605	CLA	C1D-ND	2.98	1.41	1.37
25	y	611	CLA	C3B-C2B	-2.98	1.36	1.40
25	q	602	CLA	CHC-C1C	2.98	1.42	1.35
25	b	610	CLA	CMB-C2B	-2.98	1.45	1.51
25	D	403	CLA	C1D-ND	2.98	1.41	1.37
25	a	405	CLA	C1D-ND	2.98	1.41	1.37
25	C	506	CLA	CMB-C2B	-2.98	1.45	1.51
25	7	602	CLA	C1D-ND	2.98	1.41	1.37
24	7	601	CHL	C1D-C2D	2.98	1.51	1.45
25	0	614	CLA	CHC-C1C	2.98	1.42	1.35
25	c	504	CLA	C1D-ND	2.98	1.41	1.37
25	5	604	CLA	C4D-ND	-2.98	1.33	1.37
40	f	101	HEM	CAB-C3B	2.97	1.55	1.47
25	G	612	CLA	C1D-ND	2.97	1.41	1.37
39	D	405	PL9	C21-C19	-2.97	1.45	1.51
24	7	607	CHL	MG-NA	-2.97	1.99	2.06
24	7	606	CHL	MG-NA	-2.97	1.99	2.06
25	b	605	CLA	CMB-C2B	-2.97	1.45	1.51
25	A	405	CLA	C1D-ND	2.97	1.41	1.37
24	r	608	CHL	MG-NA	-2.97	1.99	2.06
39	d	405	PL9	C21-C19	-2.96	1.45	1.51
25	A	410	CLA	C1D-ND	2.96	1.41	1.37
39	D	405	PL9	C52-C5	-2.96	1.44	1.50
28	0	1623	NEX	C7-C8	-2.96	1.27	1.32
24	1	606	CHL	MG-NA	-2.96	1.99	2.06
25	3	614	CLA	C4D-ND	-2.96	1.33	1.37
25	B	606	CLA	C1D-ND	2.96	1.41	1.37
25	4	614	CLA	CHC-C1C	2.96	1.42	1.35
24	6	608	CHL	OBD-CAD	2.96	1.27	1.22
25	2	604	CLA	CHC-C1C	2.96	1.42	1.35
25	2	602	CLA	C1D-ND	2.96	1.41	1.37
24	3	606	CHL	C1D-C2D	2.96	1.51	1.45
25	N	603	CLA	C1D-ND	2.95	1.41	1.37
25	8	614	CLA	CHC-C1C	2.95	1.42	1.35
25	C	504	CLA	C1D-ND	2.95	1.41	1.37
25	7	614	CLA	CHC-C1C	2.95	1.42	1.35
24	n	607	CHL	MG-NA	-2.95	1.99	2.06
28	q	1623	NEX	C7-C8	-2.95	1.27	1.32
25	1	614	CLA	CHC-C1C	2.95	1.42	1.35
24	8	606	CHL	C1D-C2D	2.95	1.51	1.45
25	S	602	CLA	CHC-C1C	2.95	1.42	1.35
25	0	602	CLA	CHC-C1C	2.95	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	d	405	PL9	C52-C5	-2.94	1.44	1.50
25	B	605	CLA	C1D-ND	2.94	1.41	1.37
25	4	610	CLA	CHC-C1C	2.94	1.42	1.35
24	q	606	CHL	C3D-C2D	2.94	1.47	1.39
25	3	614	CLA	CHC-C1C	2.94	1.42	1.35
25	8	602	CLA	CHC-C1C	2.94	1.42	1.35
25	S	609	CLA	C4D-ND	-2.94	1.33	1.37
24	g	609	CHL	OBD-CAD	2.94	1.27	1.22
25	a	410	CLA	C1D-ND	2.94	1.41	1.37
25	B	611	CLA	CMB-C2B	-2.94	1.45	1.51
40	F	101	HEM	CAB-C3B	2.94	1.55	1.47
24	r	607	CHL	OBD-CAD	2.94	1.27	1.22
25	c	506	CLA	C1D-ND	2.94	1.41	1.37
25	b	611	CLA	CMB-C2B	-2.94	1.45	1.51
24	g	608	CHL	MG-NA	-2.93	1.99	2.06
25	6	602	CLA	CHC-C1C	2.93	1.42	1.35
25	9	610	CLA	CHC-C1C	2.93	1.42	1.35
25	b	607	CLA	C1D-ND	2.93	1.41	1.37
25	c	510	CLA	C1D-ND	2.93	1.41	1.37
25	n	603	CLA	C1D-ND	2.93	1.41	1.37
25	3	602	CLA	CHC-C1C	2.93	1.42	1.35
25	4	602	CLA	CHC-C1C	2.93	1.42	1.35
25	C	505	CLA	CMD-C2D	-2.93	1.44	1.50
24	q	608	CHL	C3D-C2D	2.93	1.47	1.39
25	5	612	CLA	C4D-ND	-2.93	1.33	1.37
25	b	606	CLA	C1D-ND	2.93	1.41	1.37
25	c	505	CLA	CMD-C2D	-2.93	1.44	1.50
28	2	1623	NEX	C7-C8	-2.93	1.27	1.32
25	8	610	CLA	CHC-C1C	2.93	1.42	1.35
25	Y	612	CLA	C3B-C2B	-2.93	1.36	1.40
25	S	611	CLA	CHC-C1C	2.92	1.42	1.35
25	s	602	CLA	CHC-C1C	2.92	1.42	1.35
24	n	609	CHL	OBD-CAD	2.92	1.27	1.22
24	G	608	CHL	MG-NA	-2.92	1.99	2.06
24	4	607	CHL	C1D-C2D	2.92	1.51	1.45
25	c	506	CLA	C3B-C2B	-2.92	1.36	1.40
25	C	513	CLA	C1D-ND	2.92	1.41	1.37
24	q	606	CHL	C1D-C2D	2.92	1.51	1.45
25	S	610	CLA	CHC-C1C	2.92	1.42	1.35
25	r	611	CLA	C1D-ND	2.91	1.41	1.37
25	G	602	CLA	CHC-C1C	2.91	1.42	1.35
24	p	605	CHL	MG-NA	-2.91	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	606	CHL	OBD-CAD	2.91	1.27	1.22
25	s	610	CLA	CHC-C1C	2.91	1.42	1.35
24	p	606	CHL	C1D-C2D	2.91	1.51	1.45
25	q	614	CLA	CHC-C1C	2.91	1.42	1.35
25	s	609	CLA	C4D-ND	-2.91	1.33	1.37
25	c	513	CLA	C1D-ND	2.91	1.41	1.37
24	8	607	CHL	MG-NA	-2.90	1.99	2.06
24	y	609	CHL	C1C-NC	-2.90	1.33	1.37
25	C	506	CLA	C3B-C2B	-2.90	1.36	1.40
25	D	402	CLA	CMD-C2D	-2.90	1.44	1.50
25	d	402	CLA	CMD-C2D	-2.90	1.44	1.50
28	Y	1623	NEX	C7-C8	-2.90	1.27	1.32
24	0	606	CHL	MG-NA	-2.90	1.99	2.06
25	y	613	CLA	C1D-ND	2.90	1.41	1.37
24	y	606	CHL	OBD-CAD	2.90	1.27	1.22
25	9	604	CLA	CHC-C1C	2.90	1.42	1.35
24	R	607	CHL	OBD-CAD	2.90	1.27	1.22
25	B	615	CLA	CMB-C2B	-2.90	1.45	1.51
25	b	615	CLA	CMB-C2B	-2.90	1.45	1.51
25	q	610	CLA	CHC-C1C	2.89	1.42	1.35
25	3	611	CLA	CHC-C1C	2.89	1.42	1.35
25	y	611	CLA	CMB-C2B	-2.89	1.45	1.51
25	g	602	CLA	CHC-C1C	2.89	1.42	1.35
25	N	603	CLA	CMB-C2B	-2.89	1.45	1.51
25	s	611	CLA	CHC-C1C	2.89	1.42	1.35
25	Y	613	CLA	C1D-ND	2.89	1.41	1.37
24	5	601	CHL	C1D-C2D	2.89	1.51	1.45
25	Y	611	CLA	CMB-C2B	-2.89	1.45	1.51
25	Y	613	CLA	CMB-C2B	-2.89	1.45	1.51
25	C	508	CLA	CHC-C1C	2.89	1.42	1.35
25	B	606	CLA	CMB-C2B	-2.89	1.45	1.51
24	Y	609	CHL	C1C-NC	-2.88	1.33	1.37
25	g	612	CLA	C1D-ND	2.88	1.41	1.37
25	9	614	CLA	CHC-C1C	2.88	1.42	1.35
25	Y	603	CLA	CMB-C2B	-2.88	1.45	1.51
25	g	602	CLA	C1D-ND	2.88	1.41	1.37
24	N	607	CHL	MG-NA	-2.88	1.99	2.06
25	g	603	CLA	CMB-C2B	-2.88	1.45	1.51
39	D	405	PL9	C46-C44	-2.88	1.45	1.51
25	C	501	CLA	CMB-C2B	-2.87	1.45	1.51
25	p	612	CLA	C4D-ND	-2.87	1.33	1.37
25	p	614	CLA	C4D-ND	-2.87	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
28	1	1623	NEX	C7-C8	-2.87	1.27	1.32
24	2	605	CHL	C1D-C2D	2.87	1.51	1.45
25	N	602	CLA	CHC-C1C	2.87	1.42	1.35
28	y	1623	NEX	C7-C8	-2.87	1.27	1.32
25	p	611	CLA	CHC-C1C	2.87	1.42	1.35
25	n	602	CLA	CHC-C1C	2.87	1.42	1.35
25	y	613	CLA	CMB-C2B	-2.87	1.45	1.51
25	3	610	CLA	CHC-C1C	2.87	1.42	1.35
25	y	603	CLA	CMB-C2B	-2.87	1.45	1.51
24	y	609	CHL	MG-NA	-2.87	1.99	2.06
25	d	402	CLA	CMB-C2B	-2.86	1.45	1.51
25	N	602	CLA	C1D-ND	2.86	1.41	1.37
24	N	609	CHL	OBD-CAD	2.86	1.27	1.22
25	B	617	CLA	CMB-C2B	-2.86	1.45	1.51
25	4	611	CLA	CHC-C1C	2.86	1.42	1.35
24	p	609	CHL	C4C-C3C	2.86	1.50	1.45
25	s	604	CLA	CMB-C2B	-2.86	1.45	1.51
25	5	610	CLA	CHC-C1C	2.86	1.42	1.35
25	n	602	CLA	C1D-ND	2.86	1.41	1.37
28	g	1623	NEX	C7-C8	-2.86	1.27	1.32
25	p	614	CLA	CHC-C1C	2.86	1.42	1.35
25	p	610	CLA	CHC-C1C	2.86	1.42	1.35
24	2	607	CHL	MG-NA	-2.86	1.99	2.06
25	0	612	CLA	CHC-C1C	2.86	1.42	1.35
24	q	607	CHL	C1D-C2D	2.86	1.51	1.45
25	B	612	CLA	CMB-C2B	-2.86	1.45	1.51
25	8	611	CLA	CHC-C1C	2.86	1.42	1.35
24	9	605	CHL	C1D-C2D	2.86	1.51	1.45
25	2	610	CLA	CHC-C1C	2.86	1.42	1.35
25	5	614	CLA	CHC-C1C	2.86	1.42	1.35
25	B	612	CLA	C1D-ND	2.86	1.41	1.37
25	C	506	CLA	C1D-ND	2.86	1.41	1.37
25	b	612	CLA	C1D-ND	2.86	1.41	1.37
28	S	1623	NEX	C7-C8	-2.85	1.27	1.32
25	D	402	CLA	CMB-C2B	-2.85	1.45	1.51
25	a	405	CLA	CMB-C2B	-2.85	1.45	1.51
25	8	604	CLA	CHC-C1C	2.85	1.42	1.35
25	g	604	CLA	CHC-C1C	2.85	1.42	1.35
25	B	610	CLA	C1D-ND	2.85	1.41	1.37
25	c	508	CLA	CHC-C1C	2.85	1.42	1.35
25	G	603	CLA	CMB-C2B	-2.85	1.45	1.51
25	n	603	CLA	CMB-C2B	-2.85	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	604	CLA	CHC-C1C	2.85	1.42	1.35
24	3	607	CHL	MG-NA	-2.85	1.99	2.06
25	R	603	CLA	CMB-C2B	-2.85	1.45	1.51
25	r	603	CLA	CMB-C2B	-2.85	1.45	1.51
25	2	614	CLA	CHC-C1C	2.85	1.42	1.35
25	5	614	CLA	C4D-ND	-2.85	1.33	1.37
25	c	508	CLA	CMB-C2B	-2.85	1.45	1.51
25	6	612	CLA	CHC-C1C	2.85	1.42	1.35
25	p	612	CLA	CHC-C1C	2.85	1.42	1.35
25	7	612	CLA	CHC-C1C	2.85	1.42	1.35
28	R	623	NEX	C7-C8	-2.85	1.27	1.32
25	2	612	CLA	C4D-ND	-2.84	1.33	1.37
25	1	602	CLA	CHC-C1C	2.84	1.42	1.35
25	b	612	CLA	CMB-C2B	-2.84	1.45	1.51
25	N	612	CLA	C3B-C2B	-2.84	1.36	1.40
24	s	601	CHL	C1D-C2D	2.84	1.50	1.45
39	d	405	PL9	C46-C44	-2.84	1.45	1.51
25	A	405	CLA	CMB-C2B	-2.84	1.45	1.51
25	C	501	CLA	C1D-ND	2.84	1.41	1.37
24	S	601	CHL	C1D-C2D	2.84	1.50	1.45
24	6	607	CHL	MG-NA	-2.84	1.99	2.06
24	q	606	CHL	MG-NA	-2.84	1.99	2.06
25	c	512	CLA	CHC-C1C	2.84	1.42	1.35
24	Y	609	CHL	MG-NA	-2.84	1.99	2.06
25	c	501	CLA	CMB-C2B	-2.84	1.45	1.51
25	y	603	CLA	C1D-ND	2.84	1.41	1.37
24	9	609	CHL	C4C-C3C	2.83	1.49	1.45
24	6	606	CHL	MG-NA	-2.83	1.99	2.06
25	s	614	CLA	CHC-C1C	2.83	1.42	1.35
24	0	606	CHL	C1D-C2D	2.83	1.50	1.45
25	c	510	CLA	CHC-C1C	2.83	1.42	1.35
24	4	606	CHL	C3D-C2D	2.83	1.46	1.39
25	Y	610	CLA	CHC-C1C	2.83	1.42	1.35
25	C	510	CLA	CHC-C1C	2.83	1.42	1.35
33	A	409	PHO	CAC-C3C	-2.83	1.47	1.52
25	n	610	CLA	CHC-C1C	2.83	1.42	1.35
25	b	606	CLA	CMB-C2B	-2.83	1.45	1.51
24	1	605	CHL	MG-NA	-2.83	1.99	2.06
25	1	612	CLA	CHC-C1C	2.82	1.42	1.35
24	Y	609	CHL	OBD-CAD	2.82	1.27	1.22
24	p	606	CHL	MG-NA	-2.82	1.99	2.06
24	y	601	CHL	MG-NA	-2.82	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	613	CLA	CHC-C1C	2.82	1.42	1.35
25	7	602	CLA	CHC-C1C	2.82	1.42	1.35
24	y	609	CHL	OBD-CAD	2.82	1.27	1.22
28	9	1623	NEX	C7-C8	-2.82	1.27	1.32
25	b	617	CLA	CMB-C2B	-2.82	1.45	1.51
25	1	603	CLA	C3B-C2B	-2.82	1.36	1.40
25	B	602	CLA	C3B-C2B	-2.82	1.36	1.40
25	6	604	CLA	CMB-C2B	-2.82	1.45	1.51
28	G	1623	NEX	C7-C8	-2.82	1.27	1.32
25	C	510	CLA	C1D-ND	2.82	1.41	1.37
25	Y	603	CLA	C1D-ND	2.82	1.41	1.37
25	G	604	CLA	CHC-C1C	2.82	1.42	1.35
25	S	604	CLA	CMB-C2B	-2.82	1.45	1.51
25	S	614	CLA	CHC-C1C	2.81	1.42	1.35
25	q	603	CLA	CHC-C1C	2.81	1.42	1.35
25	9	612	CLA	C4D-ND	-2.81	1.33	1.37
24	q	608	CHL	C1D-C2D	2.81	1.50	1.45
25	1	603	CLA	CMB-C2B	-2.81	1.45	1.51
25	c	508	CLA	C1D-ND	2.81	1.41	1.37
24	8	605	CHL	C3D-C2D	2.81	1.46	1.39
25	0	611	CLA	CHC-C1C	2.81	1.42	1.35
24	3	605	CHL	C3D-C2D	2.81	1.46	1.39
25	C	504	CLA	CMB-C2B	-2.81	1.45	1.51
25	A	407	CLA	C1D-ND	2.81	1.41	1.37
24	y	606	CHL	MG-NA	-2.81	1.99	2.06
24	9	605	CHL	C3D-C2D	2.81	1.46	1.39
24	4	606	CHL	C1D-C2D	2.81	1.50	1.45
25	n	612	CLA	CHC-C1C	2.81	1.42	1.35
25	6	613	CLA	CHC-C1C	2.80	1.42	1.35
25	5	612	CLA	CHC-C1C	2.80	1.42	1.35
24	5	605	CHL	MG-NA	-2.80	1.99	2.06
25	D	402	CLA	CHC-C1C	2.80	1.42	1.35
24	Y	607	CHL	MG-NA	-2.80	1.99	2.06
25	0	613	CLA	C4D-ND	-2.80	1.33	1.37
25	6	610	CLA	CHC-C1C	2.80	1.42	1.35
24	4	608	CHL	C1D-C2D	2.80	1.50	1.45
25	B	616	CLA	CMB-C2B	-2.80	1.45	1.51
25	c	504	CLA	CMB-C2B	-2.80	1.45	1.51
25	b	603	CLA	C1D-ND	2.80	1.41	1.37
33	a	409	PHO	CAC-C3C	-2.80	1.47	1.52
25	N	612	CLA	CHC-C1C	2.80	1.42	1.35
25	C	508	CLA	CMB-C2B	-2.80	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	508	CLA	C1D-ND	2.80	1.41	1.37
24	6	601	CHL	MG-NA	-2.80	1.99	2.06
25	a	405	CLA	CHC-C1C	2.79	1.42	1.35
24	9	607	CHL	C1D-C2D	2.79	1.50	1.45
25	y	614	CLA	CHC-C1C	2.79	1.42	1.35
24	4	601	CHL	MG-NA	-2.79	1.99	2.06
25	0	610	CLA	CHC-C1C	2.79	1.42	1.35
24	n	606	CHL	MG-NA	-2.79	1.99	2.06
24	p	601	CHL	C1D-C2D	2.79	1.50	1.45
25	n	612	CLA	C3B-C2B	-2.79	1.36	1.40
25	a	407	CLA	C1D-ND	2.79	1.41	1.37
25	N	610	CLA	CHC-C1C	2.79	1.42	1.35
24	7	605	CHL	MG-NA	-2.79	1.99	2.06
25	q	611	CLA	CHC-C1C	2.78	1.42	1.35
25	6	604	CLA	CHC-C1C	2.78	1.42	1.35
25	5	603	CLA	CHC-C1C	2.78	1.42	1.35
25	B	608	CLA	CMB-C2B	-2.78	1.45	1.51
25	B	603	CLA	C1D-ND	2.78	1.41	1.37
28	p	1623	NEX	C7-C8	-2.78	1.27	1.32
25	B	614	CLA	CMB-C2B	-2.78	1.45	1.51
24	G	605	CHL	C1D-C2D	2.78	1.50	1.45
25	n	604	CLA	C3B-C2B	-2.78	1.36	1.40
25	b	608	CLA	CMB-C2B	-2.78	1.45	1.51
25	C	511	CLA	CMB-C2B	-2.78	1.45	1.51
24	y	607	CHL	MG-NA	-2.78	1.99	2.06
24	R	606	CHL	MG-NA	-2.78	1.99	2.06
24	r	606	CHL	MG-NA	-2.78	1.99	2.06
25	y	612	CLA	C1D-ND	2.78	1.41	1.37
25	6	611	CLA	CHC-C1C	2.78	1.42	1.35
25	N	610	CLA	CMB-C2B	-2.78	1.45	1.51
25	R	609	CLA	CMB-C2B	-2.78	1.45	1.51
25	A	405	CLA	CHC-C1C	2.78	1.42	1.35
25	7	603	CLA	CMB-C2B	-2.77	1.45	1.51
25	0	604	CLA	CMB-C2B	-2.77	1.45	1.51
24	9	607	CHL	MG-NA	-2.77	1.99	2.06
24	2	607	CHL	C1D-C2D	2.77	1.50	1.45
25	d	402	CLA	CHC-C1C	2.77	1.42	1.35
25	N	604	CLA	C3B-C2B	-2.77	1.36	1.40
25	y	613	CLA	C3B-C2B	-2.77	1.36	1.40
24	N	606	CHL	MG-NA	-2.77	1.99	2.06
24	5	609	CHL	C4C-C3C	2.77	1.49	1.45
24	4	608	CHL	MG-NA	-2.77	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	610	CLA	CHC-C1C	2.77	1.42	1.35
25	g	612	CLA	C3B-C2B	-2.77	1.36	1.40
25	c	509	CLA	CMB-C2B	-2.77	1.45	1.51
24	g	605	CHL	C1D-C2D	2.77	1.50	1.45
25	4	603	CLA	CHC-C1C	2.77	1.42	1.35
25	g	614	CLA	CHC-C1C	2.77	1.42	1.35
25	g	604	CLA	CMB-C2B	-2.77	1.45	1.51
24	5	607	CHL	MG-NA	-2.77	1.99	2.06
25	G	604	CLA	CMB-C2B	-2.77	1.45	1.51
24	2	605	CHL	C3D-C2D	2.77	1.46	1.39
25	C	509	CLA	CMB-C2B	-2.77	1.45	1.51
24	2	609	CHL	C4C-C3C	2.77	1.49	1.45
25	1	610	CLA	CHC-C1C	2.77	1.42	1.35
25	p	604	CLA	CHC-C1C	2.77	1.42	1.35
24	p	606	CHL	C3D-C2D	2.77	1.46	1.39
25	b	614	CLA	CMB-C2B	-2.77	1.45	1.51
24	p	608	CHL	C1D-C2D	2.77	1.50	1.45
25	y	610	CLA	CMB-C2B	-2.76	1.45	1.51
25	c	505	CLA	CHC-C1C	2.76	1.42	1.35
28	5	1623	NEX	C7-C8	-2.76	1.27	1.32
25	b	610	CLA	C1D-ND	2.76	1.41	1.37
24	q	606	CHL	C4B-CHC	2.76	1.48	1.41
24	Y	601	CHL	MG-NA	-2.76	1.99	2.06
25	r	604	CLA	CHC-C1C	2.76	1.42	1.35
25	Y	610	CLA	CMB-C2B	-2.76	1.45	1.51
25	S	602	CLA	CMB-C2B	-2.76	1.45	1.51
25	Y	614	CLA	CHC-C1C	2.76	1.42	1.35
25	s	613	CLA	CMB-C2B	-2.76	1.45	1.51
25	c	506	CLA	CHC-C1C	2.76	1.42	1.35
24	4	605	CHL	C3D-C2D	2.76	1.46	1.39
24	p	605	CHL	C3D-C2D	2.76	1.46	1.39
25	B	607	CLA	CHC-C1C	2.76	1.42	1.35
25	R	604	CLA	CHC-C1C	2.76	1.42	1.35
25	b	607	CLA	CHC-C1C	2.76	1.42	1.35
25	b	609	CLA	CMB-C2B	-2.76	1.45	1.51
25	r	609	CLA	CMB-C2B	-2.76	1.45	1.51
25	q	604	CLA	CHC-C1C	2.76	1.42	1.35
24	Y	605	CHL	MG-NA	-2.76	1.99	2.06
24	y	605	CHL	MG-NA	-2.76	1.99	2.06
24	5	608	CHL	C1D-C2D	2.76	1.50	1.45
25	2	613	CLA	CHC-C1C	2.75	1.42	1.35
25	R	612	CLA	CMB-C2B	-2.75	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	614	CLA	CHC-C1C	2.75	1.42	1.35
24	4	606	CHL	C4B-CHC	2.75	1.48	1.41
25	B	604	CLA	C3B-CAB	-2.75	1.42	1.47
25	C	512	CLA	CHC-C1C	2.75	1.42	1.35
25	Y	613	CLA	C3B-C2B	-2.75	1.36	1.40
25	2	611	CLA	CHC-C1C	2.75	1.42	1.35
25	C	505	CLA	CHC-C1C	2.75	1.42	1.35
25	b	616	CLA	CMB-C2B	-2.75	1.45	1.51
25	9	611	CLA	CHC-C1C	2.75	1.42	1.35
24	9	608	CHL	C1D-C2D	2.75	1.50	1.45
24	q	605	CHL	C3D-C2D	2.75	1.46	1.39
24	3	601	CHL	MG-NA	-2.75	1.99	2.06
25	b	602	CLA	C3B-C2B	-2.75	1.36	1.40
24	Y	606	CHL	MG-NA	-2.75	1.99	2.06
25	n	610	CLA	CMB-C2B	-2.75	1.45	1.51
25	7	610	CLA	CHC-C1C	2.75	1.42	1.35
25	b	614	CLA	C1D-ND	2.75	1.41	1.37
25	c	501	CLA	C1D-ND	2.75	1.41	1.37
25	4	604	CLA	CHC-C1C	2.75	1.42	1.35
25	b	612	CLA	CHC-C1C	2.75	1.42	1.35
24	q	601	CHL	MG-NA	-2.75	1.99	2.06
25	B	613	CLA	CMB-C2B	-2.75	1.45	1.51
25	b	613	CLA	CMB-C2B	-2.75	1.45	1.51
25	r	611	CLA	CMB-C2B	-2.75	1.45	1.51
25	8	613	CLA	CHC-C1C	2.75	1.42	1.35
25	B	607	CLA	C3B-C2B	-2.74	1.36	1.40
25	n	603	CLA	C3B-C2B	-2.74	1.36	1.40
25	n	614	CLA	CHC-C1C	2.74	1.42	1.35
25	c	513	CLA	CHC-C1C	2.74	1.42	1.35
25	C	506	CLA	CHC-C1C	2.74	1.42	1.35
25	S	605	CLA	CHC-C1C	2.74	1.42	1.35
28	6	1623	NEX	C7-C8	-2.74	1.27	1.32
25	9	613	CLA	CHC-C1C	2.74	1.42	1.35
35	a	412	SQD	C6-S	-2.74	1.67	1.77
24	0	609	CHL	MG-NA	-2.74	1.99	2.06
24	4	605	CHL	MG-NA	-2.74	1.99	2.06
25	c	511	CLA	CMB-C2B	-2.74	1.45	1.51
25	A	406	CLA	CMB-C2B	-2.73	1.46	1.51
25	R	602	CLA	CMB-C2B	-2.73	1.46	1.51
28	3	1623	NEX	C7-C8	-2.73	1.27	1.32
25	S	613	CLA	C3B-C2B	-2.73	1.36	1.40
25	0	613	CLA	CHC-C1C	2.73	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	p	613	CLA	CHC-C1C	2.73	1.42	1.35
25	B	615	CLA	C1D-ND	2.73	1.41	1.37
24	p	607	CHL	MG-NA	-2.73	1.99	2.06
25	b	607	CLA	CMB-C2B	-2.73	1.46	1.51
25	B	614	CLA	C1D-ND	2.73	1.41	1.37
25	S	604	CLA	CHC-C1C	2.73	1.42	1.35
25	d	403	CLA	CMB-C2B	-2.73	1.46	1.51
25	g	611	CLA	CHC-C1C	2.73	1.42	1.35
25	n	611	CLA	CHC-C1C	2.73	1.42	1.35
24	q	607	CHL	C3D-C2D	2.73	1.46	1.39
25	p	603	CLA	CHC-C1C	2.73	1.42	1.35
25	G	612	CLA	C3B-C2B	-2.72	1.36	1.40
25	S	610	CLA	CMB-C2B	-2.72	1.46	1.51
25	y	612	CLA	CHC-C1C	2.72	1.41	1.35
25	5	604	CLA	CHC-C1C	2.72	1.41	1.35
25	S	613	CLA	CMB-C2B	-2.72	1.46	1.51
35	A	412	SQD	C6-S	-2.72	1.67	1.77
25	7	603	CLA	C3B-C2B	-2.72	1.36	1.40
25	Y	612	CLA	C1D-ND	2.72	1.41	1.37
25	s	605	CLA	CHC-C1C	2.72	1.41	1.35
25	r	612	CLA	CMB-C2B	-2.72	1.46	1.51
25	2	612	CLA	CHC-C1C	2.72	1.41	1.35
25	9	612	CLA	CHC-C1C	2.72	1.41	1.35
25	s	610	CLA	CMB-C2B	-2.72	1.46	1.51
25	A	406	CLA	C1D-ND	2.72	1.41	1.37
25	a	406	CLA	C1D-ND	2.72	1.41	1.37
25	C	504	CLA	C3B-C2B	-2.72	1.36	1.40
25	s	602	CLA	CMB-C2B	-2.72	1.46	1.51
28	r	623	NEX	C7-C8	-2.72	1.27	1.32
25	s	603	CLA	CMB-C2B	-2.72	1.46	1.51
25	s	609	CLA	CHC-C1C	2.72	1.41	1.35
24	R	606	CHL	OBD-CAD	2.71	1.27	1.22
24	3	601	CHL	C1D-C2D	2.71	1.50	1.45
24	2	607	CHL	C3D-C2D	2.71	1.46	1.39
25	q	612	CLA	C4D-ND	-2.71	1.34	1.37
25	S	609	CLA	CHC-C1C	2.71	1.41	1.35
25	n	612	CLA	CMB-C2B	-2.71	1.46	1.51
25	A	405	CLA	CMC-C2C	-2.71	1.45	1.50
24	r	608	CHL	C1D-ND	-2.71	1.34	1.37
25	B	603	CLA	CHC-C1C	2.71	1.41	1.35
25	B	604	CLA	CHC-C1C	2.71	1.41	1.35
25	b	615	CLA	C1D-ND	2.71	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	611	CLA	CHC-C1C	2.71	1.41	1.35
25	D	403	CLA	CMB-C2B	-2.71	1.46	1.51
25	C	501	CLA	CMD-C2D	-2.71	1.45	1.50
24	6	606	CHL	C1D-C2D	2.71	1.50	1.45
25	G	614	CLA	CHC-C1C	2.71	1.41	1.35
25	Y	612	CLA	CHC-C1C	2.71	1.41	1.35
24	9	609	CHL	MG-NA	-2.71	1.99	2.06
25	B	612	CLA	CHC-C1C	2.71	1.41	1.35
24	4	606	CHL	MG-NA	-2.71	1.99	2.06
25	a	406	CLA	CMB-C2B	-2.71	1.46	1.51
25	G	612	CLA	CHC-C1C	2.71	1.41	1.35
25	D	402	CLA	MG-ND	-2.71	2.00	2.05
25	d	402	CLA	MG-ND	-2.71	2.00	2.05
25	b	603	CLA	CHC-C1C	2.70	1.41	1.35
25	d	403	CLA	CHC-C1C	2.70	1.41	1.35
24	N	601	CHL	MG-NA	-2.70	1.99	2.06
25	C	505	CLA	CMB-C2B	-2.70	1.46	1.51
25	3	603	CLA	CHC-C1C	2.70	1.41	1.35
25	r	602	CLA	CMB-C2B	-2.70	1.46	1.51
25	s	604	CLA	CHC-C1C	2.70	1.41	1.35
35	b	623	SQD	C6-S	-2.70	1.67	1.77
24	S	601	CHL	MG-NA	-2.70	1.99	2.06
25	B	607	CLA	CMB-C2B	-2.70	1.46	1.51
25	3	613	CLA	CHC-C1C	2.70	1.41	1.35
25	C	512	CLA	CMB-C2B	-2.70	1.46	1.51
24	0	609	CHL	C1D-C2D	2.70	1.50	1.45
25	B	609	CLA	CMB-C2B	-2.70	1.46	1.51
25	b	604	CLA	C3B-CAB	-2.70	1.42	1.47
25	n	613	CLA	CHC-C1C	2.70	1.41	1.35
25	b	602	CLA	CMB-C2B	-2.70	1.46	1.51
25	B	613	CLA	CMD-C2D	-2.70	1.45	1.50
25	a	410	CLA	CMB-C2B	-2.70	1.46	1.51
24	2	608	CHL	C1D-C2D	2.70	1.50	1.45
25	G	611	CLA	CHC-C1C	2.70	1.41	1.35
25	0	603	CLA	CHC-C1C	2.70	1.41	1.35
24	9	606	CHL	C3D-C2D	2.70	1.46	1.39
25	C	513	CLA	CHC-C1C	2.69	1.41	1.35
25	s	613	CLA	C3B-C2B	-2.69	1.36	1.40
25	1	611	CLA	CHC-C1C	2.69	1.41	1.35
25	c	501	CLA	CMD-C2D	-2.69	1.45	1.50
25	c	504	CLA	C3B-C2B	-2.69	1.36	1.40
25	4	612	CLA	CHC-C1C	2.69	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	605	CHL	C3D-C2D	2.69	1.46	1.39
24	p	607	CHL	C3D-C2D	2.69	1.46	1.39
25	Y	612	CLA	CMB-C2B	-2.69	1.46	1.51
25	y	612	CLA	CMB-C2B	-2.69	1.46	1.51
25	Y	602	CLA	CHC-C1C	2.69	1.41	1.35
25	y	614	CLA	CMB-C2B	-2.69	1.46	1.51
25	l	613	CLA	CHC-C1C	2.69	1.41	1.35
25	b	604	CLA	CHC-C1C	2.69	1.41	1.35
24	p	601	CHL	MG-NA	-2.69	1.99	2.06
24	g	606	CHL	MG-NA	-2.69	1.99	2.06
25	q	612	CLA	CHC-C1C	2.69	1.41	1.35
24	s	607	CHL	C3D-C2D	2.69	1.46	1.39
25	N	603	CLA	C3B-C2B	-2.69	1.36	1.40
25	r	616	CLA	C3B-C2B	-2.69	1.36	1.40
25	4	613	CLA	CHC-C1C	2.69	1.41	1.35
25	s	610	CLA	C3B-C2B	-2.69	1.36	1.40
25	r	602	CLA	CHC-C1C	2.69	1.41	1.35
24	6	607	CHL	C3D-C2D	2.69	1.46	1.39
25	S	610	CLA	C3B-C2B	-2.69	1.36	1.40
25	y	602	CLA	CHC-C1C	2.69	1.41	1.35
25	8	604	CLA	CMB-C2B	-2.68	1.46	1.51
35	B	623	SQD	C6-S	-2.68	1.67	1.77
25	R	610	CLA	CMB-C2B	-2.68	1.46	1.51
25	r	610	CLA	CMB-C2B	-2.68	1.46	1.51
25	R	616	CLA	CHC-C1C	2.68	1.41	1.35
25	N	614	CLA	CMB-C2B	-2.68	1.46	1.51
24	2	606	CHL	C3D-C2D	2.68	1.46	1.39
24	l	609	CHL	MG-NA	-2.68	1.99	2.06
25	C	512	CLA	C3B-C2B	-2.68	1.36	1.40
25	a	405	CLA	CMC-C2C	-2.68	1.45	1.50
24	9	609	CHL	C3D-C2D	2.68	1.46	1.39
25	c	502	CLA	C4B-CHC	-2.68	1.33	1.41
25	7	611	CLA	CHC-C1C	2.68	1.41	1.35
25	0	604	CLA	CHC-C1C	2.68	1.41	1.35
25	g	603	CLA	C3B-C2B	-2.68	1.36	1.40
25	B	605	CLA	C3B-C2B	-2.68	1.36	1.40
25	S	612	CLA	CHC-C1C	2.68	1.41	1.35
25	C	502	CLA	C4B-CHC	-2.68	1.33	1.41
25	r	613	CLA	CMB-C2B	-2.68	1.46	1.51
25	g	612	CLA	CMB-C2B	-2.68	1.46	1.51
25	n	614	CLA	CMB-C2B	-2.68	1.46	1.51
25	s	612	CLA	CHC-C1C	2.68	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	607	CHL	C3D-C2D	2.68	1.46	1.39
25	1	604	CLA	C3B-CAB	-2.68	1.42	1.47
25	2	602	CLA	CHC-C1C	2.68	1.41	1.35
25	R	613	CLA	CMB-C2B	-2.68	1.46	1.51
25	3	612	CLA	CHC-C1C	2.68	1.41	1.35
25	c	505	CLA	CMB-C2B	-2.68	1.46	1.51
25	8	612	CLA	CHC-C1C	2.68	1.41	1.35
25	B	606	CLA	CHC-C1C	2.68	1.41	1.35
25	c	501	CLA	C3B-C2B	-2.68	1.36	1.40
25	r	616	CLA	CHC-C1C	2.68	1.41	1.35
25	N	613	CLA	CMB-C2B	-2.68	1.46	1.51
24	G	605	CHL	C3D-C2D	2.68	1.46	1.39
25	B	602	CLA	CMB-C2B	-2.67	1.46	1.51
25	D	403	CLA	CHC-C1C	2.67	1.41	1.35
25	S	611	CLA	CMB-C2B	-2.67	1.46	1.51
25	S	603	CLA	C3B-C2B	-2.67	1.36	1.40
25	s	603	CLA	C3B-C2B	-2.67	1.36	1.40
25	S	603	CLA	CMB-C2B	-2.67	1.46	1.51
24	s	608	CHL	MG-NA	-2.67	1.99	2.06
25	N	612	CLA	CMB-C2B	-2.67	1.46	1.51
24	R	608	CHL	C1D-ND	-2.67	1.34	1.37
25	b	606	CLA	CHC-C1C	2.67	1.41	1.35
25	g	612	CLA	CHC-C1C	2.67	1.41	1.35
24	6	605	CHL	C3D-C2D	2.67	1.46	1.39
25	b	614	CLA	CHC-C1C	2.67	1.41	1.35
25	3	604	CLA	CMB-C2B	-2.67	1.46	1.51
25	Y	604	CLA	C1D-ND	2.67	1.41	1.37
24	r	606	CHL	OBD-CAD	2.67	1.27	1.22
25	G	612	CLA	CMB-C2B	-2.67	1.46	1.51
25	8	603	CLA	CHC-C1C	2.67	1.41	1.35
24	g	605	CHL	C3D-C2D	2.67	1.46	1.39
24	S	606	CHL	C1D-C2D	2.67	1.50	1.45
25	s	611	CLA	CMB-C2B	-2.67	1.46	1.51
25	R	611	CLA	CMB-C2B	-2.66	1.46	1.51
25	b	611	CLA	CMD-C2D	-2.66	1.45	1.50
25	y	604	CLA	C1D-ND	2.66	1.41	1.37
25	R	616	CLA	C3B-C2B	-2.66	1.36	1.40
25	B	614	CLA	CHC-C1C	2.66	1.41	1.35
25	q	613	CLA	CHC-C1C	2.66	1.41	1.35
25	7	613	CLA	CHC-C1C	2.66	1.41	1.35
24	0	601	CHL	C3D-C2D	2.66	1.46	1.39
25	b	613	CLA	CMD-C2D	-2.66	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	607	CHL	C3D-C2D	2.66	1.46	1.39
25	D	402	CLA	C3B-C2B	-2.66	1.36	1.40
25	S	603	CLA	CHC-C1C	2.66	1.41	1.35
25	4	612	CLA	C4D-ND	-2.66	1.34	1.37
25	n	611	CLA	CMB-C2B	-2.66	1.46	1.51
25	Y	613	CLA	MG-ND	-2.66	2.00	2.05
24	s	601	CHL	MG-NA	-2.65	2.00	2.06
24	q	601	CHL	C1D-C2D	2.65	1.50	1.45
25	Y	614	CLA	CMB-C2B	-2.65	1.46	1.51
39	D	405	PL9	C16-C14	-2.65	1.45	1.51
24	5	606	CHL	C1D-C2D	2.65	1.50	1.45
25	G	603	CLA	C3B-C2B	-2.65	1.36	1.40
25	A	410	CLA	CMB-C2B	-2.65	1.46	1.51
24	3	608	CHL	C1D-C2D	2.65	1.50	1.45
25	R	616	CLA	CMB-C2B	-2.65	1.46	1.51
25	b	602	CLA	CHC-C1C	2.65	1.41	1.35
25	B	604	CLA	C1D-ND	2.65	1.41	1.37
25	R	602	CLA	CHC-C1C	2.65	1.41	1.35
25	C	512	CLA	CMD-C2D	-2.65	1.45	1.50
25	B	615	CLA	CHC-C1C	2.65	1.41	1.35
25	b	607	CLA	C3B-C2B	-2.65	1.36	1.40
24	8	601	CHL	MG-NA	-2.65	2.00	2.06
25	G	614	CLA	CMB-C2B	-2.65	1.46	1.51
25	G	603	CLA	C1D-ND	2.65	1.41	1.37
25	B	608	CLA	CHC-C1C	2.65	1.41	1.35
24	4	608	CHL	C3D-C2D	2.64	1.46	1.39
25	R	610	CLA	CHC-C1C	2.64	1.41	1.35
25	r	610	CLA	CHC-C1C	2.64	1.41	1.35
25	c	513	CLA	CMB-C2B	-2.64	1.46	1.51
25	C	513	CLA	CMB-C2B	-2.64	1.46	1.51
24	s	606	CHL	C1D-C2D	2.64	1.50	1.45
25	A	410	CLA	CHC-C1C	2.64	1.41	1.35
25	a	410	CLA	CHC-C1C	2.64	1.41	1.35
25	A	407	CLA	CMB-C2B	-2.64	1.46	1.51
24	G	606	CHL	MG-NA	-2.64	2.00	2.06
25	g	611	CLA	CMB-C2B	-2.64	1.46	1.51
25	B	617	CLA	CHC-C1C	2.64	1.41	1.35
25	N	611	CLA	CMB-C2B	-2.64	1.46	1.51
25	c	512	CLA	CMB-C2B	-2.64	1.46	1.51
24	9	605	CHL	MG-NA	-2.64	2.00	2.06
25	G	611	CLA	CMB-C2B	-2.64	1.46	1.51
25	c	512	CLA	CMD-C2D	-2.64	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	603	CLA	CHC-C1C	2.64	1.41	1.35
25	C	501	CLA	C3B-C2B	-2.64	1.36	1.40
25	n	613	CLA	CMB-C2B	-2.64	1.46	1.51
39	D	405	PL9	C36-C34	-2.64	1.45	1.51
25	y	602	CLA	CMB-C2B	-2.64	1.46	1.51
24	s	608	CHL	C1D-C2D	2.64	1.50	1.45
25	B	616	CLA	C3B-C2B	-2.64	1.36	1.40
25	b	616	CLA	C3B-C2B	-2.64	1.36	1.40
24	q	605	CHL	MG-NA	-2.64	2.00	2.06
25	N	602	CLA	CMB-C2B	-2.63	1.46	1.51
24	8	601	CHL	C1D-C2D	2.63	1.50	1.45
25	S	613	CLA	CHC-C1C	2.63	1.41	1.35
25	Y	611	CLA	CHC-C1C	2.63	1.41	1.35
24	0	608	CHL	MG-NA	-2.63	2.00	2.06
25	B	606	CLA	C3B-C2B	-2.63	1.36	1.40
25	b	609	CLA	CHC-C1C	2.63	1.41	1.35
25	s	612	CLA	CMB-C2B	-2.63	1.46	1.51
25	b	606	CLA	C3B-C2B	-2.63	1.36	1.40
25	y	611	CLA	CMD-C2D	-2.63	1.45	1.50
25	d	402	CLA	C3B-C2B	-2.63	1.36	1.40
24	2	606	CHL	C1D-C2D	2.63	1.50	1.45
24	9	607	CHL	C3D-C2D	2.63	1.46	1.39
25	B	611	CLA	CMD-C2D	-2.63	1.45	1.50
25	9	603	CLA	CHC-C1C	2.63	1.41	1.35
25	c	503	CLA	CMB-C2B	-2.63	1.46	1.51
25	b	615	CLA	CHC-C1C	2.63	1.41	1.35
24	5	607	CHL	C3D-C2D	2.63	1.46	1.39
25	A	406	CLA	CHC-C1C	2.63	1.41	1.35
25	b	605	CLA	C3B-C2B	-2.63	1.36	1.40
25	s	613	CLA	CHC-C1C	2.63	1.41	1.35
25	b	604	CLA	C1D-ND	2.62	1.41	1.37
25	N	613	CLA	CHC-C1C	2.62	1.41	1.35
25	p	604	CLA	CMB-C2B	-2.62	1.46	1.51
24	q	609	CHL	C4B-CHC	2.62	1.48	1.41
24	5	606	CHL	C3D-C2D	2.62	1.46	1.39
25	g	614	CLA	CMB-C2B	-2.62	1.46	1.51
25	B	609	CLA	CHC-C1C	2.62	1.41	1.35
24	2	609	CHL	C3D-C2D	2.62	1.46	1.39
25	g	603	CLA	C1D-ND	2.62	1.41	1.37
25	B	602	CLA	CHC-C1C	2.62	1.41	1.35
39	d	405	PL9	C36-C34	-2.62	1.45	1.51
25	Y	602	CLA	CMB-C2B	-2.62	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	616	CLA	CMB-C2B	-2.62	1.46	1.51
25	y	611	CLA	CHC-C1C	2.62	1.41	1.35
24	7	605	CHL	C1D-C2D	2.62	1.50	1.45
25	C	510	CLA	CMD-C2D	-2.62	1.45	1.50
24	S	608	CHL	C1D-C2D	2.62	1.50	1.45
25	g	610	CLA	CMB-C2B	-2.61	1.46	1.51
39	d	405	PL9	C16-C14	-2.61	1.45	1.51
24	4	601	CHL	C3D-C2D	2.61	1.46	1.39
25	s	603	CLA	CHC-C1C	2.61	1.41	1.35
24	S	608	CHL	MG-NA	-2.61	2.00	2.06
24	n	601	CHL	MG-NA	-2.61	2.00	2.06
25	a	407	CLA	CMB-C2B	-2.61	1.46	1.51
25	7	603	CLA	CHC-C1C	2.61	1.41	1.35
24	p	607	CHL	C1D-C2D	2.61	1.50	1.45
25	2	603	CLA	CHC-C1C	2.61	1.41	1.35
24	0	608	CHL	C1D-C2D	2.61	1.50	1.45
25	y	613	CLA	MG-ND	-2.61	2.00	2.05
25	2	603	CLA	CMB-C2B	-2.61	1.46	1.51
24	0	605	CHL	C3D-C2D	2.61	1.46	1.39
25	1	603	CLA	CHC-C1C	2.61	1.41	1.35
25	p	603	CLA	CMB-C2B	-2.61	1.46	1.51
25	n	602	CLA	CMB-C2B	-2.61	1.46	1.51
24	6	601	CHL	C3D-C2D	2.61	1.46	1.39
24	S	606	CHL	MG-NA	-2.61	2.00	2.06
25	b	608	CLA	CHC-C1C	2.61	1.41	1.35
25	G	610	CLA	CHC-C1C	2.61	1.41	1.35
39	d	405	PL9	C7-C8	-2.61	1.46	1.50
25	B	610	CLA	CHC-C1C	2.60	1.41	1.35
25	c	507	CLA	CMB-C2B	-2.60	1.46	1.51
25	B	604	CLA	CMD-C2D	-2.60	1.45	1.50
24	9	601	CHL	MG-NA	-2.60	2.00	2.06
25	c	510	CLA	CMD-C2D	-2.60	1.45	1.50
25	C	503	CLA	CMB-C2B	-2.60	1.46	1.51
25	G	610	CLA	CMB-C2B	-2.60	1.46	1.51
24	2	601	CHL	MG-NA	-2.60	2.00	2.06
25	C	504	CLA	CHC-C1C	2.60	1.41	1.35
25	9	603	CLA	CMB-C2B	-2.60	1.46	1.51
24	p	601	CHL	C3D-C2D	2.60	1.46	1.39
25	N	604	CLA	CHC-C1C	2.60	1.41	1.35
25	n	604	CLA	CHC-C1C	2.60	1.41	1.35
25	N	614	CLA	C3B-C2B	-2.60	1.36	1.40
25	R	610	CLA	CMC-C2C	-2.60	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	612	CLA	CMB-C2B	-2.60	1.46	1.51
24	8	605	CHL	C4B-CHC	2.60	1.48	1.41
24	8	609	CHL	C3D-C2D	2.60	1.46	1.39
25	2	604	CLA	CMB-C2B	-2.60	1.46	1.51
25	7	612	CLA	CMB-C2B	-2.60	1.46	1.51
24	6	605	CHL	C1D-C2D	2.60	1.50	1.45
25	g	610	CLA	CHC-C1C	2.60	1.41	1.35
25	r	609	CLA	CHC-C1C	2.60	1.41	1.35
25	C	507	CLA	CMB-C2B	-2.59	1.46	1.51
25	a	406	CLA	CHC-C1C	2.59	1.41	1.35
25	4	604	CLA	CMB-C2B	-2.59	1.46	1.51
25	8	602	CLA	CMB-C2B	-2.59	1.46	1.51
28	n	1623	NEX	C7-C8	-2.59	1.27	1.32
25	R	609	CLA	CHC-C1C	2.59	1.41	1.35
24	8	608	CHL	C1D-C2D	2.59	1.50	1.45
24	s	607	CHL	C1D-C2D	2.59	1.50	1.45
25	b	617	CLA	CHC-C1C	2.59	1.41	1.35
24	S	607	CHL	C1D-C2D	2.59	1.50	1.45
25	9	602	CLA	CHC-C1C	2.59	1.41	1.35
24	7	601	CHL	MG-NA	-2.59	2.00	2.06
24	4	609	CHL	C4B-CHC	2.59	1.48	1.41
24	9	606	CHL	MG-NA	-2.59	2.00	2.06
24	3	606	CHL	C3D-C2D	2.59	1.46	1.39
25	r	610	CLA	CMC-C2C	-2.59	1.45	1.50
24	3	605	CHL	C4B-CHC	2.59	1.48	1.41
24	4	605	CHL	C4C-C3C	2.59	1.49	1.45
25	S	605	CLA	CMB-C2B	-2.59	1.46	1.51
25	R	609	CLA	C3B-C2B	-2.59	1.36	1.40
25	b	615	CLA	C3B-C2B	-2.59	1.36	1.40
25	r	609	CLA	C3B-C2B	-2.59	1.36	1.40
25	5	604	CLA	CMB-C2B	-2.59	1.46	1.51
25	9	604	CLA	CMB-C2B	-2.59	1.46	1.51
24	2	605	CHL	MG-NA	-2.58	2.00	2.06
25	3	612	CLA	CMB-C2B	-2.58	1.46	1.51
24	5	609	CHL	C3D-C2D	2.58	1.46	1.39
25	p	613	CLA	CMB-C2B	-2.58	1.46	1.51
25	3	602	CLA	CMB-C2B	-2.58	1.46	1.51
25	Y	611	CLA	CMD-C2D	-2.58	1.45	1.50
24	6	609	CHL	C1D-C2D	2.58	1.50	1.45
24	9	601	CHL	C1D-C2D	2.58	1.50	1.45
25	c	512	CLA	C3B-C2B	-2.58	1.36	1.40
25	b	610	CLA	CHC-C1C	2.58	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	c	504	CLA	CHC-C1C	2.58	1.41	1.35
25	2	612	CLA	CMB-C2B	-2.58	1.46	1.51
25	8	612	CLA	CMB-C2B	-2.58	1.46	1.51
25	0	610	CLA	CMB-C2B	-2.58	1.46	1.51
24	2	605	CHL	C4C-C3C	2.57	1.49	1.45
24	g	607	CHL	C1D-C2D	2.57	1.50	1.45
25	1	610	CLA	CMB-C2B	-2.57	1.46	1.51
25	B	605	CLA	CMD-C2D	-2.57	1.45	1.50
25	6	612	CLA	CMB-C2B	-2.57	1.46	1.51
25	B	603	CLA	CMB-C2B	-2.57	1.46	1.51
24	8	606	CHL	C3D-C2D	2.57	1.46	1.39
25	c	510	CLA	CMB-C2B	-2.57	1.46	1.51
24	0	609	CHL	C3D-C2D	2.57	1.46	1.39
25	1	602	CLA	CMB-C2B	-2.57	1.46	1.51
25	b	611	CLA	CMC-C2C	-2.57	1.45	1.50
25	9	602	CLA	CMB-C2B	-2.57	1.46	1.51
25	b	604	CLA	CMD-C2D	-2.57	1.45	1.50
24	s	608	CHL	C3D-C2D	2.57	1.46	1.39
24	q	609	CHL	C1B-CHB	2.57	1.48	1.41
24	7	609	CHL	MG-NA	-2.57	2.00	2.06
25	q	603	CLA	CMB-C2B	-2.57	1.46	1.51
25	b	605	CLA	CMD-C2D	-2.57	1.45	1.50
24	5	601	CHL	MG-NA	-2.56	2.00	2.06
24	p	609	CHL	C3D-C2D	2.56	1.46	1.39
24	G	605	CHL	MG-NA	-2.56	2.00	2.06
24	6	608	CHL	MG-NA	-2.56	2.00	2.06
25	1	611	CLA	CMB-C2B	-2.56	1.46	1.51
24	n	601	CHL	C1D-C2D	2.56	1.50	1.45
25	R	611	CLA	CHC-C1C	2.56	1.41	1.35
25	6	603	CLA	CMB-C2B	-2.56	1.46	1.51
24	6	609	CHL	C3D-C2D	2.56	1.46	1.39
24	1	605	CHL	C1D-C2D	2.56	1.50	1.45
24	6	601	CHL	C1D-C2D	2.56	1.50	1.45
24	s	606	CHL	MG-NA	-2.56	2.00	2.06
25	7	611	CLA	CMB-C2B	-2.56	1.46	1.51
25	B	609	CLA	C1D-ND	2.56	1.40	1.37
25	b	609	CLA	C1D-ND	2.56	1.40	1.37
24	1	601	CHL	MG-NA	-2.56	2.00	2.06
24	6	607	CHL	C1D-C2D	2.56	1.50	1.45
24	G	607	CHL	MG-NA	-2.56	2.00	2.06
25	C	505	CLA	MG-ND	-2.55	2.00	2.05
25	q	604	CLA	CMB-C2B	-2.55	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	5	609	CHL	MG-NA	-2.55	2.00	2.06
24	2	609	CHL	MG-NA	-2.55	2.00	2.06
25	5	603	CLA	CMB-C2B	-2.55	1.46	1.51
25	R	613	CLA	CHC-C1C	2.55	1.41	1.35
24	3	609	CHL	MG-NA	-2.55	2.00	2.06
25	y	603	CLA	MG-ND	-2.55	2.00	2.05
25	B	611	CLA	CMC-C2C	-2.55	1.45	1.50
24	6	605	CHL	MG-NA	-2.55	2.00	2.06
25	7	610	CLA	CMB-C2B	-2.55	1.46	1.51
25	C	510	CLA	CMB-C2B	-2.55	1.46	1.51
24	0	607	CHL	C3D-C2D	2.54	1.46	1.39
25	1	612	CLA	CMB-C2B	-2.54	1.46	1.51
24	p	606	CHL	C4C-C3C	2.54	1.49	1.45
25	c	502	CLA	CMC-C2C	-2.54	1.45	1.50
25	C	503	CLA	CHC-C1C	2.54	1.41	1.35
39	D	405	PL9	C7-C8	-2.54	1.47	1.50
25	4	611	CLA	CMB-C2B	-2.54	1.46	1.51
25	1	613	CLA	CMB-C2B	-2.54	1.46	1.51
24	3	608	CHL	MG-NA	-2.54	2.00	2.06
25	b	603	CLA	CMB-C2B	-2.54	1.46	1.51
25	R	612	CLA	CHC-C1C	2.54	1.41	1.35
25	r	612	CLA	CHC-C1C	2.54	1.41	1.35
25	S	609	CLA	CMB-C2B	-2.54	1.46	1.51
24	9	605	CHL	C4C-C3C	2.54	1.49	1.45
24	G	605	CHL	C4C-C3C	2.54	1.49	1.45
24	7	605	CHL	C3D-C2D	2.53	1.46	1.39
25	s	605	CLA	CMB-C2B	-2.53	1.46	1.51
25	C	502	CLA	CMC-C2C	-2.53	1.45	1.50
25	Y	603	CLA	MG-ND	-2.53	2.00	2.05
25	c	505	CLA	C1D-ND	2.53	1.40	1.37
25	9	614	CLA	CMB-C2B	-2.53	1.46	1.51
24	5	601	CHL	C3D-C2D	2.53	1.46	1.39
25	r	613	CLA	CHC-C1C	2.53	1.41	1.35
24	s	606	CHL	C3D-C2D	2.53	1.46	1.39
25	G	603	CLA	CHC-C1C	2.53	1.41	1.35
25	g	603	CLA	CHC-C1C	2.53	1.41	1.35
24	0	605	CHL	C1D-C2D	2.53	1.50	1.45
24	3	609	CHL	C3D-C2D	2.53	1.46	1.39
24	Y	605	CHL	C3D-C2D	2.53	1.46	1.39
24	y	605	CHL	C3D-C2D	2.53	1.46	1.39
24	G	609	CHL	C1D-C2D	2.53	1.50	1.45
25	0	612	CLA	CMB-C2B	-2.53	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	605	CHL	C3D-C2D	2.53	1.46	1.39
25	C	511	CLA	CHC-C1C	2.53	1.41	1.35
24	q	608	CHL	C4B-CHC	2.53	1.48	1.41
33	a	408	PHO	CMC-C2C	-2.53	1.45	1.51
25	B	615	CLA	C3B-C2B	-2.53	1.36	1.40
24	4	601	CHL	C1D-C2D	2.53	1.50	1.45
39	d	405	PL9	C26-C24	-2.53	1.46	1.51
24	2	601	CHL	C1D-C2D	2.53	1.50	1.45
24	g	607	CHL	MG-NA	-2.53	2.00	2.06
25	Y	613	CLA	CHC-C1C	2.53	1.41	1.35
25	Y	611	CLA	C1D-ND	2.53	1.40	1.37
25	G	603	CLA	MG-ND	-2.53	2.00	2.05
39	D	405	PL9	C26-C24	-2.53	1.46	1.51
25	n	613	CLA	C3B-C2B	-2.53	1.36	1.40
24	N	601	CHL	C1D-C2D	2.52	1.50	1.45
24	1	608	CHL	MG-NA	-2.52	2.00	2.06
25	c	503	CLA	CHC-C1C	2.52	1.41	1.35
28	r	623	NEX	C1-C6	-2.52	1.50	1.54
33	a	409	PHO	CMD-C2D	-2.52	1.45	1.51
24	5	606	CHL	C4B-CHC	2.52	1.48	1.41
24	S	606	CHL	C3D-C2D	2.52	1.46	1.39
25	7	602	CLA	CMB-C2B	-2.52	1.46	1.51
24	g	609	CHL	C1D-C2D	2.52	1.50	1.45
25	C	505	CLA	C1D-ND	2.52	1.40	1.37
25	4	614	CLA	CMB-C2B	-2.52	1.46	1.51
25	g	613	CLA	CMB-C2B	-2.52	1.46	1.51
24	6	608	CHL	C1D-C2D	2.52	1.50	1.45
25	2	602	CLA	CMB-C2B	-2.52	1.46	1.51
25	B	608	CLA	C3B-C2B	-2.52	1.36	1.40
24	Y	605	CHL	C1D-C2D	2.52	1.50	1.45
24	y	605	CHL	C1D-C2D	2.52	1.50	1.45
25	6	610	CLA	CMB-C2B	-2.51	1.46	1.51
24	p	605	CHL	C1B-CHB	2.51	1.48	1.41
25	Y	614	CLA	C3B-C2B	-2.51	1.36	1.40
25	y	614	CLA	C3B-C2B	-2.51	1.36	1.40
25	G	613	CLA	CMB-C2B	-2.51	1.46	1.51
25	s	609	CLA	CMB-C2B	-2.51	1.46	1.51
24	8	609	CHL	MG-NA	-2.51	2.00	2.06
24	g	605	CHL	MG-NA	-2.51	2.00	2.06
25	p	611	CLA	CMB-C2B	-2.51	1.46	1.51
25	p	602	CLA	CMB-C2B	-2.51	1.46	1.51
25	g	603	CLA	MG-ND	-2.51	2.00	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	S	608	CHL	C3D-C2D	2.51	1.46	1.39
25	q	614	CLA	CMB-C2B	-2.51	1.46	1.51
25	B	610	CLA	CMD-C2D	-2.51	1.45	1.50
25	c	505	CLA	MG-ND	-2.51	2.00	2.05
28	s	1623	NEX	C1-C6	-2.51	1.50	1.54
24	5	606	CHL	MG-NA	-2.51	2.00	2.06
24	p	605	CHL	C4B-CHC	2.51	1.48	1.41
25	9	612	CLA	CMB-C2B	-2.51	1.46	1.51
25	6	613	CLA	CMB-C2B	-2.50	1.46	1.51
25	5	613	CLA	CMB-C2B	-2.50	1.46	1.51
25	d	403	CLA	C3B-C2B	-2.50	1.36	1.40
25	0	603	CLA	CMB-C2B	-2.50	1.46	1.51
25	y	613	CLA	CHC-C1C	2.50	1.41	1.35
24	8	608	CHL	MG-NA	-2.50	2.00	2.06
25	G	611	CLA	C3B-C2B	-2.50	1.36	1.40
25	g	611	CLA	C3B-C2B	-2.50	1.36	1.40
25	r	611	CLA	CHC-C1C	2.50	1.41	1.35
33	A	408	PHO	CMC-C2C	-2.50	1.45	1.51
25	p	614	CLA	CMB-C2B	-2.50	1.46	1.51
25	B	615	CLA	CMD-C2D	-2.50	1.45	1.50
25	b	617	CLA	C3B-C2B	-2.50	1.36	1.40
24	0	607	CHL	MG-NA	-2.50	2.00	2.06
24	4	607	CHL	C4B-CHC	2.50	1.47	1.41
25	3	611	CLA	CMB-C2B	-2.50	1.46	1.51
25	8	611	CLA	CMB-C2B	-2.50	1.46	1.51
25	2	611	CLA	CMB-C2B	-2.50	1.46	1.51
25	7	604	CLA	CHC-C1C	2.49	1.41	1.35
33	A	409	PHO	CMD-C2D	-2.49	1.45	1.51
24	0	608	CHL	C3D-C2D	2.49	1.45	1.39
25	c	511	CLA	CHC-C1C	2.49	1.41	1.35
25	2	614	CLA	CMB-C2B	-2.49	1.46	1.51
24	4	609	CHL	C1B-CHB	2.49	1.47	1.41
25	A	406	CLA	C3B-C2B	-2.49	1.36	1.40
25	a	406	CLA	C3B-C2B	-2.49	1.36	1.40
25	S	610	CLA	CMD-C2D	-2.49	1.45	1.50
25	3	610	CLA	CMB-C2B	-2.49	1.46	1.51
25	9	611	CLA	CMB-C2B	-2.49	1.46	1.51
25	r	613	CLA	C3B-C2B	-2.49	1.36	1.40
24	N	608	CHL	MG-NA	-2.49	2.00	2.06
25	5	612	CLA	CMB-C2B	-2.49	1.46	1.51
25	8	610	CLA	CMB-C2B	-2.49	1.46	1.51
24	7	606	CHL	C1D-C2D	2.49	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	613	CLA	CMB-C2B	-2.49	1.46	1.51
25	1	614	CLA	CMB-C2B	-2.49	1.46	1.51
25	7	614	CLA	CMB-C2B	-2.48	1.46	1.51
24	g	605	CHL	C4C-C3C	2.48	1.49	1.45
25	g	603	CLA	CMD-C2D	-2.48	1.45	1.50
33	A	408	PHO	CMB-C2B	-2.48	1.45	1.51
25	7	604	CLA	C3B-CAB	-2.48	1.42	1.47
24	Y	608	CHL	MG-NA	-2.48	2.00	2.06
25	c	508	CLA	CMD-C2D	-2.48	1.45	1.50
24	9	606	CHL	C1D-C2D	2.48	1.50	1.45
25	5	614	CLA	CMB-C2B	-2.48	1.46	1.51
25	0	602	CLA	CMB-C2B	-2.48	1.46	1.51
25	5	611	CLA	CMB-C2B	-2.48	1.46	1.51
25	y	611	CLA	C1D-ND	2.48	1.40	1.37
24	9	605	CHL	C4B-CHC	2.48	1.47	1.41
25	7	612	CLA	C3B-C2B	-2.48	1.36	1.40
25	s	610	CLA	CMD-C2D	-2.48	1.45	1.50
25	b	604	CLA	CMC-C2C	-2.48	1.45	1.50
25	S	614	CLA	CMB-C2B	-2.48	1.46	1.51
25	q	611	CLA	CMB-C2B	-2.48	1.46	1.51
25	b	615	CLA	CMD-C2D	-2.47	1.45	1.50
24	6	609	CHL	MG-NA	-2.47	2.00	2.06
25	N	613	CLA	C3B-C2B	-2.47	1.36	1.40
25	n	611	CLA	C3B-C2B	-2.47	1.36	1.40
24	q	607	CHL	C4C-C3C	2.47	1.49	1.45
25	g	602	CLA	CMB-C2B	-2.47	1.46	1.51
25	c	513	CLA	CMD-C2D	-2.47	1.45	1.50
24	q	605	CHL	C4C-C3C	2.47	1.49	1.45
24	1	606	CHL	C1D-C2D	2.47	1.50	1.45
25	C	509	CLA	CHC-C1C	2.47	1.41	1.35
25	c	509	CLA	CHC-C1C	2.47	1.41	1.35
25	n	614	CLA	C3B-C2B	-2.47	1.36	1.40
25	Y	612	CLA	CMD-C2D	-2.47	1.45	1.50
25	G	602	CLA	CMB-C2B	-2.47	1.46	1.51
24	0	605	CHL	MG-NA	-2.47	2.00	2.06
25	s	614	CLA	CMB-C2B	-2.47	1.46	1.51
24	G	608	CHL	C1D-C2D	2.47	1.50	1.45
25	A	405	CLA	CMD-C2D	-2.47	1.45	1.50
25	a	405	CLA	CMD-C2D	-2.47	1.45	1.50
24	y	608	CHL	MG-NA	-2.47	2.00	2.06
25	7	613	CLA	CMB-C2B	-2.47	1.46	1.51
25	B	617	CLA	C3B-C2B	-2.47	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	0	611	CLA	CMB-C2B	-2.46	1.46	1.51
24	2	605	CHL	C4B-CHC	2.46	1.47	1.41
25	C	508	CLA	C3B-C2B	-2.46	1.36	1.40
33	A	408	PHO	C3B-C2B	-2.46	1.36	1.40
33	a	408	PHO	C3B-C2B	-2.46	1.36	1.40
24	q	607	CHL	C4B-CHC	2.46	1.47	1.41
34	C	515	BCR	C30-C25	-2.46	1.50	1.53
24	5	605	CHL	C1B-CHB	2.46	1.47	1.41
25	Y	612	CLA	MG-ND	-2.46	2.00	2.05
25	N	602	CLA	C3B-C2B	-2.46	1.37	1.40
26	y	1620	LUT	C10-C9	-2.46	1.32	1.35
25	r	612	CLA	C3B-C2B	-2.46	1.37	1.40
33	a	408	PHO	CMB-C2B	-2.46	1.45	1.51
25	6	604	CLA	C3B-C2B	-2.46	1.37	1.40
24	g	606	CHL	C1D-C2D	2.46	1.50	1.45
24	p	606	CHL	C4B-CHC	2.46	1.47	1.41
25	r	603	CLA	C3B-C2B	-2.46	1.37	1.40
25	3	603	CLA	CMB-C2B	-2.46	1.46	1.51
25	4	612	CLA	CMB-C2B	-2.46	1.46	1.51
25	Y	604	CLA	CMD-C2D	-2.46	1.45	1.50
25	b	610	CLA	CMD-C2D	-2.46	1.45	1.50
25	r	602	CLA	C3B-C2B	-2.46	1.37	1.40
25	G	603	CLA	CMD-C2D	-2.46	1.45	1.50
24	4	605	CHL	C1B-CHB	2.46	1.47	1.41
24	g	608	CHL	C1D-C2D	2.46	1.50	1.45
25	B	606	CLA	CMD-C2D	-2.45	1.45	1.50
25	B	607	CLA	CMD-C2D	-2.45	1.45	1.50
25	R	613	CLA	C3B-C2B	-2.45	1.37	1.40
25	C	508	CLA	CMD-C2D	-2.45	1.45	1.50
24	G	607	CHL	C1D-C2D	2.45	1.50	1.45
25	C	512	CLA	C3B-CAB	-2.45	1.42	1.47
24	G	608	CHL	C3D-C2D	2.45	1.45	1.39
25	6	602	CLA	CMB-C2B	-2.45	1.46	1.51
25	B	604	CLA	CMC-C2C	-2.45	1.45	1.50
25	C	513	CLA	CMD-C2D	-2.45	1.45	1.50
24	q	601	CHL	C3D-C2D	2.45	1.45	1.39
24	7	608	CHL	MG-NA	-2.45	2.00	2.06
25	c	507	CLA	CMD-C2D	-2.45	1.45	1.50
25	g	613	CLA	CHC-C1C	2.45	1.41	1.35
25	8	614	CLA	CMB-C2B	-2.45	1.46	1.51
26	Y	1620	LUT	C10-C9	-2.45	1.32	1.35
24	8	605	CHL	C1B-CHB	2.45	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	604	CLA	CMD-C2D	-2.45	1.45	1.50
24	8	607	CHL	C1D-C2D	2.45	1.50	1.45
25	b	609	CLA	CMD-C2D	-2.45	1.45	1.50
24	3	605	CHL	C1B-CHB	2.44	1.47	1.41
24	8	601	CHL	C3D-C2D	2.44	1.45	1.39
24	4	605	CHL	C4B-CHC	2.44	1.47	1.41
24	q	608	CHL	C1B-CHB	2.44	1.47	1.41
24	S	601	CHL	C3D-C2D	2.44	1.45	1.39
25	D	402	CLA	CMC-C2C	-2.44	1.45	1.50
25	Y	604	CLA	CHC-C1C	2.44	1.41	1.35
25	C	507	CLA	MG-ND	-2.44	2.00	2.05
25	B	613	CLA	CMC-C2C	-2.44	1.45	1.50
25	b	613	CLA	CMC-C2C	-2.44	1.45	1.50
24	5	605	CHL	C4B-CHC	2.44	1.47	1.41
25	b	608	CLA	C3B-C2B	-2.44	1.37	1.40
25	C	512	CLA	MG-ND	-2.44	2.01	2.05
25	6	611	CLA	CMB-C2B	-2.44	1.46	1.51
25	y	612	CLA	MG-ND	-2.44	2.01	2.05
25	b	605	CLA	CHC-C1C	2.44	1.41	1.35
24	n	608	CHL	MG-NA	-2.44	2.00	2.06
25	B	612	CLA	CMD-C2D	-2.44	1.45	1.50
25	b	612	CLA	CMD-C2D	-2.44	1.45	1.50
24	4	608	CHL	C4B-CHC	2.44	1.47	1.41
25	y	612	CLA	CMD-C2D	-2.44	1.45	1.50
25	3	614	CLA	CMB-C2B	-2.43	1.46	1.51
25	5	602	CLA	CMB-C2B	-2.43	1.46	1.51
24	3	601	CHL	C3D-C2D	2.43	1.45	1.39
25	0	612	CLA	C3B-C2B	-2.43	1.37	1.40
25	b	616	CLA	CHC-C1C	2.43	1.41	1.35
25	3	613	CLA	CMB-C2B	-2.43	1.46	1.51
25	b	607	CLA	CMD-C2D	-2.43	1.45	1.50
25	4	604	CLA	C3B-C2B	-2.43	1.37	1.40
25	1	612	CLA	C3B-C2B	-2.43	1.37	1.40
25	G	613	CLA	CHC-C1C	2.43	1.41	1.35
25	R	602	CLA	C3B-C2B	-2.43	1.37	1.40
25	c	509	CLA	CMD-C2D	-2.43	1.45	1.50
25	B	605	CLA	CHC-C1C	2.43	1.41	1.35
25	N	611	CLA	C3B-C2B	-2.43	1.37	1.40
25	c	504	CLA	CMD-C2D	-2.43	1.45	1.50
25	B	613	CLA	CHC-C1C	2.43	1.41	1.35
25	b	613	CLA	CHC-C1C	2.43	1.41	1.35
25	0	613	CLA	CMB-C2B	-2.43	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	608	CHL	C3D-C2D	2.43	1.45	1.39
25	S	613	CLA	MG-ND	-2.43	2.01	2.05
25	1	604	CLA	CHC-C1C	2.43	1.41	1.35
24	9	601	CHL	C3D-C2D	2.43	1.45	1.39
25	a	407	CLA	CMD-C2D	-2.43	1.45	1.50
25	8	603	CLA	CMB-C2B	-2.43	1.46	1.51
25	n	603	CLA	CHC-C1C	2.42	1.41	1.35
25	q	610	CLA	CMB-C2B	-2.42	1.46	1.51
24	9	606	CHL	C1B-CHB	2.42	1.47	1.41
25	b	604	CLA	MG-ND	-2.42	2.01	2.05
25	8	613	CLA	CMB-C2B	-2.42	1.46	1.51
25	B	612	CLA	C3B-C2B	-2.42	1.37	1.40
25	b	612	CLA	C3B-C2B	-2.42	1.37	1.40
24	g	608	CHL	C3D-C2D	2.42	1.45	1.39
25	b	606	CLA	CMD-C2D	-2.42	1.45	1.50
24	5	607	CHL	C1D-C2D	2.42	1.50	1.45
24	q	606	CHL	C1B-CHB	2.42	1.47	1.41
24	G	607	CHL	C3D-C2D	2.42	1.45	1.39
24	3	607	CHL	C1D-C2D	2.42	1.50	1.45
33	a	409	PHO	CMC-C2C	-2.42	1.45	1.51
25	2	603	CLA	C3B-C2B	-2.42	1.37	1.40
24	p	609	CHL	MG-NA	-2.42	2.00	2.06
25	c	508	CLA	C3B-C2B	-2.42	1.37	1.40
24	9	608	CHL	C3D-C2D	2.42	1.45	1.39
24	6	608	CHL	C3D-C2D	2.42	1.45	1.39
25	n	602	CLA	C3B-C2B	-2.41	1.37	1.40
28	R	623	NEX	O24-C25	-2.41	1.42	1.46
25	A	410	CLA	C3B-C2B	-2.41	1.37	1.40
25	C	504	CLA	CMD-C2D	-2.41	1.45	1.50
25	Y	610	CLA	CMD-C2D	-2.41	1.45	1.50
25	9	610	CLA	CMC-C2C	-2.41	1.45	1.50
25	0	604	CLA	C3B-C2B	-2.41	1.37	1.40
24	g	601	CHL	MG-NA	-2.41	2.00	2.06
25	d	402	CLA	CMC-C2C	-2.41	1.45	1.50
24	0	607	CHL	C1D-C2D	2.41	1.50	1.45
25	a	405	CLA	C3B-CAB	-2.41	1.43	1.47
25	R	612	CLA	C3B-C2B	-2.41	1.37	1.40
25	b	602	CLA	C3B-CAB	-2.41	1.43	1.47
24	q	605	CHL	C4B-CHC	2.41	1.47	1.41
25	q	611	CLA	CMD-C2D	-2.41	1.45	1.50
25	c	510	CLA	MG-ND	-2.41	2.01	2.05
24	2	605	CHL	C1B-CHB	2.41	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	604	CLA	CHC-C1C	2.41	1.41	1.35
25	r	603	CLA	CHC-C1C	2.41	1.41	1.35
25	Y	610	CLA	C3B-C2B	-2.41	1.37	1.40
24	2	606	CHL	MG-NA	-2.40	2.00	2.06
25	q	613	CLA	CMB-C2B	-2.40	1.46	1.51
25	c	503	CLA	C3B-C2B	-2.40	1.37	1.40
25	N	603	CLA	MG-ND	-2.40	2.01	2.05
25	p	612	CLA	CMB-C2B	-2.40	1.46	1.51
25	R	603	CLA	C3B-C2B	-2.40	1.37	1.40
33	A	408	PHO	CMD-C2D	-2.40	1.45	1.51
25	c	507	CLA	CHC-C1C	2.40	1.41	1.35
25	C	507	CLA	CMD-C2D	-2.40	1.45	1.50
25	c	511	CLA	CMD-C2D	-2.40	1.45	1.50
25	c	501	CLA	MG-ND	-2.40	2.01	2.05
25	B	616	CLA	CHC-C1C	2.40	1.41	1.35
33	A	409	PHO	CMC-C2C	-2.40	1.45	1.51
25	C	510	CLA	MG-ND	-2.40	2.01	2.05
25	B	604	CLA	MG-ND	-2.40	2.01	2.05
25	a	407	CLA	CHC-C1C	2.40	1.41	1.35
25	C	501	CLA	CMC-C2C	-2.40	1.45	1.50
25	B	616	CLA	C4B-CHC	-2.40	1.34	1.41
25	2	610	CLA	CMC-C2C	-2.40	1.45	1.50
24	N	609	CHL	C1C-NC	-2.40	1.34	1.37
25	s	613	CLA	MG-ND	-2.40	2.01	2.05
25	A	407	CLA	CMD-C2D	-2.40	1.45	1.50
24	4	601	CHL	C4B-CHC	2.40	1.47	1.41
25	R	609	CLA	CMD-C2D	-2.40	1.45	1.50
25	r	609	CLA	CMD-C2D	-2.40	1.45	1.50
25	C	511	CLA	CMD-C2D	-2.40	1.45	1.50
24	p	606	CHL	C1B-CHB	2.39	1.47	1.41
25	n	610	CLA	C3B-C2B	-2.39	1.37	1.40
25	4	603	CLA	CMB-C2B	-2.39	1.46	1.51
25	4	610	CLA	CMB-C2B	-2.39	1.46	1.51
25	b	617	CLA	CMC-C2C	-2.39	1.45	1.50
25	R	603	CLA	CHC-C1C	2.39	1.41	1.35
24	4	607	CHL	C4C-C3C	2.39	1.49	1.45
25	N	603	CLA	CMD-C2D	-2.39	1.45	1.50
34	c	515	BCR	C30-C25	-2.39	1.50	1.53
24	G	601	CHL	MG-NA	-2.39	2.00	2.06
25	b	616	CLA	C4B-CHC	-2.39	1.34	1.41
25	b	603	CLA	CMD-C2D	-2.39	1.45	1.50
25	c	512	CLA	C3B-CAB	-2.39	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	606	CHL	C1B-CHB	2.39	1.47	1.41
25	9	610	CLA	CMB-C2B	-2.39	1.46	1.51
25	q	612	CLA	CMB-C2B	-2.39	1.46	1.51
25	c	507	CLA	MG-ND	-2.39	2.01	2.05
24	3	608	CHL	C3D-C2D	2.39	1.45	1.39
25	y	603	CLA	C3B-C2B	-2.39	1.37	1.40
25	C	509	CLA	CMD-C2D	-2.39	1.45	1.50
25	b	608	CLA	CMD-C2D	-2.39	1.45	1.50
25	B	602	CLA	C3B-CAB	-2.39	1.43	1.47
25	B	609	CLA	CMD-C2D	-2.39	1.45	1.50
24	G	606	CHL	C1D-C2D	2.39	1.50	1.45
24	9	605	CHL	C1B-CHB	2.39	1.47	1.41
25	R	603	CLA	CMD-C2D	-2.38	1.45	1.50
24	q	605	CHL	C1B-CHB	2.38	1.47	1.41
25	l	602	CLA	CMC-C2C	-2.38	1.45	1.50
25	B	611	CLA	CHC-C1C	2.38	1.41	1.35
25	Y	613	CLA	CMC-C2C	-2.38	1.45	1.50
25	c	504	CLA	CMC-C2C	-2.38	1.45	1.50
25	y	613	CLA	CMC-C2C	-2.38	1.45	1.50
24	p	608	CHL	C3D-C2D	2.38	1.45	1.39
25	D	403	CLA	C3B-C2B	-2.38	1.37	1.40
25	G	610	CLA	CMC-C2C	-2.38	1.45	1.50
25	Y	612	CLA	C3B-CAB	-2.38	1.43	1.47
24	5	606	CHL	C4C-C3C	2.38	1.49	1.45
25	Y	612	CLA	CMC-C2C	-2.38	1.45	1.50
24	5	606	CHL	C1B-CHB	2.38	1.47	1.41
25	r	601	CLA	CMB-C2B	-2.38	1.46	1.51
25	B	617	CLA	CMC-C2C	-2.38	1.45	1.50
25	a	406	CLA	CMD-C2D	-2.38	1.45	1.50
25	G	610	CLA	C3B-C2B	-2.38	1.37	1.40
25	9	603	CLA	C3B-C2B	-2.38	1.37	1.40
28	r	623	NEX	O24-C25	-2.38	1.42	1.46
25	S	614	CLA	CMD-C2D	-2.38	1.45	1.50
25	c	512	CLA	MG-ND	-2.38	2.01	2.05
24	8	608	CHL	C3D-C2D	2.38	1.45	1.39
25	r	603	CLA	CMD-C2D	-2.38	1.45	1.50
24	s	607	CHL	C4B-CHC	2.38	1.47	1.41
25	A	407	CLA	CHC-C1C	2.38	1.41	1.35
24	5	608	CHL	C3D-C2D	2.38	1.45	1.39
25	N	603	CLA	CHC-C1C	2.38	1.41	1.35
25	p	610	CLA	CMB-C2B	-2.38	1.46	1.51
25	Y	613	CLA	CMD-C2D	-2.38	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	601	CLA	CHC-C1C	2.38	1.41	1.35
25	y	611	CLA	C3B-CAB	-2.38	1.43	1.47
25	R	601	CLA	CHC-C1C	2.38	1.41	1.35
25	B	608	CLA	CMD-C2D	-2.38	1.45	1.50
25	g	610	CLA	CMC-C2C	-2.38	1.45	1.50
33	a	408	PHO	CMD-C2D	-2.37	1.45	1.51
25	Y	603	CLA	C3B-C2B	-2.37	1.37	1.40
25	7	602	CLA	CMC-C2C	-2.37	1.45	1.50
25	g	613	CLA	CMD-C2D	-2.37	1.45	1.50
25	Y	611	CLA	MG-ND	-2.37	2.01	2.05
25	g	602	CLA	CMC-C2C	-2.37	1.45	1.50
25	C	507	CLA	CHC-C1C	2.37	1.41	1.35
25	n	603	CLA	C4B-CHC	-2.37	1.34	1.41
25	s	614	CLA	CMD-C2D	-2.37	1.45	1.50
25	6	612	CLA	C3B-C2B	-2.37	1.37	1.40
25	q	610	CLA	C3B-C2B	-2.37	1.37	1.40
24	n	609	CHL	C1D-C2D	2.37	1.50	1.45
25	b	611	CLA	MG-ND	-2.37	2.01	2.05
25	0	603	CLA	CMD-C2D	-2.37	1.45	1.50
25	Y	611	CLA	C3B-CAB	-2.37	1.43	1.47
27	r	622	XAT	O4-C5	-2.37	1.42	1.46
25	n	603	CLA	MG-ND	-2.37	2.01	2.05
24	q	606	CHL	C2C-C1C	2.37	1.49	1.44
24	r	606	CHL	C1D-C2D	2.36	1.50	1.45
25	N	610	CLA	C3B-C2B	-2.36	1.37	1.40
24	y	609	CHL	C1B-NB	-2.36	1.33	1.35
24	8	606	CHL	C4B-CHC	2.36	1.47	1.41
25	2	613	CLA	CMB-C2B	-2.36	1.46	1.51
25	b	614	CLA	CMC-C2C	-2.36	1.45	1.50
25	1	614	CLA	CMD-C2D	-2.36	1.45	1.50
25	B	614	CLA	CMC-C2C	-2.36	1.45	1.50
25	7	611	CLA	CMD-C2D	-2.36	1.45	1.50
24	3	605	CHL	C4C-C3C	2.36	1.49	1.45
24	6	606	CHL	C3D-C2D	2.36	1.45	1.39
25	c	509	CLA	CMC-C2C	-2.36	1.45	1.50
25	A	405	CLA	C3B-CAB	-2.36	1.43	1.47
24	8	606	CHL	C4C-C3C	2.36	1.49	1.45
25	y	610	CLA	CMD-C2D	-2.36	1.45	1.50
25	R	601	CLA	CMB-C2B	-2.36	1.46	1.51
25	2	610	CLA	CMB-C2B	-2.36	1.46	1.51
24	N	605	CHL	C1D-C2D	2.36	1.50	1.45
25	C	504	CLA	CMC-C2C	-2.36	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	4	606	CHL	C2C-C1C	2.36	1.49	1.44
25	A	406	CLA	CMD-C2D	-2.36	1.45	1.50
25	b	616	CLA	CMD-C2D	-2.36	1.45	1.50
25	y	611	CLA	MG-ND	-2.36	2.01	2.05
25	y	610	CLA	C3B-C2B	-2.36	1.37	1.40
24	8	607	CHL	C3D-C2D	2.36	1.45	1.39
25	1	611	CLA	CMD-C2D	-2.36	1.45	1.50
25	b	611	CLA	CHC-C1C	2.36	1.41	1.35
24	n	607	CHL	C1D-ND	-2.36	1.34	1.37
24	S	607	CHL	C4B-CHC	2.36	1.47	1.41
25	B	615	CLA	CMC-C2C	-2.36	1.45	1.50
25	5	610	CLA	CMB-C2B	-2.36	1.46	1.51
24	9	608	CHL	MG-NA	-2.36	2.00	2.06
25	G	613	CLA	CMD-C2D	-2.36	1.45	1.50
25	s	611	CLA	CMD-C2D	-2.36	1.45	1.50
25	B	614	CLA	MG-ND	-2.35	2.01	2.05
24	3	606	CHL	C4B-CHC	2.35	1.47	1.41
24	R	606	CHL	C1D-C2D	2.35	1.50	1.45
24	8	605	CHL	C4C-C3C	2.35	1.49	1.45
25	y	610	CLA	CMC-C2C	-2.35	1.45	1.50
24	3	607	CHL	C3D-C2D	2.35	1.45	1.39
25	r	604	CLA	CMD-C2D	-2.35	1.45	1.50
24	q	606	CHL	C4C-C3C	2.35	1.49	1.45
25	G	602	CLA	CMC-C2C	-2.35	1.45	1.50
25	Y	610	CLA	CMC-C2C	-2.35	1.45	1.50
25	Y	614	CLA	CMD-C2D	-2.35	1.45	1.50
25	b	615	CLA	CMC-C2C	-2.35	1.45	1.50
25	b	614	CLA	MG-ND	-2.35	2.01	2.05
24	4	608	CHL	C1B-CHB	2.35	1.47	1.41
25	G	602	CLA	CMD-C2D	-2.35	1.45	1.50
25	c	502	CLA	CMD-C2D	-2.35	1.45	1.50
25	c	501	CLA	CHC-C1C	2.35	1.41	1.35
25	2	613	CLA	CMD-C2D	-2.35	1.45	1.50
25	n	603	CLA	CMD-C2D	-2.35	1.45	1.50
24	5	607	CHL	C4B-CHC	2.35	1.47	1.41
25	r	601	CLA	CMD-C2D	-2.35	1.45	1.50
24	s	601	CHL	C3D-C2D	2.35	1.45	1.39
25	6	603	CLA	C3B-C2B	-2.35	1.37	1.40
25	g	614	CLA	CMD-C2D	-2.35	1.45	1.50
24	n	609	CHL	C4B-NB	-2.35	1.33	1.35
25	C	501	CLA	MG-ND	-2.35	2.01	2.05
24	1	607	CHL	C3D-C2D	2.34	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	Y	1622	XAT	O24-C25	-2.34	1.42	1.46
25	n	602	CLA	CMD-C2D	-2.34	1.45	1.50
25	4	611	CLA	CMD-C2D	-2.34	1.45	1.50
25	g	610	CLA	C3B-C2B	-2.34	1.37	1.40
25	4	602	CLA	CMB-C2B	-2.34	1.46	1.51
27	n	1622	XAT	O4-C5	-2.34	1.42	1.46
25	B	617	CLA	CMD-C2D	-2.34	1.45	1.50
24	0	606	CHL	C3D-C2D	2.34	1.45	1.39
25	S	602	CLA	CMD-C2D	-2.34	1.45	1.50
25	r	604	CLA	C3B-C2B	-2.34	1.37	1.40
25	N	603	CLA	C4B-CHC	-2.34	1.34	1.41
25	y	612	CLA	CMC-C2C	-2.34	1.45	1.50
24	N	607	CHL	C4B-CHC	2.34	1.47	1.41
25	a	410	CLA	C3B-C2B	-2.34	1.37	1.40
25	9	613	CLA	CMB-C2B	-2.34	1.46	1.51
25	0	610	CLA	CMD-C2D	-2.34	1.45	1.50
25	y	612	CLA	C3B-CAB	-2.34	1.43	1.47
25	Y	603	CLA	CMC-C2C	-2.33	1.45	1.50
27	N	1622	XAT	O4-C5	-2.33	1.42	1.46
25	R	610	CLA	C3B-C2B	-2.33	1.37	1.40
25	a	410	CLA	CMC-C2C	-2.33	1.45	1.50
24	Y	609	CHL	C1B-NB	-2.33	1.33	1.35
24	2	608	CHL	MG-NA	-2.33	2.00	2.06
24	y	601	CHL	C1D-ND	-2.33	1.34	1.37
25	9	611	CLA	CMD-C2D	-2.33	1.45	1.50
25	4	614	CLA	CMD-C2D	-2.33	1.45	1.50
25	R	604	CLA	CMD-C2D	-2.33	1.45	1.50
25	7	614	CLA	CMD-C2D	-2.33	1.45	1.50
25	Y	603	CLA	CMD-C2D	-2.33	1.45	1.50
25	7	603	CLA	MG-ND	-2.33	2.01	2.05
24	2	606	CHL	C1B-CHB	2.33	1.47	1.41
25	c	503	CLA	CMD-C2D	-2.33	1.45	1.50
25	6	614	CLA	CMB-C2B	-2.33	1.46	1.51
24	S	601	CHL	C4B-CHC	2.33	1.47	1.41
25	D	403	CLA	C3B-CAB	-2.33	1.43	1.47
25	b	606	CLA	CMC-C2C	-2.33	1.45	1.50
25	B	611	CLA	MG-ND	-2.32	2.01	2.05
25	B	616	CLA	CMD-C2D	-2.32	1.45	1.50
25	A	410	CLA	MG-ND	-2.32	2.01	2.05
25	c	511	CLA	CMC-C2C	-2.32	1.45	1.50
25	G	612	CLA	CMD-C2D	-2.32	1.45	1.50
25	c	509	CLA	C3B-C2B	-2.32	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	603	CLA	CMD-C2D	-2.32	1.45	1.50
25	R	601	CLA	CMD-C2D	-2.32	1.45	1.50
25	9	613	CLA	CMD-C2D	-2.32	1.45	1.50
25	b	605	CLA	CMC-C2C	-2.32	1.45	1.50
24	q	609	CHL	C4C-C3C	2.32	1.49	1.45
25	B	606	CLA	CMC-C2C	-2.32	1.45	1.50
24	7	607	CHL	C3D-C2D	2.32	1.45	1.39
25	0	614	CLA	CMB-C2B	-2.32	1.46	1.51
25	S	611	CLA	CMD-C2D	-2.32	1.45	1.50
25	A	410	CLA	CMC-C2C	-2.32	1.45	1.50
24	s	601	CHL	C4B-CHC	2.32	1.47	1.41
25	n	611	CLA	CMD-C2D	-2.32	1.45	1.50
25	q	614	CLA	CMD-C2D	-2.32	1.45	1.50
25	B	609	CLA	C3B-CAB	-2.32	1.43	1.47
25	b	609	CLA	C3B-CAB	-2.32	1.43	1.47
25	C	502	CLA	CMD-C2D	-2.32	1.45	1.50
25	b	609	CLA	CMC-C2C	-2.31	1.45	1.50
25	n	613	CLA	CMD-C2D	-2.31	1.45	1.50
27	R	622	XAT	O4-C5	-2.31	1.42	1.46
25	y	603	CLA	CMC-C2C	-2.31	1.45	1.50
25	y	613	CLA	CMD-C2D	-2.31	1.45	1.50
25	B	605	CLA	CMC-C2C	-2.31	1.45	1.50
25	r	610	CLA	CMD-C2D	-2.31	1.45	1.50
25	7	613	CLA	CMD-C2D	-2.31	1.45	1.50
34	b	620	BCR	C1-C6	-2.31	1.50	1.53
25	C	503	CLA	CMD-C2D	-2.31	1.45	1.50
25	y	614	CLA	CMD-C2D	-2.31	1.45	1.50
24	n	607	CHL	C4B-CHC	2.31	1.47	1.41
34	B	620	BCR	C1-C6	-2.31	1.50	1.53
25	C	511	CLA	CMC-C2C	-2.31	1.45	1.50
24	3	606	CHL	C4C-C3C	2.31	1.49	1.45
25	G	613	CLA	C4B-CHC	-2.31	1.34	1.41
25	2	602	CLA	CMD-C2D	-2.31	1.45	1.50
25	6	603	CLA	CMD-C2D	-2.31	1.45	1.50
25	C	509	CLA	C3B-C2B	-2.31	1.37	1.40
25	R	616	CLA	CMD-C2D	-2.30	1.45	1.50
24	7	607	CHL	C4B-CHC	2.30	1.47	1.41
25	B	607	CLA	CMC-C2C	-2.30	1.45	1.50
25	N	611	CLA	CMD-C2D	-2.30	1.45	1.50
25	g	602	CLA	CMD-C2D	-2.30	1.45	1.50
24	5	608	CHL	MG-NA	-2.30	2.00	2.06
24	N	607	CHL	C1D-ND	-2.30	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	602	CLA	CMD-C2D	-2.30	1.45	1.50
24	g	607	CHL	C3D-C2D	2.30	1.45	1.39
27	g	1622	XAT	O4-C5	-2.30	1.42	1.46
25	N	604	CLA	CMD-C2D	-2.30	1.45	1.50
25	6	610	CLA	CMD-C2D	-2.30	1.45	1.50
25	q	604	CLA	C3B-C2B	-2.30	1.37	1.40
25	6	613	CLA	CMD-C2D	-2.30	1.45	1.50
24	0	601	CHL	C1D-C2D	2.30	1.49	1.45
25	S	613	CLA	CMD-C2D	-2.30	1.45	1.50
25	s	613	CLA	CMD-C2D	-2.30	1.45	1.50
24	p	607	CHL	C4B-CHC	2.30	1.47	1.41
27	Y	1622	XAT	O4-C5	-2.30	1.42	1.46
25	b	617	CLA	CMD-C2D	-2.30	1.45	1.50
25	A	406	CLA	C4B-CHC	-2.30	1.34	1.41
25	C	501	CLA	C4B-CHC	-2.30	1.34	1.41
25	C	509	CLA	CMC-C2C	-2.30	1.45	1.50
26	R	620	LUT	C1-C6	-2.30	1.50	1.53
25	B	603	CLA	C3B-C2B	-2.30	1.37	1.40
25	G	614	CLA	CMD-C2D	-2.30	1.45	1.50
25	q	602	CLA	CMB-C2B	-2.29	1.46	1.51
24	q	601	CHL	C4B-CHC	2.29	1.47	1.41
24	q	607	CHL	C1B-CHB	2.29	1.47	1.41
25	B	609	CLA	CMC-C2C	-2.29	1.45	1.50
25	r	616	CLA	CMD-C2D	-2.29	1.45	1.50
24	N	606	CHL	C1D-C2D	2.29	1.49	1.45
24	S	608	CHL	C4C-C3C	2.29	1.49	1.45
25	y	614	CLA	C3B-CAB	-2.29	1.43	1.47
25	n	612	CLA	CMD-C2D	-2.29	1.45	1.50
24	1	606	CHL	C3D-C2D	2.29	1.45	1.39
24	1	609	CHL	C3D-C2D	2.29	1.45	1.39
25	C	506	CLA	CMC-C2C	-2.29	1.45	1.50
25	9	614	CLA	C3B-C2B	-2.29	1.37	1.40
25	g	614	CLA	C3B-C2B	-2.29	1.37	1.40
25	7	612	CLA	CMD-C2D	-2.29	1.45	1.50
24	1	606	CHL	C4B-CHC	2.29	1.47	1.41
25	b	607	CLA	CMC-C2C	-2.29	1.45	1.50
25	Y	603	CLA	CHC-C1C	2.29	1.40	1.35
24	0	606	CHL	C1B-CHB	2.29	1.47	1.41
25	B	616	CLA	MG-ND	-2.29	2.01	2.05
25	N	613	CLA	CMD-C2D	-2.29	1.45	1.50
24	s	607	CHL	C1B-CHB	2.29	1.47	1.41
24	Y	601	CHL	C1D-ND	-2.29	1.35	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	607	CHL	C4B-CHC	2.29	1.47	1.41
25	4	610	CLA	C3B-C2B	-2.29	1.37	1.40
25	5	603	CLA	CMD-C2D	-2.29	1.46	1.50
25	Y	614	CLA	C3B-CAB	-2.29	1.43	1.47
24	n	605	CHL	C1D-C2D	2.29	1.49	1.45
25	B	616	CLA	CMC-C2C	-2.29	1.46	1.50
25	B	612	CLA	MG-ND	-2.29	2.01	2.05
25	b	612	CLA	MG-ND	-2.29	2.01	2.05
24	7	606	CHL	C3D-C2D	2.28	1.45	1.39
24	p	608	CHL	MG-NA	-2.28	2.00	2.06
24	6	606	CHL	C1B-CHB	2.28	1.47	1.41
25	g	613	CLA	C4B-CHC	-2.28	1.34	1.41
25	4	610	CLA	CMC-C2C	-2.28	1.46	1.50
25	s	605	CLA	CMD-C2D	-2.28	1.46	1.50
25	a	406	CLA	C4B-CHC	-2.28	1.34	1.41
28	8	1623	NEX	C7-C8	-2.28	1.28	1.32
25	8	602	CLA	CMD-C2D	-2.28	1.46	1.50
25	y	603	CLA	CHC-C1C	2.28	1.40	1.35
27	y	1622	XAT	O4-C5	-2.28	1.42	1.46
25	p	613	CLA	C3B-C2B	-2.28	1.37	1.40
25	B	608	CLA	CMC-C2C	-2.28	1.46	1.50
25	S	605	CLA	CMD-C2D	-2.28	1.46	1.50
25	1	603	CLA	MG-ND	-2.28	2.01	2.05
25	a	407	CLA	C3B-C2B	-2.28	1.37	1.40
25	y	603	CLA	CMD-C2D	-2.28	1.46	1.50
24	N	609	CHL	C1D-C2D	2.28	1.49	1.45
25	2	614	CLA	C3B-C2B	-2.28	1.37	1.40
24	3	609	CHL	C1C-NC	-2.28	1.34	1.37
25	c	501	CLA	C4B-CHC	-2.28	1.34	1.41
24	7	609	CHL	C3D-C2D	2.28	1.45	1.39
24	3	606	CHL	C1B-CHB	2.28	1.47	1.41
25	r	611	CLA	C3B-C2B	-2.28	1.37	1.40
25	b	602	CLA	CMC-C2C	-2.28	1.46	1.50
24	5	609	CHL	C1B-CHB	2.28	1.47	1.41
24	7	607	CHL	C1D-C2D	2.28	1.49	1.45
25	S	605	CLA	C3B-C2B	-2.28	1.37	1.40
25	1	613	CLA	CMD-C2D	-2.27	1.46	1.50
25	g	612	CLA	CMD-C2D	-2.27	1.46	1.50
25	B	602	CLA	CMD-C2D	-2.27	1.46	1.50
27	y	1622	XAT	O24-C25	-2.27	1.43	1.46
25	B	613	CLA	MG-ND	-2.27	2.01	2.05
25	b	613	CLA	MG-ND	-2.27	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	614	CLA	CMD-C2D	-2.27	1.46	1.50
24	4	607	CHL	C1B-CHB	2.27	1.47	1.41
25	D	402	CLA	C1D-ND	2.27	1.40	1.37
25	2	611	CLA	CMD-C2D	-2.27	1.46	1.50
25	R	602	CLA	C3B-CAB	-2.27	1.43	1.47
24	8	606	CHL	C1B-CHB	2.27	1.47	1.41
25	c	511	CLA	C3B-C2B	-2.27	1.37	1.40
34	C	515	BCR	C1-C6	-2.27	1.50	1.53
25	B	610	CLA	C3B-C2B	-2.27	1.37	1.40
25	9	612	CLA	CMD-C2D	-2.27	1.46	1.50
25	d	402	CLA	C1D-ND	2.27	1.40	1.37
25	Y	602	CLA	CMD-C2D	-2.27	1.46	1.50
25	a	410	CLA	MG-ND	-2.27	2.01	2.05
27	G	1622	XAT	O4-C5	-2.27	1.43	1.46
25	b	603	CLA	C3B-C2B	-2.27	1.37	1.40
25	b	616	CLA	MG-ND	-2.27	2.01	2.05
25	A	406	CLA	MG-ND	-2.27	2.01	2.05
25	D	403	CLA	CMD-C2D	-2.27	1.46	1.50
25	g	611	CLA	CMD-C2D	-2.27	1.46	1.50
25	C	509	CLA	MG-ND	-2.27	2.01	2.05
25	N	602	CLA	C3B-CAB	-2.27	1.43	1.47
25	G	612	CLA	C3B-CAB	-2.27	1.43	1.47
25	R	610	CLA	CMD-C2D	-2.27	1.46	1.50
25	S	613	CLA	C3B-CAB	-2.27	1.43	1.47
24	s	608	CHL	C4C-C3C	2.26	1.48	1.45
25	d	403	CLA	C3B-CAB	-2.26	1.43	1.47
25	3	603	CLA	MG-ND	-2.26	2.01	2.05
25	c	506	CLA	CMC-C2C	-2.26	1.46	1.50
24	G	606	CHL	C3D-C2D	2.26	1.45	1.39
25	p	603	CLA	CMD-C2D	-2.26	1.46	1.50
24	4	606	CHL	C4C-C3C	2.26	1.48	1.45
24	2	601	CHL	C3D-C2D	2.26	1.45	1.39
25	c	506	CLA	CMD-C2D	-2.26	1.46	1.50
24	6	607	CHL	C4C-C3C	2.26	1.48	1.45
24	y	601	CHL	C1D-C2D	2.26	1.49	1.45
25	6	610	CLA	C3B-C2B	-2.26	1.37	1.40
25	Y	613	CLA	C3B-CAB	-2.26	1.43	1.47
25	y	604	CLA	C4B-CHC	-2.26	1.34	1.41
25	1	612	CLA	CMD-C2D	-2.26	1.46	1.50
24	S	607	CHL	C1B-CHB	2.26	1.47	1.41
25	s	605	CLA	C3B-C2B	-2.26	1.37	1.40
24	g	606	CHL	C3D-C2D	2.26	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	606	CHL	C4C-C3C	2.26	1.48	1.45
25	y	602	CLA	CMD-C2D	-2.26	1.46	1.50
25	n	602	CLA	C3B-CAB	-2.26	1.43	1.47
25	G	610	CLA	CMD-C2D	-2.26	1.46	1.50
25	c	509	CLA	MG-ND	-2.26	2.01	2.05
26	r	620	LUT	C1-C6	-2.26	1.50	1.53
25	n	604	CLA	CMD-C2D	-2.25	1.46	1.50
26	Y	1621	LUT	C22-C21	-2.25	1.51	1.54
25	b	616	CLA	CMC-C2C	-2.25	1.46	1.50
25	3	603	CLA	CMD-C2D	-2.25	1.46	1.50
25	N	612	CLA	CMD-C2D	-2.25	1.46	1.50
25	c	503	CLA	CMC-C2C	-2.25	1.46	1.50
25	7	614	CLA	C3B-C2B	-2.25	1.37	1.40
25	2	603	CLA	CMD-C2D	-2.25	1.46	1.50
25	G	611	CLA	CMD-C2D	-2.25	1.46	1.50
24	1	607	CHL	C1D-C2D	2.25	1.49	1.45
25	G	604	CLA	CMD-C2D	-2.25	1.46	1.50
25	C	501	CLA	CHC-C1C	2.25	1.40	1.35
24	2	607	CHL	C4B-CHC	2.25	1.47	1.41
25	1	614	CLA	C3B-C2B	-2.25	1.37	1.40
25	0	610	CLA	C3B-C2B	-2.25	1.37	1.40
25	b	610	CLA	C3B-C2B	-2.25	1.37	1.40
33	A	408	PHO	C3B-CAB	-2.25	1.43	1.47
33	a	408	PHO	C3B-CAB	-2.25	1.43	1.47
25	d	403	CLA	CMD-C2D	-2.25	1.46	1.50
25	C	502	CLA	MG-ND	-2.25	2.01	2.05
25	q	611	CLA	CMC-C2C	-2.25	1.46	1.50
24	5	608	CHL	C4B-CHC	2.25	1.47	1.41
25	B	603	CLA	CMC-C2C	-2.25	1.46	1.50
25	a	407	CLA	MG-ND	-2.25	2.01	2.05
25	b	603	CLA	CMC-C2C	-2.25	1.46	1.50
25	A	407	CLA	MG-ND	-2.25	2.01	2.05
25	C	506	CLA	CMD-C2D	-2.24	1.46	1.50
25	G	611	CLA	CMC-C2C	-2.24	1.46	1.50
25	g	611	CLA	CMC-C2C	-2.24	1.46	1.50
24	3	608	CHL	C4B-CHC	2.24	1.47	1.41
24	9	606	CHL	C4C-C3C	2.24	1.48	1.45
25	g	613	CLA	MG-ND	-2.24	2.01	2.05
25	b	608	CLA	CMC-C2C	-2.24	1.46	1.50
34	c	515	BCR	C1-C6	-2.24	1.50	1.53
24	G	605	CHL	C1B-CHB	2.24	1.47	1.41
24	2	606	CHL	C4B-CHC	2.24	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	C	506	CLA	C3B-CAB	-2.24	1.43	1.47
24	g	609	CHL	MG-ND	-2.24	2.01	2.05
25	B	609	CLA	C3B-C2B	-2.24	1.37	1.40
25	b	609	CLA	C3B-C2B	-2.24	1.37	1.40
25	B	614	CLA	CMD-C2D	-2.24	1.46	1.50
25	b	614	CLA	CMD-C2D	-2.24	1.46	1.50
25	s	612	CLA	CMD-C2D	-2.24	1.46	1.50
25	r	610	CLA	C3B-C2B	-2.24	1.37	1.40
25	s	602	CLA	CMD-C2D	-2.24	1.46	1.50
25	3	602	CLA	CMD-C2D	-2.24	1.46	1.50
25	B	602	CLA	CMC-C2C	-2.24	1.46	1.50
25	b	602	CLA	CMD-C2D	-2.24	1.46	1.50
24	7	606	CHL	C4B-CHC	2.24	1.47	1.41
25	2	612	CLA	CMD-C2D	-2.24	1.46	1.50
25	R	604	CLA	CMC-C2C	-2.24	1.46	1.50
25	R	601	CLA	C3B-C2B	-2.24	1.37	1.40
25	R	604	CLA	C3B-C2B	-2.24	1.37	1.40
24	0	601	CHL	C4B-CHC	2.24	1.47	1.41
25	S	602	CLA	C3B-C2B	-2.24	1.37	1.40
25	c	513	CLA	C3B-C2B	-2.24	1.37	1.40
24	N	609	CHL	C3D-C2D	2.24	1.45	1.39
25	C	511	CLA	C4B-CHC	-2.23	1.34	1.41
25	c	511	CLA	C4B-CHC	-2.23	1.34	1.41
24	6	608	CHL	C4B-CHC	2.23	1.47	1.41
25	s	602	CLA	C3B-C2B	-2.23	1.37	1.40
25	S	612	CLA	CMD-C2D	-2.23	1.46	1.50
25	y	613	CLA	C3B-CAB	-2.23	1.43	1.47
27	r	622	XAT	O24-C25	-2.23	1.43	1.46
25	A	405	CLA	MG-ND	-2.23	2.01	2.05
25	a	405	CLA	MG-ND	-2.23	2.01	2.05
25	R	611	CLA	CMC-C2C	-2.23	1.46	1.50
24	G	609	CHL	MG-ND	-2.23	2.01	2.05
25	c	502	CLA	MG-ND	-2.23	2.01	2.05
24	9	607	CHL	C4B-CHC	2.23	1.47	1.41
25	Y	604	CLA	C4B-CHC	-2.23	1.34	1.41
25	C	503	CLA	CMC-C2C	-2.23	1.46	1.50
25	b	606	CLA	MG-ND	-2.23	2.01	2.05
25	r	602	CLA	C3B-CAB	-2.23	1.43	1.47
25	0	603	CLA	C3B-C2B	-2.23	1.37	1.40
24	R	607	CHL	C3D-C2D	2.23	1.45	1.39
25	R	602	CLA	CMD-C2D	-2.23	1.46	1.50
25	s	609	CLA	C3B-C2B	-2.23	1.37	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	612	CLA	C3B-C2B	-2.23	1.37	1.40
25	A	410	CLA	CMD-C2D	-2.23	1.46	1.50
25	a	410	CLA	CMD-C2D	-2.23	1.46	1.50
25	C	511	CLA	C3B-C2B	-2.23	1.37	1.40
25	y	611	CLA	CMC-C2C	-2.23	1.46	1.50
24	3	607	CHL	C4B-CHC	2.22	1.47	1.41
25	G	613	CLA	MG-ND	-2.22	2.01	2.05
25	a	406	CLA	MG-ND	-2.22	2.01	2.05
25	y	603	CLA	C4B-CHC	-2.22	1.34	1.41
25	D	403	CLA	CMC-C2C	-2.22	1.46	1.50
25	B	610	CLA	MG-ND	-2.22	2.01	2.05
25	8	603	CLA	MG-ND	-2.22	2.01	2.05
24	1	608	CHL	C3D-C2D	2.22	1.45	1.39
25	s	613	CLA	C3B-CAB	-2.22	1.43	1.47
25	7	603	CLA	CMD-C2D	-2.22	1.46	1.50
25	y	602	CLA	CMC-C2C	-2.22	1.46	1.50
25	4	612	CLA	C3B-C2B	-2.22	1.37	1.40
24	N	608	CHL	C1D-C2D	2.22	1.49	1.45
24	n	609	CHL	C3D-C2D	2.22	1.45	1.39
24	1	608	CHL	C4B-CHC	2.22	1.47	1.41
24	1	609	CHL	C1D-C2D	2.22	1.49	1.45
25	n	602	CLA	CMC-C2C	-2.22	1.46	1.50
25	A	405	CLA	C3B-C2B	-2.22	1.37	1.40
25	a	405	CLA	C3B-C2B	-2.22	1.37	1.40
24	6	605	CHL	C4B-CHC	2.22	1.47	1.41
24	g	609	CHL	C1B-NB	-2.22	1.33	1.35
24	9	606	CHL	C4B-CHC	2.22	1.47	1.41
25	c	504	CLA	C3B-CAB	-2.22	1.43	1.47
25	Y	602	CLA	CMC-C2C	-2.22	1.46	1.50
25	r	611	CLA	CMC-C2C	-2.22	1.46	1.50
24	n	606	CHL	C1D-C2D	2.22	1.49	1.45
25	A	407	CLA	C3B-CAB	-2.22	1.43	1.47
24	8	608	CHL	C4B-CHC	2.22	1.47	1.41
24	n	606	CHL	C4B-CHC	2.22	1.47	1.41
25	a	407	CLA	C4B-CHC	-2.22	1.34	1.41
24	4	609	CHL	MG-ND	-2.22	2.01	2.05
25	A	407	CLA	C3B-C2B	-2.22	1.37	1.40
25	S	609	CLA	C3B-C2B	-2.22	1.37	1.40
24	Y	601	CHL	C1D-C2D	2.22	1.49	1.45
24	n	609	CHL	C1C-NC	-2.22	1.34	1.37
25	Y	604	CLA	CMC-C2C	-2.22	1.46	1.50
25	Y	614	CLA	CMC-C2C	-2.22	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	604	CLA	CMC-C2C	-2.22	1.46	1.50
25	y	614	CLA	CMC-C2C	-2.22	1.46	1.50
24	1	605	CHL	C1B-CHB	2.21	1.47	1.41
25	Y	603	CLA	C4B-CHC	-2.21	1.34	1.41
33	a	409	PHO	C1C-NC	-2.21	1.31	1.38
25	R	603	CLA	C3B-CAB	-2.21	1.43	1.47
24	Y	606	CHL	C1C-NC	-2.21	1.34	1.37
25	b	615	CLA	MG-ND	-2.21	2.01	2.05
25	G	614	CLA	CMC-C2C	-2.21	1.46	1.50
24	9	607	CHL	C4C-C3C	2.21	1.48	1.45
25	G	614	CLA	C3B-C2B	-2.21	1.37	1.40
25	R	611	CLA	C3B-C2B	-2.21	1.37	1.40
25	n	613	CLA	C3B-CAB	-2.21	1.43	1.47
24	0	606	CHL	C4B-CHC	2.21	1.47	1.41
24	y	607	CHL	C4B-CHC	2.21	1.47	1.41
24	Y	601	CHL	C1C-NC	-2.21	1.34	1.37
25	R	616	CLA	CMC-C2C	-2.21	1.46	1.50
25	g	614	CLA	CMC-C2C	-2.21	1.46	1.50
24	8	609	CHL	C1C-NC	-2.21	1.34	1.37
25	6	604	CLA	CMD-C2D	-2.21	1.46	1.50
25	C	512	CLA	CMC-C2C	-2.21	1.46	1.50
24	7	606	CHL	C1B-CHB	2.21	1.47	1.41
25	6	611	CLA	CMD-C2D	-2.21	1.46	1.50
25	c	506	CLA	C3B-CAB	-2.21	1.43	1.47
24	0	605	CHL	C4B-CHC	2.21	1.47	1.41
25	9	612	CLA	C3B-C2B	-2.21	1.37	1.40
25	2	602	CLA	MG-ND	-2.21	2.01	2.05
25	g	610	CLA	CMD-C2D	-2.21	1.46	1.50
24	q	609	CHL	C2C-C1C	2.21	1.49	1.44
25	q	610	CLA	C3B-CAB	-2.21	1.43	1.47
24	8	607	CHL	C4B-CHC	2.21	1.47	1.41
24	p	608	CHL	C4B-CHC	2.21	1.47	1.41
25	7	604	CLA	C4B-CHC	-2.20	1.34	1.41
25	q	612	CLA	CMD-C2D	-2.20	1.46	1.50
25	g	612	CLA	C3B-CAB	-2.20	1.43	1.47
24	N	609	CHL	C4B-NB	-2.20	1.33	1.35
24	2	608	CHL	C2C-C1C	2.20	1.49	1.44
27	N	1622	XAT	C22-C21	-2.20	1.51	1.54
25	0	611	CLA	CMD-C2D	-2.20	1.46	1.50
25	C	505	CLA	CMC-C2C	-2.20	1.46	1.50
25	C	513	CLA	C3B-C2B	-2.20	1.37	1.40
25	R	611	CLA	CMD-C2D	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	B	609	CLA	MG-ND	-2.20	2.01	2.05
25	b	609	CLA	MG-ND	-2.20	2.01	2.05
25	b	610	CLA	MG-ND	-2.20	2.01	2.05
25	c	507	CLA	C3B-CAB	-2.20	1.43	1.47
25	S	613	CLA	CMC-C2C	-2.20	1.46	1.50
24	Y	607	CHL	C4B-CHC	2.20	1.47	1.41
25	a	410	CLA	C3B-CAB	-2.20	1.43	1.47
25	1	611	CLA	MG-ND	-2.20	2.01	2.05
25	3	613	CLA	CMD-C2D	-2.20	1.46	1.50
25	R	612	CLA	CMD-C2D	-2.20	1.46	1.50
25	a	407	CLA	C3B-CAB	-2.20	1.43	1.47
25	A	407	CLA	C4B-CHC	-2.20	1.34	1.41
25	r	601	CLA	C3B-C2B	-2.20	1.37	1.40
25	Y	611	CLA	CMC-C2C	-2.20	1.46	1.50
25	B	606	CLA	MG-ND	-2.20	2.01	2.05
25	r	603	CLA	MG-ND	-2.20	2.01	2.05
25	4	604	CLA	CMC-C2C	-2.20	1.46	1.50
25	n	603	CLA	CMC-C2C	-2.20	1.46	1.50
25	r	611	CLA	CMD-C2D	-2.20	1.46	1.50
24	7	605	CHL	C1B-CHB	2.20	1.47	1.41
24	p	609	CHL	C1B-CHB	2.20	1.47	1.41
25	r	616	CLA	CMC-C2C	-2.20	1.46	1.50
33	A	409	PHO	C1C-NC	-2.20	1.31	1.38
25	8	610	CLA	CMD-C2D	-2.20	1.46	1.50
24	g	601	CHL	C1D-C2D	2.20	1.49	1.45
25	d	403	CLA	CMC-C2C	-2.20	1.46	1.50
25	r	603	CLA	C4B-CHC	-2.20	1.34	1.41
24	r	607	CHL	C3D-C2D	2.20	1.45	1.39
25	q	613	CLA	CMD-C2D	-2.19	1.46	1.50
24	y	606	CHL	C1C-NC	-2.19	1.34	1.37
25	4	612	CLA	CMD-C2D	-2.19	1.46	1.50
25	c	505	CLA	CMC-C2C	-2.19	1.46	1.50
25	b	603	CLA	C3B-CAB	-2.19	1.43	1.47
24	2	607	CHL	C4C-C3C	2.19	1.48	1.45
25	0	604	CLA	C3B-CAB	-2.19	1.43	1.47
25	c	508	CLA	C3B-CAB	-2.19	1.43	1.47
25	b	611	CLA	C4B-CHC	-2.19	1.34	1.41
25	7	611	CLA	MG-ND	-2.19	2.01	2.05
25	C	507	CLA	C4B-CHC	-2.19	1.34	1.41
25	1	602	CLA	CMD-C2D	-2.19	1.46	1.50
25	c	510	CLA	CMC-C2C	-2.19	1.46	1.50
25	g	604	CLA	CMD-C2D	-2.19	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	607	CHL	C1B-CHB	2.19	1.47	1.41
25	n	613	CLA	CMC-C2C	-2.19	1.46	1.50
25	n	603	CLA	CAC-C3C	-2.19	1.45	1.51
25	B	611	CLA	C4B-CHC	-2.19	1.34	1.41
25	N	603	CLA	CMC-C2C	-2.19	1.46	1.50
25	8	603	CLA	CMD-C2D	-2.19	1.46	1.50
25	c	501	CLA	CMC-C2C	-2.19	1.46	1.50
25	c	512	CLA	CMC-C2C	-2.19	1.46	1.50
25	B	610	CLA	C4B-CHC	-2.19	1.34	1.41
25	2	602	CLA	CMC-C2C	-2.19	1.46	1.50
25	n	610	CLA	CMD-C2D	-2.19	1.46	1.50
25	r	604	CLA	CMC-C2C	-2.19	1.46	1.50
24	g	605	CHL	C1B-CHB	2.19	1.47	1.41
25	4	602	CLA	CMC-C2C	-2.19	1.46	1.50
25	r	611	CLA	C3B-CAB	-2.18	1.43	1.47
24	2	601	CHL	C4C-C3C	2.18	1.48	1.45
24	q	608	CHL	C4C-C3C	2.18	1.48	1.45
25	8	613	CLA	CMD-C2D	-2.18	1.46	1.50
25	B	605	CLA	C3B-CAB	-2.18	1.43	1.47
25	r	601	CLA	C4B-CHC	-2.18	1.34	1.41
25	R	603	CLA	MG-ND	-2.18	2.01	2.05
24	n	607	CHL	C1D-C2D	2.18	1.49	1.45
25	2	611	CLA	MG-ND	-2.18	2.01	2.05
24	n	606	CHL	C3D-C2D	2.18	1.45	1.39
24	G	609	CHL	C1B-NB	-2.18	1.33	1.35
25	3	610	CLA	CMD-C2D	-2.18	1.46	1.50
25	R	602	CLA	CMC-C2C	-2.18	1.46	1.50
25	y	613	CLA	C4B-CHC	-2.18	1.34	1.41
24	R	607	CHL	C1D-ND	-2.18	1.35	1.37
25	4	611	CLA	CMC-C2C	-2.18	1.46	1.50
25	n	604	CLA	CMC-C2C	-2.18	1.46	1.50
24	2	605	CHL	C4D-CHA	2.18	1.46	1.38
24	N	606	CHL	C3D-C2D	2.18	1.45	1.39
25	D	402	CLA	C3B-CAB	-2.18	1.43	1.47
25	d	402	CLA	C3B-CAB	-2.18	1.43	1.47
24	p	608	CHL	C4C-C3C	2.18	1.48	1.45
25	r	602	CLA	CMD-C2D	-2.18	1.46	1.50
25	C	504	CLA	C3B-CAB	-2.18	1.43	1.47
25	N	613	CLA	C3B-CAB	-2.18	1.43	1.47
24	4	608	CHL	C4C-C3C	2.18	1.48	1.45
25	B	615	CLA	MG-ND	-2.18	2.01	2.05
25	S	612	CLA	MG-ND	-2.18	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	604	CLA	C3B-C2B	-2.18	1.37	1.40
24	9	609	CHL	CMC-C2C	2.18	1.49	1.45
25	S	602	CLA	CMC-C2C	-2.18	1.46	1.50
25	b	610	CLA	C4B-CHC	-2.18	1.34	1.41
25	9	611	CLA	MG-ND	-2.18	2.01	2.05
25	c	502	CLA	CHC-C1C	2.18	1.40	1.35
24	N	605	CHL	C3D-C2D	2.18	1.45	1.39
25	C	502	CLA	CHC-C1C	2.18	1.40	1.35
25	N	603	CLA	CAC-C3C	-2.17	1.45	1.51
24	G	601	CHL	C1D-C2D	2.17	1.49	1.45
25	7	611	CLA	C3B-C2B	-2.17	1.37	1.40
25	9	603	CLA	CMD-C2D	-2.17	1.46	1.50
24	r	607	CHL	C1D-ND	-2.17	1.35	1.37
25	7	602	CLA	CMD-C2D	-2.17	1.46	1.50
24	y	601	CHL	C1C-NC	-2.17	1.34	1.37
25	c	513	CLA	CMC-C2C	-2.17	1.46	1.50
33	A	408	PHO	CBD-CGD	-2.17	1.49	1.52
25	R	603	CLA	C4B-CHC	-2.17	1.35	1.41
25	R	611	CLA	C3B-CAB	-2.17	1.43	1.47
28	1	1623	NEX	O24-C25	-2.17	1.43	1.46
25	R	613	CLA	C4B-CHC	-2.17	1.35	1.41
25	B	610	CLA	CMC-C2C	-2.17	1.46	1.50
25	N	602	CLA	CMC-C2C	-2.17	1.46	1.50
25	p	610	CLA	CMD-C2D	-2.17	1.46	1.50
25	1	610	CLA	C3B-C2B	-2.17	1.37	1.40
33	a	409	PHO	CMB-C2B	-2.17	1.46	1.51
24	2	608	CHL	C4B-CHC	2.17	1.47	1.41
25	r	612	CLA	CMD-C2D	-2.17	1.46	1.50
24	9	607	CHL	C1B-CHB	2.17	1.47	1.41
25	b	615	CLA	C3B-CAB	-2.17	1.43	1.47
25	r	613	CLA	C3B-CAB	-2.17	1.43	1.47
24	N	607	CHL	C1D-C2D	2.17	1.49	1.45
25	5	604	CLA	C3B-C2B	-2.17	1.37	1.40
24	0	608	CHL	C4B-CHC	2.17	1.47	1.41
25	B	608	CLA	C4B-CHC	-2.17	1.35	1.41
25	r	610	CLA	C3B-CAB	-2.17	1.43	1.47
25	q	604	CLA	CMC-C2C	-2.17	1.46	1.50
25	N	613	CLA	CMC-C2C	-2.17	1.46	1.50
24	y	608	CHL	C4B-CHC	2.17	1.47	1.41
25	C	509	CLA	C4B-CHC	-2.16	1.35	1.41
26	N	1621	LUT	C22-C21	-2.16	1.52	1.54
25	B	603	CLA	C3B-CAB	-2.16	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	602	CLA	CMC-C2C	-2.16	1.46	1.50
24	6	605	CHL	C4C-C3C	2.16	1.48	1.45
25	s	611	CLA	MG-ND	-2.16	2.01	2.05
25	b	617	CLA	MG-ND	-2.16	2.01	2.05
25	C	508	CLA	C3B-CAB	-2.16	1.43	1.47
25	1	612	CLA	MG-ND	-2.16	2.01	2.05
25	0	604	CLA	CMD-C2D	-2.16	1.46	1.50
25	C	507	CLA	C3B-CAB	-2.16	1.43	1.47
27	R	622	XAT	O24-C25	-2.16	1.43	1.46
24	s	601	CHL	C1B-CHB	2.16	1.47	1.41
25	c	504	CLA	MG-ND	-2.16	2.01	2.05
25	N	604	CLA	CMC-C2C	-2.16	1.46	1.50
25	s	612	CLA	MG-ND	-2.16	2.01	2.05
25	1	603	CLA	CMD-C2D	-2.16	1.46	1.50
25	4	603	CLA	CMD-C2D	-2.16	1.46	1.50
25	b	610	CLA	CMC-C2C	-2.16	1.46	1.50
24	7	608	CHL	C3D-C2D	2.16	1.45	1.39
25	s	610	CLA	CMC-C2C	-2.16	1.46	1.50
24	G	608	CHL	C4B-CHC	2.16	1.47	1.41
25	N	611	CLA	CMC-C2C	-2.16	1.46	1.50
25	S	610	CLA	CMC-C2C	-2.16	1.46	1.50
24	9	605	CHL	C4D-CHA	2.16	1.46	1.38
33	A	409	PHO	CMB-C2B	-2.16	1.46	1.51
25	6	604	CLA	C3B-CAB	-2.16	1.43	1.47
25	2	612	CLA	C3B-C2B	-2.16	1.37	1.40
25	S	612	CLA	C4B-CHC	-2.16	1.35	1.41
25	1	610	CLA	CMD-C2D	-2.16	1.46	1.50
25	7	604	CLA	CMC-C2C	-2.16	1.46	1.50
24	6	607	CHL	C4B-CHC	2.16	1.47	1.41
24	S	601	CHL	C1B-CHB	2.16	1.47	1.41
24	9	608	CHL	C4B-CHC	2.16	1.47	1.41
27	n	1622	XAT	C22-C21	-2.16	1.51	1.54
25	S	603	CLA	CMD-C2D	-2.16	1.46	1.50
24	s	606	CHL	C1B-CHB	2.16	1.47	1.41
25	R	601	CLA	C4B-CHC	-2.15	1.35	1.41
25	Y	613	CLA	C4B-CHC	-2.15	1.35	1.41
25	7	610	CLA	CMD-C2D	-2.15	1.46	1.50
24	0	609	CHL	C4C-C3C	2.15	1.48	1.45
25	b	608	CLA	C4B-CHC	-2.15	1.35	1.41
25	6	603	CLA	MG-ND	-2.15	2.01	2.05
25	C	513	CLA	CMC-C2C	-2.15	1.46	1.50
25	b	616	CLA	C3B-CAB	-2.15	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	6	606	CHL	C4B-CHC	2.15	1.47	1.41
25	r	603	CLA	C3B-CAB	-2.15	1.43	1.47
24	6	609	CHL	C4C-C3C	2.15	1.48	1.45
25	C	503	CLA	MG-ND	-2.15	2.01	2.05
25	b	609	CLA	C4B-CHC	-2.15	1.35	1.41
25	6	610	CLA	C3B-CAB	-2.15	1.43	1.47
24	N	606	CHL	C4B-CHC	2.15	1.47	1.41
25	S	611	CLA	CMC-C2C	-2.15	1.46	1.50
25	B	615	CLA	C3B-CAB	-2.15	1.43	1.47
25	c	507	CLA	C4B-CHC	-2.15	1.35	1.41
24	S	608	CHL	C4B-CHC	2.15	1.47	1.41
25	B	616	CLA	C3B-CAB	-2.15	1.43	1.47
25	C	503	CLA	C4B-CHC	-2.15	1.35	1.41
25	r	602	CLA	CMC-C2C	-2.15	1.46	1.50
25	n	602	CLA	MG-ND	-2.15	2.01	2.05
25	c	507	CLA	C3B-C2B	-2.15	1.37	1.40
25	p	614	CLA	CMD-C2D	-2.15	1.46	1.50
25	C	510	CLA	CMC-C2C	-2.15	1.46	1.50
25	3	603	CLA	C3B-C2B	-2.15	1.37	1.40
25	y	604	CLA	MG-ND	-2.15	2.01	2.05
25	N	614	CLA	CMD-C2D	-2.15	1.46	1.50
25	S	604	CLA	CMD-C2D	-2.15	1.46	1.50
25	A	410	CLA	C3B-CAB	-2.15	1.43	1.47
25	c	509	CLA	C4B-CHC	-2.15	1.35	1.41
25	n	614	CLA	CMD-C2D	-2.15	1.46	1.50
25	s	613	CLA	CMC-C2C	-2.15	1.46	1.50
25	N	610	CLA	C3B-CAB	-2.15	1.43	1.47
24	2	608	CHL	C4C-C3C	2.14	1.48	1.45
24	G	609	CHL	C3D-C2D	2.14	1.45	1.39
25	8	603	CLA	C3B-C2B	-2.14	1.37	1.40
24	7	609	CHL	C1D-C2D	2.14	1.49	1.45
24	9	608	CHL	C2C-C1C	2.14	1.49	1.44
25	G	612	CLA	MG-ND	-2.14	2.01	2.05
25	g	612	CLA	MG-ND	-2.14	2.01	2.05
24	s	608	CHL	C4B-CHC	2.14	1.46	1.41
25	3	611	CLA	CMD-C2D	-2.14	1.46	1.50
25	R	613	CLA	CMC-C2C	-2.14	1.46	1.50
24	S	606	CHL	C1B-CHB	2.14	1.46	1.41
25	N	602	CLA	MG-ND	-2.14	2.01	2.05
25	c	503	CLA	C4B-CHC	-2.14	1.35	1.41
25	s	611	CLA	CMC-C2C	-2.14	1.46	1.50
25	s	610	CLA	MG-ND	-2.14	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	608	CHL	C4B-CHC	2.14	1.46	1.41
24	4	605	CHL	C2C-C1C	2.14	1.49	1.44
25	B	603	CLA	MG-ND	-2.14	2.01	2.05
24	y	608	CHL	C1C-NC	-2.14	1.34	1.37
25	r	603	CLA	CMC-C2C	-2.14	1.46	1.50
25	C	507	CLA	C3B-C2B	-2.14	1.37	1.40
25	Y	604	CLA	MG-ND	-2.14	2.01	2.05
26	y	1621	LUT	C22-C21	-2.14	1.52	1.54
24	g	605	CHL	C4B-CHC	2.14	1.46	1.41
24	s	608	CHL	C1B-CHB	2.14	1.46	1.41
25	r	612	CLA	MG-ND	-2.14	2.01	2.05
25	5	610	CLA	CMC-C2C	-2.14	1.46	1.50
25	N	610	CLA	CMD-C2D	-2.14	1.46	1.50
25	y	604	CLA	C3B-CAB	-2.14	1.43	1.47
24	g	607	CHL	C4B-CHC	2.14	1.46	1.41
25	A	406	CLA	CMC-C2C	-2.14	1.46	1.50
25	a	406	CLA	CMC-C2C	-2.14	1.46	1.50
25	n	610	CLA	C3B-CAB	-2.14	1.43	1.47
25	s	612	CLA	C4B-CHC	-2.14	1.35	1.41
25	l	611	CLA	C3B-C2B	-2.14	1.37	1.40
25	G	611	CLA	C3B-CAB	-2.14	1.43	1.47
25	g	611	CLA	C3B-CAB	-2.14	1.43	1.47
25	g	603	CLA	C4B-CHC	-2.14	1.35	1.41
24	9	601	CHL	C4C-C3C	2.13	1.48	1.45
25	R	612	CLA	MG-ND	-2.13	2.01	2.05
25	A	407	CLA	CMC-C2C	-2.13	1.46	1.50
24	n	608	CHL	C1D-C2D	2.13	1.49	1.45
25	7	610	CLA	C3B-C2B	-2.13	1.37	1.40
25	S	611	CLA	MG-ND	-2.13	2.01	2.05
25	a	407	CLA	CMC-C2C	-2.13	1.46	1.50
24	l	606	CHL	C1B-CHB	2.13	1.46	1.41
25	r	601	CLA	CMC-C2C	-2.13	1.46	1.50
24	g	606	CHL	C4B-CHC	2.13	1.46	1.41
24	R	606	CHL	C3D-C2D	2.13	1.44	1.39
25	0	603	CLA	MG-ND	-2.13	2.01	2.05
25	q	612	CLA	C3B-C2B	-2.13	1.37	1.40
25	R	603	CLA	CMC-C2C	-2.13	1.46	1.50
25	s	604	CLA	CMD-C2D	-2.13	1.46	1.50
25	r	613	CLA	C4B-CHC	-2.13	1.35	1.41
25	B	607	CLA	C3B-CAB	-2.13	1.43	1.47
25	Y	604	CLA	C3B-CAB	-2.13	1.43	1.47
25	b	607	CLA	C3B-CAB	-2.13	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	0	604	CLA	CMC-C2C	-2.13	1.46	1.50
26	n	1621	LUT	C22-C21	-2.13	1.52	1.54
25	1	603	CLA	C3B-CAB	-2.13	1.43	1.47
25	R	613	CLA	C3B-CAB	-2.13	1.43	1.47
25	b	605	CLA	C3B-CAB	-2.13	1.43	1.47
25	c	513	CLA	MG-ND	-2.13	2.01	2.05
25	l	612	CLA	C3B-CAB	-2.13	1.43	1.47
25	s	611	CLA	C3B-C2B	-2.13	1.37	1.40
25	b	603	CLA	MG-ND	-2.13	2.01	2.05
25	1	604	CLA	C4B-CHC	-2.13	1.35	1.41
25	g	613	CLA	CMC-C2C	-2.13	1.46	1.50
25	7	613	CLA	MG-ND	-2.13	2.01	2.05
34	C	517	BCR	C30-C25	-2.13	1.50	1.53
24	G	608	CHL	C1B-CHB	2.13	1.46	1.41
25	S	610	CLA	MG-ND	-2.13	2.01	2.05
24	G	605	CHL	C4B-CHC	2.13	1.46	1.41
25	9	614	CLA	CMD-C2D	-2.13	1.46	1.50
25	n	611	CLA	MG-ND	-2.13	2.01	2.05
25	5	613	CLA	CMD-C2D	-2.13	1.46	1.50
33	A	409	PHO	C3B-C2B	-2.13	1.37	1.40
25	9	602	CLA	CMD-C2D	-2.12	1.46	1.50
25	R	610	CLA	C3B-CAB	-2.12	1.43	1.47
28	g	1623	NEX	O24-C25	-2.12	1.43	1.46
25	s	602	CLA	CMC-C2C	-2.12	1.46	1.50
24	1	605	CHL	C4B-CHC	2.12	1.46	1.41
25	G	604	CLA	C3B-C2B	-2.12	1.37	1.40
25	4	604	CLA	CMD-C2D	-2.12	1.46	1.50
25	C	505	CLA	C3B-C2B	-2.12	1.37	1.40
25	c	505	CLA	C3B-C2B	-2.12	1.37	1.40
25	4	613	CLA	CMD-C2D	-2.12	1.46	1.50
25	B	609	CLA	C4B-CHC	-2.12	1.35	1.41
33	a	408	PHO	CBD-CGD	-2.12	1.49	1.52
25	D	403	CLA	MG-ND	-2.12	2.01	2.05
25	S	610	CLA	C3B-CAB	-2.12	1.43	1.47
25	g	613	CLA	C3B-C2B	-2.12	1.37	1.40
24	4	609	CHL	C4C-C3C	2.12	1.48	1.45
25	g	614	CLA	C3B-CAB	-2.12	1.43	1.47
24	G	606	CHL	C4B-CHC	2.12	1.46	1.41
25	C	504	CLA	MG-ND	-2.12	2.01	2.05
25	S	611	CLA	C3B-CAB	-2.12	1.43	1.47
25	s	610	CLA	C3B-CAB	-2.12	1.43	1.47
25	8	611	CLA	CMD-C2D	-2.12	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	p	607	CHL	C4C-C3C	2.12	1.48	1.45
24	5	607	CHL	C1B-CHB	2.12	1.46	1.41
25	d	403	CLA	MG-ND	-2.12	2.01	2.05
25	q	614	CLA	C3B-C2B	-2.12	1.37	1.40
24	G	607	CHL	C4B-CHC	2.11	1.46	1.41
25	G	613	CLA	C3B-C2B	-2.11	1.37	1.40
25	N	614	CLA	CMC-C2C	-2.11	1.46	1.50
25	s	603	CLA	CMD-C2D	-2.11	1.46	1.50
25	R	601	CLA	CMC-C2C	-2.11	1.46	1.50
25	p	611	CLA	CMD-C2D	-2.11	1.46	1.50
24	6	605	CHL	C1B-CHB	2.11	1.46	1.41
24	g	608	CHL	C4B-CHC	2.11	1.46	1.41
24	y	607	CHL	C1D-C2D	2.11	1.49	1.45
24	4	601	CHL	C1B-CHB	2.11	1.46	1.41
24	G	606	CHL	C1B-CHB	2.11	1.46	1.41
24	Y	608	CHL	C1C-NC	-2.11	1.34	1.37
25	G	603	CLA	C4B-CHC	-2.11	1.35	1.41
24	p	605	CHL	C4C-C3C	2.11	1.48	1.45
25	n	611	CLA	CMC-C2C	-2.11	1.46	1.50
24	7	608	CHL	C1D-C2D	2.11	1.49	1.45
27	0	1622	XAT	O24-C25	-2.11	1.43	1.46
25	c	507	CLA	CMC-C2C	-2.11	1.46	1.50
25	G	613	CLA	CMC-C2C	-2.11	1.46	1.50
24	q	607	CHL	C4D-CHA	2.11	1.45	1.38
24	S	608	CHL	C1B-CHB	2.11	1.46	1.41
24	y	605	CHL	C4B-CHC	2.11	1.46	1.41
24	r	606	CHL	C3D-C2D	2.11	1.44	1.39
24	y	601	CHL	C4B-CHC	2.11	1.46	1.41
33	a	409	PHO	C3B-C2B	-2.11	1.37	1.40
25	n	610	CLA	CMC-C2C	-2.11	1.46	1.50
25	N	614	CLA	C3B-CAB	-2.11	1.43	1.47
25	s	611	CLA	C3B-CAB	-2.11	1.43	1.47
25	B	617	CLA	MG-ND	-2.11	2.01	2.05
25	R	609	CLA	C3B-CAB	-2.11	1.43	1.47
25	r	609	CLA	C3B-CAB	-2.11	1.43	1.47
25	2	603	CLA	MG-ND	-2.11	2.01	2.05
24	S	606	CHL	C4C-C3C	2.11	1.48	1.45
25	1	604	CLA	CMD-C2D	-2.10	1.46	1.50
25	0	612	CLA	CMD-C2D	-2.10	1.46	1.50
25	7	612	CLA	C3B-CAB	-2.10	1.43	1.47
24	0	606	CHL	C4C-C3C	2.10	1.48	1.45
28	Y	1623	NEX	O24-C25	-2.10	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	A	406	CLA	C3B-CAB	-2.10	1.43	1.47
25	a	406	CLA	C3B-CAB	-2.10	1.43	1.47
24	Y	607	CHL	C1D-C2D	2.10	1.49	1.45
25	C	507	CLA	CMC-C2C	-2.10	1.46	1.50
27	n	1622	XAT	O24-C25	-2.10	1.43	1.46
25	r	611	CLA	MG-ND	-2.10	2.01	2.05
24	y	606	CHL	C3D-C2D	2.10	1.44	1.39
25	6	610	CLA	CMC-C2C	-2.10	1.46	1.50
25	n	612	CLA	MG-ND	-2.10	2.01	2.05
25	b	611	CLA	C3B-CAB	-2.10	1.43	1.47
25	4	614	CLA	C3B-C2B	-2.10	1.37	1.40
25	5	603	CLA	C3B-C2B	-2.10	1.37	1.40
25	S	604	CLA	MG-ND	-2.10	2.01	2.05
25	R	613	CLA	CMD-C2D	-2.10	1.46	1.50
24	9	608	CHL	C4C-C3C	2.10	1.48	1.45
24	7	605	CHL	C4B-CHC	2.10	1.46	1.41
25	C	513	CLA	MG-ND	-2.10	2.01	2.05
25	C	513	CLA	C3B-CAB	-2.10	1.43	1.47
25	B	612	CLA	C3B-CAB	-2.10	1.43	1.47
25	b	612	CLA	C3B-CAB	-2.10	1.43	1.47
25	n	614	CLA	C3B-CAB	-2.10	1.43	1.47
25	p	612	CLA	C3B-C2B	-2.10	1.37	1.40
25	G	604	CLA	CMC-C2C	-2.09	1.46	1.50
24	n	605	CHL	C3D-C2D	2.09	1.44	1.39
25	c	508	CLA	MG-ND	-2.09	2.01	2.05
25	N	612	CLA	CMC-C2C	-2.09	1.46	1.50
24	Y	601	CHL	C4B-CHC	2.09	1.46	1.41
25	7	612	CLA	MG-ND	-2.09	2.01	2.05
25	b	608	CLA	MG-ND	-2.09	2.01	2.05
25	r	601	CLA	MG-ND	-2.09	2.01	2.05
25	6	612	CLA	CMD-C2D	-2.09	1.46	1.50
25	S	602	CLA	C3B-CAB	-2.09	1.43	1.47
34	c	517	BCR	C30-C25	-2.09	1.50	1.53
25	q	611	CLA	C3B-C2B	-2.09	1.37	1.40
25	N	611	CLA	MG-ND	-2.09	2.01	2.05
25	0	610	CLA	C3B-CAB	-2.09	1.43	1.47
25	R	611	CLA	MG-ND	-2.09	2.01	2.05
24	Y	606	CHL	C3D-C2D	2.09	1.44	1.39
25	c	503	CLA	C3B-CAB	-2.09	1.43	1.47
24	g	606	CHL	C1B-CHB	2.09	1.46	1.41
25	2	614	CLA	CMD-C2D	-2.09	1.46	1.50
25	r	613	CLA	CMC-C2C	-2.09	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	603	CLA	C4B-CHC	-2.09	1.35	1.41
25	B	605	CLA	MG-ND	-2.09	2.01	2.05
28	n	1623	NEX	O24-C25	-2.09	1.43	1.46
24	s	606	CHL	C4C-C3C	2.09	1.48	1.45
24	0	607	CHL	C4B-CHC	2.09	1.46	1.41
25	s	609	CLA	CMD-C2D	-2.09	1.46	1.50
25	b	602	CLA	MG-ND	-2.09	2.01	2.05
24	1	608	CHL	C1D-C2D	2.09	1.49	1.45
25	1	603	CLA	C4B-CHC	-2.09	1.35	1.41
25	p	612	CLA	CMD-C2D	-2.09	1.46	1.50
25	1	613	CLA	MG-ND	-2.09	2.01	2.05
24	y	609	CHL	C1D-ND	-2.09	1.35	1.37
25	3	612	CLA	C3B-C2B	-2.09	1.37	1.40
24	5	605	CHL	C4C-C3C	2.09	1.48	1.45
25	p	610	CLA	CMC-C2C	-2.09	1.46	1.50
25	s	603	CLA	C3B-CAB	-2.09	1.43	1.47
25	C	503	CLA	C3B-C2B	-2.09	1.37	1.40
25	B	613	CLA	C4B-CHC	-2.09	1.35	1.41
25	b	613	CLA	C4B-CHC	-2.09	1.35	1.41
24	g	608	CHL	C1B-CHB	2.09	1.46	1.41
25	8	604	CLA	CMD-C2D	-2.09	1.46	1.50
25	1	604	CLA	CMC-C2C	-2.08	1.46	1.50
25	3	603	CLA	C3B-CAB	-2.08	1.43	1.47
24	R	608	CHL	MG-ND	-2.08	2.01	2.05
26	1	1620	LUT	C22-C21	-2.08	1.52	1.54
26	7	1620	LUT	C22-C21	-2.08	1.52	1.54
25	n	604	CLA	C3B-CAB	-2.08	1.43	1.47
25	C	503	CLA	C3B-CAB	-2.08	1.43	1.47
25	p	603	CLA	C3B-C2B	-2.08	1.37	1.40
25	c	513	CLA	C3B-CAB	-2.08	1.43	1.47
25	3	610	CLA	CMC-C2C	-2.08	1.46	1.50
25	C	511	CLA	MG-ND	-2.08	2.01	2.05
25	n	614	CLA	CMC-C2C	-2.08	1.46	1.50
25	1	604	CLA	MG-ND	-2.08	2.01	2.05
25	s	612	CLA	CMC-C2C	-2.08	1.46	1.50
25	g	604	CLA	CMC-C2C	-2.08	1.46	1.50
25	3	603	CLA	C4B-CHC	-2.08	1.35	1.41
25	B	603	CLA	C4B-CHC	-2.08	1.35	1.41
25	B	611	CLA	C3B-CAB	-2.08	1.43	1.47
25	n	603	CLA	C3B-CAB	-2.08	1.43	1.47
28	N	1623	NEX	O24-C25	-2.08	1.43	1.46
24	6	605	CHL	C4D-CHA	2.08	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	612	CLA	CMC-C2C	-2.08	1.46	1.50
24	9	609	CHL	C1B-CHB	2.08	1.46	1.41
25	1	614	CLA	CMC-C2C	-2.08	1.46	1.50
25	B	608	CLA	MG-ND	-2.08	2.01	2.05
24	Y	605	CHL	C4B-CHC	2.08	1.46	1.41
25	N	613	CLA	C4B-CHC	-2.08	1.35	1.41
25	7	612	CLA	CMC-C2C	-2.08	1.46	1.50
25	r	613	CLA	CMD-C2D	-2.08	1.46	1.50
25	c	506	CLA	MG-ND	-2.08	2.01	2.05
24	6	601	CHL	C4B-CHC	2.08	1.46	1.41
24	7	607	CHL	C1B-CHB	2.08	1.46	1.41
24	g	609	CHL	C1B-CHB	2.08	1.46	1.41
25	s	602	CLA	C3B-CAB	-2.08	1.43	1.47
25	8	603	CLA	C3B-CAB	-2.07	1.43	1.47
25	0	602	CLA	C3B-C2B	-2.07	1.37	1.40
25	C	501	CLA	C3B-CAB	-2.07	1.43	1.47
25	C	502	CLA	C3B-CAB	-2.07	1.43	1.47
25	q	612	CLA	C4B-CHC	-2.07	1.35	1.41
25	q	613	CLA	C4B-CHC	-2.07	1.35	1.41
25	1	603	CLA	CMC-C2C	-2.07	1.46	1.50
24	5	605	CHL	C2C-C1C	2.07	1.49	1.44
25	N	604	CLA	C3B-CAB	-2.07	1.43	1.47
24	p	601	CHL	C4B-CHC	2.07	1.46	1.41
25	7	604	CLA	CMD-C2D	-2.07	1.46	1.50
25	7	603	CLA	C3B-CAB	-2.07	1.43	1.47
24	0	609	CHL	C1B-CHB	2.07	1.46	1.41
25	7	603	CLA	C4B-CHC	-2.07	1.35	1.41
25	B	602	CLA	MG-ND	-2.07	2.01	2.05
25	1	612	CLA	CMC-C2C	-2.07	1.46	1.50
25	p	602	CLA	CMC-C2C	-2.07	1.46	1.50
25	g	602	CLA	C3B-C2B	-2.07	1.37	1.40
25	G	603	CLA	CMC-C2C	-2.07	1.46	1.50
25	g	603	CLA	CMC-C2C	-2.07	1.46	1.50
24	Y	609	CHL	C1D-ND	-2.07	1.35	1.37
24	2	601	CHL	MG-ND	-2.07	2.01	2.05
25	2	613	CLA	MG-ND	-2.07	2.01	2.05
25	5	613	CLA	C3B-C2B	-2.07	1.37	1.40
25	c	503	CLA	MG-ND	-2.07	2.01	2.05
24	3	601	CHL	C1B-CHB	2.07	1.46	1.41
25	G	614	CLA	C3B-CAB	-2.07	1.43	1.47
25	5	611	CLA	CMD-C2D	-2.07	1.46	1.50
25	N	610	CLA	CMC-C2C	-2.07	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	602	CLA	C3B-CAB	-2.07	1.43	1.47
24	5	608	CHL	C4C-C3C	2.07	1.48	1.45
25	N	612	CLA	MG-ND	-2.07	2.01	2.05
24	g	609	CHL	C3D-C2D	2.07	1.44	1.39
24	0	605	CHL	C1B-CHB	2.07	1.46	1.41
25	b	603	CLA	C4B-CHC	-2.07	1.35	1.41
25	2	614	CLA	C3B-CAB	-2.07	1.43	1.47
25	4	602	CLA	CMD-C2D	-2.07	1.46	1.50
25	r	616	CLA	MG-ND	-2.07	2.01	2.05
24	N	608	CHL	C1B-CHB	2.07	1.46	1.41
25	4	614	CLA	CMC-C2C	-2.07	1.46	1.50
24	r	608	CHL	C1B-CHB	2.07	1.46	1.41
25	r	612	CLA	CMC-C2C	-2.07	1.46	1.50
25	n	604	CLA	MG-ND	-2.06	2.01	2.05
25	3	604	CLA	CMD-C2D	-2.06	1.46	1.50
24	G	609	CHL	C1B-CHB	2.06	1.46	1.41
25	s	604	CLA	MG-ND	-2.06	2.01	2.05
25	S	603	CLA	C3B-CAB	-2.06	1.43	1.47
25	s	614	CLA	CMC-C2C	-2.06	1.46	1.50
26	g	1621	LUT	C22-C21	-2.06	1.52	1.54
27	N	1622	XAT	O24-C25	-2.06	1.43	1.46
25	s	612	CLA	C3B-CAB	-2.06	1.43	1.47
25	y	602	CLA	C3B-CAB	-2.06	1.43	1.47
25	S	613	CLA	C4B-CHC	-2.06	1.35	1.41
24	y	606	CHL	MG-ND	-2.06	2.01	2.05
24	0	609	CHL	C4B-CHC	2.06	1.46	1.41
24	N	608	CHL	C3D-C2D	2.06	1.44	1.39
25	G	602	CLA	MG-ND	-2.06	2.01	2.05
25	0	602	CLA	CMC-C2C	-2.06	1.46	1.50
24	4	601	CHL	C4C-C3C	2.06	1.48	1.45
25	4	603	CLA	CMC-C2C	-2.06	1.46	1.50
25	9	611	CLA	C3B-C2B	-2.06	1.37	1.40
25	7	604	CLA	MG-ND	-2.06	2.01	2.05
24	q	601	CHL	C4C-C3C	2.06	1.48	1.45
25	S	614	CLA	CMC-C2C	-2.06	1.46	1.50
25	q	604	CLA	CMD-C2D	-2.06	1.46	1.50
24	9	601	CHL	MG-ND	-2.06	2.01	2.05
25	R	601	CLA	MG-ND	-2.06	2.01	2.05
25	c	511	CLA	MG-ND	-2.06	2.01	2.05
25	N	604	CLA	MG-ND	-2.06	2.01	2.05
28	2	1623	NEX	O24-C25	-2.06	1.43	1.46
25	g	610	CLA	C3B-CAB	-2.06	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	610	CLA	CMC-C2C	-2.06	1.46	1.50
25	S	609	CLA	CMD-C2D	-2.06	1.46	1.50
25	7	614	CLA	CMC-C2C	-2.06	1.46	1.50
25	7	613	CLA	C4B-CHC	-2.06	1.35	1.41
25	r	609	CLA	CMC-C2C	-2.06	1.46	1.50
34	B	619	BCR	C1-C6	-2.06	1.50	1.53
34	b	619	BCR	C1-C6	-2.06	1.50	1.53
25	8	604	CLA	CMC-C2C	-2.06	1.46	1.50
25	q	610	CLA	CMC-C2C	-2.06	1.46	1.50
25	5	610	CLA	CMD-C2D	-2.05	1.46	1.50
25	R	609	CLA	CMC-C2C	-2.05	1.46	1.50
25	6	602	CLA	CMC-C2C	-2.05	1.46	1.50
25	7	610	CLA	CMC-C2C	-2.05	1.46	1.50
25	0	603	CLA	C4B-CHC	-2.05	1.35	1.41
25	R	612	CLA	CMC-C2C	-2.05	1.46	1.50
25	7	613	CLA	CMC-C2C	-2.05	1.46	1.50
25	6	602	CLA	CMD-C2D	-2.05	1.46	1.50
28	s	1623	NEX	O24-C25	-2.05	1.43	1.46
33	A	408	PHO	C1C-NC	-2.05	1.32	1.38
33	a	408	PHO	C1C-NC	-2.05	1.32	1.38
24	5	601	CHL	C4B-CHC	2.05	1.46	1.41
25	4	612	CLA	C4B-CHC	-2.05	1.35	1.41
25	2	612	CLA	MG-ND	-2.05	2.01	2.05
28	G	1623	NEX	O24-C25	-2.05	1.43	1.46
25	p	602	CLA	CMD-C2D	-2.05	1.46	1.50
24	Y	601	CHL	C4B-NB	-2.05	1.33	1.35
24	Y	606	CHL	C4B-CHC	2.05	1.46	1.41
25	G	602	CLA	C3B-C2B	-2.05	1.37	1.40
25	p	604	CLA	C3B-C2B	-2.05	1.37	1.40
25	S	604	CLA	C3B-C2B	-2.05	1.37	1.40
25	c	509	CLA	C3B-CAB	-2.05	1.43	1.47
24	1	609	CHL	C1B-CHB	2.05	1.46	1.41
25	8	611	CLA	C3B-C2B	-2.05	1.37	1.40
25	S	612	CLA	C3B-CAB	-2.05	1.43	1.47
25	D	403	CLA	C4B-CHC	-2.05	1.35	1.41
24	2	609	CHL	CMC-C2C	2.05	1.49	1.45
25	b	605	CLA	MG-ND	-2.05	2.01	2.05
25	c	502	CLA	CAC-C3C	-2.05	1.45	1.51
25	s	605	CLA	CMC-C2C	-2.05	1.46	1.50
24	4	609	CHL	C1D-ND	-2.05	1.35	1.37
24	3	607	CHL	C2C-C1C	2.05	1.49	1.44
27	0	1622	XAT	O4-C5	-2.05	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	2	608	CHL	CMC-C2C	2.04	1.49	1.45
25	B	614	CLA	C4B-CHC	-2.04	1.35	1.41
25	b	614	CLA	C4B-CHC	-2.04	1.35	1.41
25	r	611	CLA	C4B-CHC	-2.04	1.35	1.41
25	0	602	CLA	CMD-C2D	-2.04	1.46	1.50
27	6	1622	XAT	O4-C5	-2.04	1.43	1.46
24	y	607	CHL	C3A-C2A	-2.04	1.48	1.54
25	N	603	CLA	C3B-CAB	-2.04	1.43	1.47
24	9	608	CHL	C1B-CHB	2.04	1.46	1.41
25	9	610	CLA	CMD-C2D	-2.04	1.46	1.50
25	6	602	CLA	C3B-C2B	-2.04	1.37	1.40
25	4	604	CLA	C3B-CAB	-2.04	1.43	1.47
25	c	502	CLA	C3B-CAB	-2.04	1.43	1.47
24	S	606	CHL	C4B-CHC	2.04	1.46	1.41
25	6	604	CLA	CMC-C2C	-2.04	1.46	1.50
25	9	614	CLA	C3B-CAB	-2.04	1.43	1.47
24	5	606	CHL	C2C-C1C	2.04	1.48	1.44
25	5	602	CLA	CMD-C2D	-2.04	1.46	1.50
25	q	602	CLA	CMC-C2C	-2.04	1.46	1.50
25	8	613	CLA	C3B-C2B	-2.04	1.37	1.40
28	q	1623	NEX	O24-C25	-2.04	1.43	1.46
25	5	612	CLA	CMC-C2C	-2.04	1.46	1.50
25	1	613	CLA	C4B-CHC	-2.04	1.35	1.41
24	r	606	CHL	C4C-C3C	2.04	1.48	1.45
28	7	1623	NEX	O24-C25	-2.04	1.43	1.46
27	6	1622	XAT	O24-C25	-2.04	1.43	1.46
24	6	609	CHL	C4B-CHC	2.04	1.46	1.41
24	0	601	CHL	C1B-CHB	2.04	1.46	1.41
24	6	608	CHL	C1B-CHB	2.04	1.46	1.41
24	0	605	CHL	C4C-C3C	2.04	1.48	1.45
24	g	601	CHL	C1C-NC	-2.04	1.34	1.37
24	7	601	CHL	C3D-C2D	2.04	1.44	1.39
28	4	1623	NEX	O24-C25	-2.04	1.43	1.46
24	y	606	CHL	C4B-CHC	2.04	1.46	1.41
25	C	508	CLA	MG-ND	-2.04	2.01	2.05
25	G	612	CLA	CMC-C2C	-2.04	1.46	1.50
24	2	608	CHL	C1B-CHB	2.04	1.46	1.41
24	7	609	CHL	C4B-CHC	2.04	1.46	1.41
25	Y	612	CLA	C4B-CHC	-2.04	1.35	1.41
25	s	613	CLA	C4B-CHC	-2.03	1.35	1.41
25	g	612	CLA	CMC-C2C	-2.03	1.46	1.50
24	2	608	CHL	C4D-CHA	2.03	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	1	601	CHL	C3D-C2D	2.03	1.44	1.39
25	q	603	CLA	CMD-C2D	-2.03	1.46	1.50
25	7	602	CLA	MG-ND	-2.03	2.01	2.05
25	3	612	CLA	CMD-C2D	-2.03	1.46	1.50
25	4	603	CLA	MG-ND	-2.03	2.01	2.05
24	N	608	CHL	C4B-CHC	2.03	1.46	1.41
24	p	607	CHL	C1B-CHB	2.03	1.46	1.41
25	0	612	CLA	MG-ND	-2.03	2.01	2.05
24	q	609	CHL	C1D-ND	-2.03	1.35	1.37
25	p	604	CLA	CMD-C2D	-2.03	1.46	1.50
25	n	611	CLA	C4B-CHC	-2.03	1.35	1.41
24	Y	607	CHL	C3D-C2D	2.03	1.44	1.39
25	3	611	CLA	C3B-C2B	-2.03	1.37	1.40
25	B	615	CLA	C4B-CHC	-2.03	1.35	1.41
25	q	603	CLA	C3B-C2B	-2.03	1.37	1.40
24	p	608	CHL	C1B-CHB	2.03	1.46	1.41
25	G	610	CLA	C3B-CAB	-2.03	1.43	1.47
24	Y	606	CHL	C1D-ND	-2.03	1.35	1.37
25	8	612	CLA	C3B-C2B	-2.03	1.37	1.40
25	C	511	CLA	C3B-CAB	-2.03	1.43	1.47
24	1	607	CHL	C1B-CHB	2.03	1.46	1.41
24	0	608	CHL	C1B-CHB	2.03	1.46	1.41
24	n	608	CHL	C1B-CHB	2.03	1.46	1.41
25	8	602	CLA	CMC-C2C	-2.03	1.46	1.50
25	S	612	CLA	CMC-C2C	-2.03	1.46	1.50
25	B	615	CLA	CAC-C3C	-2.03	1.45	1.51
25	b	615	CLA	CAC-C3C	-2.03	1.45	1.51
34	D	404	BCR	C1-C6	-2.03	1.51	1.53
25	8	612	CLA	CMD-C2D	-2.03	1.46	1.50
39	d	405	PL9	C40-C39	-2.03	1.45	1.50
24	R	608	CHL	C1B-CHB	2.03	1.46	1.41
25	c	501	CLA	C3B-CAB	-2.03	1.43	1.47
34	c	517	BCR	C1-C6	-2.03	1.51	1.53
28	9	1623	NEX	O24-C25	-2.03	1.43	1.46
25	9	604	CLA	CMD-C2D	-2.03	1.46	1.50
25	4	611	CLA	C3B-C2B	-2.03	1.37	1.40
25	4	613	CLA	C4B-CHC	-2.03	1.35	1.41
24	Y	609	CHL	C4B-NB	-2.03	1.33	1.35
25	q	602	CLA	CMD-C2D	-2.03	1.46	1.50
25	s	603	CLA	C4B-CHC	-2.03	1.35	1.41
25	C	506	CLA	MG-ND	-2.03	2.01	2.05
25	S	605	CLA	MG-ND	-2.03	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	612	CLA	CMC-C2C	-2.03	1.46	1.50
24	n	608	CHL	C3D-C2D	2.03	1.44	1.39
25	N	611	CLA	C4B-CHC	-2.03	1.35	1.41
25	C	502	CLA	CAC-C3C	-2.03	1.45	1.51
25	q	604	CLA	C3B-CAB	-2.03	1.43	1.47
25	a	410	CLA	C4B-CHC	-2.03	1.35	1.41
25	0	612	CLA	CMC-C2C	-2.03	1.46	1.50
25	2	604	CLA	CMC-C2C	-2.02	1.46	1.50
25	9	602	CLA	CMC-C2C	-2.02	1.46	1.50
25	9	603	CLA	MG-ND	-2.02	2.01	2.05
25	d	402	CLA	CAA-C2A	-2.02	1.50	1.54
24	Y	608	CHL	C1D-C2D	2.02	1.49	1.45
34	C	517	BCR	C1-C6	-2.02	1.51	1.53
24	6	606	CHL	C4C-C3C	2.02	1.48	1.45
25	R	611	CLA	C4B-CHC	-2.02	1.35	1.41
24	R	606	CHL	C3A-C2A	-2.02	1.48	1.54
24	7	608	CHL	C1B-CHB	2.02	1.46	1.41
24	0	609	CHL	C2C-C1C	2.02	1.48	1.44
25	9	612	CLA	C4B-CHC	-2.02	1.35	1.41
25	5	604	CLA	CMD-C2D	-2.02	1.46	1.50
28	S	1623	NEX	O24-C25	-2.02	1.43	1.46
25	S	603	CLA	C4B-CHC	-2.02	1.35	1.41
24	r	608	CHL	MG-ND	-2.02	2.01	2.05
24	7	608	CHL	C4B-CHC	2.02	1.46	1.41
24	8	609	CHL	C4B-CHC	2.02	1.46	1.41
25	2	610	CLA	CMD-C2D	-2.02	1.46	1.50
25	9	602	CLA	C4B-CHC	-2.02	1.35	1.41
25	d	403	CLA	C4B-CHC	-2.02	1.35	1.41
24	Y	606	CHL	MG-ND	-2.02	2.01	2.05
25	B	614	CLA	C3B-CAB	-2.02	1.43	1.47
24	p	601	CHL	C4C-C3C	2.02	1.48	1.45
25	5	612	CLA	C3B-CAB	-2.02	1.43	1.47
24	8	607	CHL	C2C-C1C	2.02	1.48	1.44
25	2	611	CLA	C3B-CAB	-2.02	1.43	1.47
25	N	612	CLA	C3B-CAB	-2.02	1.43	1.47
25	n	612	CLA	C3B-CAB	-2.02	1.43	1.47
24	r	606	CHL	C3A-C2A	-2.02	1.48	1.54
25	3	604	CLA	CMC-C2C	-2.02	1.46	1.50
25	y	612	CLA	C4B-CHC	-2.02	1.35	1.41
25	r	609	CLA	C4B-CHC	-2.02	1.35	1.41
25	G	604	CLA	MG-ND	-2.02	2.01	2.05
25	9	604	CLA	C3B-CAB	-2.02	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
24	Y	607	CHL	C3A-C2A	-2.02	1.48	1.54
25	y	603	CLA	CAC-C3C	-2.02	1.45	1.51
24	6	607	CHL	C1B-CHB	2.02	1.46	1.41
25	3	613	CLA	C4B-CHC	-2.02	1.35	1.41
25	5	612	CLA	CMD-C2D	-2.01	1.46	1.50
25	S	611	CLA	C3B-C2B	-2.01	1.37	1.40
27	1	1622	XAT	O4-C5	-2.01	1.43	1.46
25	n	613	CLA	C4B-CHC	-2.01	1.35	1.41
25	1	611	CLA	CMC-C2C	-2.01	1.46	1.50
25	6	612	CLA	C3B-CAB	-2.01	1.43	1.47
25	2	611	CLA	C3B-C2B	-2.01	1.37	1.40
25	5	611	CLA	C3B-C2B	-2.01	1.37	1.40
24	y	608	CHL	C1B-CHB	2.01	1.46	1.41
25	6	603	CLA	C4B-CHC	-2.01	1.35	1.41
25	7	602	CLA	C3B-C2B	-2.01	1.37	1.40
25	R	616	CLA	MG-ND	-2.01	2.01	2.05
25	b	608	CLA	C3B-CAB	-2.01	1.43	1.47
25	C	504	CLA	CAC-C3C	-2.01	1.46	1.51
25	2	613	CLA	CMC-C2C	-2.01	1.46	1.50
25	2	612	CLA	C4B-CHC	-2.01	1.35	1.41
25	R	609	CLA	C4B-CHC	-2.01	1.35	1.41
24	7	609	CHL	C1B-CHB	2.01	1.46	1.41
39	D	405	PL9	C40-C39	-2.01	1.45	1.50
25	3	614	CLA	CMD-C2D	-2.01	1.46	1.50
28	y	1623	NEX	C22-C21	-2.01	1.51	1.54
25	4	610	CLA	CMD-C2D	-2.01	1.46	1.50
25	C	509	CLA	C3B-CAB	-2.01	1.43	1.47
25	0	613	CLA	CMD-C2D	-2.01	1.46	1.50
24	R	607	CHL	MG-ND	-2.01	2.01	2.05
24	0	605	CHL	C4D-CHA	2.01	1.45	1.38
25	S	605	CLA	CMC-C2C	-2.01	1.46	1.50
28	Y	1623	NEX	C22-C21	-2.01	1.51	1.54
25	0	610	CLA	CMC-C2C	-2.01	1.46	1.50
25	8	610	CLA	CMC-C2C	-2.01	1.46	1.50
25	9	603	CLA	CMC-C2C	-2.01	1.46	1.50
25	B	608	CLA	C3B-CAB	-2.01	1.43	1.47
25	R	604	CLA	C4B-CHC	-2.01	1.35	1.41
25	Y	603	CLA	CAC-C3C	-2.01	1.46	1.51
24	Y	606	CHL	C1D-C2D	2.01	1.49	1.45
25	9	613	CLA	CMC-C2C	-2.01	1.46	1.50
25	9	611	CLA	C3B-CAB	-2.01	1.43	1.47
24	s	606	CHL	C4B-CHC	2.01	1.46	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	0	613	CLA	C3B-C2B	-2.01	1.37	1.40
24	2	607	CHL	C4D-CHA	2.01	1.45	1.38
24	y	607	CHL	C3D-C2D	2.01	1.44	1.39
37	c	524	DGD	O2G-C2G	-2.01	1.41	1.46
24	8	608	CHL	C4C-C3C	2.01	1.48	1.45
25	G	604	CLA	C3B-CAB	-2.01	1.43	1.47
25	r	604	CLA	C4B-CHC	-2.01	1.35	1.41
24	1	609	CHL	C1C-NC	-2.01	1.34	1.37
24	r	608	CHL	C1D-C2D	2.00	1.49	1.45
27	1	1622	XAT	O24-C25	-2.00	1.43	1.46
24	y	608	CHL	C1D-C2D	2.00	1.49	1.45
24	Y	608	CHL	C1B-CHB	2.00	1.46	1.41
25	9	604	CLA	CMC-C2C	-2.00	1.46	1.50
34	d	404	BCR	C1-C6	-2.00	1.51	1.53
24	1	608	CHL	C1B-CHB	2.00	1.46	1.41
25	7	603	CLA	CMC-C2C	-2.00	1.46	1.50
25	p	613	CLA	CMD-C2D	-2.00	1.46	1.50
24	N	607	CHL	C2C-C1C	2.00	1.48	1.44
25	0	613	CLA	C4B-CHC	-2.00	1.35	1.41
24	r	608	CHL	C3D-C2D	2.00	1.44	1.39
25	A	410	CLA	C4B-CHC	-2.00	1.35	1.41
25	q	603	CLA	CMC-C2C	-2.00	1.46	1.50
24	1	609	CHL	C4B-CHC	2.00	1.46	1.41
25	G	603	CLA	C3B-CAB	-2.00	1.43	1.47
25	S	609	CLA	CMC-C2C	-2.00	1.46	1.50
25	7	611	CLA	CMC-C2C	-2.00	1.46	1.50
37	C	524	DGD	O2G-C2G	-2.00	1.41	1.46

All (6324) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	a	412	SQD	O9-S-C6	-19.98	83.20	106.94
35	A	412	SQD	O9-S-C6	-19.85	83.34	106.94
27	Y	1622	XAT	C37-C21-C36	-17.70	81.26	107.37
27	y	1622	XAT	C37-C21-C36	-17.70	81.26	107.37
27	6	1622	XAT	C37-C21-C36	-17.56	81.47	107.37
27	0	1622	XAT	C37-C21-C36	-17.49	81.58	107.37
27	1	1622	XAT	C37-C21-C36	-17.00	82.29	107.37
27	7	1622	XAT	C37-C21-C36	-16.64	82.82	107.37
27	Y	1622	XAT	C37-C21-C22	-15.26	82.46	108.98
27	y	1622	XAT	C37-C21-C22	-15.26	82.46	108.98
27	1	1622	XAT	C37-C21-C22	-15.05	82.82	108.98

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	7	1622	XAT	C37-C21-C22	-15.05	82.84	108.98
27	6	1622	XAT	C37-C21-C22	-14.93	83.04	108.98
27	0	1622	XAT	C37-C21-C22	-14.84	83.20	108.98
35	A	412	SQD	O8-S-O9	-11.92	82.14	111.27
35	a	412	SQD	O8-S-O9	-11.90	82.20	111.27
28	2	1623	NEX	O24-C25-C24	11.26	121.84	113.38
28	9	1623	NEX	O24-C25-C24	10.64	121.38	113.38
28	5	1623	NEX	O24-C25-C24	10.44	121.22	113.38
24	1	601	CHL	CMD-C2D-C1D	10.43	143.09	124.71
24	7	601	CHL	CMD-C2D-C1D	10.35	142.95	124.71
28	s	1623	NEX	O24-C25-C24	10.33	121.14	113.38
28	S	1623	NEX	O24-C25-C24	10.29	121.11	113.38
27	n	1622	XAT	O24-C25-C24	10.29	121.11	113.38
27	N	1622	XAT	O24-C25-C24	10.24	121.08	113.38
24	G	601	CHL	CMD-C2D-C1D	10.24	142.76	124.71
24	q	609	CHL	CHD-C1D-ND	-10.17	115.11	124.45
35	a	412	SQD	O7-S-C6	9.89	118.69	106.94
28	0	1623	NEX	O24-C25-C24	9.87	120.80	113.38
28	p	1623	NEX	O24-C25-C24	9.85	120.78	113.38
24	g	601	CHL	CMD-C2D-C1D	9.82	142.02	124.71
28	R	623	NEX	O24-C25-C24	9.81	120.75	113.38
35	A	412	SQD	O7-S-C6	9.79	118.58	106.94
28	r	623	NEX	O24-C25-C24	9.79	120.74	113.38
24	g	609	CHL	CMD-C2D-C1D	9.60	141.63	124.71
24	G	609	CHL	CMD-C2D-C1D	9.59	141.61	124.71
24	N	601	CHL	CMD-C2D-C1D	9.45	141.36	124.71
28	8	1623	NEX	O24-C25-C24	9.43	120.47	113.38
24	n	601	CHL	CMD-C2D-C1D	9.39	141.27	124.71
28	3	1623	NEX	O24-C25-C24	9.25	120.33	113.38
24	4	609	CHL	CHD-C1D-ND	-9.22	115.98	124.45
27	5	1622	XAT	O24-C25-C24	9.21	120.30	113.38
24	s	601	CHL	CMD-C2D-C1D	9.08	140.72	124.71
25	c	502	CLA	C4A-NA-C1A	9.08	110.79	106.71
24	N	607	CHL	CMD-C2D-C1D	9.06	140.67	124.71
28	q	1623	NEX	O24-C25-C24	9.04	120.17	113.38
24	n	607	CHL	CMD-C2D-C1D	9.02	140.61	124.71
28	n	1623	NEX	O24-C25-C24	9.01	120.15	113.38
24	n	605	CHL	CMD-C2D-C1D	9.01	140.59	124.71
24	2	601	CHL	CMD-C2D-C1D	9.00	140.57	124.71
25	C	502	CLA	C4A-NA-C1A	8.95	110.73	106.71
24	N	605	CHL	CMD-C2D-C1D	8.94	140.47	124.71
35	A	412	SQD	O9-S-O7	-8.93	83.04	113.95

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	N	1623	NEX	O24-C25-C24	8.89	120.06	113.38
35	a	412	SQD	O9-S-O7	-8.89	83.18	113.95
24	y	606	CHL	C2C-C3C-C4C	-8.89	100.15	106.49
28	4	1623	NEX	O24-C25-C24	8.88	120.05	113.38
24	9	601	CHL	CMD-C2D-C1D	8.88	140.36	124.71
24	8	607	CHL	C1D-ND-C4D	-8.87	100.03	106.33
24	5	609	CHL	CMD-C2D-C1D	8.87	140.34	124.71
24	r	606	CHL	CMD-C2D-C1D	8.84	140.29	124.71
24	S	601	CHL	CMD-C2D-C1D	8.82	140.26	124.71
24	p	609	CHL	CMD-C2D-C1D	8.82	140.26	124.71
24	9	608	CHL	CMD-C2D-C1D	8.82	140.26	124.71
24	R	606	CHL	CMD-C2D-C1D	8.82	140.25	124.71
24	3	607	CHL	C1D-ND-C4D	-8.82	100.07	106.33
24	Y	606	CHL	C2C-C3C-C4C	-8.81	100.21	106.49
24	9	609	CHL	CMD-C2D-C1D	8.81	140.24	124.71
24	p	605	CHL	CMD-C2D-C1D	8.81	140.23	124.71
24	y	608	CHL	C1D-ND-C4D	-8.80	100.08	106.33
24	3	609	CHL	C2C-C3C-C4C	-8.78	100.23	106.49
24	Y	607	CHL	CMD-C2D-C1D	8.76	140.15	124.71
24	5	601	CHL	CMD-C2D-C1D	8.75	140.14	124.71
24	y	607	CHL	CMD-C2D-C1D	8.75	140.13	124.71
24	Y	608	CHL	C1D-ND-C4D	-8.74	100.12	106.33
24	0	606	CHL	CMD-C2D-C1D	8.74	140.12	124.71
24	2	608	CHL	CMD-C2D-C1D	8.74	140.12	124.71
27	3	1622	XAT	O24-C25-C24	8.73	119.94	113.38
24	7	601	CHL	C1D-ND-C4D	-8.72	100.14	106.33
24	2	609	CHL	CMD-C2D-C1D	8.71	140.07	124.71
28	6	1623	NEX	O24-C25-C24	8.71	119.92	113.38
24	7	608	CHL	C2C-C3C-C4C	-8.70	100.28	106.49
24	Y	606	CHL	CMD-C2D-C1D	8.70	140.05	124.71
24	3	606	CHL	CMD-C2D-C1D	8.70	140.04	124.71
24	8	606	CHL	CMD-C2D-C1D	8.69	140.03	124.71
24	6	609	CHL	CMD-C2D-C1D	8.68	140.01	124.71
24	q	605	CHL	CMD-C2D-C1D	8.68	140.00	124.71
24	y	606	CHL	CMD-C2D-C1D	8.67	139.99	124.71
24	N	608	CHL	CMD-C2D-C1D	8.67	139.99	124.71
24	y	601	CHL	CMD-C2D-C1D	8.67	139.99	124.71
24	n	608	CHL	CMD-C2D-C1D	8.67	139.99	124.71
24	y	608	CHL	CMD-C2D-C1D	8.66	139.98	124.71
24	Y	608	CHL	CMD-C2D-C1D	8.66	139.98	124.71
27	8	1622	XAT	O24-C25-C24	8.66	119.89	113.38
24	N	607	CHL	C1D-ND-C4D	-8.66	100.19	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	3	601	CHL	CMD-C2D-C1D	8.65	139.95	124.71
24	1	601	CHL	C1D-ND-C4D	-8.64	100.19	106.33
24	7	606	CHL	CMD-C2D-C1D	8.62	139.91	124.71
24	1	608	CHL	C2C-C3C-C4C	-8.62	100.34	106.49
24	n	607	CHL	C1D-ND-C4D	-8.62	100.21	106.33
28	g	1623	NEX	O24-C25-C24	8.60	119.84	113.38
24	y	609	CHL	C2C-C3C-C4C	-8.59	100.36	106.49
24	4	607	CHL	CMD-C2D-C1D	8.59	139.85	124.71
24	1	606	CHL	CMD-C2D-C1D	8.58	139.84	124.71
24	5	605	CHL	CMD-C2D-C1D	8.58	139.84	124.71
24	6	608	CHL	CMD-C2D-C1D	8.58	139.83	124.71
24	0	608	CHL	CMD-C2D-C1D	8.58	139.83	124.71
24	Y	609	CHL	C2C-C3C-C4C	-8.57	100.38	106.49
24	8	608	CHL	CMD-C2D-C1D	8.57	139.81	124.71
24	4	605	CHL	CMD-C2D-C1D	8.56	139.79	124.71
24	q	609	CHL	CMD-C2D-C1D	8.56	139.79	124.71
27	2	1622	XAT	O4-C5-C4	8.55	119.80	113.38
24	p	608	CHL	CMD-C2D-C1D	8.55	139.78	124.71
24	5	608	CHL	C1D-ND-C4D	-8.54	100.27	106.33
27	y	1622	XAT	C36-C21-C22	8.54	123.82	108.98
27	Y	1622	XAT	C36-C21-C22	8.53	123.81	108.98
24	0	609	CHL	CMD-C2D-C1D	8.53	139.75	124.71
24	7	608	CHL	CMD-C2D-C1D	8.53	139.74	124.71
24	1	609	CHL	CMD-C2D-C1D	8.52	139.74	124.71
28	G	1623	NEX	O24-C25-C24	8.52	119.78	113.38
24	5	608	CHL	CMD-C2D-C1D	8.51	139.72	124.71
24	N	606	CHL	CMD-C2D-C1D	8.51	139.71	124.71
24	8	601	CHL	CMD-C2D-C1D	8.51	139.71	124.71
24	g	607	CHL	CMD-C2D-C1D	8.51	139.70	124.71
24	p	608	CHL	C1D-ND-C4D	-8.51	100.29	106.33
24	8	609	CHL	C2C-C3C-C4C	-8.50	100.43	106.49
24	Y	601	CHL	CMD-C2D-C1D	8.49	139.68	124.71
24	8	607	CHL	CMD-C2D-C1D	8.48	139.66	124.71
24	n	606	CHL	CMD-C2D-C1D	8.47	139.65	124.71
24	7	609	CHL	CMD-C2D-C1D	8.47	139.64	124.71
24	p	605	CHL	CHD-C1D-ND	-8.47	116.67	124.45
24	3	607	CHL	CMD-C2D-C1D	8.46	139.63	124.71
24	7	605	CHL	CMD-C2D-C1D	8.45	139.61	124.71
24	3	608	CHL	CMD-C2D-C1D	8.45	139.60	124.71
24	p	601	CHL	CMD-C2D-C1D	8.43	139.58	124.71
24	Y	607	CHL	C1D-ND-C4D	-8.43	100.34	106.33
24	4	608	CHL	CMD-C2D-C1D	8.42	139.56	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	1	1623	NEX	O24-C25-C24	8.42	119.71	113.38
24	q	601	CHL	CMD-C2D-C1D	8.42	139.56	124.71
24	Y	609	CHL	CMD-C2D-C1D	8.42	139.55	124.71
24	y	607	CHL	C1D-ND-C4D	-8.41	100.36	106.33
24	9	607	CHL	CMD-C2D-C1D	8.41	139.54	124.71
24	6	601	CHL	C1D-ND-C4D	-8.41	100.36	106.33
24	n	601	CHL	C1D-ND-C4D	-8.40	100.37	106.33
24	g	606	CHL	CMD-C2D-C1D	8.39	139.50	124.71
24	s	608	CHL	CMD-C2D-C1D	8.39	139.50	124.71
24	n	609	CHL	CMD-C2D-C1D	8.38	139.48	124.71
24	G	606	CHL	CMD-C2D-C1D	8.38	139.48	124.71
27	9	1622	XAT	O4-C5-C4	8.37	119.67	113.38
24	1	608	CHL	CMD-C2D-C1D	8.37	139.47	124.71
24	G	608	CHL	CMD-C2D-C1D	8.37	139.46	124.71
24	8	605	CHL	CMD-C2D-C1D	8.37	139.46	124.71
24	q	608	CHL	CHD-C1D-ND	-8.36	116.77	124.45
24	6	606	CHL	CMD-C2D-C1D	8.36	139.44	124.71
24	N	609	CHL	CMD-C2D-C1D	8.35	139.44	124.71
24	S	608	CHL	CMD-C2D-C1D	8.35	139.42	124.71
24	g	608	CHL	CMD-C2D-C1D	8.34	139.40	124.71
24	n	606	CHL	C1D-ND-C4D	-8.33	100.42	106.33
24	p	606	CHL	CMD-C2D-C1D	8.32	139.37	124.71
24	1	605	CHL	CMD-C2D-C1D	8.32	139.37	124.71
24	0	607	CHL	C1D-ND-C4D	-8.31	100.43	106.33
24	5	605	CHL	CHD-C1D-ND	-8.31	116.82	124.45
24	3	605	CHL	CMD-C2D-C1D	8.30	139.34	124.71
24	y	609	CHL	CMD-C2D-C1D	8.29	139.32	124.71
24	q	607	CHL	CMD-C2D-C1D	8.27	139.29	124.71
24	8	601	CHL	C1D-ND-C4D	-8.27	100.46	106.33
27	p	1622	XAT	O24-C25-C24	8.26	119.59	113.38
24	N	601	CHL	C1D-ND-C4D	-8.26	100.47	106.33
24	8	605	CHL	CHD-C1D-ND	-8.24	116.88	124.45
24	5	605	CHL	C1D-ND-C4D	-8.24	100.48	106.33
24	4	609	CHL	CMD-C2D-C1D	8.22	139.20	124.71
24	q	608	CHL	C2C-C3C-C4C	-8.22	100.63	106.49
24	p	601	CHL	C1D-ND-C4D	-8.21	100.50	106.33
24	g	601	CHL	C1D-ND-C4D	-8.21	100.50	106.33
24	8	609	CHL	C1D-ND-C4D	-8.21	100.50	106.33
24	G	605	CHL	CMD-C2D-C1D	8.21	139.18	124.71
24	9	605	CHL	CMD-C2D-C1D	8.20	139.17	124.71
24	3	605	CHL	CHD-C1D-ND	-8.19	116.93	124.45
24	0	605	CHL	CMD-C2D-C1D	8.19	139.15	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	g	605	CHL	CMD-C2D-C1D	8.19	139.15	124.71
24	2	605	CHL	CMD-C2D-C1D	8.19	139.15	124.71
24	S	606	CHL	C2C-C3C-C4C	-8.18	100.66	106.49
24	R	607	CHL	C2C-C3C-C4C	-8.17	100.67	106.49
24	s	606	CHL	C2C-C3C-C4C	-8.17	100.67	106.49
24	Y	609	CHL	C1D-ND-C4D	-8.16	100.53	106.33
24	r	608	CHL	CMD-C2D-C1D	8.16	139.10	124.71
24	N	608	CHL	C1D-ND-C4D	-8.15	100.55	106.33
24	9	609	CHL	C2C-C3C-C4C	-8.15	100.68	106.49
24	R	608	CHL	CMD-C2D-C1D	8.15	139.07	124.71
24	N	606	CHL	C1D-ND-C4D	-8.15	100.55	106.33
24	g	606	CHL	C1D-ND-C4D	-8.15	100.55	106.33
24	G	606	CHL	C1D-ND-C4D	-8.14	100.55	106.33
24	r	607	CHL	C2C-C3C-C4C	-8.14	100.69	106.49
24	6	605	CHL	CMD-C2D-C1D	8.11	139.01	124.71
24	2	609	CHL	C2C-C3C-C4C	-8.11	100.71	106.49
24	S	606	CHL	CMD-C2D-C1D	8.11	139.00	124.71
24	0	609	CHL	C2C-C3C-C4C	-8.10	100.71	106.49
24	3	601	CHL	C1D-ND-C4D	-8.10	100.58	106.33
24	y	609	CHL	C1D-ND-C4D	-8.10	100.58	106.33
24	1	608	CHL	C1D-ND-C4D	-8.10	100.58	106.33
24	G	601	CHL	C1D-ND-C4D	-8.09	100.58	106.33
24	5	606	CHL	CMD-C2D-C1D	8.09	138.97	124.71
24	s	606	CHL	CMD-C2D-C1D	8.08	138.96	124.71
24	S	608	CHL	C2C-C3C-C4C	-8.07	100.73	106.49
24	3	609	CHL	C1D-ND-C4D	-8.07	100.60	106.33
24	2	607	CHL	CMD-C2D-C1D	8.07	138.94	124.71
24	y	608	CHL	C2C-C3C-C4C	-8.06	100.74	106.49
24	2	606	CHL	CMD-C2D-C1D	8.05	138.91	124.71
24	G	607	CHL	CMD-C2D-C1D	8.04	138.89	124.71
24	s	608	CHL	C2C-C3C-C4C	-8.03	100.76	106.49
24	n	608	CHL	C2C-C3C-C4C	-8.03	100.77	106.49
24	n	608	CHL	C1D-ND-C4D	-8.01	100.64	106.33
24	R	607	CHL	CMD-C2D-C1D	8.01	138.83	124.71
24	r	607	CHL	CMD-C2D-C1D	8.01	138.83	124.71
24	5	607	CHL	C1D-ND-C4D	-8.01	100.65	106.33
24	6	608	CHL	C2C-C3C-C4C	-8.00	100.78	106.49
24	S	606	CHL	C1D-ND-C4D	-8.00	100.66	106.33
24	4	608	CHL	C2C-C3C-C4C	-7.99	100.79	106.49
24	y	601	CHL	C1D-ND-C4D	-7.99	100.66	106.33
24	Y	605	CHL	CMD-C2D-C1D	7.98	138.78	124.71
24	y	605	CHL	CMD-C2D-C1D	7.98	138.78	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	7	608	CHL	C1D-ND-C4D	-7.98	100.67	106.33
24	4	606	CHL	CMD-C2D-C1D	7.98	138.77	124.71
24	Y	608	CHL	C2C-C3C-C4C	-7.97	100.81	106.49
24	q	606	CHL	CMD-C2D-C1D	7.96	138.74	124.71
24	R	608	CHL	C2C-C3C-C4C	-7.94	100.83	106.49
24	r	608	CHL	C2C-C3C-C4C	-7.94	100.83	106.49
24	9	608	CHL	C1D-ND-C4D	-7.94	100.69	106.33
24	6	607	CHL	C2C-C3C-C4C	-7.94	100.83	106.49
24	6	606	CHL	C1D-ND-C4D	-7.94	100.70	106.33
24	2	608	CHL	C1D-ND-C4D	-7.93	100.70	106.33
24	s	606	CHL	C1D-ND-C4D	-7.93	100.70	106.33
24	N	608	CHL	C2C-C3C-C4C	-7.93	100.84	106.49
24	q	605	CHL	CHD-C1D-ND	-7.93	117.17	124.45
24	R	606	CHL	C2C-C3C-C4C	-7.93	100.84	106.49
24	r	606	CHL	C2C-C3C-C4C	-7.92	100.84	106.49
24	5	601	CHL	C1D-ND-C4D	-7.91	100.71	106.33
24	Y	601	CHL	C1D-ND-C4D	-7.89	100.73	106.33
24	6	607	CHL	CMD-C2D-C1D	7.89	138.61	124.71
24	q	608	CHL	CMD-C2D-C1D	7.88	138.60	124.71
24	Y	607	CHL	C2C-C3C-C4C	-7.87	100.88	106.49
27	0	1622	XAT	O4-C5-C4	7.87	119.29	113.38
24	S	607	CHL	CMD-C2D-C1D	7.86	138.57	124.71
24	6	601	CHL	CMD-C2D-C1D	7.84	138.53	124.71
24	0	607	CHL	CMD-C2D-C1D	7.84	138.53	124.71
24	q	601	CHL	C1D-ND-C4D	-7.84	100.77	106.33
24	y	607	CHL	C2C-C3C-C4C	-7.84	100.90	106.49
24	p	609	CHL	C2C-C3C-C4C	-7.84	100.90	106.49
24	s	607	CHL	CMD-C2D-C1D	7.83	138.51	124.71
27	1	1622	XAT	C36-C21-C22	7.82	122.57	108.98
24	7	607	CHL	CMD-C2D-C1D	7.81	138.49	124.71
24	4	601	CHL	CMD-C2D-C1D	7.81	138.48	124.71
28	y	1623	NEX	O24-C25-C24	7.81	119.25	113.38
24	1	605	CHL	C2C-C3C-C4C	-7.80	100.93	106.49
24	g	607	CHL	C2C-C3C-C4C	-7.79	100.94	106.49
28	Y	1623	NEX	O24-C25-C24	7.79	119.23	113.38
24	9	606	CHL	CMD-C2D-C1D	7.78	138.43	124.71
24	G	607	CHL	C1D-ND-C4D	-7.77	100.81	106.33
24	8	605	CHL	C2C-C3C-C4C	-7.77	100.95	106.49
24	4	605	CHL	CHD-C1D-ND	-7.77	117.31	124.45
24	G	607	CHL	C2C-C3C-C4C	-7.77	100.95	106.49
24	6	609	CHL	C2C-C3C-C4C	-7.76	100.96	106.49
24	0	601	CHL	C1D-ND-C4D	-7.76	100.82	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	7	605	CHL	C2C-C3C-C4C	-7.74	100.97	106.49
24	1	607	CHL	CMD-C2D-C1D	7.74	138.35	124.71
24	7	609	CHL	C1D-ND-C4D	-7.74	100.84	106.33
24	3	605	CHL	C2C-C3C-C4C	-7.73	100.98	106.49
24	5	607	CHL	CMD-C2D-C1D	7.73	138.34	124.71
27	6	1622	XAT	O4-C5-C4	7.73	119.19	113.38
27	7	1622	XAT	C36-C21-C22	7.72	122.40	108.98
27	6	1622	XAT	C36-C21-C22	7.72	122.39	108.98
24	p	607	CHL	C1D-ND-C4D	-7.72	100.85	106.33
24	8	607	CHL	C2D-C1D-ND	7.71	115.79	110.10
24	p	607	CHL	CMD-C2D-C1D	7.71	138.31	124.71
24	7	607	CHL	C1D-ND-C4D	-7.71	100.86	106.33
24	y	608	CHL	C2D-C1D-ND	7.70	115.78	110.10
24	9	609	CHL	CHD-C1D-ND	-7.70	117.38	124.45
24	0	607	CHL	C2C-C3C-C4C	-7.70	101.00	106.49
35	a	412	SQD	O8-S-C6	7.69	118.00	105.74
27	0	1622	XAT	C36-C21-C22	7.69	122.35	108.98
24	0	606	CHL	C1D-ND-C4D	-7.69	100.87	106.33
35	A	412	SQD	O8-S-C6	7.69	118.00	105.74
24	g	607	CHL	C1D-ND-C4D	-7.69	100.88	106.33
24	7	609	CHL	C2C-C3C-C4C	-7.68	101.02	106.49
24	8	608	CHL	C1D-ND-C4D	-7.68	100.88	106.33
24	Y	608	CHL	C2D-C1D-ND	7.67	115.75	110.10
24	g	608	CHL	C1D-ND-C4D	-7.66	100.89	106.33
24	N	609	CHL	C2C-C3C-C4C	-7.66	101.03	106.49
24	1	601	CHL	CHD-C1D-ND	-7.65	117.43	124.45
24	1	609	CHL	C1D-ND-C4D	-7.64	100.91	106.33
24	3	607	CHL	C2D-C1D-ND	7.64	115.73	110.10
24	3	608	CHL	C1D-ND-C4D	-7.63	100.91	106.33
24	1	609	CHL	C2C-C3C-C4C	-7.63	101.05	106.49
24	g	605	CHL	C1D-ND-C4D	-7.62	100.92	106.33
24	2	609	CHL	C1D-ND-C4D	-7.61	100.93	106.33
24	5	609	CHL	C2C-C3C-C4C	-7.60	101.07	106.49
24	R	606	CHL	C1D-ND-C4D	-7.60	100.93	106.33
24	r	606	CHL	C1D-ND-C4D	-7.60	100.93	106.33
24	7	601	CHL	CHD-C1D-ND	-7.60	117.47	124.45
24	R	608	CHL	C1D-ND-C4D	-7.60	100.94	106.33
24	2	606	CHL	C2C-C3C-C4C	-7.60	101.08	106.49
24	3	607	CHL	C2C-C3C-C4C	-7.59	101.08	106.49
24	n	606	CHL	C2C-C3C-C4C	-7.58	101.09	106.49
24	5	605	CHL	C2C-C3C-C4C	-7.57	101.09	106.49
24	0	605	CHL	C2C-C3C-C4C	-7.56	101.10	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	S	601	CHL	C1D-ND-C4D	-7.56	100.97	106.33
24	1	606	CHL	C1D-ND-C4D	-7.55	100.97	106.33
24	4	601	CHL	C2C-C3C-C4C	-7.55	101.11	106.49
24	4	601	CHL	C1D-ND-C4D	-7.54	100.98	106.33
24	s	608	CHL	C1D-ND-C4D	-7.54	100.98	106.33
24	S	608	CHL	C1D-ND-C4D	-7.54	100.98	106.33
24	1	607	CHL	C1D-ND-C4D	-7.53	100.99	106.33
24	1	608	CHL	C2D-C1D-ND	7.53	115.65	110.10
24	2	609	CHL	CHD-C1D-ND	-7.52	117.54	124.45
24	3	608	CHL	C2C-C3C-C4C	-7.52	101.13	106.49
24	8	608	CHL	C2C-C3C-C4C	-7.51	101.14	106.49
24	q	607	CHL	C2C-C3C-C4C	-7.51	101.14	106.49
24	p	608	CHL	C2C-C3C-C4C	-7.51	101.14	106.49
24	Y	606	CHL	C1D-ND-C4D	-7.50	101.00	106.33
24	G	605	CHL	C1D-ND-C4D	-7.50	101.01	106.33
24	R	607	CHL	C1D-ND-C4D	-7.50	101.01	106.33
24	0	608	CHL	C1D-ND-C4D	-7.49	101.01	106.33
24	s	607	CHL	C2C-C3C-C4C	-7.49	101.15	106.49
24	5	609	CHL	CHD-C1D-ND	-7.49	117.57	124.45
24	s	601	CHL	C1D-ND-C4D	-7.49	101.01	106.33
24	r	607	CHL	C1D-ND-C4D	-7.49	101.02	106.33
24	1	606	CHL	C2C-C3C-C4C	-7.48	101.15	106.49
24	y	606	CHL	C1D-ND-C4D	-7.48	101.02	106.33
24	9	606	CHL	C2C-C3C-C4C	-7.48	101.16	106.49
24	r	608	CHL	C1D-ND-C4D	-7.48	101.02	106.33
24	4	607	CHL	C2C-C3C-C4C	-7.48	101.16	106.49
24	Y	605	CHL	C2C-C3C-C4C	-7.47	101.17	106.49
24	g	606	CHL	C2C-C3C-C4C	-7.46	101.17	106.49
24	S	607	CHL	C2C-C3C-C4C	-7.46	101.17	106.49
24	G	606	CHL	C2C-C3C-C4C	-7.45	101.18	106.49
24	8	607	CHL	C2C-C3C-C4C	-7.43	101.19	106.49
24	y	605	CHL	C2C-C3C-C4C	-7.42	101.20	106.49
24	4	608	CHL	CHD-C1D-ND	-7.41	117.64	124.45
24	7	606	CHL	C2C-C3C-C4C	-7.41	101.20	106.49
24	5	608	CHL	C2C-C3C-C4C	-7.41	101.21	106.49
25	c	509	CLA	C4A-NA-C1A	7.40	110.03	106.71
24	0	601	CHL	C2C-C3C-C4C	-7.40	101.21	106.49
24	6	607	CHL	C1D-ND-C4D	-7.39	101.08	106.33
25	C	509	CLA	C4A-NA-C1A	7.39	110.03	106.71
24	7	608	CHL	C2D-C1D-ND	7.38	115.55	110.10
24	7	607	CHL	C2C-C3C-C4C	-7.38	101.23	106.49
24	0	609	CHL	CHD-C1D-ND	-7.37	117.68	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	N	607	CHL	C2C-C3C-C4C	-7.36	101.24	106.49
24	p	605	CHL	C1D-ND-C4D	-7.36	101.11	106.33
24	6	605	CHL	C2C-C3C-C4C	-7.36	101.24	106.49
24	6	608	CHL	C1D-ND-C4D	-7.36	101.11	106.33
24	N	606	CHL	C2C-C3C-C4C	-7.35	101.25	106.49
24	G	605	CHL	C2C-C3C-C4C	-7.34	101.25	106.49
24	G	608	CHL	C1D-ND-C4D	-7.34	101.12	106.33
24	p	609	CHL	CHD-C1D-ND	-7.34	117.71	124.45
24	q	605	CHL	C1D-ND-C4D	-7.33	101.12	106.33
24	g	609	CHL	CHD-C1D-ND	-7.32	117.72	124.45
24	8	606	CHL	CHD-C1D-ND	-7.31	117.73	124.45
24	4	608	CHL	C1D-ND-C4D	-7.31	101.14	106.33
24	0	608	CHL	C2C-C3C-C4C	-7.31	101.28	106.49
24	p	605	CHL	C2C-C3C-C4C	-7.30	101.28	106.49
24	G	609	CHL	CHD-C1D-ND	-7.29	117.76	124.45
24	3	606	CHL	CHD-C1D-ND	-7.28	117.76	124.45
27	Y	1622	XAT	O24-C25-C24	7.28	118.85	113.38
24	n	605	CHL	C1D-ND-C4D	-7.27	101.17	106.33
24	g	605	CHL	C2C-C3C-C4C	-7.27	101.31	106.49
24	4	609	CHL	C2C-C3C-C4C	-7.26	101.31	106.49
24	5	606	CHL	C1D-ND-C4D	-7.25	101.18	106.33
24	5	606	CHL	C2C-C3C-C4C	-7.23	101.33	106.49
24	p	607	CHL	C2C-C3C-C4C	-7.22	101.34	106.49
25	B	613	CLA	C4A-NA-C1A	7.22	109.95	106.71
25	b	613	CLA	C4A-NA-C1A	7.22	109.95	106.71
24	5	601	CHL	CHD-C1D-ND	-7.22	117.82	124.45
25	5	613	CLA	C4A-NA-C1A	7.22	109.95	106.71
24	9	608	CHL	C2C-C3C-C4C	-7.21	101.35	106.49
27	y	1622	XAT	O24-C25-C24	7.21	118.80	113.38
24	n	607	CHL	C2C-C3C-C4C	-7.20	101.36	106.49
24	0	601	CHL	CMD-C2D-C1D	7.20	137.40	124.71
24	q	601	CHL	C2C-C3C-C4C	-7.19	101.37	106.49
24	5	608	CHL	C2D-C1D-ND	7.18	115.40	110.10
24	7	606	CHL	C1D-ND-C4D	-7.18	101.23	106.33
24	q	605	CHL	C2C-C3C-C4C	-7.15	101.39	106.49
24	N	609	CHL	C1D-ND-C4D	-7.15	101.25	106.33
24	2	608	CHL	C2C-C3C-C4C	-7.14	101.40	106.49
24	N	605	CHL	C1D-ND-C4D	-7.14	101.26	106.33
24	y	605	CHL	C1D-ND-C4D	-7.14	101.26	106.33
24	0	607	CHL	C2D-C1D-ND	7.13	115.36	110.10
24	n	609	CHL	CHD-C1D-ND	-7.13	117.91	124.45
24	6	601	CHL	C2C-C3C-C4C	-7.13	101.41	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	p	608	CHL	C2D-C1D-ND	7.12	115.35	110.10
24	y	609	CHL	C2D-C1D-ND	7.12	115.35	110.10
24	l	607	CHL	C2C-C3C-C4C	-7.11	101.42	106.49
24	Y	607	CHL	C2D-C1D-ND	7.11	115.34	110.10
24	g	608	CHL	C2C-C3C-C4C	-7.10	101.43	106.49
24	n	609	CHL	C1D-ND-C4D	-7.10	101.29	106.33
24	8	609	CHL	C2D-C1D-ND	7.10	115.33	110.10
24	y	601	CHL	CHD-C1D-ND	-7.09	117.94	124.45
24	G	608	CHL	C2C-C3C-C4C	-7.09	101.44	106.49
24	p	609	CHL	C1D-ND-C4D	-7.08	101.31	106.33
24	S	601	CHL	C2C-C3C-C4C	-7.08	101.44	106.49
24	Y	605	CHL	C1D-ND-C4D	-7.07	101.31	106.33
24	2	607	CHL	C2C-C3C-C4C	-7.07	101.45	106.49
24	0	605	CHL	C1D-ND-C4D	-7.05	101.32	106.33
24	2	605	CHL	C1D-ND-C4D	-7.05	101.33	106.33
24	Y	609	CHL	C2D-C1D-ND	7.04	115.29	110.10
24	y	607	CHL	C2D-C1D-ND	7.04	115.29	110.10
24	6	606	CHL	C2C-C3C-C4C	-7.04	101.47	106.49
24	2	606	CHL	C1D-ND-C4D	-7.02	101.35	106.33
24	4	606	CHL	C2C-C3C-C4C	-7.02	101.49	106.49
24	s	601	CHL	CHD-C1D-ND	-7.00	118.02	124.45
27	r	622	XAT	O4-C5-C4	7.00	118.64	113.38
24	9	601	CHL	CHD-C1D-ND	-7.00	118.03	124.45
24	n	608	CHL	C2D-C1D-ND	6.99	115.26	110.10
24	9	606	CHL	C1D-ND-C4D	-6.99	101.37	106.33
25	C	506	CLA	C4A-NA-C1A	6.99	109.85	106.71
24	9	605	CHL	C1D-ND-C4D	-6.99	101.37	106.33
24	9	607	CHL	C2C-C3C-C4C	-6.98	101.51	106.49
24	5	607	CHL	C2C-C3C-C4C	-6.98	101.52	106.49
24	9	609	CHL	C1D-ND-C4D	-6.97	101.38	106.33
24	3	609	CHL	C2D-C1D-ND	6.97	115.24	110.10
25	c	506	CLA	C4A-NA-C1A	6.97	109.84	106.71
24	S	601	CHL	CHD-C1D-ND	-6.97	118.05	124.45
24	2	601	CHL	C2C-C3C-C4C	-6.97	101.52	106.49
27	q	1622	XAT	O24-C25-C24	6.96	118.61	113.38
24	n	607	CHL	C2D-C1D-ND	6.95	115.23	110.10
27	R	622	XAT	O4-C5-C4	6.95	118.61	113.38
24	Y	601	CHL	CHD-C1D-ND	-6.95	118.06	124.45
24	n	609	CHL	C2C-C3C-C4C	-6.95	101.54	106.49
24	4	605	CHL	C1D-ND-C4D	-6.94	101.40	106.33
24	9	607	CHL	C1D-ND-C4D	-6.94	101.40	106.33
24	s	601	CHL	C2C-C3C-C4C	-6.94	101.54	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	n	613	CLA	C4A-NA-C1A	6.93	109.82	106.71
24	4	607	CHL	C1D-ND-C4D	-6.93	101.41	106.33
24	N	608	CHL	C2D-C1D-ND	6.92	115.21	110.10
24	4	605	CHL	C2C-C3C-C4C	-6.92	101.56	106.49
24	3	609	CHL	CMD-C2D-C1D	6.92	136.90	124.71
24	6	601	CHL	C2D-C1D-ND	6.91	115.19	110.10
24	9	601	CHL	C2C-C3C-C4C	-6.90	101.57	106.49
24	4	607	CHL	CHD-C1D-ND	-6.90	118.11	124.45
24	5	609	CHL	C1D-ND-C4D	-6.89	101.44	106.33
24	q	609	CHL	C2C-C3C-C4C	-6.89	101.58	106.49
24	q	606	CHL	C2C-C3C-C4C	-6.88	101.58	106.49
24	2	605	CHL	C2C-C3C-C4C	-6.87	101.59	106.49
24	N	607	CHL	C2D-C1D-ND	6.87	115.17	110.10
24	n	606	CHL	C2D-C1D-ND	6.86	115.16	110.10
24	9	607	CHL	CHD-C1D-ND	-6.85	118.16	124.45
24	0	606	CHL	C2C-C3C-C4C	-6.84	101.61	106.49
24	9	605	CHL	C2C-C3C-C4C	-6.84	101.61	106.49
24	6	609	CHL	C1D-ND-C4D	-6.84	101.48	106.33
24	5	607	CHL	C2D-C1D-ND	6.84	115.14	110.10
25	r	601	CLA	C4A-NA-C1A	6.83	109.78	106.71
24	2	607	CHL	CHD-C1D-ND	-6.83	118.17	124.45
24	q	607	CHL	CHD-C1D-ND	-6.83	118.18	124.45
24	7	609	CHL	C2D-C1D-ND	6.83	115.14	110.10
24	1	605	CHL	C1D-ND-C4D	-6.83	101.48	106.33
25	r	603	CLA	C4A-NA-C1A	6.82	109.77	106.71
24	6	609	CHL	CHD-C1D-ND	-6.82	118.18	124.45
24	N	609	CHL	CHD-C1D-ND	-6.82	118.18	124.45
25	R	603	CLA	C4A-NA-C1A	6.82	109.77	106.71
24	8	609	CHL	CMD-C2D-C1D	6.81	136.71	124.71
24	7	605	CHL	CHD-C1D-ND	-6.81	118.20	124.45
24	q	606	CHL	CHD-C1D-ND	-6.80	118.20	124.45
24	2	607	CHL	C1D-ND-C4D	-6.80	101.51	106.33
24	0	608	CHL	CHD-C1D-ND	-6.78	118.23	124.45
24	p	601	CHL	C2D-C1D-ND	6.77	115.09	110.10
24	r	607	CHL	C2D-C1D-ND	6.76	115.08	110.10
25	8	613	CLA	C4A-NA-C1A	6.75	109.74	106.71
25	N	613	CLA	C4A-NA-C1A	6.75	109.74	106.71
24	1	605	CHL	CHD-C1D-ND	-6.75	118.25	124.45
24	p	601	CHL	CHD-C1D-ND	-6.75	118.25	124.45
24	7	605	CHL	C1D-ND-C4D	-6.74	101.55	106.33
28	7	1623	NEX	O24-C25-C24	6.74	118.44	113.38
24	N	606	CHL	C2D-C1D-ND	6.72	115.05	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	2	608	CHL	C2D-C1D-ND	6.72	115.05	110.10
24	9	608	CHL	C2D-C1D-ND	6.72	115.05	110.10
24	R	607	CHL	C2D-C1D-ND	6.70	115.04	110.10
24	4	606	CHL	C1D-ND-C4D	-6.69	101.58	106.33
24	Y	606	CHL	C2D-C1D-ND	6.69	115.03	110.10
25	R	601	CLA	C4A-NA-C1A	6.68	109.71	106.71
24	3	606	CHL	C2C-C3C-C4C	-6.68	101.73	106.49
24	n	607	CHL	CHD-C1D-ND	-6.68	118.32	124.45
24	G	607	CHL	C2D-C1D-ND	6.67	115.02	110.10
24	p	601	CHL	C2C-C3C-C4C	-6.67	101.73	106.49
24	8	606	CHL	C2C-C3C-C4C	-6.67	101.73	106.49
24	0	601	CHL	C2D-C1D-ND	6.66	115.01	110.10
24	s	607	CHL	C1D-ND-C4D	-6.65	101.61	106.33
24	8	601	CHL	C2C-C3C-C4C	-6.65	101.75	106.49
24	p	606	CHL	CHD-C1D-ND	-6.64	118.35	124.45
24	8	606	CHL	C1D-ND-C4D	-6.63	101.62	106.33
24	y	606	CHL	C2D-C1D-ND	6.63	114.99	110.10
24	5	601	CHL	C2C-C3C-C4C	-6.63	101.76	106.49
25	r	602	CLA	C4A-NA-C1A	6.63	109.69	106.71
27	y	1622	XAT	O4-C5-C4	6.62	118.35	113.38
24	G	601	CHL	C2C-C3C-C4C	-6.62	101.77	106.49
24	Y	601	CHL	C2C-C3C-C4C	-6.61	101.77	106.49
24	S	607	CHL	C1D-ND-C4D	-6.61	101.64	106.33
27	p	1622	XAT	O4-C5-C4	6.61	118.34	113.38
24	s	608	CHL	C2D-C1D-ND	6.60	114.97	110.10
24	1	609	CHL	C2D-C1D-ND	6.60	114.97	110.10
25	R	602	CLA	C4A-NA-C1A	6.60	109.67	106.71
27	Y	1622	XAT	O4-C5-C4	6.59	118.33	113.38
24	3	601	CHL	CHD-C1D-ND	-6.58	118.40	124.45
24	2	601	CHL	CHD-C1D-ND	-6.57	118.42	124.45
24	0	609	CHL	C1D-ND-C4D	-6.57	101.67	106.33
24	n	601	CHL	CHD-C1D-ND	-6.56	118.43	124.45
24	5	605	CHL	C2D-C1D-ND	6.56	114.94	110.10
24	G	609	CHL	C1D-ND-C4D	-6.55	101.68	106.33
25	3	613	CLA	C4A-NA-C1A	6.55	109.65	106.71
24	R	608	CHL	C2D-C1D-ND	6.55	114.93	110.10
24	N	607	CHL	CHD-C1D-ND	-6.55	118.44	124.45
24	S	608	CHL	C2D-C1D-ND	6.54	114.93	110.10
24	g	601	CHL	C2C-C3C-C4C	-6.54	101.83	106.49
24	s	608	CHL	CHD-C1D-ND	-6.53	118.45	124.45
24	S	608	CHL	CHD-C1D-ND	-6.53	118.45	124.45
24	r	608	CHL	C2D-C1D-ND	6.53	114.91	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	605	CHL	C1D-ND-C4D	-6.52	101.70	106.33
24	S	606	CHL	C2D-C1D-ND	6.52	114.91	110.10
24	9	606	CHL	CHD-C1D-ND	-6.52	118.46	124.45
27	g	1622	XAT	O24-C25-C24	6.51	118.28	113.38
24	g	606	CHL	C2D-C1D-ND	6.51	114.90	110.10
25	B	611	CLA	C4A-NA-C1A	6.51	109.63	106.71
24	0	601	CHL	CHD-C1D-ND	-6.50	118.48	124.45
24	8	601	CHL	C2D-C1D-ND	6.50	114.89	110.10
24	g	609	CHL	C1D-ND-C4D	-6.49	101.72	106.33
24	2	606	CHL	CHD-C1D-ND	-6.48	118.50	124.45
25	c	512	CLA	C4A-NA-C1A	6.48	109.62	106.71
24	6	608	CHL	CHD-C1D-ND	-6.48	118.50	124.45
24	y	601	CHL	C2C-C3C-C4C	-6.48	101.87	106.49
24	3	606	CHL	C1D-ND-C4D	-6.48	101.73	106.33
24	G	606	CHL	C2D-C1D-ND	6.47	114.88	110.10
24	0	605	CHL	C2D-C1D-ND	6.46	114.87	110.10
25	C	512	CLA	C4A-NA-C1A	6.46	109.61	106.71
24	6	601	CHL	CHD-C1D-ND	-6.45	118.52	124.45
24	g	605	CHL	C2D-C1D-ND	6.45	114.86	110.10
24	g	608	CHL	C2D-C1D-ND	6.45	114.86	110.10
24	p	606	CHL	C2C-C3C-C4C	-6.44	101.90	106.49
24	g	607	CHL	CHD-C1D-ND	-6.44	118.54	124.45
27	G	1622	XAT	O24-C25-C24	6.43	118.21	113.38
27	3	1622	XAT	O4-C5-C4	6.42	118.21	113.38
24	s	606	CHL	C2D-C1D-ND	6.42	114.84	110.10
24	g	609	CHL	C2C-C3C-C4C	-6.42	101.91	106.49
24	4	606	CHL	CHD-C1D-ND	-6.42	118.55	124.45
24	N	601	CHL	C2C-C3C-C4C	-6.41	101.92	106.49
24	G	609	CHL	C2C-C3C-C4C	-6.40	101.92	106.49
24	0	606	CHL	CHD-C1D-ND	-6.39	118.58	124.45
24	8	601	CHL	CHD-C1D-ND	-6.39	118.58	124.45
24	7	606	CHL	CHD-C1D-ND	-6.39	118.58	124.45
27	4	1622	XAT	O24-C25-C24	6.39	118.18	113.38
24	8	605	CHL	C1D-ND-C4D	-6.38	101.80	106.33
24	3	601	CHL	C2D-C1D-ND	6.38	114.80	110.10
25	b	611	CLA	C4A-NA-C1A	6.37	109.57	106.71
24	2	601	CHL	C1D-ND-C4D	-6.37	101.81	106.33
24	n	601	CHL	C2D-C1D-ND	6.37	114.80	110.10
24	g	607	CHL	C2D-C1D-ND	6.35	114.78	110.10
24	p	606	CHL	C1D-ND-C4D	-6.35	101.82	106.33
27	8	1622	XAT	O4-C5-C4	6.35	118.15	113.38
24	q	606	CHL	C1D-ND-C4D	-6.35	101.82	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	8	608	CHL	C2D-C1D-ND	6.34	114.78	110.10
24	5	601	CHL	C2D-C1D-ND	6.32	114.76	110.10
24	6	607	CHL	C2D-C1D-ND	6.31	114.76	110.10
24	G	605	CHL	C2D-C1D-ND	6.31	114.75	110.10
24	1	606	CHL	CHD-C1D-ND	-6.31	118.66	124.45
24	3	608	CHL	C2D-C1D-ND	6.30	114.75	110.10
24	q	608	CHL	C1D-ND-C4D	-6.29	101.87	106.33
24	6	608	CHL	C2D-C1D-ND	6.29	114.74	110.10
24	N	601	CHL	CHD-C1D-ND	-6.29	118.68	124.45
25	1	613	CLA	C4A-NA-C1A	6.28	109.53	106.71
24	N	605	CHL	C2C-C3C-C4C	-6.28	102.01	106.49
27	N	1622	XAT	O4-C5-C4	6.28	118.10	113.38
24	G	607	CHL	CHD-C1D-ND	-6.28	118.69	124.45
24	3	605	CHL	C1D-ND-C4D	-6.28	101.88	106.33
24	p	607	CHL	C2D-C1D-ND	6.27	114.72	110.10
24	7	607	CHL	C2D-C1D-ND	6.26	114.72	110.10
24	q	601	CHL	C2D-C1D-ND	6.25	114.71	110.10
24	y	605	CHL	C2D-C1D-ND	6.25	114.71	110.10
24	0	608	CHL	C2D-C1D-ND	6.25	114.71	110.10
24	q	601	CHL	CHD-C1D-ND	-6.25	118.71	124.45
25	7	613	CLA	C4A-NA-C1A	6.24	109.51	106.71
24	n	605	CHL	C2C-C3C-C4C	-6.23	102.05	106.49
24	4	601	CHL	C2D-C1D-ND	6.23	114.69	110.10
24	y	608	CHL	CHD-C1D-ND	-6.23	118.73	124.45
24	Y	608	CHL	CHD-C1D-ND	-6.22	118.73	124.45
24	Y	605	CHL	C2D-C1D-ND	6.22	114.69	110.10
24	5	608	CHL	CHD-C1D-ND	-6.22	118.74	124.45
24	6	607	CHL	CHD-C1D-ND	-6.22	118.74	124.45
24	2	608	CHL	CHD-C1D-ND	-6.19	118.77	124.45
27	7	1622	XAT	O24-C25-C38	6.16	122.44	115.06
25	9	603	CLA	C4A-NA-C1A	6.15	109.47	106.71
27	6	1622	XAT	C38-C25-C26	-6.15	111.95	122.26
24	p	607	CHL	CHD-C1D-ND	-6.15	118.80	124.45
24	R	606	CHL	C2D-C1D-ND	6.15	114.64	110.10
24	3	601	CHL	C2C-C3C-C4C	-6.15	102.11	106.49
24	q	607	CHL	C1D-ND-C4D	-6.15	101.97	106.33
24	r	606	CHL	C2D-C1D-ND	6.14	114.63	110.10
24	6	606	CHL	CHD-C1D-ND	-6.14	118.81	124.45
24	6	609	CHL	C2D-C1D-ND	6.13	114.62	110.10
27	n	1622	XAT	O4-C5-C4	6.12	117.98	113.38
24	q	609	CHL	C1D-ND-C4D	-6.12	101.99	106.33
25	2	603	CLA	C4A-NA-C1A	6.11	109.45	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	9	608	CHL	CHD-C1D-ND	-6.11	118.84	124.45
25	1	611	CLA	C4A-NA-C1A	6.10	109.45	106.71
24	g	605	CHL	CHD-C1D-ND	-6.08	118.87	124.45
25	R	610	CLA	C4A-NA-C1A	6.07	109.44	106.71
25	0	614	CLA	C4A-NA-C1A	6.07	109.43	106.71
25	r	612	CLA	C4A-NA-C1A	6.06	109.43	106.71
24	9	605	CHL	C2D-C1D-ND	6.06	114.57	110.10
24	N	601	CHL	C2D-C1D-ND	6.05	114.56	110.10
24	G	605	CHL	CHD-C1D-ND	-6.04	118.90	124.45
24	4	608	CHL	C2D-C1D-ND	6.04	114.56	110.10
24	G	608	CHL	C2D-C1D-ND	6.03	114.55	110.10
25	p	613	CLA	C4A-NA-C1A	6.03	109.42	106.71
24	s	607	CHL	CHD-C1D-ND	-6.03	118.92	124.45
24	S	607	CHL	CHD-C1D-ND	-6.03	118.92	124.45
34	D	404	BCR	C7-C8-C9	-6.02	117.13	126.23
24	2	609	CHL	C2D-C1D-ND	6.02	114.54	110.10
34	d	404	BCR	C7-C8-C9	-6.02	117.14	126.23
24	1	607	CHL	C2D-C1D-ND	6.01	114.54	110.10
24	y	601	CHL	C2D-C1D-ND	6.01	114.53	110.10
24	p	608	CHL	CHD-C1D-ND	-6.01	118.93	124.45
24	4	601	CHL	CHD-C1D-ND	-6.01	118.93	124.45
24	y	608	CHL	C3C-C4C-NC	6.01	117.31	110.57
25	r	610	CLA	C4A-NA-C1A	6.01	109.41	106.71
24	3	609	CHL	C3C-C4C-NC	6.00	117.31	110.57
24	2	605	CHL	C2D-C1D-ND	6.00	114.53	110.10
25	G	603	CLA	C4A-NA-C1A	6.00	109.40	106.71
25	N	603	CLA	C4A-NA-C1A	6.00	109.40	106.71
25	g	603	CLA	C4A-NA-C1A	6.00	109.40	106.71
24	8	607	CHL	CHD-C1D-ND	-6.00	118.94	124.45
24	y	606	CHL	CHD-C1D-ND	-5.99	118.95	124.45
24	Y	606	CHL	CHD-C1D-ND	-5.98	118.96	124.45
24	7	609	CHL	CHD-C1D-ND	-5.98	118.96	124.45
24	q	608	CHL	C1B-CHB-C4A	-5.98	118.28	130.12
24	1	609	CHL	CHD-C1D-ND	-5.98	118.96	124.45
24	p	605	CHL	O2D-CGD-CBD	5.97	121.88	111.27
24	g	601	CHL	CHD-C1D-ND	-5.97	118.96	124.45
25	G	611	CLA	C4A-NA-C1A	5.97	109.39	106.71
24	9	605	CHL	CHD-C1D-ND	-5.97	118.97	124.45
24	Y	601	CHL	C2D-C1D-ND	5.97	114.50	110.10
25	7	611	CLA	C4A-NA-C1A	5.96	109.39	106.71
27	q	1622	XAT	C18-C5-C6	-5.96	112.27	122.26
24	R	606	CHL	CHD-C1D-ND	-5.96	118.98	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	612	CLA	C4A-NA-C1A	5.95	109.38	106.71
24	y	606	CHL	C3C-C4C-NC	5.95	117.25	110.57
24	R	606	CHL	CAC-C3C-C4C	5.95	132.53	124.81
25	C	511	CLA	C4A-NA-C1A	5.94	109.38	106.71
25	n	603	CLA	C4A-NA-C1A	5.94	109.38	106.71
24	3	607	CHL	CHD-C1D-ND	-5.94	119.00	124.45
24	Y	608	CHL	C3C-C4C-NC	5.93	117.22	110.57
24	r	606	CHL	CHD-C1D-ND	-5.92	119.02	124.45
24	2	605	CHL	CHD-C1D-ND	-5.92	119.02	124.45
24	Y	607	CHL	CHD-C1D-ND	-5.92	119.02	124.45
24	g	601	CHL	C2D-C1D-ND	5.91	114.46	110.10
24	S	606	CHL	CHD-C1D-ND	-5.91	119.03	124.45
24	Y	606	CHL	C3C-C4C-NC	5.91	117.19	110.57
24	5	605	CHL	O2D-CGD-CBD	5.90	121.76	111.27
24	g	606	CHL	CHD-C1D-ND	-5.90	119.03	124.45
24	Y	609	CHL	CHD-C1D-ND	-5.90	119.03	124.45
24	y	607	CHL	CHD-C1D-ND	-5.90	119.03	124.45
24	5	607	CHL	CHD-C1D-ND	-5.89	119.04	124.45
24	n	606	CHL	CHD-C1D-ND	-5.89	119.04	124.45
24	q	605	CHL	C2D-C1D-ND	5.89	114.44	110.10
27	1	1622	XAT	O24-C25-C38	5.89	122.11	115.06
24	r	606	CHL	CAC-C3C-C4C	5.89	132.45	124.81
24	N	606	CHL	CHD-C1D-ND	-5.89	119.05	124.45
24	n	601	CHL	C2C-C3C-C4C	-5.88	102.30	106.49
24	7	601	CHL	C2D-C1D-ND	5.88	114.44	110.10
24	G	601	CHL	CHD-C1D-ND	-5.88	119.05	124.45
25	g	611	CLA	C4A-NA-C1A	5.88	109.35	106.71
24	6	606	CHL	C2D-C1D-ND	5.88	114.44	110.10
27	5	1622	XAT	O4-C5-C4	5.87	117.80	113.38
24	1	606	CHL	C2D-C1D-ND	5.87	114.43	110.10
24	6	605	CHL	C2D-C1D-ND	5.87	114.43	110.10
27	q	1622	XAT	O4-C5-C18	5.87	122.09	115.06
25	c	511	CLA	C4A-NA-C1A	5.87	109.35	106.71
27	r	622	XAT	O24-C25-C24	5.87	117.79	113.38
24	s	606	CHL	CHD-C1D-ND	-5.87	119.06	124.45
24	7	608	CHL	C3C-C4C-NC	5.86	117.14	110.57
24	Y	605	CHL	CHD-C1D-ND	-5.85	119.08	124.45
24	5	606	CHL	CHD-C1D-ND	-5.85	119.08	124.45
24	8	609	CHL	C3C-C4C-NC	5.85	117.13	110.57
24	q	608	CHL	C2D-C1D-ND	5.84	114.41	110.10
27	9	1622	XAT	C38-C25-C26	-5.84	112.47	122.26
27	0	1622	XAT	C38-C25-C26	-5.84	112.48	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	R	622	XAT	O24-C25-C24	5.83	117.77	113.38
24	4	609	CHL	C1B-CHB-C4A	-5.83	118.57	130.12
24	y	605	CHL	CHD-C1D-ND	-5.83	119.09	124.45
25	q	613	CLA	C4A-NA-C1A	5.83	109.33	106.71
34	H	101	BCR	C7-C8-C9	-5.83	117.43	126.23
25	2	612	CLA	C4A-NA-C1A	5.83	109.33	106.71
24	1	601	CHL	C2D-C1D-ND	5.82	114.39	110.10
24	y	601	CHL	O2D-CGD-CBD	5.82	121.61	111.27
34	h	101	BCR	C7-C8-C9	-5.81	117.45	126.23
24	G	608	CHL	CHD-C1D-ND	-5.81	119.11	124.45
24	G	606	CHL	CHD-C1D-ND	-5.80	119.12	124.45
24	0	607	CHL	CHD-C1D-ND	-5.80	119.13	124.45
24	R	608	CHL	CHD-C1D-ND	-5.79	119.13	124.45
24	1	608	CHL	C3C-C4C-NC	5.79	117.06	110.57
24	9	607	CHL	C2D-C1D-ND	5.79	114.37	110.10
24	N	609	CHL	C2D-C1D-ND	5.78	114.37	110.10
24	N	605	CHL	C2D-C1D-ND	5.78	114.36	110.10
24	8	608	CHL	CHD-C1D-ND	-5.77	119.15	124.45
24	9	601	CHL	C1D-ND-C4D	-5.77	102.23	106.33
25	q	611	CLA	C4A-NA-C1A	5.76	109.30	106.71
24	n	605	CHL	C2D-C1D-ND	5.76	114.35	110.10
24	g	608	CHL	CHD-C1D-ND	-5.76	119.16	124.45
25	Y	611	CLA	C4A-NA-C1A	5.75	109.29	106.71
25	3	604	CLA	CMB-C2B-C1B	-5.75	119.63	128.46
24	N	605	CHL	CHD-C1D-ND	-5.74	119.17	124.45
27	7	1622	XAT	C38-C25-C26	-5.74	112.63	122.26
24	2	607	CHL	C2D-C1D-ND	5.74	114.34	110.10
24	Y	608	CHL	C3D-C2D-C1D	-5.74	98.00	105.83
24	3	607	CHL	C3C-C4C-NC	5.73	117.00	110.57
25	8	603	CLA	C4A-NA-C1A	5.73	109.28	106.71
27	1	1622	XAT	C38-C25-C26	-5.73	112.66	122.26
24	7	601	CHL	C2C-C3C-C4C	-5.73	102.41	106.49
24	y	608	CHL	C3D-C2D-C1D	-5.72	98.02	105.83
24	0	609	CHL	C2D-C1D-ND	5.72	114.32	110.10
24	3	608	CHL	CHD-C1D-ND	-5.72	119.20	124.45
27	4	1622	XAT	C18-C5-C6	-5.72	112.68	122.26
24	6	605	CHL	CHD-C1D-ND	-5.72	119.20	124.45
24	S	601	CHL	C2D-C1D-ND	5.71	114.31	110.10
24	1	605	CHL	C2D-C1D-ND	5.71	114.31	110.10
24	r	608	CHL	CHD-C1D-ND	-5.71	119.21	124.45
27	5	1622	XAT	C18-C5-C6	-5.71	112.69	122.26
27	2	1622	XAT	C38-C25-C26	-5.71	112.69	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	8	605	CHL	C2D-C1D-ND	5.70	114.31	110.10
24	y	609	CHL	C3D-C2D-C1D	-5.70	98.05	105.83
24	0	605	CHL	CHD-C1D-ND	-5.70	119.21	124.45
24	N	607	CHL	C3C-C4C-NC	5.70	116.97	110.57
24	1	601	CHL	C2C-C3C-C4C	-5.70	102.43	106.49
27	6	1622	XAT	O24-C25-C38	5.70	121.89	115.06
24	9	606	CHL	C2D-C1D-ND	5.70	114.30	110.10
24	N	608	CHL	CHD-C1D-ND	-5.70	119.22	124.45
24	n	605	CHL	CHD-C1D-ND	-5.69	119.22	124.45
27	y	1622	XAT	C38-C25-C26	-5.69	112.72	122.26
24	4	607	CHL	C2D-C1D-ND	5.69	114.30	110.10
24	y	609	CHL	CHD-C1D-ND	-5.69	119.23	124.45
25	y	611	CLA	C4A-NA-C1A	5.68	109.26	106.71
24	N	601	CHL	O2D-CGD-CBD	5.68	121.36	111.27
24	p	609	CHL	C2D-C1D-ND	5.68	114.29	110.10
27	Y	1622	XAT	C38-C25-C26	-5.68	112.75	122.26
27	4	1622	XAT	C38-C25-C26	-5.68	112.75	122.26
24	n	609	CHL	C2D-C1D-ND	5.68	114.29	110.10
24	R	608	CHL	O2D-CGD-CBD	5.67	121.35	111.27
24	n	608	CHL	C3C-C4C-NC	5.67	116.93	110.57
24	r	608	CHL	O2D-CGD-CBD	5.67	121.33	111.27
25	8	604	CLA	CMB-C2B-C1B	-5.66	119.76	128.46
24	8	607	CHL	C3C-C4C-NC	5.66	116.92	110.57
25	2	613	CLA	C4A-NA-C1A	5.66	109.25	106.71
24	Y	609	CHL	C3D-C2D-C1D	-5.66	98.11	105.83
25	6	611	CLA	C4A-NA-C1A	5.66	109.25	106.71
24	n	606	CHL	C3C-C4C-NC	5.65	116.91	110.57
25	9	612	CLA	C4A-NA-C1A	5.65	109.25	106.71
25	p	603	CLA	C4A-NA-C1A	5.65	109.25	106.71
24	7	606	CHL	C2D-C1D-ND	5.65	114.27	110.10
24	5	606	CHL	C2D-C1D-ND	5.64	114.26	110.10
24	y	609	CHL	C3C-C4C-NC	5.64	116.89	110.57
24	3	605	CHL	C2D-C1D-ND	5.64	114.26	110.10
24	n	601	CHL	O2D-CGD-CBD	5.63	121.27	111.27
28	5	1623	NEX	C27-C28-C29	-5.63	116.80	125.53
24	4	605	CHL	C2D-C1D-ND	5.62	114.25	110.10
25	6	613	CLA	C4A-NA-C1A	5.62	109.23	106.71
24	4	606	CHL	C2D-C1D-ND	5.62	114.24	110.10
27	2	1622	XAT	O24-C25-C24	5.61	117.60	113.38
24	r	607	CHL	O2D-CGD-CBD	5.61	121.23	111.27
24	7	608	CHL	C3D-C2D-C1D	-5.60	98.18	105.83
25	4	603	CLA	C4A-NA-C1A	5.60	109.22	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	614	CLA	C4A-NA-C1A	5.59	109.22	106.71
24	3	606	CHL	O2D-CGD-CBD	5.59	121.20	111.27
24	s	601	CHL	C2D-C1D-ND	5.59	114.22	110.10
24	2	606	CHL	C2D-C1D-ND	5.59	114.22	110.10
24	4	601	CHL	O2D-CGD-CBD	5.58	121.19	111.27
24	Y	607	CHL	C3C-C4C-NC	5.58	116.83	110.57
24	Y	601	CHL	O2D-CGD-CBD	5.58	121.17	111.27
24	R	607	CHL	O2D-CGD-CBD	5.57	121.17	111.27
24	N	608	CHL	C3C-C4C-NC	5.57	116.82	110.57
24	y	607	CHL	C3C-C4C-NC	5.57	116.82	110.57
24	1	608	CHL	C3D-C2D-C1D	-5.57	98.23	105.83
25	C	504	CLA	C4A-NA-C1A	5.56	109.20	106.71
24	N	606	CHL	C3C-C4C-NC	5.55	116.79	110.57
25	C	510	CLA	CMB-C2B-C1B	-5.55	119.94	128.46
24	q	601	CHL	O2D-CGD-CBD	5.55	121.12	111.27
25	q	603	CLA	C4A-NA-C1A	5.54	109.20	106.71
24	Y	609	CHL	C3C-C4C-NC	5.54	116.78	110.57
24	G	601	CHL	C2D-C1D-ND	5.54	114.18	110.10
38	D	401	BCT	O2-C-O1	5.52	133.87	119.55
24	R	608	CHL	C3C-C4C-NC	5.52	116.76	110.57
24	r	608	CHL	C3C-C4C-NC	5.52	116.76	110.57
25	5	603	CLA	C4A-NA-C1A	5.52	109.19	106.71
24	8	609	CHL	O2D-CGD-CBD	5.51	121.07	111.27
38	d	401	BCT	O2-C-O1	5.51	133.83	119.55
27	g	1622	XAT	O4-C5-C4	5.50	117.52	113.38
24	n	607	CHL	C3C-C4C-NC	5.50	116.74	110.57
25	c	510	CLA	CMB-C2B-C1B	-5.50	120.01	128.46
24	9	609	CHL	C2D-C1D-ND	5.50	114.16	110.10
25	3	603	CLA	C4A-NA-C1A	5.49	109.18	106.71
25	c	504	CLA	C4A-NA-C1A	5.49	109.17	106.71
25	4	611	CLA	C4A-NA-C1A	5.49	109.17	106.71
25	0	611	CLA	C4A-NA-C1A	5.49	109.17	106.71
27	7	1622	XAT	C18-C5-C6	-5.48	113.07	122.26
24	q	607	CHL	C1B-CHB-C4A	-5.48	119.27	130.12
24	3	609	CHL	O2D-CGD-CBD	5.48	121.01	111.27
24	R	607	CHL	C3C-C4C-NC	5.47	116.70	110.57
24	5	609	CHL	C2D-C1D-ND	5.47	114.13	110.10
34	B	618	BCR	C28-C27-C26	-5.47	104.32	114.08
24	7	609	CHL	C3C-C4C-NC	5.47	116.70	110.57
24	r	607	CHL	C3C-C4C-NC	5.47	116.70	110.57
34	b	618	BCR	C28-C27-C26	-5.46	104.33	114.08
25	4	613	CLA	C4A-NA-C1A	5.46	109.16	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	1	1622	XAT	C18-C5-C6	-5.46	113.12	122.26
27	4	1622	XAT	O4-C5-C18	5.45	121.59	115.06
24	8	606	CHL	O2D-CGD-CBD	5.45	120.96	111.27
24	0	606	CHL	C2D-C1D-ND	5.45	114.12	110.10
24	7	609	CHL	C3D-C2D-C1D	-5.44	98.40	105.83
27	9	1622	XAT	O24-C25-C38	5.44	121.58	115.06
28	Y	1623	NEX	C38-C25-C26	-5.44	113.14	122.26
28	y	1623	NEX	C38-C25-C26	-5.44	113.15	122.26
24	p	605	CHL	C2D-C1D-ND	5.44	114.11	110.10
27	9	1622	XAT	O24-C25-C24	5.44	117.47	113.38
27	g	1622	XAT	C38-C25-C26	-5.43	113.16	122.26
27	G	1622	XAT	O4-C5-C4	5.43	117.46	113.38
25	s	613	CLA	C4A-NA-C1A	5.42	109.14	106.71
24	s	607	CHL	C2D-C1D-ND	5.42	114.10	110.10
24	s	608	CHL	C3D-C2D-C1D	-5.42	98.43	105.83
25	0	603	CLA	C4A-NA-C1A	5.42	109.14	106.71
24	n	608	CHL	C3D-C2D-C1D	-5.42	98.44	105.83
24	7	605	CHL	C2D-C1D-ND	5.41	114.09	110.10
25	R	613	CLA	C4A-NA-C1A	5.41	109.14	106.71
25	b	617	CLA	C4A-NA-C1A	5.41	109.14	106.71
25	B	617	CLA	C4A-NA-C1A	5.40	109.13	106.71
25	9	613	CLA	C4A-NA-C1A	5.40	109.13	106.71
24	N	605	CHL	O2D-CGD-CBD	5.39	120.85	111.27
27	1	1622	XAT	O4-C5-C18	5.39	121.51	115.06
24	6	608	CHL	C3C-C4C-NC	5.39	116.61	110.57
24	S	606	CHL	O2D-CGD-CBD	5.39	120.84	111.27
27	q	1622	XAT	C38-C25-C26	-5.39	113.23	122.26
24	S	607	CHL	C2D-C1D-ND	5.38	114.07	110.10
25	b	616	CLA	C4A-NA-C1A	5.38	109.12	106.71
27	7	1622	XAT	O4-C5-C18	5.37	121.50	115.06
25	r	613	CLA	C4A-NA-C1A	5.37	109.12	106.71
24	S	608	CHL	C3D-C2D-C1D	-5.37	98.50	105.83
25	S	613	CLA	C4A-NA-C1A	5.37	109.12	106.71
24	N	608	CHL	C3D-C2D-C1D	-5.37	98.50	105.83
24	1	605	CHL	C3C-C4C-NC	5.37	116.59	110.57
27	0	1622	XAT	O24-C25-C24	5.37	117.42	113.38
27	G	1622	XAT	C38-C25-C26	-5.37	113.27	122.26
27	p	1622	XAT	C18-C5-C6	-5.36	113.27	122.26
27	4	1622	XAT	O4-C5-C4	5.36	117.41	113.38
27	2	1622	XAT	O24-C25-C38	5.36	121.48	115.06
24	s	606	CHL	O2D-CGD-CBD	5.36	120.79	111.27
27	5	1622	XAT	O4-C5-C18	5.35	121.47	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	7	601	CHL	O2D-CGD-CBD	5.35	120.78	111.27
25	R	616	CLA	C4A-NA-C1A	5.35	109.11	106.71
27	r	622	XAT	C6-C7-C8	-5.35	114.69	125.99
25	N	604	CLA	C4A-NA-C1A	5.34	109.11	106.71
27	R	622	XAT	C6-C7-C8	-5.34	114.69	125.99
24	g	605	CHL	O2D-CGD-CBD	5.34	120.76	111.27
25	B	610	CLA	CMB-C2B-C1B	-5.34	120.26	128.46
24	7	607	CHL	CHD-C1D-ND	-5.34	119.55	124.45
24	y	601	CHL	C4A-NA-C1A	-5.33	104.31	106.71
24	Y	606	CHL	C3D-C2D-C1D	-5.33	98.55	105.83
24	Y	607	CHL	C3D-C2D-C1D	-5.32	98.56	105.83
24	n	608	CHL	CHD-C1D-ND	-5.32	119.56	124.45
28	S	1623	NEX	C15-C14-C13	-5.32	119.71	127.31
24	7	605	CHL	C3C-C4C-NC	5.32	116.54	110.57
24	n	609	CHL	O2D-CGD-CBD	5.32	120.72	111.27
24	8	607	CHL	C3D-C2D-C1D	-5.32	98.57	105.83
24	1	609	CHL	C3D-C2D-C1D	-5.32	98.57	105.83
24	y	607	CHL	C3D-C2D-C1D	-5.32	98.58	105.83
28	7	1623	NEX	C38-C25-C26	-5.32	113.35	122.26
25	b	610	CLA	CMB-C2B-C1B	-5.32	120.29	128.46
25	R	609	CLA	C4A-NA-C1A	5.32	109.10	106.71
25	r	609	CLA	C4A-NA-C1A	5.32	109.10	106.71
24	6	608	CHL	C3D-C2D-C1D	-5.31	98.58	105.83
24	G	606	CHL	C3C-C4C-NC	5.31	116.53	110.57
28	N	1623	NEX	C38-C25-C26	-5.31	113.36	122.26
24	s	606	CHL	C3C-C4C-NC	5.30	116.52	110.57
24	y	606	CHL	C3D-C2D-C1D	-5.30	98.59	105.83
24	S	606	CHL	C3C-C4C-NC	5.30	116.52	110.57
24	5	609	CHL	O2D-CGD-CBD	5.29	120.67	111.27
25	r	616	CLA	C4A-NA-C1A	5.29	109.08	106.71
24	p	608	CHL	C3C-C4C-NC	5.29	116.50	110.57
24	3	601	CHL	O2D-CGD-CBD	5.29	120.66	111.27
24	7	601	CHL	C3D-C4D-ND	5.29	118.79	110.24
28	n	1623	NEX	C38-C25-C26	-5.28	113.40	122.26
24	2	601	CHL	C2D-C1D-ND	5.28	114.00	110.10
25	S	603	CLA	C4A-NA-C1A	5.28	109.08	106.71
25	p	611	CLA	C4A-NA-C1A	5.28	109.08	106.71
24	1	601	CHL	O2D-CGD-CBD	5.28	120.64	111.27
24	G	607	CHL	C3C-C4C-NC	5.28	116.49	110.57
25	n	604	CLA	C4A-NA-C1A	5.27	109.08	106.71
24	g	606	CHL	C3C-C4C-NC	5.27	116.48	110.57
24	6	609	CHL	C3D-C2D-C1D	-5.27	98.64	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	614	CLA	CMB-C2B-C1B	-5.27	120.36	128.46
24	3	605	CHL	C1B-CHB-C4A	-5.27	119.68	130.12
27	6	1622	XAT	C31-C30-C29	-5.27	119.79	127.31
25	6	603	CLA	C4A-NA-C1A	5.26	109.07	106.71
27	p	1622	XAT	C38-C25-C26	-5.26	113.44	122.26
24	1	601	CHL	C3D-C4D-ND	5.26	118.75	110.24
34	C	517	BCR	C20-C21-C22	-5.26	119.80	127.31
25	b	614	CLA	CMB-C2B-C1B	-5.26	120.38	128.46
24	p	601	CHL	O2D-CGD-CBD	5.26	120.62	111.27
25	c	501	CLA	C4A-NA-C1A	5.26	109.07	106.71
24	g	601	CHL	O2D-CGD-CBD	5.26	120.61	111.27
24	2	608	CHL	O2D-CGD-CBD	5.26	120.61	111.27
24	5	608	CHL	C3C-C4C-NC	5.25	116.46	110.57
24	G	605	CHL	O2D-CGD-CBD	5.25	120.60	111.27
24	1	609	CHL	C3C-C4C-NC	5.25	116.46	110.57
24	3	607	CHL	C3D-C2D-C1D	-5.24	98.67	105.83
25	d	402	CLA	C4A-NA-C1A	5.24	109.06	106.71
24	9	608	CHL	C3D-C2D-C1D	-5.24	98.68	105.83
24	r	608	CHL	C3D-C2D-C1D	-5.24	98.69	105.83
24	8	605	CHL	C1B-CHB-C4A	-5.24	119.75	130.12
24	2	609	CHL	C3C-C4C-NC	5.23	116.44	110.57
24	Y	601	CHL	C4A-NA-C1A	-5.23	104.35	106.71
24	5	607	CHL	C3C-C4C-NC	5.23	116.44	110.57
27	6	1622	XAT	C18-C5-C6	-5.23	113.50	122.26
24	2	608	CHL	C3D-C2D-C1D	-5.23	98.70	105.83
34	c	517	BCR	C20-C21-C22	-5.23	119.85	127.31
24	5	605	CHL	C3D-C4D-ND	5.23	118.69	110.24
24	9	608	CHL	C3C-C4C-NC	5.22	116.43	110.57
25	s	603	CLA	C4A-NA-C1A	5.22	109.05	106.71
24	2	608	CHL	C3C-C4C-NC	5.22	116.42	110.57
24	p	609	CHL	O2D-CGD-CBD	5.22	120.53	111.27
25	8	611	CLA	C4A-NA-C1A	5.21	109.05	106.71
24	q	606	CHL	C2D-C1D-ND	5.21	113.94	110.10
24	2	607	CHL	O2D-CGD-CBD	5.20	120.52	111.27
24	R	608	CHL	C3D-C2D-C1D	-5.20	98.73	105.83
24	1	607	CHL	CHD-C1D-ND	-5.20	119.67	124.45
24	q	607	CHL	C2D-C1D-ND	5.20	113.94	110.10
24	6	606	CHL	O2D-CGD-CBD	5.20	120.50	111.27
24	p	605	CHL	C3D-C4D-ND	5.20	118.64	110.24
24	0	608	CHL	C3D-C2D-C1D	-5.20	98.74	105.83
25	B	609	CLA	CMB-C2B-C1B	-5.19	120.48	128.46
27	G	1622	XAT	C18-C5-C6	-5.19	113.56	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	5	601	CHL	O2D-CGD-CBD	5.19	120.49	111.27
28	Y	1623	NEX	O24-C25-C38	5.19	121.27	115.06
24	9	609	CHL	C3C-C4C-NC	5.19	116.39	110.57
24	n	607	CHL	C3D-C2D-C1D	-5.18	98.76	105.83
24	G	607	CHL	C3D-C2D-C1D	-5.18	98.76	105.83
27	R	622	XAT	C38-C25-C26	-5.18	113.57	122.26
25	b	609	CLA	CMB-C2B-C1B	-5.18	120.50	128.46
24	5	608	CHL	C3D-C2D-C1D	-5.18	98.76	105.83
27	y	1622	XAT	C6-C7-C8	-5.18	115.04	125.99
25	c	508	CLA	C4A-NA-C1A	5.18	109.03	106.71
27	8	1622	XAT	C18-C5-C6	-5.18	113.58	122.26
25	s	611	CLA	C4A-NA-C1A	5.18	109.03	106.71
24	g	607	CHL	C3C-C4C-NC	5.17	116.37	110.57
24	p	608	CHL	C3D-C2D-C1D	-5.17	98.77	105.83
27	7	1622	XAT	C37-C21-C26	-5.17	96.08	110.05
24	Y	605	CHL	C3C-C4C-NC	5.17	116.37	110.57
24	q	601	CHL	C3D-C2D-C1D	-5.17	98.78	105.83
25	N	614	CLA	C4A-NA-C1A	5.17	109.03	106.71
25	b	608	CLA	C4A-NA-C1A	5.17	109.03	106.71
25	3	611	CLA	C4A-NA-C1A	5.16	109.03	106.71
25	S	602	CLA	C4A-NA-C1A	5.16	109.03	106.71
24	Y	605	CHL	C3D-C2D-C1D	-5.16	98.78	105.83
24	y	605	CHL	C3D-C2D-C1D	-5.16	98.78	105.83
24	S	608	CHL	C3C-C4C-NC	5.16	116.36	110.57
27	Y	1622	XAT	C6-C7-C8	-5.16	115.08	125.99
27	r	622	XAT	C38-C25-C26	-5.16	113.61	122.26
24	y	605	CHL	C3C-C4C-NC	5.16	116.36	110.57
27	N	1622	XAT	C6-C7-C8	-5.16	115.09	125.99
24	2	606	CHL	C3C-C4C-NC	5.16	116.36	110.57
27	3	1622	XAT	C18-C5-C6	-5.16	113.62	122.26
27	g	1622	XAT	C18-C5-C6	-5.16	113.62	122.26
25	B	614	CLA	C4A-NA-C1A	5.16	109.02	106.71
24	g	607	CHL	C3D-C2D-C1D	-5.15	98.80	105.83
25	D	402	CLA	C4A-NA-C1A	5.15	109.02	106.71
24	R	607	CHL	C3D-C2D-C1D	-5.15	98.80	105.83
28	y	1623	NEX	O24-C25-C38	5.15	121.22	115.06
25	B	616	CLA	C4A-NA-C1A	5.14	109.02	106.71
27	1	1622	XAT	C37-C21-C26	-5.14	96.15	110.05
24	s	608	CHL	C3C-C4C-NC	5.14	116.34	110.57
27	y	1622	XAT	C15-C14-C13	-5.13	119.98	127.31
24	0	609	CHL	C3C-C4C-NC	5.13	116.33	110.57
25	C	508	CLA	C4A-NA-C1A	5.13	109.01	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	N	609	CHL	O2D-CGD-CBD	5.13	120.39	111.27
25	a	405	CLA	CMB-C2B-C1B	-5.13	120.58	128.46
24	r	607	CHL	C3D-C2D-C1D	-5.13	98.83	105.83
24	n	606	CHL	C3D-C2D-C1D	-5.13	98.83	105.83
24	g	609	CHL	C3D-C2D-C1D	-5.13	98.83	105.83
25	s	602	CLA	C4A-NA-C1A	5.13	109.01	106.71
24	G	609	CHL	C3D-C2D-C1D	-5.13	98.83	105.83
28	G	1623	NEX	C38-C25-C26	-5.13	113.67	122.26
25	5	612	CLA	C4A-NA-C1A	5.13	109.01	106.71
24	N	607	CHL	C3D-C2D-C1D	-5.13	98.84	105.83
24	0	601	CHL	C3C-C4C-NC	5.12	116.31	110.57
25	r	611	CLA	C4A-NA-C1A	5.12	109.01	106.71
27	n	1622	XAT	C6-C7-C8	-5.12	115.17	125.99
27	Y	1622	XAT	C15-C14-C13	-5.11	120.01	127.31
24	N	606	CHL	C3D-C2D-C1D	-5.11	98.85	105.83
24	8	601	CHL	C3D-C4D-ND	5.11	118.51	110.24
27	1	1622	XAT	O24-C25-C24	5.11	117.22	113.38
24	0	606	CHL	C3D-C4D-ND	5.11	118.51	110.24
25	C	501	CLA	C4A-NA-C1A	5.11	109.00	106.71
24	r	606	CHL	C3D-C2D-C1D	-5.11	98.86	105.83
24	0	605	CHL	C3D-C2D-C1D	-5.11	98.86	105.83
25	3	612	CLA	C4A-NA-C1A	5.10	109.00	106.71
28	1	1623	NEX	C11-C10-C9	-5.10	120.03	127.31
27	8	1622	XAT	O4-C5-C18	5.10	121.17	115.06
28	s	1623	NEX	C15-C14-C13	-5.10	120.03	127.31
24	g	606	CHL	C3D-C2D-C1D	-5.10	98.87	105.83
27	8	1622	XAT	C38-C25-C26	-5.10	113.72	122.26
24	0	607	CHL	C3C-C4C-NC	5.09	116.28	110.57
25	G	613	CLA	C4A-NA-C1A	5.09	109.00	106.71
28	7	1623	NEX	C15-C14-C13	-5.09	120.04	127.31
24	8	608	CHL	C3C-C4C-NC	5.09	116.28	110.57
24	6	601	CHL	C3C-C4C-NC	5.09	116.28	110.57
24	9	606	CHL	C3C-C4C-NC	5.09	116.28	110.57
25	A	405	CLA	CMB-C2B-C1B	-5.09	120.64	128.46
25	b	607	CLA	C4A-NA-C1A	5.09	109.00	106.71
24	5	605	CHL	C3C-C4C-NC	5.09	116.28	110.57
25	6	604	CLA	C4A-NA-C1A	5.09	108.99	106.71
24	p	601	CHL	C3D-C2D-C1D	-5.08	98.89	105.83
24	S	606	CHL	C3D-C2D-C1D	-5.08	98.90	105.83
24	R	606	CHL	C3D-C2D-C1D	-5.08	98.90	105.83
24	7	608	CHL	CHD-C1D-ND	-5.08	119.78	124.45
24	1	609	CHL	O2D-CGD-CBD	5.08	120.29	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	3	608	CHL	C3C-C4C-NC	5.08	116.26	110.57
27	3	1622	XAT	C38-C25-C26	-5.07	113.75	122.26
24	0	607	CHL	C3D-C2D-C1D	-5.07	98.91	105.83
25	q	614	CLA	C4A-NA-C1A	5.07	108.98	106.71
24	G	601	CHL	O2D-CGD-CBD	5.07	120.27	111.27
28	g	1623	NEX	C38-C25-C26	-5.07	113.77	122.26
28	4	1623	NEX	C11-C10-C9	-5.07	120.08	127.31
27	0	1622	XAT	O24-C25-C38	5.06	121.12	115.06
25	g	613	CLA	C4A-NA-C1A	5.06	108.98	106.71
24	8	601	CHL	O2D-CGD-CBD	5.06	120.26	111.27
25	q	604	CLA	C4A-NA-C1A	5.06	108.98	106.71
24	3	601	CHL	C3D-C4D-ND	5.06	118.42	110.24
24	6	609	CHL	C3C-C4C-NC	5.06	116.25	110.57
24	6	601	CHL	C3D-C4D-ND	5.06	118.42	110.24
27	3	1622	XAT	O4-C5-C18	5.06	121.11	115.06
24	0	609	CHL	C3D-C2D-C1D	-5.06	98.93	105.83
24	1	608	CHL	CHD-C1D-ND	-5.05	119.81	124.45
25	Y	603	CLA	C4A-NA-C1A	5.05	108.98	106.71
25	b	614	CLA	C4A-NA-C1A	5.05	108.98	106.71
28	R	623	NEX	C27-C28-C29	-5.05	117.70	125.53
25	q	613	CLA	CMB-C2B-C1B	-5.04	120.71	128.46
25	A	410	CLA	CMB-C2B-C1B	-5.04	120.71	128.46
24	N	605	CHL	C3D-C2D-C1D	-5.04	98.95	105.83
24	4	601	CHL	C3D-C2D-C1D	-5.04	98.95	105.83
24	y	601	CHL	C3D-C4D-ND	5.04	118.39	110.24
24	q	608	CHL	C3D-C2D-C1D	-5.04	98.96	105.83
27	4	1622	XAT	O24-C25-C38	5.03	121.09	115.06
24	G	606	CHL	C3D-C2D-C1D	-5.03	98.96	105.83
24	6	606	CHL	C3D-C4D-ND	5.03	118.38	110.24
27	2	1622	XAT	C31-C30-C29	-5.03	120.13	127.31
24	7	609	CHL	O2D-CGD-CBD	5.03	120.20	111.27
24	0	605	CHL	C3C-C4C-NC	5.03	116.21	110.57
28	r	623	NEX	C27-C28-C29	-5.02	117.73	125.53
24	N	601	CHL	C3D-C4D-ND	5.02	118.36	110.24
24	0	608	CHL	C3C-C4C-NC	5.02	116.20	110.57
25	R	611	CLA	C4A-NA-C1A	5.02	108.96	106.71
24	4	608	CHL	O2D-CGD-CBD	5.02	120.19	111.27
25	a	410	CLA	CMB-C2B-C1B	-5.02	120.75	128.46
24	9	607	CHL	O2D-CGD-CBD	5.02	120.19	111.27
24	s	606	CHL	C3D-C2D-C1D	-5.02	98.98	105.83
24	N	609	CHL	C3D-C2D-C1D	-5.01	98.99	105.83
25	Y	604	CLA	CMB-C2B-C1B	-5.01	120.76	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	605	CHL	O2D-CGD-CBD	5.01	120.17	111.27
24	y	605	CHL	O2D-CGD-CBD	5.01	120.17	111.27
28	l	1623	NEX	C38-C25-C26	-5.01	113.87	122.26
24	N	607	CHL	CHD-C4C-C3C	-5.01	117.48	124.84
24	q	609	CHL	O2D-CGD-CBD	5.01	120.16	111.27
25	c	510	CLA	C4A-NA-C1A	5.00	108.96	106.71
34	c	517	BCR	C24-C23-C22	-5.00	118.67	126.23
27	l	1622	XAT	O4-C5-C4	5.00	117.14	113.38
25	y	604	CLA	CMB-C2B-C1B	-5.00	120.78	128.46
28	4	1623	NEX	C15-C14-C13	-5.00	120.17	127.31
24	n	601	CHL	C3D-C4D-ND	5.00	118.33	110.24
24	g	605	CHL	C3C-C4C-NC	5.00	116.18	110.57
24	6	601	CHL	C3D-C2D-C1D	-5.00	99.01	105.83
25	B	608	CLA	C4A-NA-C1A	5.00	108.95	106.71
24	Y	601	CHL	C3D-C4D-ND	4.99	118.32	110.24
25	8	612	CLA	C4A-NA-C1A	4.99	108.95	106.71
24	g	608	CHL	C3C-C4C-NC	4.99	116.17	110.57
25	S	611	CLA	C4A-NA-C1A	4.99	108.95	106.71
24	g	608	CHL	C3D-C2D-C1D	-4.99	99.02	105.83
25	y	603	CLA	C4A-NA-C1A	4.99	108.95	106.71
24	5	605	CHL	C3D-C2D-C1D	-4.99	99.03	105.83
24	S	601	CHL	C3D-C4D-ND	4.98	118.30	110.24
24	R	606	CHL	C3C-C4C-NC	4.98	116.16	110.57
25	c	511	CLA	CMB-C2B-C1B	-4.98	120.81	128.46
24	p	609	CHL	C3D-C2D-C1D	-4.98	99.03	105.83
25	B	607	CLA	C4A-NA-C1A	4.98	108.94	106.71
24	q	605	CHL	C3D-C2D-C1D	-4.98	99.03	105.83
24	0	606	CHL	O2D-CGD-CBD	4.97	120.11	111.27
24	0	607	CHL	O2D-CGD-CBD	4.97	120.11	111.27
24	2	609	CHL	C3D-C2D-C1D	-4.97	99.05	105.83
25	Y	610	CLA	CMB-C2B-C1B	-4.97	120.82	128.46
24	g	605	CHL	C3D-C2D-C1D	-4.97	99.05	105.83
34	C	517	BCR	C24-C23-C22	-4.97	118.73	126.23
24	8	605	CHL	C3D-C2D-C1D	-4.97	99.06	105.83
24	n	601	CHL	C3D-C2D-C1D	-4.96	99.06	105.83
24	n	609	CHL	C3D-C2D-C1D	-4.96	99.06	105.83
24	6	607	CHL	C3D-C2D-C1D	-4.96	99.06	105.83
25	n	614	CLA	C4A-NA-C1A	4.96	108.94	106.71
24	N	607	CHL	C3D-C4D-ND	4.96	118.27	110.24
24	Y	609	CHL	O2D-CGD-CBD	4.96	120.08	111.27
24	G	609	CHL	C2D-C1D-ND	4.96	113.76	110.10
24	l	605	CHL	C3D-C2D-C1D	-4.96	99.06	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	7	1622	XAT	O4-C5-C4	4.96	117.11	113.38
24	q	609	CHL	C3D-C4D-ND	4.96	118.26	110.24
24	9	605	CHL	O2D-CGD-CBD	4.95	120.07	111.27
28	p	1623	NEX	C27-C28-C29	-4.95	117.85	125.53
25	9	604	CLA	C4A-NA-C1A	4.95	108.93	106.71
24	3	605	CHL	C3D-C2D-C1D	-4.95	99.07	105.83
24	n	607	CHL	C3D-C4D-ND	4.95	118.25	110.24
24	8	608	CHL	C3D-C2D-C1D	-4.95	99.08	105.83
27	5	1622	XAT	C38-C25-C26	-4.95	113.97	122.26
24	n	605	CHL	C3D-C2D-C1D	-4.95	99.08	105.83
24	p	609	CHL	C3C-C4C-NC	4.95	116.12	110.57
25	y	610	CLA	CMB-C2B-C1B	-4.94	120.86	128.46
24	5	601	CHL	C3D-C2D-C1D	-4.94	99.08	105.83
24	3	608	CHL	C3D-C2D-C1D	-4.94	99.09	105.83
24	6	606	CHL	C3C-C4C-NC	4.94	116.11	110.57
24	4	608	CHL	C3D-C2D-C1D	-4.94	99.09	105.83
24	G	605	CHL	C3D-C2D-C1D	-4.94	99.09	105.83
28	G	1623	NEX	C15-C14-C13	-4.94	120.27	127.31
24	g	609	CHL	C2D-C1D-ND	4.93	113.74	110.10
24	Y	601	CHL	C3D-C2D-C1D	-4.93	99.10	105.83
24	G	605	CHL	C3C-C4C-NC	4.93	116.10	110.57
24	y	601	CHL	C3D-C2D-C1D	-4.93	99.11	105.83
25	C	505	CLA	CMB-C2B-C1B	-4.93	120.89	128.46
25	A	407	CLA	C4A-NA-C1A	4.93	108.92	106.71
25	C	511	CLA	CMB-C2B-C1B	-4.93	120.89	128.46
24	8	607	CHL	C3D-C4D-ND	4.92	118.20	110.24
25	a	407	CLA	C4A-NA-C1A	4.92	108.92	106.71
25	c	505	CLA	CMB-C2B-C1B	-4.92	120.90	128.46
24	5	609	CHL	C3D-C2D-C1D	-4.92	99.12	105.83
24	3	607	CHL	CHD-C4C-C3C	-4.92	117.61	124.84
24	3	601	CHL	C3D-C2D-C1D	-4.92	99.12	105.83
24	s	601	CHL	C3D-C4D-ND	4.92	118.19	110.24
24	7	605	CHL	O2D-CGD-CBD	4.92	120.00	111.27
24	3	607	CHL	C3D-C4D-ND	4.91	118.19	110.24
27	6	1622	XAT	C37-C21-C26	-4.91	96.78	110.05
24	8	609	CHL	C3D-C4D-ND	4.91	118.18	110.24
25	a	405	CLA	C4A-NA-C1A	4.91	108.91	106.71
27	G	1622	XAT	O4-C5-C18	4.91	120.94	115.06
24	2	601	CHL	C3D-C2D-C1D	-4.91	99.13	105.83
24	g	601	CHL	C3D-C2D-C1D	-4.91	99.13	105.83
24	q	609	CHL	C1B-CHB-C4A	-4.91	120.40	130.12
24	s	606	CHL	C3D-C4D-ND	4.91	118.17	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	0	1623	NEX	C27-C28-C29	-4.90	117.92	125.53
28	6	1623	NEX	C27-C28-C29	-4.90	117.92	125.53
28	6	1623	NEX	C38-C25-C26	-4.90	114.04	122.26
24	n	605	CHL	O2D-CGD-CBD	4.90	119.98	111.27
24	6	605	CHL	C3D-C2D-C1D	-4.90	99.14	105.83
24	2	605	CHL	O2D-CGD-CBD	4.90	119.97	111.27
28	q	1623	NEX	C15-C14-C13	-4.90	120.32	127.31
24	r	606	CHL	C3C-C4C-NC	4.89	116.06	110.57
24	8	601	CHL	C3D-C2D-C1D	-4.89	99.15	105.83
24	2	609	CHL	C3D-C4D-ND	4.89	118.15	110.24
24	p	607	CHL	C3D-C4D-ND	4.89	118.15	110.24
24	6	605	CHL	O2D-CGD-CBD	4.89	119.96	111.27
24	1	606	CHL	C3C-C4C-NC	4.89	116.06	110.57
25	n	611	CLA	C4A-NA-C1A	4.89	108.90	106.71
24	S	606	CHL	C3D-C4D-ND	4.89	118.14	110.24
24	7	606	CHL	O2D-CGD-CBD	4.88	119.95	111.27
27	g	1622	XAT	O4-C5-C18	4.88	120.91	115.06
24	4	605	CHL	C3D-C2D-C1D	-4.88	99.17	105.83
24	3	609	CHL	C3D-C2D-C1D	-4.88	99.17	105.83
24	0	608	CHL	O2D-CGD-CBD	4.88	119.94	111.27
26	8	1620	LUT	C35-C34-C33	-4.88	120.35	127.31
27	0	1622	XAT	C37-C21-C26	-4.88	96.87	110.05
28	9	1623	NEX	C11-C10-C9	-4.88	120.35	127.31
25	C	507	CLA	C4A-NA-C1A	4.88	108.90	106.71
28	5	1623	NEX	C15-C14-C13	-4.88	120.35	127.31
27	y	1622	XAT	C18-C5-C6	-4.88	114.09	122.26
34	D	404	BCR	C11-C10-C9	-4.87	120.35	127.31
24	4	601	CHL	C3D-C4D-ND	4.87	118.12	110.24
24	7	606	CHL	C3D-C2D-C1D	-4.87	99.18	105.83
24	n	607	CHL	CHD-C4C-C3C	-4.87	117.68	124.84
24	q	609	CHL	C2D-C1D-ND	4.87	113.69	110.10
25	b	612	CLA	CMB-C2B-C1B	-4.87	120.98	128.46
24	6	607	CHL	C3C-C4C-NC	4.87	116.03	110.57
27	r	622	XAT	C18-C5-C6	-4.87	114.11	122.26
34	h	101	BCR	C28-C27-C26	-4.87	105.39	114.08
24	4	607	CHL	C3D-C2D-C1D	-4.86	99.19	105.83
24	G	606	CHL	C3D-C4D-ND	4.86	118.11	110.24
24	1	606	CHL	C3D-C2D-C1D	-4.86	99.19	105.83
24	6	608	CHL	O2D-CGD-CBD	4.86	119.91	111.27
24	0	607	CHL	C3D-C4D-ND	4.86	118.10	110.24
24	9	609	CHL	C3D-C2D-C1D	-4.86	99.20	105.83
27	R	622	XAT	C18-C5-C6	-4.86	114.12	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	606	CHL	C3D-C4D-ND	4.86	118.10	110.24
27	Y	1622	XAT	C18-C5-C6	-4.86	114.12	122.26
24	p	601	CHL	C3D-C4D-ND	4.85	118.09	110.24
24	g	606	CHL	C3D-C4D-ND	4.85	118.09	110.24
24	S	601	CHL	C3D-C2D-C1D	-4.85	99.21	105.83
34	H	101	BCR	C28-C27-C26	-4.85	105.41	114.08
25	Y	602	CLA	CMB-C2B-C1B	-4.85	121.00	128.46
24	s	601	CHL	C3D-C2D-C1D	-4.85	99.21	105.83
24	N	601	CHL	C3C-C4C-NC	4.85	116.01	110.57
24	n	607	CHL	O2D-CGD-CBD	4.85	119.89	111.27
27	9	1622	XAT	C18-C5-C6	-4.85	114.13	122.26
24	7	605	CHL	C3D-C2D-C1D	-4.85	99.22	105.83
25	A	410	CLA	C4A-NA-C1A	4.84	108.88	106.71
24	8	609	CHL	C3D-C2D-C1D	-4.84	99.22	105.83
25	b	603	CLA	C4A-NA-C1A	4.84	108.88	106.71
28	4	1623	NEX	C38-C25-C26	-4.84	114.14	122.26
24	5	607	CHL	C3D-C4D-ND	4.84	118.07	110.24
25	B	612	CLA	CMB-C2B-C1B	-4.84	121.03	128.46
24	9	605	CHL	C3D-C2D-C1D	-4.84	99.23	105.83
27	p	1622	XAT	O4-C5-C18	4.84	120.85	115.06
28	3	1623	NEX	C38-C25-C26	-4.84	114.15	122.26
24	n	606	CHL	C3D-C4D-ND	4.84	118.06	110.24
24	9	601	CHL	C2D-C1D-ND	4.84	113.67	110.10
24	8	606	CHL	C3D-C4D-ND	4.84	118.06	110.24
24	1	601	CHL	C3D-C2D-C1D	-4.83	99.23	105.83
24	0	601	CHL	C3D-C4D-ND	4.83	118.06	110.24
24	0	601	CHL	C3D-C2D-C1D	-4.83	99.24	105.83
24	1	605	CHL	O2D-CGD-CBD	4.83	119.85	111.27
25	C	510	CLA	C4A-NA-C1A	4.83	108.88	106.71
24	7	601	CHL	C3D-C2D-C1D	-4.83	99.24	105.83
24	7	607	CHL	C3C-C4C-NC	4.83	115.99	110.57
25	y	602	CLA	CMB-C2B-C1B	-4.83	121.04	128.46
28	5	1623	NEX	C11-C10-C9	-4.83	120.42	127.31
24	7	606	CHL	C3C-C4C-NC	4.83	115.98	110.57
24	3	606	CHL	C3D-C4D-ND	4.83	118.04	110.24
24	9	607	CHL	C3D-C2D-C1D	-4.83	99.25	105.83
34	d	404	BCR	C11-C10-C9	-4.82	120.42	127.31
24	4	601	CHL	C3C-C4C-NC	4.82	115.98	110.57
27	N	1622	XAT	C38-C25-C26	-4.82	114.18	122.26
24	5	608	CHL	C3D-C4D-ND	4.82	118.04	110.24
25	C	510	CLA	CMB-C2B-C3B	4.82	133.69	124.68
24	G	608	CHL	C3D-C2D-C1D	-4.82	99.25	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	C	515	BCR	C7-C8-C9	-4.82	118.95	126.23
24	p	601	CHL	C3C-C4C-NC	4.82	115.97	110.57
27	n	1622	XAT	C38-C25-C26	-4.82	114.19	122.26
28	8	1623	NEX	C38-C25-C26	-4.82	114.19	122.26
24	9	609	CHL	C3D-C4D-ND	4.82	118.03	110.24
24	5	607	CHL	C3D-C2D-C1D	-4.82	99.26	105.83
24	N	601	CHL	C3D-C2D-C1D	-4.82	99.26	105.83
24	4	609	CHL	C3D-C2D-C1D	-4.82	99.26	105.83
24	q	605	CHL	C3D-C4D-ND	4.81	118.03	110.24
24	G	608	CHL	C3C-C4C-NC	4.81	115.97	110.57
27	q	1622	XAT	O24-C25-C38	4.81	120.82	115.06
27	2	1622	XAT	C18-C5-C6	-4.81	114.20	122.26
24	5	601	CHL	C3D-C4D-ND	4.81	118.02	110.24
25	q	612	CLA	C4A-NA-C1A	4.81	108.87	106.71
24	8	606	CHL	C2D-C1D-ND	4.81	113.65	110.10
27	5	1622	XAT	C15-C14-C13	-4.81	120.45	127.31
24	q	609	CHL	C3D-C2D-C1D	-4.80	99.27	105.83
24	s	607	CHL	C3D-C2D-C1D	-4.80	99.27	105.83
24	N	606	CHL	C3D-C4D-ND	4.80	118.01	110.24
24	2	605	CHL	C3D-C2D-C1D	-4.80	99.28	105.83
27	0	1622	XAT	C18-C5-C6	-4.80	114.22	122.26
24	2	607	CHL	C3D-C2D-C1D	-4.80	99.28	105.83
34	c	515	BCR	C7-C8-C9	-4.80	118.98	126.23
28	3	1623	NEX	C27-C28-C29	-4.80	118.08	125.53
25	r	604	CLA	C4A-NA-C1A	4.80	108.86	106.71
24	8	607	CHL	CHD-C4C-C3C	-4.80	117.79	124.84
24	2	606	CHL	O2D-CGD-CBD	4.80	119.79	111.27
24	3	609	CHL	C3D-C4D-ND	4.80	118.00	110.24
24	Y	607	CHL	O2D-CGD-CBD	4.79	119.79	111.27
24	4	606	CHL	C3D-C2D-C1D	-4.79	99.29	105.83
25	B	609	CLA	C4A-NA-C1A	4.79	108.86	106.71
25	b	609	CLA	C4A-NA-C1A	4.79	108.86	106.71
24	q	601	CHL	C3D-C4D-ND	4.79	117.99	110.24
25	N	611	CLA	C4A-NA-C1A	4.79	108.86	106.71
28	q	1623	NEX	C38-C25-C26	-4.79	114.24	122.26
24	7	607	CHL	C3D-C4D-ND	4.79	117.98	110.24
24	S	607	CHL	C3D-C2D-C1D	-4.78	99.30	105.83
24	5	606	CHL	C3C-C4C-NC	4.78	115.94	110.57
25	B	613	CLA	CMB-C2B-C1B	-4.78	121.12	128.46
25	b	613	CLA	CMB-C2B-C1B	-4.78	121.12	128.46
24	2	606	CHL	C3D-C4D-ND	4.78	117.97	110.24
24	5	606	CHL	C3D-C4D-ND	4.78	117.96	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	8	609	CHL	CHD-C1D-ND	-4.78	120.06	124.45
24	4	607	CHL	C1B-CHB-C4A	-4.78	120.66	130.12
24	s	607	CHL	O2D-CGD-CBD	4.77	119.75	111.27
25	R	604	CLA	C4A-NA-C1A	4.77	108.85	106.71
24	S	607	CHL	O2D-CGD-CBD	4.77	119.75	111.27
24	p	608	CHL	C3D-C4D-ND	4.77	117.96	110.24
25	A	405	CLA	C4A-NA-C1A	4.77	108.85	106.71
25	a	410	CLA	C4A-NA-C1A	4.77	108.85	106.71
25	3	604	CLA	CMB-C2B-C3B	4.77	133.60	124.68
25	c	510	CLA	CMB-C2B-C3B	4.77	133.60	124.68
24	y	608	CHL	CHD-C4C-C3C	-4.77	117.83	124.84
24	y	607	CHL	O2D-CGD-CBD	4.76	119.73	111.27
24	n	606	CHL	CHD-C4C-C3C	-4.76	117.84	124.84
27	n	1622	XAT	C18-C5-C6	-4.75	114.29	122.26
24	y	606	CHL	CHD-C4C-C3C	-4.75	117.86	124.84
25	c	507	CLA	C4A-NA-C1A	4.75	108.84	106.71
24	4	608	CHL	C3C-C4C-NC	4.75	115.90	110.57
28	0	1623	NEX	C38-C25-C26	-4.75	114.30	122.26
24	S	601	CHL	O2D-CGD-CBD	4.74	119.70	111.27
24	p	605	CHL	C3C-C4C-NC	4.74	115.89	110.57
24	p	607	CHL	C3C-C4C-NC	4.74	115.89	110.57
24	y	609	CHL	O2D-CGD-CBD	4.74	119.69	111.27
24	9	606	CHL	C3D-C4D-ND	4.74	117.90	110.24
24	9	601	CHL	C3D-C2D-C1D	-4.74	99.37	105.83
24	G	601	CHL	C3D-C4D-ND	4.74	117.90	110.24
24	l	607	CHL	O2D-CGD-CBD	4.74	119.68	111.27
24	g	601	CHL	C3D-C4D-ND	4.74	117.90	110.24
27	9	1622	XAT	C31-C30-C29	-4.73	120.55	127.31
27	N	1622	XAT	C18-C5-C6	-4.73	114.33	122.26
28	p	1623	NEX	C38-C25-C26	-4.73	114.33	122.26
24	p	606	CHL	C3D-C4D-ND	4.73	117.89	110.24
25	4	614	CLA	C4A-NA-C1A	4.73	108.83	106.71
24	7	606	CHL	C3D-C4D-ND	4.73	117.89	110.24
24	4	608	CHL	C3D-C4D-ND	4.73	117.88	110.24
28	q	1623	NEX	C11-C10-C9	-4.73	120.56	127.31
24	1	607	CHL	C3D-C4D-ND	4.72	117.88	110.24
24	0	605	CHL	O2D-CGD-CBD	4.72	119.66	111.27
24	3	605	CHL	C3C-C4C-NC	4.72	115.87	110.57
25	p	612	CLA	C4A-NA-C1A	4.72	108.83	106.71
28	g	1623	NEX	C15-C14-C13	-4.72	120.57	127.31
24	s	607	CHL	C3D-C4D-ND	4.72	117.87	110.24
24	Y	607	CHL	C3D-C4D-ND	4.72	117.87	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	q	607	CHL	C3D-C2D-C1D	-4.71	99.40	105.83
24	2	609	CHL	O2D-CGD-CBD	4.71	119.64	111.27
25	5	602	CLA	CMB-C2B-C1B	-4.71	121.22	128.46
24	s	601	CHL	O2D-CGD-CBD	4.71	119.64	111.27
24	y	607	CHL	C3D-C4D-ND	4.71	117.86	110.24
24	5	609	CHL	C3C-C4C-NC	4.71	115.85	110.57
24	8	605	CHL	C3C-C4C-NC	4.71	115.85	110.57
24	G	607	CHL	C3D-C4D-ND	4.71	117.85	110.24
26	3	1620	LUT	C35-C34-C33	-4.71	120.59	127.31
24	7	607	CHL	O2D-CGD-CBD	4.71	119.63	111.27
24	q	605	CHL	C3C-C4C-NC	4.70	115.85	110.57
25	5	604	CLA	C4A-NA-C1A	4.70	108.82	106.71
26	p	1620	LUT	C31-C30-C29	-4.70	120.60	127.31
24	S	607	CHL	C3D-C4D-ND	4.70	117.85	110.24
24	n	606	CHL	O2D-CGD-CBD	4.70	119.62	111.27
25	r	604	CLA	CMB-C2B-C1B	-4.70	121.24	128.46
24	4	605	CHL	C3D-C4D-ND	4.70	117.84	110.24
24	6	605	CHL	C3C-C4C-NC	4.70	115.84	110.57
25	B	603	CLA	C4A-NA-C1A	4.70	108.82	106.71
24	Y	606	CHL	CHD-C4C-C3C	-4.70	117.93	124.84
25	c	508	CLA	CMB-C2B-C1B	-4.70	121.24	128.46
25	R	604	CLA	CMB-C2B-C1B	-4.70	121.24	128.46
29	d	410	LHG	O7-C7-C8	4.70	121.62	111.50
24	8	601	CHL	C3C-C4C-NC	4.70	115.84	110.57
24	G	607	CHL	O2D-CGD-CBD	4.70	119.61	111.27
24	N	609	CHL	C3D-C4D-ND	4.70	117.83	110.24
29	D	410	LHG	O7-C7-C8	4.69	121.62	111.50
24	4	605	CHL	O2D-CGD-CBD	4.69	119.61	111.27
24	G	601	CHL	C3D-C2D-C1D	-4.69	99.43	105.83
27	7	1622	XAT	O24-C25-C24	4.69	116.91	113.38
24	g	607	CHL	C3D-C4D-ND	4.69	117.82	110.24
24	5	601	CHL	C3C-C4C-NC	4.69	115.83	110.57
24	4	609	CHL	C1D-ND-C4D	-4.68	103.01	106.33
24	6	607	CHL	O2D-CGD-CBD	4.68	119.59	111.27
24	n	609	CHL	C3D-C4D-ND	4.68	117.81	110.24
24	N	605	CHL	C3C-C4C-NC	4.68	115.82	110.57
26	2	1621	LUT	C35-C34-C33	-4.68	120.63	127.31
24	6	607	CHL	C3D-C4D-ND	4.68	117.80	110.24
24	N	607	CHL	O2D-CGD-CBD	4.67	119.57	111.27
27	y	1622	XAT	C37-C21-C26	-4.67	97.43	110.05
25	C	508	CLA	CMB-C2B-C1B	-4.67	121.29	128.46
24	9	606	CHL	O2D-CGD-CBD	4.66	119.56	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	g	608	CHL	C3D-C4D-ND	4.66	117.78	110.24
24	l	607	CHL	C3C-C4C-NC	4.66	115.80	110.57
27	Y	1622	XAT	C37-C21-C26	-4.66	97.46	110.05
24	N	608	CHL	O2D-CGD-CBD	4.66	119.55	111.27
24	2	607	CHL	C3C-C4C-NC	4.66	115.80	110.57
24	p	605	CHL	C3D-C2D-C1D	-4.66	99.47	105.83
24	R	606	CHL	C3D-C4D-ND	4.66	117.77	110.24
28	y	1623	NEX	C35-C34-C33	-4.66	120.66	127.31
25	8	604	CLA	CMB-C2B-C3B	4.66	133.39	124.68
25	4	603	CLA	CMB-C2B-C1B	-4.66	121.31	128.46
24	3	606	CHL	C1B-CHB-C4A	-4.65	120.91	130.12
25	5	611	CLA	C4A-NA-C1A	4.65	108.80	106.71
24	p	606	CHL	C2D-C1D-ND	4.65	113.53	110.10
24	5	607	CHL	O2D-CGD-CBD	4.65	119.53	111.27
24	g	609	CHL	O2D-CGD-CBD	4.65	119.53	111.27
25	G	602	CLA	C4A-NA-C1A	4.65	108.80	106.71
24	N	606	CHL	CHD-C4C-C3C	-4.65	118.01	124.84
24	5	609	CHL	C3D-C4D-ND	4.64	117.75	110.24
24	p	609	CHL	C3D-C4D-ND	4.64	117.75	110.24
34	c	515	BCR	C15-C14-C13	-4.64	120.68	127.31
28	N	1623	NEX	C27-C28-C29	-4.64	118.33	125.53
24	n	605	CHL	C3C-C4C-NC	4.64	115.78	110.57
25	A	406	CLA	CMB-C2B-C1B	-4.64	121.33	128.46
25	N	612	CLA	C4A-NA-C1A	4.64	108.79	106.71
24	7	607	CHL	C3D-C2D-C1D	-4.64	99.50	105.83
24	N	606	CHL	O2D-CGD-CBD	4.64	119.51	111.27
25	a	406	CLA	CMB-C2B-C1B	-4.64	121.33	128.46
24	r	606	CHL	C3D-C4D-ND	4.64	117.74	110.24
24	0	606	CHL	C3C-C4C-NC	4.64	115.77	110.57
24	1	606	CHL	O2D-CGD-CBD	4.64	119.51	111.27
24	0	608	CHL	C3D-C4D-ND	4.63	117.73	110.24
25	b	603	CLA	CMB-C2B-C1B	-4.63	121.34	128.46
24	4	605	CHL	C3C-C4C-NC	4.63	115.76	110.57
24	r	606	CHL	O2D-CGD-CBD	4.63	119.50	111.27
24	r	607	CHL	CHD-C1D-ND	-4.63	120.20	124.45
24	G	608	CHL	C3D-C4D-ND	4.63	117.73	110.24
25	g	602	CLA	C4A-NA-C1A	4.63	108.79	106.71
24	3	606	CHL	C2D-C1D-ND	4.63	113.52	110.10
34	c	516	BCR	C16-C17-C18	-4.63	120.71	127.31
25	B	603	CLA	CMB-C2B-C1B	-4.62	121.36	128.46
27	g	1622	XAT	O24-C25-C38	4.62	120.60	115.06
24	Y	608	CHL	CHD-C4C-C3C	-4.62	118.04	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	G	604	CLA	CMB-C2B-C1B	-4.62	121.36	128.46
24	R	606	CHL	O2D-CGD-CBD	4.62	119.48	111.27
24	q	606	CHL	C1B-CHB-C4A	-4.62	120.97	130.12
25	B	605	CLA	C4A-NA-C1A	4.62	108.78	106.71
24	q	606	CHL	C3D-C2D-C1D	-4.62	99.53	105.83
25	2	602	CLA	C4A-NA-C1A	4.62	108.78	106.71
24	7	605	CHL	C3D-C4D-ND	4.62	117.70	110.24
25	5	614	CLA	C4A-NA-C1A	4.62	108.78	106.71
24	9	607	CHL	C3C-C4C-NC	4.62	115.75	110.57
24	q	605	CHL	O2D-CGD-CBD	4.61	119.47	111.27
28	Y	1623	NEX	C35-C34-C33	-4.61	120.73	127.31
24	5	606	CHL	C3D-C2D-C1D	-4.61	99.54	105.83
24	0	601	CHL	O2D-CGD-CBD	4.61	119.46	111.27
27	G	1622	XAT	O24-C25-C38	4.61	120.58	115.06
34	C	516	BCR	C16-C17-C18	-4.60	120.74	127.31
24	1	609	CHL	C3D-C4D-ND	4.60	117.68	110.24
25	4	612	CLA	C4A-NA-C1A	4.60	108.77	106.71
28	n	1623	NEX	C35-C34-C33	-4.60	120.75	127.31
24	g	605	CHL	C3D-C4D-ND	4.60	117.67	110.24
24	q	606	CHL	C3D-C4D-ND	4.59	117.67	110.24
25	G	602	CLA	CMB-C2B-C1B	-4.59	121.40	128.46
24	Y	608	CHL	C3D-C4D-ND	4.59	117.66	110.24
24	9	607	CHL	C3D-C4D-ND	4.59	117.66	110.24
24	s	608	CHL	C3D-C4D-ND	4.59	117.66	110.24
28	n	1623	NEX	C27-C28-C29	-4.59	118.41	125.53
24	G	605	CHL	C3D-C4D-ND	4.59	117.66	110.24
24	y	608	CHL	C3D-C4D-ND	4.59	117.66	110.24
24	G	601	CHL	C3C-C4C-NC	4.59	115.71	110.57
25	8	602	CLA	CMB-C2B-C1B	-4.59	121.42	128.46
24	p	607	CHL	C3D-C2D-C1D	-4.58	99.57	105.83
24	2	606	CHL	C3D-C2D-C1D	-4.58	99.58	105.83
24	8	608	CHL	C3D-C4D-ND	4.58	117.65	110.24
34	C	515	BCR	C15-C14-C13	-4.58	120.77	127.31
27	0	1622	XAT	C31-C30-C29	-4.58	120.77	127.31
25	7	613	CLA	CMB-C2B-C1B	-4.58	121.42	128.46
25	b	614	CLA	CMB-C2B-C3B	4.58	133.25	124.68
24	q	601	CHL	C3C-C4C-NC	4.58	115.70	110.57
26	r	620	LUT	C15-C14-C13	-4.57	120.78	127.31
25	B	614	CLA	CMB-C2B-C3B	4.57	133.23	124.68
24	6	606	CHL	C3D-C2D-C1D	-4.57	99.59	105.83
34	b	619	BCR	C15-C14-C13	-4.57	120.79	127.31
27	q	1622	XAT	C6-C7-C8	-4.57	116.34	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	604	CLA	CMB-C2B-C1B	-4.57	121.44	128.46
24	N	609	CHL	CAC-C3C-C4C	4.57	130.73	124.81
24	9	608	CHL	C3D-C4D-ND	4.56	117.62	110.24
24	3	608	CHL	C3D-C4D-ND	4.56	117.62	110.24
24	1	605	CHL	C3D-C4D-ND	4.56	117.62	110.24
24	7	608	CHL	CHD-C4C-C3C	-4.56	118.13	124.84
24	4	607	CHL	C3D-C4D-ND	4.56	117.61	110.24
24	g	601	CHL	C3C-C4C-NC	4.56	115.68	110.57
26	R	620	LUT	C15-C14-C13	-4.56	120.81	127.31
24	9	606	CHL	C3D-C2D-C1D	-4.56	99.61	105.83
25	2	611	CLA	C4A-NA-C1A	4.55	108.75	106.71
34	B	619	BCR	C15-C14-C13	-4.55	120.81	127.31
25	3	602	CLA	CMB-C2B-C1B	-4.55	121.47	128.46
24	4	609	CHL	O2D-CGD-CBD	4.55	119.36	111.27
24	S	608	CHL	C3D-C4D-ND	4.55	117.60	110.24
28	g	1623	NEX	C27-C28-C29	-4.55	118.47	125.53
25	b	605	CLA	C4A-NA-C1A	4.55	108.75	106.71
24	1	607	CHL	C3D-C2D-C1D	-4.55	99.62	105.83
24	5	607	CHL	CHD-C4C-C3C	-4.55	118.16	124.84
25	1	613	CLA	CMB-C2B-C1B	-4.55	121.47	128.46
28	9	1623	NEX	C38-C25-C26	-4.55	114.64	122.26
24	2	607	CHL	C3D-C4D-ND	4.54	117.59	110.24
29	q	2630	LHG	O7-C7-C8	4.54	121.29	111.50
27	R	622	XAT	O4-C5-C18	4.54	120.49	115.06
24	9	601	CHL	C1B-CHB-C4A	-4.54	121.14	130.12
24	R	608	CHL	C3D-C4D-ND	4.53	117.57	110.24
24	Y	609	CHL	C3D-C4D-ND	4.53	117.57	110.24
25	p	602	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
24	R	607	CHL	CHD-C1D-ND	-4.53	120.29	124.45
26	5	1620	LUT	C31-C30-C29	-4.53	120.84	127.31
28	r	623	NEX	C38-C25-C26	-4.53	114.67	122.26
24	G	609	CHL	O2D-CGD-CBD	4.53	119.32	111.27
29	9	2630	LHG	O7-C7-C8	4.53	121.26	111.50
25	g	604	CLA	CMB-C2B-C1B	-4.53	121.50	128.46
27	r	622	XAT	O4-C5-C18	4.53	120.48	115.06
25	B	610	CLA	C4A-NA-C1A	4.53	108.74	106.71
25	b	610	CLA	C4A-NA-C1A	4.53	108.74	106.71
24	8	606	CHL	C3D-C2D-C1D	-4.53	99.66	105.83
28	5	1623	NEX	C38-C25-C26	-4.52	114.68	122.26
24	y	606	CHL	O2D-CGD-CBD	4.52	119.30	111.27
26	5	1620	LUT	C15-C14-C13	-4.52	120.86	127.31
24	G	609	CHL	C3D-C4D-ND	4.52	117.55	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	n	601	CHL	C3C-C4C-NC	4.52	115.64	110.57
24	r	608	CHL	C3D-C4D-ND	4.51	117.54	110.24
24	1	608	CHL	CHD-C4C-C3C	-4.51	118.20	124.84
24	2	608	CHL	C3D-C4D-ND	4.51	117.54	110.24
24	4	606	CHL	C3D-C4D-ND	4.51	117.54	110.24
26	p	1620	LUT	C15-C14-C13	-4.51	120.87	127.31
25	7	603	CLA	C4A-NA-C1A	4.51	108.73	106.71
25	s	604	CLA	CMB-C2B-C1B	-4.51	121.53	128.46
24	7	609	CHL	C3D-C4D-ND	4.51	117.53	110.24
28	R	623	NEX	C38-C25-C26	-4.51	114.71	122.26
27	4	1622	XAT	C26-C27-C28	-4.50	116.47	125.99
34	H	101	BCR	C11-C10-C9	-4.50	120.89	127.31
27	R	622	XAT	O24-C25-C38	4.50	120.45	115.06
25	1	603	CLA	C4A-NA-C1A	4.50	108.73	106.71
24	Y	606	CHL	O2D-CGD-CBD	4.50	119.26	111.27
24	3	609	CHL	CHD-C1D-ND	-4.50	120.32	124.45
27	N	1622	XAT	C15-C14-C13	-4.49	120.89	127.31
24	q	608	CHL	C3D-C4D-ND	4.49	117.51	110.24
25	2	604	CLA	C4A-NA-C1A	4.49	108.72	106.71
25	p	604	CLA	C4A-NA-C1A	4.49	108.72	106.71
27	r	622	XAT	O24-C25-C38	4.49	120.43	115.06
24	9	609	CHL	O2D-CGD-CBD	4.48	119.23	111.27
24	y	609	CHL	C3D-C4D-ND	4.48	117.48	110.24
25	B	612	CLA	C4A-NA-C1A	4.48	108.72	106.71
25	b	612	CLA	C4A-NA-C1A	4.48	108.72	106.71
26	5	1621	LUT	C35-C34-C33	-4.48	120.92	127.31
24	N	608	CHL	C3D-C4D-ND	4.47	117.48	110.24
24	3	606	CHL	C3D-C2D-C1D	-4.47	99.72	105.83
27	p	1622	XAT	C15-C14-C13	-4.47	120.92	127.31
25	C	503	CLA	CMB-C2B-C1B	-4.47	121.59	128.46
28	p	1623	NEX	C15-C14-C13	-4.47	120.93	127.31
24	y	607	CHL	CHD-C4C-C3C	-4.47	118.27	124.84
25	S	602	CLA	CMB-C2B-C1B	-4.47	121.60	128.46
24	6	608	CHL	C3D-C4D-ND	4.47	117.46	110.24
28	N	1623	NEX	O24-C25-C38	4.47	120.41	115.06
28	7	1623	NEX	O24-C25-C38	4.47	120.41	115.06
34	h	101	BCR	C11-C10-C9	-4.47	120.94	127.31
24	0	606	CHL	C3D-C2D-C1D	-4.46	99.74	105.83
24	Y	607	CHL	CHD-C4C-C3C	-4.46	118.28	124.84
24	n	608	CHL	O2D-CGD-CBD	4.46	119.19	111.27
28	S	1623	NEX	C38-C25-C26	-4.45	114.79	122.26
24	8	605	CHL	C3D-C4D-ND	4.45	117.44	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	605	CHL	C3D-C4D-ND	4.45	117.44	110.24
25	B	607	CLA	CMB-C2B-C1B	-4.45	121.63	128.46
24	Y	608	CHL	O2D-CGD-CBD	4.45	119.17	111.27
25	s	602	CLA	CMB-C2B-C1B	-4.45	121.63	128.46
24	n	605	CHL	C3D-C4D-ND	4.44	117.41	110.24
28	2	1623	NEX	C38-C25-C26	-4.43	114.83	122.26
24	G	608	CHL	O2D-CGD-CBD	4.43	119.14	111.27
24	3	605	CHL	C3D-C4D-ND	4.43	117.40	110.24
24	2	601	CHL	C3C-C4C-NC	4.43	115.53	110.57
24	5	608	CHL	O2D-CGD-CBD	4.42	119.13	111.27
28	g	1623	NEX	C11-C10-C9	-4.42	121.00	127.31
27	7	1622	XAT	C6-C7-C8	-4.42	116.64	125.99
24	p	607	CHL	O2D-CGD-CBD	4.42	119.13	111.27
24	n	608	CHL	CHD-C4C-C3C	-4.42	118.34	124.84
24	g	609	CHL	C3D-C4D-ND	4.42	117.38	110.24
25	4	604	CLA	C4A-NA-C1A	4.42	108.69	106.71
25	b	610	CLA	CMB-C2B-C3B	4.41	132.94	124.68
25	b	607	CLA	CMB-C2B-C1B	-4.41	121.68	128.46
24	4	606	CHL	C3C-C4C-NC	4.41	115.52	110.57
25	B	610	CLA	CMB-C2B-C3B	4.41	132.93	124.68
24	2	605	CHL	C3D-C4D-ND	4.41	117.37	110.24
24	Y	605	CHL	C3D-C4D-ND	4.41	117.37	110.24
25	1	610	CLA	CMB-C2B-C1B	-4.41	121.69	128.46
27	R	622	XAT	C26-C27-C28	-4.41	116.68	125.99
25	9	602	CLA	C4A-NA-C1A	4.40	108.69	106.71
24	q	608	CHL	C3C-C4C-NC	4.40	115.51	110.57
28	s	1623	NEX	C38-C25-C26	-4.40	114.89	122.26
28	2	1623	NEX	C11-C10-C9	-4.40	121.03	127.31
24	Y	606	CHL	C3D-C4D-ND	4.40	117.35	110.24
24	4	607	CHL	CAC-C3C-C4C	4.40	130.51	124.81
27	6	1622	XAT	O24-C25-C24	4.40	116.69	113.38
24	N	609	CHL	C3C-C4C-NC	4.40	115.50	110.57
28	8	1623	NEX	C27-C28-C29	-4.40	118.71	125.53
24	y	608	CHL	O2D-CGD-CBD	4.39	119.08	111.27
26	s	1621	LUT	C35-C34-C33	-4.39	121.04	127.31
25	9	611	CLA	C4A-NA-C1A	4.39	108.68	106.71
27	r	622	XAT	C26-C27-C28	-4.39	116.71	125.99
25	D	403	CLA	C4A-NA-C1A	4.39	108.68	106.71
26	S	1621	LUT	C35-C34-C33	-4.39	121.05	127.31
24	2	605	CHL	C3C-C4C-NC	4.39	115.49	110.57
24	G	609	CHL	C3C-C4C-NC	4.39	115.49	110.57
25	n	612	CLA	C4A-NA-C1A	4.39	108.68	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	G	1621	LUT	C15-C14-C13	-4.39	121.05	127.31
26	9	1620	LUT	C35-C34-C33	-4.38	121.05	127.31
24	0	609	CHL	C3D-C4D-ND	4.38	117.33	110.24
24	y	606	CHL	C3D-C4D-ND	4.38	117.33	110.24
28	n	1623	NEX	O24-C25-C38	4.38	120.31	115.06
25	1	602	CLA	C4A-NA-C1A	4.38	108.68	106.71
24	9	605	CHL	C3C-C4C-NC	4.38	115.48	110.57
25	B	613	CLA	CMB-C2B-C3B	4.38	132.88	124.68
25	b	613	CLA	CMB-C2B-C3B	4.38	132.88	124.68
24	g	609	CHL	C3C-C4C-NC	4.37	115.48	110.57
26	p	1620	LUT	C35-C34-C33	-4.37	121.07	127.31
24	s	607	CHL	C3C-C4C-NC	4.37	115.48	110.57
24	3	608	CHL	O2D-CGD-CBD	4.37	119.04	111.27
28	1	1623	NEX	C35-C34-C33	-4.37	121.07	127.31
28	y	1623	NEX	C27-C28-C29	-4.37	118.75	125.53
28	N	1623	NEX	C35-C34-C33	-4.37	121.07	127.31
24	q	607	CHL	CAC-C3C-C4C	4.37	130.48	124.81
24	R	607	CHL	C3D-C4D-ND	4.37	117.31	110.24
28	Y	1623	NEX	C27-C28-C29	-4.37	118.75	125.53
24	9	605	CHL	C3D-C4D-ND	4.37	117.30	110.24
25	g	602	CLA	CMB-C2B-C1B	-4.36	121.75	128.46
27	n	1622	XAT	C15-C14-C13	-4.36	121.08	127.31
25	2	602	CLA	CMB-C2B-C1B	-4.36	121.76	128.46
24	N	605	CHL	C3D-C4D-ND	4.36	117.29	110.24
24	g	608	CHL	O2D-CGD-CBD	4.36	119.02	111.27
25	b	605	CLA	CMB-C2B-C1B	-4.36	121.76	128.46
25	b	608	CLA	CMB-C2B-C1B	-4.36	121.76	128.46
25	y	602	CLA	C4A-NA-C1A	4.36	108.67	106.71
26	p	1621	LUT	C35-C34-C33	-4.36	121.09	127.31
25	2	610	CLA	CMB-C2B-C1B	-4.36	121.77	128.46
39	d	405	PL9	C7-C3-C4	4.36	120.42	116.88
24	N	608	CHL	CHD-C4C-C3C	-4.36	118.44	124.84
25	4	602	CLA	CMB-C2B-C1B	-4.35	121.77	128.46
27	q	1622	XAT	C15-C14-C13	-4.35	121.10	127.31
25	1	612	CLA	CMB-C2B-C1B	-4.35	121.78	128.46
24	6	609	CHL	C3D-C4D-ND	4.35	117.28	110.24
24	6	601	CHL	O2D-CGD-CBD	4.35	119.00	111.27
26	G	1621	LUT	C35-C34-C33	-4.35	121.10	127.31
28	G	1623	NEX	C27-C28-C29	-4.35	118.78	125.53
25	0	613	CLA	C4A-NA-C1A	4.35	108.66	106.71
24	8	608	CHL	O2D-CGD-CBD	4.35	118.99	111.27
24	3	601	CHL	C3C-C4C-NC	4.34	115.44	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	405	CLA	CMB-C2B-C3B	4.34	132.80	124.68
25	Y	603	CLA	CMB-C2B-C1B	-4.34	121.79	128.46
24	q	607	CHL	C3C-C4C-NC	4.34	115.44	110.57
25	q	603	CLA	CMB-C2B-C1B	-4.34	121.80	128.46
36	s	2631	LMG	O7-C10-C11	4.34	120.85	111.50
25	q	613	CLA	CMB-C2B-C3B	4.34	132.79	124.68
25	q	602	CLA	CMB-C2B-C1B	-4.34	121.80	128.46
24	4	606	CHL	O2D-CGD-CBD	4.33	118.97	111.27
24	y	607	CHL	CHB-C4A-NA	4.33	130.50	124.51
34	B	619	BCR	C1-C6-C5	-4.33	116.51	122.61
25	y	603	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
25	A	405	CLA	CMB-C2B-C3B	4.33	132.78	124.68
27	N	1622	XAT	C27-C28-C29	-4.33	118.82	125.53
29	2	2630	LHG	O7-C7-C8	4.32	120.82	111.50
24	1	601	CHL	CMD-C2D-C3D	-4.32	117.67	127.61
26	2	1620	LUT	C35-C34-C33	-4.32	121.14	127.31
36	D	411	LMG	O7-C10-C11	4.32	120.82	111.50
24	S	607	CHL	C3C-C4C-NC	4.32	115.42	110.57
25	9	602	CLA	CMB-C2B-C1B	-4.32	121.83	128.46
25	4	613	CLA	CMB-C2B-C1B	-4.31	121.83	128.46
24	Y	607	CHL	CHB-C4A-NA	4.31	130.47	124.51
25	d	403	CLA	C4A-NA-C1A	4.31	108.64	106.71
24	0	609	CHL	O2D-CGD-CBD	4.31	118.93	111.27
24	p	608	CHL	O2D-CGD-CBD	4.31	118.92	111.27
24	r	607	CHL	C3D-C4D-ND	4.31	117.20	110.24
24	4	607	CHL	C3C-C4C-NC	4.30	115.40	110.57
24	p	606	CHL	C3D-C2D-C1D	-4.30	99.96	105.83
34	b	619	BCR	C1-C6-C5	-4.30	116.55	122.61
36	d	411	LMG	O7-C10-C11	4.30	120.77	111.50
27	N	1622	XAT	C31-C30-C29	-4.30	121.17	127.31
25	7	610	CLA	CMB-C2B-C1B	-4.30	121.85	128.46
27	1	1622	XAT	C6-C7-C8	-4.30	116.90	125.99
24	4	609	CHL	C3D-C4D-ND	4.30	117.19	110.24
34	b	618	BCR	C15-C14-C13	-4.29	121.18	127.31
24	6	609	CHL	O2D-CGD-CBD	4.29	118.89	111.27
24	1	608	CHL	C3D-C4D-ND	4.29	117.18	110.24
26	q	1621	LUT	C15-C14-C13	-4.29	121.19	127.31
24	1	608	CHL	O2D-CGD-CBD	4.29	118.88	111.27
25	d	402	CLA	CMB-C2B-C1B	-4.28	121.88	128.46
24	n	608	CHL	C3D-C4D-ND	4.28	117.16	110.24
39	D	405	PL9	C7-C3-C4	4.28	120.36	116.88
27	p	1622	XAT	O24-C25-C38	4.28	120.18	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	q	1621	LUT	C35-C34-C33	-4.28	121.20	127.31
24	q	607	CHL	C3D-C4D-ND	4.28	117.16	110.24
25	Y	602	CLA	C4A-NA-C1A	4.28	108.63	106.71
29	s	2630	LHG	O7-C7-C8	4.27	120.71	111.50
25	Y	610	CLA	CMB-C2B-C3B	4.27	132.67	124.68
29	5	2630	LHG	O7-C7-C8	4.27	120.71	111.50
25	D	402	CLA	CMB-C2B-C1B	-4.27	121.90	128.46
29	4	2630	LHG	O7-C7-C8	4.27	120.70	111.50
26	5	1620	LUT	C35-C34-C33	-4.27	121.22	127.31
24	7	601	CHL	CMD-C2D-C3D	-4.27	117.80	127.61
24	Y	601	CHL	C3C-C4C-NC	4.26	115.35	110.57
34	d	404	BCR	C24-C23-C22	-4.26	119.79	126.23
24	G	601	CHL	CMD-C2D-C3D	-4.26	117.80	127.61
25	B	609	CLA	CMB-C2B-C3B	4.26	132.66	124.68
25	y	610	CLA	CMB-C2B-C3B	4.26	132.66	124.68
28	1	1623	NEX	C15-C14-C13	-4.26	121.23	127.31
34	D	404	BCR	C24-C23-C22	-4.26	119.80	126.23
34	B	618	BCR	C15-C14-C13	-4.26	121.23	127.31
25	B	605	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
25	b	609	CLA	CMB-C2B-C3B	4.26	132.65	124.68
25	s	614	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
25	9	610	CLA	CMB-C2B-C1B	-4.26	121.92	128.46
26	g	1621	LUT	C15-C14-C13	-4.25	121.24	127.31
36	S	2631	LMG	O7-C10-C11	4.25	120.66	111.50
29	S	2630	LHG	O7-C7-C8	4.25	120.66	111.50
24	n	609	CHL	C3C-C4C-NC	4.25	115.34	110.57
25	c	503	CLA	C4A-NA-C1A	4.25	108.62	106.71
25	S	614	CLA	CMB-C2B-C1B	-4.25	121.94	128.46
28	s	1623	NEX	C35-C34-C33	-4.25	121.25	127.31
24	3	609	CHL	CHD-C4C-C3C	-4.24	118.60	124.84
25	A	410	CLA	CMB-C2B-C3B	4.24	132.61	124.68
24	2	601	CHL	C3D-C4D-ND	4.24	117.10	110.24
25	a	410	CLA	CMB-C2B-C3B	4.24	132.61	124.68
27	0	1622	XAT	O4-C5-C18	4.24	120.13	115.06
24	3	605	CHL	O2D-CGD-CBD	4.23	118.79	111.27
25	b	616	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
34	B	620	BCR	C24-C23-C22	-4.23	119.84	126.23
24	6	607	CHL	CAC-C3C-C4C	4.23	130.30	124.81
25	B	608	CLA	CMB-C2B-C1B	-4.23	121.96	128.46
24	g	606	CHL	O2D-CGD-CBD	4.23	118.78	111.27
27	8	1622	XAT	C6-C7-C8	-4.23	117.06	125.99
24	p	606	CHL	O2D-CGD-CBD	4.23	118.78	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	0	605	CHL	C3D-C4D-ND	4.23	117.07	110.24
24	5	606	CHL	O2D-CGD-CBD	4.22	118.77	111.27
29	y	2630	LHG	O7-C7-C8	4.22	120.60	111.50
28	1	1623	NEX	C39-C29-C30	-4.22	117.02	122.92
36	A	413	LMG	O7-C10-C11	4.22	120.59	111.50
24	7	608	CHL	C3D-C4D-ND	4.22	117.06	110.24
25	B	616	CLA	CMB-C2B-C1B	-4.21	121.99	128.46
28	r	623	NEX	C11-C10-C9	-4.21	121.30	127.31
24	5	608	CHL	CHD-C4C-C3C	-4.21	118.65	124.84
28	6	1623	NEX	O24-C25-C38	4.21	120.10	115.06
24	y	609	CHL	CHD-C4C-C3C	-4.20	118.66	124.84
24	n	609	CHL	CAC-C3C-C4C	4.20	130.26	124.81
25	C	505	CLA	CMB-C2B-C3B	4.20	132.53	124.68
36	a	413	LMG	O7-C10-C11	4.20	120.55	111.50
25	7	612	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
34	H	101	BCR	C15-C14-C13	-4.20	121.32	127.31
25	Y	602	CLA	CMB-C2B-C3B	4.20	132.53	124.68
27	2	1622	XAT	C15-C14-C13	-4.19	121.33	127.31
35	b	623	SQD	O47-C7-C8	4.19	120.53	111.50
27	g	1622	XAT	C26-C27-C28	-4.19	117.14	125.99
27	G	1622	XAT	C26-C27-C28	-4.19	117.14	125.99
25	b	617	CLA	CMB-C2B-C1B	-4.19	122.03	128.46
25	B	617	CLA	CMB-C2B-C1B	-4.18	122.03	128.46
35	B	623	SQD	O47-C7-C8	4.18	120.52	111.50
34	b	620	BCR	C24-C23-C22	-4.18	119.92	126.23
25	b	602	CLA	C4A-NA-C1A	4.18	108.59	106.71
24	q	605	CHL	CAC-C3C-C4C	4.18	130.23	124.81
36	h	102	LMG	O7-C10-C11	4.18	120.51	111.50
25	y	602	CLA	CMB-C2B-C3B	4.18	132.50	124.68
25	c	505	CLA	CMB-C2B-C3B	4.18	132.50	124.68
25	6	614	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
25	y	613	CLA	C4A-NA-C1A	4.18	108.58	106.71
27	5	1622	XAT	O24-C25-C38	4.17	120.06	115.06
24	g	607	CHL	O2D-CGD-CBD	4.17	118.68	111.27
24	Y	605	CHL	CHD-C4C-C3C	-4.17	118.71	124.84
24	0	609	CHL	C1B-CHB-C4A	-4.17	121.86	130.12
26	9	1621	LUT	C35-C34-C33	-4.17	121.36	127.31
34	h	101	BCR	C15-C14-C13	-4.17	121.36	127.31
24	8	605	CHL	O2D-CGD-CBD	4.17	118.67	111.27
24	g	607	CHL	CAC-C3C-C4C	4.16	130.21	124.81
24	6	605	CHL	C3D-C4D-ND	4.16	116.97	110.24
24	7	608	CHL	O2D-CGD-CBD	4.16	118.66	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	G	606	CHL	O2D-CGD-CBD	4.16	118.66	111.27
34	b	619	BCR	C28-C27-C26	-4.16	106.65	114.08
36	H	102	LMG	O7-C10-C11	4.16	120.47	111.50
24	2	605	CHL	C1B-CHB-C4A	-4.16	121.88	130.12
24	R	607	CHL	CHD-C4C-C3C	-4.16	118.73	124.84
27	n	1622	XAT	C27-C28-C29	-4.15	119.09	125.53
24	y	605	CHL	CHD-C4C-C3C	-4.15	118.74	124.84
24	9	601	CHL	C3D-C4D-ND	4.15	116.95	110.24
24	4	609	CHL	C2D-C1D-ND	4.15	113.16	110.10
34	B	619	BCR	C28-C27-C26	-4.14	106.68	114.08
25	r	601	CLA	C2A-C1A-CHA	4.14	131.10	123.86
29	7	2630	LHG	O7-C7-C8	4.14	120.42	111.50
27	q	1622	XAT	O4-C5-C4	4.14	116.49	113.38
25	p	614	CLA	C4A-NA-C1A	4.14	108.57	106.71
27	n	1622	XAT	C31-C30-C29	-4.13	121.41	127.31
24	r	607	CHL	CHD-C4C-C3C	-4.13	118.76	124.84
25	S	611	CLA	CMB-C2B-C1B	-4.13	122.11	128.46
24	6	601	CHL	CHD-C4C-C3C	-4.13	118.77	124.84
24	Y	609	CHL	CHD-C4C-C3C	-4.13	118.77	124.84
24	y	601	CHL	C3C-C4C-NC	4.13	115.20	110.57
24	9	605	CHL	C1B-CHB-C4A	-4.13	121.94	130.12
25	4	612	CLA	CMB-C2B-C1B	-4.13	122.12	128.46
29	R	2630	LHG	O7-C7-C8	4.12	120.39	111.50
25	n	604	CLA	CMB-C2B-C1B	-4.12	122.12	128.46
27	3	1622	XAT	C6-C7-C8	-4.12	117.27	125.99
24	q	606	CHL	C3C-C4C-NC	4.12	115.20	110.57
24	8	609	CHL	CHD-C4C-C3C	-4.12	118.78	124.84
28	S	1623	NEX	C27-C28-C29	-4.12	119.14	125.53
25	R	601	CLA	C2A-C1A-CHA	4.12	131.06	123.86
25	b	615	CLA	CMB-C2B-C1B	-4.12	122.13	128.46
27	q	1622	XAT	C26-C27-C28	-4.12	117.29	125.99
26	6	1620	LUT	C15-C14-C13	-4.11	121.44	127.31
24	9	608	CHL	O2D-CGD-CBD	4.11	118.58	111.27
29	r	2630	LHG	O7-C7-C8	4.11	120.36	111.50
35	a	412	SQD	O47-C7-C8	4.11	120.36	111.50
28	s	1623	NEX	C2-C1-C6	4.11	113.21	109.21
28	N	1623	NEX	C15-C14-C13	-4.11	121.44	127.31
25	y	612	CLA	CMB-C2B-C1B	-4.11	122.14	128.46
25	G	604	CLA	C4A-NA-C1A	4.11	108.55	106.71
27	G	1622	XAT	C6-C7-C8	-4.11	117.31	125.99
25	7	604	CLA	CAC-C3C-C4C	4.11	130.14	124.81
34	c	516	BCR	C24-C23-C22	-4.11	120.03	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	407	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
27	g	1622	XAT	C6-C7-C8	-4.11	117.31	125.99
24	p	606	CHL	CAC-C3C-C4C	4.11	130.14	124.81
25	6	602	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
24	4	605	CHL	C1B-CHB-C4A	-4.10	121.99	130.12
25	B	615	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
24	S	606	CHL	CAC-C3C-C4C	4.10	130.13	124.81
28	S	1623	NEX	C35-C34-C33	-4.10	121.45	127.31
24	s	608	CHL	O2D-CGD-CBD	4.10	118.56	111.27
34	D	404	BCR	C16-C15-C14	-4.10	115.07	123.47
24	g	606	CHL	CAC-C3C-C4C	4.10	130.13	124.81
29	Y	2630	LHG	O7-C7-C8	4.10	120.34	111.50
25	Y	613	CLA	C4A-NA-C1A	4.10	108.55	106.71
26	n	1621	LUT	C35-C34-C33	-4.10	121.46	127.31
35	A	412	SQD	O47-C7-C8	4.10	120.34	111.50
24	G	606	CHL	CHD-C4C-C3C	-4.10	118.82	124.84
25	c	511	CLA	CMB-C2B-C3B	4.09	132.34	124.68
27	6	1622	XAT	O4-C5-C18	4.09	119.96	115.06
34	d	404	BCR	C16-C15-C14	-4.09	115.09	123.47
28	s	1623	NEX	C27-C28-C29	-4.09	119.18	125.53
25	B	602	CLA	C4A-NA-C1A	4.09	108.55	106.71
26	g	1621	LUT	C35-C34-C33	-4.09	121.47	127.31
36	B	622	LMG	O7-C10-C11	4.09	120.32	111.50
24	p	608	CHL	CHD-C4C-C3C	-4.09	118.83	124.84
24	4	606	CHL	C1B-CHB-C4A	-4.09	122.02	130.12
29	1	2630	LHG	O7-C7-C8	4.09	120.32	111.50
24	9	601	CHL	C3C-C4C-NC	4.09	115.16	110.57
27	6	1622	XAT	C6-C7-C8	-4.09	117.35	125.99
25	A	407	CLA	CMB-C2B-C1B	-4.09	122.18	128.46
27	1	1622	XAT	C15-C14-C13	-4.09	121.48	127.31
27	7	1622	XAT	C15-C14-C13	-4.08	121.48	127.31
34	C	516	BCR	C24-C23-C22	-4.08	120.06	126.23
24	G	607	CHL	CAC-C3C-C4C	4.08	130.11	124.81
24	3	601	CHL	C3B-C4B-NB	4.08	114.48	109.21
25	Y	612	CLA	CMB-C2B-C1B	-4.08	122.19	128.46
27	G	1622	XAT	C31-C30-C29	-4.08	121.49	127.31
25	4	603	CLA	CMB-C2B-C3B	4.08	132.31	124.68
29	g	2630	LHG	O7-C7-C8	4.08	120.29	111.50
24	q	608	CHL	O2D-CGD-CBD	4.08	118.51	111.27
28	S	1623	NEX	C31-C30-C29	-4.07	121.50	127.31
25	b	611	CLA	CAA-C2A-C3A	-4.07	101.62	112.78
36	b	622	LMG	O7-C10-C11	4.07	120.28	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	9	1621	LUT	C15-C14-C13	-4.07	121.50	127.31
37	c	523	DGD	O2G-C1B-C2B	4.07	120.28	111.50
25	6	604	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
25	0	612	CLA	CMB-C2B-C1B	-4.07	122.21	128.46
24	G	606	CHL	CAC-C3C-C4C	4.07	130.09	124.81
24	s	606	CHL	CAC-C3C-C4C	4.07	130.09	124.81
27	6	1622	XAT	C27-C28-C29	-4.07	119.22	125.53
24	S	608	CHL	O2D-CGD-CBD	4.07	118.50	111.27
25	C	503	CLA	C4A-NA-C1A	4.07	108.53	106.71
25	S	614	CLA	C4A-NA-C1A	4.07	108.53	106.71
25	c	507	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
29	G	2630	LHG	O7-C7-C8	4.06	120.26	111.50
25	q	612	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
24	r	608	CHL	CHD-C4C-C3C	-4.06	118.87	124.84
25	B	611	CLA	CAA-C2A-C3A	-4.06	101.66	112.78
25	7	602	CLA	C4A-NA-C1A	4.06	108.53	106.71
25	0	602	CLA	CMB-C2B-C1B	-4.06	122.23	128.46
25	C	503	CLA	CMB-C2B-C3B	4.06	132.27	124.68
37	C	523	DGD	O2G-C1B-C2B	4.05	120.24	111.50
25	C	511	CLA	CMB-C2B-C3B	4.05	132.26	124.68
27	4	1622	XAT	C11-C10-C9	-4.05	121.53	127.31
25	C	507	CLA	CMB-C2B-C1B	-4.05	122.23	128.46
24	R	608	CHL	CHD-C4C-C3C	-4.05	118.89	124.84
28	R	623	NEX	C11-C10-C9	-4.05	121.53	127.31
27	9	1622	XAT	C15-C14-C13	-4.05	121.53	127.31
26	2	1621	LUT	C15-C14-C13	-4.04	121.54	127.31
34	c	517	BCR	C7-C8-C9	-4.04	120.13	126.23
25	8	610	CLA	CMB-C2B-C1B	-4.04	122.25	128.46
24	R	607	CHL	CAC-C3C-C4C	4.04	130.05	124.81
27	4	1622	XAT	C15-C14-C13	-4.04	121.55	127.31
34	B	620	BCR	C7-C8-C9	-4.03	120.14	126.23
27	8	1622	XAT	C15-C14-C13	-4.03	121.55	127.31
25	g	604	CLA	C4A-NA-C1A	4.03	108.52	106.71
25	7	613	CLA	CMB-C2B-C3B	4.03	132.22	124.68
34	b	620	BCR	C7-C8-C9	-4.03	120.14	126.23
35	B	623	SQD	O9-S-C6	4.03	111.73	106.94
25	6	612	CLA	CMB-C2B-C1B	-4.03	122.28	128.46
25	7	614	CLA	C4A-NA-C1A	4.03	108.52	106.71
25	C	506	CLA	CMB-C2B-C1B	-4.03	122.28	128.46
25	1	604	CLA	C4A-NA-C1A	4.02	108.51	106.71
24	5	609	CHL	CAC-C3C-C4C	4.02	130.02	124.81
34	C	514	BCR	C16-C17-C18	-4.02	121.58	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	q	606	CHL	CAC-C3C-C4C	4.02	130.02	124.81
24	p	606	CHL	C3C-C4C-NC	4.02	115.08	110.57
25	B	603	CLA	CMB-C2B-C3B	4.02	132.19	124.68
26	N	1621	LUT	C35-C34-C33	-4.01	121.58	127.31
25	n	602	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
24	g	606	CHL	CHD-C4C-C3C	-4.01	118.94	124.84
25	d	403	CLA	CMB-C2B-C1B	-4.01	122.30	128.46
24	3	607	CHL	O2D-CGD-CBD	4.01	118.39	111.27
24	7	609	CHL	CHD-C4C-C3C	-4.01	118.95	124.84
24	r	607	CHL	CAC-C3C-C4C	4.01	130.01	124.81
27	y	1622	XAT	C31-C30-C29	-4.01	121.59	127.31
28	0	1623	NEX	C39-C29-C30	-4.01	117.31	122.92
24	p	609	CHL	CAC-C3C-C4C	4.00	130.01	124.81
24	S	601	CHL	C3C-C4C-NC	4.00	115.06	110.57
25	c	508	CLA	CMB-C2B-C3B	4.00	132.17	124.68
25	s	614	CLA	C4A-NA-C1A	4.00	108.51	106.71
34	c	514	BCR	C16-C17-C18	-4.00	121.60	127.31
25	1	613	CLA	CMB-C2B-C3B	4.00	132.17	124.68
34	C	517	BCR	C7-C8-C9	-4.00	120.19	126.23
37	C	520	DGD	O2G-C1B-C2B	4.00	120.13	111.50
25	Y	604	CLA	C4A-NA-C1A	4.00	108.50	106.71
28	n	1623	NEX	C15-C14-C13	-4.00	121.60	127.31
25	s	612	CLA	C4A-NA-C1A	4.00	108.50	106.71
24	3	607	CHL	CHB-C4A-NA	4.00	130.04	124.51
25	N	604	CLA	CMB-C2B-C1B	-4.00	122.32	128.46
24	6	608	CHL	CHD-C4C-C3C	-4.00	118.96	124.84
25	b	603	CLA	CMB-C2B-C3B	4.00	132.16	124.68
27	q	1622	XAT	C11-C10-C9	-3.99	121.61	127.31
29	n	2630	LHG	O7-C7-C8	3.99	120.10	111.50
25	3	610	CLA	C4A-NA-C1A	3.99	108.50	106.71
25	C	508	CLA	CMB-C2B-C3B	3.99	132.14	124.68
25	0	614	CLA	CMB-C2B-C1B	-3.99	122.34	128.46
24	9	608	CHL	CHD-C4C-C3C	-3.99	118.98	124.84
25	D	403	CLA	CMB-C2B-C1B	-3.98	122.34	128.46
28	8	1623	NEX	C11-C10-C9	-3.98	121.63	127.31
37	c	520	DGD	O2G-C1B-C2B	3.98	120.08	111.50
27	3	1622	XAT	C15-C14-C13	-3.98	121.63	127.31
24	2	608	CHL	CHD-C4C-C3C	-3.98	118.99	124.84
25	G	602	CLA	CMB-C2B-C3B	3.98	132.12	124.68
24	q	608	CHL	C4A-NA-C1A	3.98	108.50	106.71
25	q	610	CLA	C4A-NA-C1A	3.98	108.50	106.71
24	7	601	CHL	C3C-C4C-NC	3.98	115.03	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	9	1622	XAT	O4-C5-C18	3.98	119.82	115.06
24	1	609	CHL	CAC-C3C-C4C	3.98	129.97	124.81
29	p	2630	LHG	O7-C7-C8	3.98	120.07	111.50
24	G	607	CHL	O2A-CGA-CBA	3.97	124.38	111.91
25	N	602	CLA	CMB-C2B-C1B	-3.97	122.36	128.46
24	8	607	CHL	O2D-CGD-CBD	3.97	118.33	111.27
35	b	623	SQD	O9-S-C6	3.97	111.66	106.94
28	Y	1623	NEX	C15-C14-C13	-3.97	121.64	127.31
24	6	605	CHL	C1B-CHB-C4A	-3.97	122.26	130.12
25	2	604	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
25	G	610	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
25	c	506	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
24	8	607	CHL	CHB-C4A-NA	3.97	130.00	124.51
25	0	610	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
24	5	606	CHL	CAC-C3C-C4C	3.97	129.96	124.81
24	n	601	CHL	CHD-C4C-C3C	-3.96	119.01	124.84
24	4	605	CHL	CAC-C3C-C4C	3.96	129.95	124.81
25	c	503	CLA	CMB-C2B-C1B	-3.96	122.37	128.46
24	s	601	CHL	C3C-C4C-NC	3.96	115.02	110.57
25	9	613	CLA	CMB-C2B-C1B	-3.96	122.38	128.46
25	c	513	CLA	C4A-NA-C1A	3.96	108.49	106.71
24	N	601	CHL	CHD-C4C-C3C	-3.96	119.02	124.84
25	S	612	CLA	C4A-NA-C1A	3.96	108.48	106.71
27	Y	1622	XAT	C31-C30-C29	-3.96	121.66	127.31
24	p	601	CHL	CHD-C4C-C3C	-3.96	119.03	124.84
25	3	613	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
27	7	1622	XAT	C26-C27-C28	-3.95	117.63	125.99
29	N	2630	LHG	O7-C7-C8	3.95	120.02	111.50
25	A	406	CLA	CMB-C2B-C3B	3.95	132.07	124.68
24	4	607	CHL	O2D-CGD-CBD	3.95	118.29	111.27
34	D	404	BCR	C16-C17-C18	-3.95	121.67	127.31
25	s	604	CLA	C4A-NA-C1A	3.95	108.48	106.71
25	s	603	CLA	CAA-C2A-C3A	-3.95	104.39	114.26
25	a	406	CLA	CMB-C2B-C3B	3.95	132.07	124.68
25	y	614	CLA	CMB-C2B-C1B	-3.95	122.39	128.46
34	a	411	BCR	C7-C8-C9	-3.95	120.27	126.23
26	1	1620	LUT	C15-C14-C13	-3.95	121.68	127.31
25	s	611	CLA	CMB-C2B-C1B	-3.95	122.40	128.46
24	G	608	CHL	C1B-CHB-C4A	-3.95	122.30	130.12
25	g	610	CLA	CMB-C2B-C1B	-3.94	122.40	128.46
25	c	507	CLA	CMB-C2B-C3B	3.94	132.06	124.68
25	S	603	CLA	CAA-C2A-C3A	-3.94	104.41	114.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	614	CLA	C4A-NA-C1A	3.94	108.48	106.71
25	g	613	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
24	1	601	CHL	C3C-C4C-NC	3.94	114.99	110.57
25	b	606	CLA	C4A-NA-C1A	3.94	108.48	106.71
34	d	404	BCR	C16-C17-C18	-3.94	121.69	127.31
29	l	101	LHG	O7-C7-C8	3.93	119.98	111.50
25	C	507	CLA	CMB-C2B-C3B	3.93	132.03	124.68
24	2	601	CHL	O2D-CGD-CBD	3.93	118.25	111.27
24	p	605	CHL	C1B-CHB-C4A	-3.93	122.34	130.12
25	5	602	CLA	CMB-C2B-C3B	3.93	132.02	124.68
25	4	610	CLA	C4A-NA-C1A	3.93	108.47	106.71
25	3	610	CLA	CMB-C2B-C1B	-3.93	122.43	128.46
29	L	101	LHG	O7-C7-C8	3.92	119.96	111.50
25	S	612	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
34	A	411	BCR	C7-C8-C9	-3.92	120.31	126.23
36	d	412	LMG	O7-C10-C11	3.92	119.95	111.50
27	7	1622	XAT	C35-C34-C33	-3.92	121.72	127.31
25	G	613	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
26	6	1621	LUT	C35-C34-C33	-3.92	121.72	127.31
26	0	1620	LUT	C15-C14-C13	-3.92	121.72	127.31
24	8	601	CHL	C3B-C4B-NB	3.91	114.27	109.21
36	D	412	LMG	O7-C10-C11	3.91	119.94	111.50
25	b	612	CLA	CMB-C2B-C3B	3.91	132.00	124.68
25	r	610	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
25	Y	614	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
24	2	609	CHL	C3B-C4B-NB	3.91	114.27	109.21
25	2	613	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
24	N	609	CHL	OMC-CMC-C2C	-3.91	116.85	125.69
24	9	601	CHL	O2D-CGD-CBD	3.91	118.21	111.27
26	3	1621	LUT	C35-C34-C33	-3.91	121.73	127.31
25	R	610	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
25	q	604	CLA	O2D-CGD-O1D	-3.91	116.20	123.84
25	B	611	CLA	CMB-C2B-C1B	-3.90	122.46	128.46
25	C	513	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
27	1	1622	XAT	C35-C34-C33	-3.90	121.74	127.31
24	g	607	CHL	O2A-CGA-CBA	3.90	124.13	111.91
25	B	612	CLA	CMB-C2B-C3B	3.89	131.96	124.68
27	Y	1622	XAT	O4-C5-C18	3.89	119.72	115.06
24	2	601	CHL	C3B-C4B-NB	3.89	114.24	109.21
27	r	622	XAT	C4-C3-C2	-3.89	103.27	110.77
24	9	609	CHL	C3B-C4B-NB	3.88	114.23	109.21
25	B	615	CLA	C4A-NA-C1A	3.88	108.45	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	6	1623	NEX	C39-C29-C30	-3.88	117.49	122.92
25	b	611	CLA	CMB-C2B-C1B	-3.88	122.50	128.46
28	0	1623	NEX	C35-C34-C33	-3.88	121.78	127.31
34	c	514	BCR	C15-C14-C13	-3.88	121.78	127.31
25	B	606	CLA	C4A-NA-C1A	3.87	108.45	106.71
25	y	614	CLA	C4A-NA-C1A	3.87	108.45	106.71
25	4	602	CLA	C4A-NA-C1A	3.87	108.45	106.71
25	S	609	CLA	C4A-NA-C1A	3.87	108.45	106.71
25	b	617	CLA	CMB-C2B-C3B	3.87	131.92	124.68
24	4	606	CHL	CAC-C3C-C4C	3.87	129.83	124.81
24	0	601	CHL	CHD-C4C-C3C	-3.87	119.15	124.84
24	4	608	CHL	CAC-C3C-C4C	3.87	129.83	124.81
37	C	519	DGD	O2G-C1B-C2B	3.87	119.84	111.50
27	2	1622	XAT	O4-C5-C18	3.87	119.69	115.06
25	8	602	CLA	CMB-C2B-C3B	3.87	131.91	124.68
25	s	612	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
25	6	613	CLA	CMB-C2B-C1B	-3.87	122.52	128.46
29	D	408	LHG	O7-C7-C8	3.86	119.83	111.50
26	7	1621	LUT	C15-C14-C13	-3.86	121.80	127.31
26	7	1620	LUT	C15-C14-C13	-3.86	121.80	127.31
25	B	617	CLA	CMB-C2B-C3B	3.86	131.90	124.68
25	3	612	CLA	CMB-C2B-C1B	-3.86	122.53	128.46
37	c	519	DGD	O2G-C1B-C2B	3.86	119.81	111.50
25	2	610	CLA	CMB-C2B-C3B	3.86	131.90	124.68
27	R	622	XAT	C4-C3-C2	-3.86	103.33	110.77
25	3	602	CLA	CMB-C2B-C3B	3.85	131.89	124.68
28	6	1623	NEX	C15-C14-C13	-3.85	121.81	127.31
28	5	1623	NEX	C35-C34-C33	-3.85	121.81	127.31
24	3	606	CHL	CAC-C3C-C4C	3.85	129.81	124.81
28	3	1623	NEX	C39-C29-C30	-3.85	117.53	122.92
25	y	604	CLA	C4A-NA-C1A	3.85	108.44	106.71
27	1	1622	XAT	C27-C28-C29	-3.85	119.56	125.53
27	y	1622	XAT	O4-C5-C18	3.85	119.67	115.06
34	C	517	BCR	C15-C14-C13	-3.85	121.82	127.31
25	6	610	CLA	CMB-C2B-C1B	-3.84	122.56	128.46
24	G	607	CHL	CHD-C4C-C3C	-3.84	119.19	124.84
25	3	604	CLA	C4A-NA-C1A	3.84	108.43	106.71
24	4	609	CHL	C3C-C4C-NC	3.84	114.88	110.57
27	g	1622	XAT	C31-C30-C29	-3.84	121.83	127.31
25	s	612	CLA	C1B-CHB-C4A	-3.84	122.51	130.12
27	4	1622	XAT	C31-C30-C29	-3.84	121.83	127.31
24	6	606	CHL	CHD-C4C-C3C	-3.84	119.20	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	513	CLA	CMB-C2B-C1B	-3.83	122.57	128.46
28	Y	1623	NEX	C24-C23-C22	-3.83	103.37	110.77
28	y	1623	NEX	C24-C23-C22	-3.83	103.37	110.77
24	p	601	CHL	C3B-C4B-NB	3.83	114.16	109.21
25	0	612	CLA	C4A-NA-C1A	3.83	108.43	106.71
24	N	607	CHL	CAA-C2A-C3A	-3.83	102.29	112.78
24	R	607	CHL	CHB-C4A-NA	3.83	129.81	124.51
24	8	608	CHL	CHD-C4C-C3C	-3.83	119.22	124.84
25	7	602	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
25	Y	614	CLA	C4A-NA-C1A	3.83	108.43	106.71
29	d	408	LHG	O7-C7-C8	3.82	119.74	111.50
25	1	610	CLA	CMB-C2B-C3B	3.82	131.83	124.68
25	S	604	CLA	C4A-NA-C1A	3.82	108.42	106.71
25	b	615	CLA	C4A-NA-C1A	3.82	108.42	106.71
24	0	607	CHL	CHD-C4C-C3C	-3.82	119.22	124.84
27	8	1622	XAT	C26-C27-C28	-3.82	117.92	125.99
24	g	601	CHL	CMD-C2D-C3D	-3.82	118.83	127.61
28	1	1623	NEX	C27-C28-C29	-3.82	119.61	125.53
40	f	101	HEM	CMC-C2C-C3C	3.82	131.82	124.68
26	g	1620	LUT	C35-C34-C33	-3.82	121.86	127.31
24	g	605	CHL	C3B-C4B-NB	3.82	114.14	109.21
24	3	608	CHL	CHD-C4C-C3C	-3.82	119.23	124.84
24	7	609	CHL	CAC-C3C-C4C	3.81	129.76	124.81
26	7	1621	LUT	C35-C34-C33	-3.81	121.87	127.31
25	8	612	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
26	y	1621	LUT	C15-C14-C13	-3.81	121.87	127.31
34	C	514	BCR	C15-C14-C13	-3.81	121.87	127.31
34	A	411	BCR	C16-C17-C18	-3.81	121.88	127.31
34	a	411	BCR	C16-C17-C18	-3.81	121.88	127.31
25	8	604	CLA	C4A-NA-C1A	3.81	108.42	106.71
26	0	1621	LUT	C35-C34-C33	-3.81	121.88	127.31
34	c	517	BCR	C15-C14-C13	-3.81	121.88	127.31
40	F	101	HEM	CMC-C2C-C3C	3.80	131.80	124.68
25	N	610	CLA	CMB-C2B-C1B	-3.80	122.62	128.46
25	q	602	CLA	CMB-C2B-C3B	3.80	131.79	124.68
28	p	1623	NEX	C11-C10-C9	-3.80	121.88	127.31
24	8	606	CHL	C3C-C4C-NC	3.80	114.84	110.57
25	S	612	CLA	C1B-CHB-C4A	-3.80	122.59	130.12
26	9	1620	LUT	C7-C8-C9	-3.80	120.49	126.23
24	q	606	CHL	O2D-CGD-CBD	3.80	118.02	111.27
28	7	1623	NEX	C27-C28-C29	-3.80	119.63	125.53
26	6	1620	LUT	C35-C34-C33	-3.80	121.89	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	G	1620	LUT	C35-C34-C33	-3.80	121.89	127.31
25	8	613	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
24	p	609	CHL	C3B-C4B-NB	3.79	114.12	109.21
25	1	612	CLA	CMB-C2B-C3B	3.79	131.78	124.68
24	n	608	CHL	CAC-C3C-C4C	3.79	129.73	124.81
27	n	1622	XAT	O4-C5-C18	3.79	119.60	115.06
25	b	613	CLA	CHB-C4A-NA	3.79	129.76	124.51
24	6	609	CHL	CAC-C3C-C4C	3.79	129.73	124.81
24	G	601	CHL	C3B-C4B-NB	3.79	114.11	109.21
24	1	606	CHL	CHD-C4C-C3C	-3.79	119.27	124.84
24	1	609	CHL	CHD-C4C-C3C	-3.79	119.27	124.84
26	y	1620	LUT	C35-C34-C33	-3.79	121.90	127.31
25	R	601	CLA	C1B-CHB-C4A	-3.79	122.61	130.12
25	g	610	CLA	C4A-NA-C1A	3.79	108.41	106.71
26	0	1620	LUT	C35-C34-C33	-3.79	121.90	127.31
24	r	607	CHL	CHB-C4A-NA	3.79	129.75	124.51
24	g	601	CHL	C3B-C4B-NB	3.79	114.11	109.21
28	s	1623	NEX	C31-C30-C29	-3.78	121.91	127.31
25	1	602	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
28	s	1623	NEX	C11-C10-C9	-3.78	121.91	127.31
24	8	606	CHL	CAC-C3C-C4C	3.78	129.72	124.81
26	n	1621	LUT	C15-C14-C13	-3.78	121.92	127.31
25	2	612	CLA	CMB-C2B-C1B	-3.78	122.66	128.46
24	s	608	CHL	CAC-C3C-C4C	3.78	129.71	124.81
28	g	1623	NEX	O24-C25-C38	3.78	119.58	115.06
34	B	620	BCR	C33-C5-C6	-3.77	120.29	124.53
27	8	1622	XAT	O24-C25-C38	3.77	119.58	115.06
24	5	601	CHL	C3B-C4B-NB	3.77	114.09	109.21
25	1	610	CLA	C1B-CHB-C4A	-3.77	122.64	130.12
25	9	610	CLA	CMB-C2B-C3B	3.77	131.74	124.68
24	R	608	CHL	CAC-C3C-C4C	3.77	129.70	124.81
25	0	604	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
25	g	602	CLA	CMB-C2B-C3B	3.77	131.73	124.68
24	1	608	CHL	CAC-C3C-C4C	3.77	129.70	124.81
25	q	603	CLA	CMB-C2B-C3B	3.77	131.72	124.68
34	b	620	BCR	C33-C5-C6	-3.77	120.30	124.53
24	n	609	CHL	C1B-CHB-C4A	-3.76	122.66	130.12
25	n	610	CLA	CMB-C2B-C1B	-3.76	122.68	128.46
28	G	1623	NEX	O24-C25-C38	3.76	119.56	115.06
25	3	614	CLA	C4A-NA-C1A	3.76	108.40	106.71
28	G	1623	NEX	C11-C10-C9	-3.76	121.94	127.31
26	Y	1620	LUT	C35-C34-C33	-3.76	121.94	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	G	612	CLA	C4A-NA-C1A	3.76	108.40	106.71
25	g	612	CLA	C4A-NA-C1A	3.76	108.40	106.71
25	B	613	CLA	CHB-C4A-NA	3.76	129.71	124.51
24	S	608	CHL	CAC-C3C-C4C	3.76	129.69	124.81
25	C	513	CLA	C4A-NA-C1A	3.76	108.39	106.71
24	r	608	CHL	CAC-C3C-C4C	3.76	129.68	124.81
27	5	1622	XAT	C27-C28-C29	-3.75	119.70	125.53
24	0	608	CHL	CHD-C4C-C3C	-3.75	119.32	124.84
26	Y	1621	LUT	C15-C14-C13	-3.75	121.96	127.31
24	0	607	CHL	CAC-C3C-C4C	3.75	129.68	124.81
28	7	1623	NEX	C39-C29-C30	-3.75	117.67	122.92
26	g	1620	LUT	C15-C14-C13	-3.75	121.96	127.31
25	G	610	CLA	C4A-NA-C1A	3.75	108.39	106.71
26	G	1620	LUT	C15-C14-C13	-3.75	121.96	127.31
25	b	604	CLA	C1B-CHB-C4A	-3.75	122.70	130.12
25	7	612	CLA	C4A-NA-C1A	3.75	108.39	106.71
24	g	607	CHL	CHD-C4C-C3C	-3.75	119.33	124.84
25	g	614	CLA	CMB-C2B-C1B	-3.74	122.71	128.46
24	s	606	CHL	CHD-C4C-C3C	-3.74	119.34	124.84
25	2	610	CLA	C4A-NA-C1A	3.74	108.39	106.71
25	p	602	CLA	CMB-C2B-C3B	3.74	131.68	124.68
24	9	601	CHL	C3B-C4B-NB	3.74	114.05	109.21
25	4	602	CLA	CMB-C2B-C3B	3.74	131.68	124.68
40	f	101	HEM	CBA-CAA-C2A	-3.74	106.23	112.62
25	9	602	CLA	CMB-C2B-C3B	3.74	131.68	124.68
25	G	604	CLA	CMB-C2B-C3B	3.74	131.67	124.68
24	S	606	CHL	CHD-C4C-C3C	-3.74	119.34	124.84
25	8	610	CLA	C4A-NA-C1A	3.74	108.39	106.71
26	8	1621	LUT	C35-C34-C33	-3.74	121.97	127.31
25	s	605	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
24	N	608	CHL	CAC-C3C-C4C	3.73	129.66	124.81
24	G	605	CHL	C3B-C4B-NB	3.73	114.04	109.21
24	1	607	CHL	CAC-C3C-C4C	3.73	129.66	124.81
24	N	606	CHL	CAC-C3C-C4C	3.73	129.65	124.81
24	7	608	CHL	CAC-C3C-C4C	3.73	129.65	124.81
24	q	609	CHL	C3C-C4C-NC	3.73	114.75	110.57
37	c	518	DGD	O2G-C1B-C2B	3.73	119.53	111.50
27	3	1622	XAT	O24-C25-C38	3.73	119.52	115.06
27	6	1622	XAT	C15-C14-C13	-3.73	121.99	127.31
25	r	601	CLA	C1B-CHB-C4A	-3.72	122.74	130.12
27	4	1622	XAT	C6-C7-C8	-3.72	118.12	125.99
24	1	605	CHL	CHD-C4C-C3C	-3.72	119.37	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	7	610	CLA	CMB-C2B-C3B	3.72	131.64	124.68
27	9	1622	XAT	C11-C10-C9	-3.72	122.00	127.31
34	b	619	BCR	C11-C10-C9	-3.72	122.00	127.31
28	G	1623	NEX	C2-C1-C6	3.72	112.82	109.21
25	g	604	CLA	CMB-C2B-C3B	3.72	131.63	124.68
25	s	609	CLA	C4A-NA-C1A	3.72	108.38	106.71
24	0	605	CHL	CHD-C4C-C3C	-3.72	119.38	124.84
24	q	607	CHL	O2D-CGD-CBD	3.71	117.87	111.27
25	B	604	CLA	C4A-NA-C1A	3.71	108.38	106.71
25	S	610	CLA	C1B-CHB-C4A	-3.71	122.76	130.12
25	9	610	CLA	C1B-CHB-C4A	-3.71	122.77	130.12
24	n	605	CHL	C1C-C2C-C3C	-3.71	104.17	107.11
34	A	411	BCR	C15-C14-C13	-3.71	122.01	127.31
25	9	604	CLA	CMB-C2B-C1B	-3.71	122.76	128.46
24	6	606	CHL	C4-C3-C5	3.71	121.51	115.27
25	4	613	CLA	CMB-C2B-C3B	3.71	131.61	124.68
34	B	619	BCR	C11-C10-C9	-3.71	122.02	127.31
25	R	613	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
26	8	1621	LUT	C7-C8-C9	-3.70	120.64	126.23
25	B	607	CLA	CMB-C2B-C3B	3.70	131.61	124.68
33	A	409	PHO	CMB-C2B-C3B	3.70	131.61	124.68
25	0	603	CLA	CMB-C2B-C1B	-3.70	122.78	128.46
24	N	605	CHL	CHD-C4C-C3C	-3.70	119.40	124.84
24	4	608	CHL	C1B-CHB-C4A	-3.70	122.79	130.12
25	B	604	CLA	C1B-CHB-C4A	-3.70	122.79	130.12
37	C	518	DGD	O2G-C1B-C2B	3.70	119.47	111.50
33	a	409	PHO	CMB-C2B-C3B	3.70	131.60	124.68
25	s	610	CLA	C1B-CHB-C4A	-3.70	122.80	130.12
27	1	1622	XAT	C11-C10-C9	-3.70	122.03	127.31
34	H	101	BCR	C16-C17-C18	-3.70	122.04	127.31
34	a	411	BCR	C15-C14-C13	-3.70	122.04	127.31
35	b	621	SQD	O47-C7-C8	3.69	119.46	111.50
25	G	614	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
34	h	101	BCR	C16-C17-C18	-3.69	122.04	127.31
28	Y	1623	NEX	C39-C29-C30	-3.69	117.75	122.92
28	y	1623	NEX	C39-C29-C30	-3.69	117.75	122.92
28	y	1623	NEX	C15-C14-C13	-3.69	122.04	127.31
25	r	613	CLA	CMB-C2B-C1B	-3.69	122.79	128.46
25	b	615	CLA	C1B-CHB-C4A	-3.69	122.81	130.12
24	0	607	CHL	C3B-C4B-NB	3.69	113.98	109.21
24	0	606	CHL	C4-C3-C5	3.69	121.48	115.27
25	S	602	CLA	CMB-C2B-C3B	3.69	131.58	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	7	1623	NEX	C11-C10-C9	-3.69	122.05	127.31
25	7	610	CLA	C1B-CHB-C4A	-3.69	122.82	130.12
25	Y	612	CLA	C4A-NA-C1A	3.69	108.36	106.71
25	Y	604	CLA	C1B-CHB-C4A	-3.69	122.82	130.12
24	3	606	CHL	C3C-C4C-NC	3.68	114.70	110.57
24	y	607	CHL	C1-O2A-CGA	3.68	126.11	116.44
25	C	505	CLA	C1B-CHB-C4A	-3.68	122.82	130.12
25	b	607	CLA	CMB-C2B-C3B	3.68	131.57	124.68
24	n	607	CHL	CAA-C2A-C3A	-3.68	102.69	112.78
24	Y	601	CHL	CAC-C3C-C4C	3.68	129.59	124.81
27	N	1622	XAT	O4-C5-C18	3.68	119.47	115.06
25	c	512	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
24	8	608	CHL	CAC-C3C-C4C	3.67	129.58	124.81
24	8	606	CHL	C1B-CHB-C4A	-3.67	122.84	130.12
25	y	604	CLA	C1B-CHB-C4A	-3.67	122.84	130.12
25	2	602	CLA	CMB-C2B-C3B	3.67	131.55	124.68
24	8	601	CHL	CHD-C4C-C3C	-3.67	119.44	124.84
24	4	609	CHL	CAC-C3C-C4C	3.67	129.57	124.81
25	N	613	CLA	C1B-CHB-C4A	-3.67	122.85	130.12
25	s	610	CLA	CMB-C2B-C1B	-3.67	122.83	128.46
25	8	602	CLA	C4A-NA-C1A	3.67	108.35	106.71
24	n	605	CHL	CHD-C4C-C3C	-3.67	119.45	124.84
27	N	1622	XAT	C11-C10-C9	-3.67	122.08	127.31
25	S	610	CLA	CMB-C2B-C1B	-3.66	122.83	128.46
25	p	610	CLA	C4A-NA-C1A	3.66	108.35	106.71
26	N	1621	LUT	C15-C14-C13	-3.66	122.08	127.31
25	7	612	CLA	CMB-C2B-C3B	3.66	131.53	124.68
35	B	621	SQD	O47-C7-C8	3.66	119.39	111.50
26	S	1621	LUT	C7-C8-C9	-3.66	120.71	126.23
25	0	604	CLA	C4A-NA-C1A	3.66	108.35	106.71
27	2	1622	XAT	C11-C10-C9	-3.66	122.09	127.31
34	C	515	BCR	C24-C23-C22	-3.65	120.72	126.23
34	c	515	BCR	C24-C23-C22	-3.65	120.72	126.23
24	0	606	CHL	CAC-C3C-C4C	3.65	129.55	124.81
25	8	614	CLA	C4A-NA-C1A	3.65	108.35	106.71
25	c	505	CLA	C4A-NA-C1A	3.65	108.35	106.71
27	7	1622	XAT	C11-C10-C9	-3.65	122.10	127.31
27	n	1622	XAT	C11-C10-C9	-3.65	122.10	127.31
27	q	1622	XAT	C31-C30-C29	-3.65	122.10	127.31
35	b	623	SQD	O7-S-C6	3.65	111.27	106.94
24	g	608	CHL	C1B-CHB-C4A	-3.65	122.89	130.12
25	A	406	CLA	C1B-CHB-C4A	-3.65	122.89	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	406	CLA	C1B-CHB-C4A	-3.65	122.89	130.12
24	5	601	CHL	CHD-C4C-C3C	-3.65	119.48	124.84
28	0	1623	NEX	O24-C25-C38	3.64	119.42	115.06
25	2	610	CLA	C1B-CHB-C4A	-3.64	122.90	130.12
27	y	1622	XAT	O24-C25-C38	3.64	119.42	115.06
24	1	601	CHL	CAC-C3C-C4C	3.64	129.53	124.81
24	y	601	CHL	CAC-C3C-C4C	3.64	129.53	124.81
25	S	605	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
25	B	615	CLA	C1B-CHB-C4A	-3.64	122.91	130.12
25	s	614	CLA	CMB-C2B-C3B	3.64	131.48	124.68
25	a	410	CLA	C1B-CHB-C4A	-3.64	122.91	130.12
25	c	505	CLA	C1B-CHB-C4A	-3.64	122.92	130.12
25	s	602	CLA	CMB-C2B-C3B	3.64	131.48	124.68
26	7	1620	LUT	C35-C34-C33	-3.63	122.12	127.31
28	8	1623	NEX	C15-C14-C13	-3.63	122.13	127.31
24	5	609	CHL	C3B-C4B-NB	3.63	113.91	109.21
26	s	1621	LUT	C7-C8-C9	-3.63	120.75	126.23
25	6	612	CLA	C4A-NA-C1A	3.63	108.34	106.71
27	3	1622	XAT	C26-C27-C28	-3.63	118.32	125.99
24	3	608	CHL	CAC-C3C-C4C	3.63	129.52	124.81
25	p	611	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
24	6	601	CHL	C3B-C4B-NB	3.62	113.90	109.21
34	B	619	BCR	C33-C5-C6	-3.62	120.46	124.53
25	b	608	CLA	CMB-C2B-C3B	3.62	131.46	124.68
28	6	1623	NEX	C35-C34-C33	-3.62	122.14	127.31
24	2	605	CHL	CAC-C3C-C4C	3.62	129.51	124.81
24	N	601	CHL	C3B-C4B-NB	3.62	113.89	109.21
25	S	614	CLA	CMB-C2B-C3B	3.62	131.46	124.68
25	9	612	CLA	CMB-C2B-C1B	-3.62	122.90	128.46
34	b	618	BCR	C24-C23-C22	-3.62	120.76	126.23
25	q	602	CLA	C4A-NA-C1A	3.62	108.33	106.71
36	c	521	LMG	O7-C10-C11	3.62	119.30	111.50
25	6	604	CLA	C1B-CHB-C4A	-3.62	122.95	130.12
24	N	605	CHL	C1C-C2C-C3C	-3.62	104.24	107.11
24	7	608	CHL	C3B-C4B-NB	3.62	113.89	109.21
27	N	1622	XAT	C35-C34-C33	-3.62	122.15	127.31
25	B	616	CLA	CMB-C2B-C3B	3.62	131.45	124.68
25	Y	603	CLA	CMB-C2B-C3B	3.62	131.45	124.68
27	Y	1622	XAT	O24-C25-C38	3.62	119.39	115.06
26	4	1620	LUT	C35-C34-C33	-3.62	122.15	127.31
25	y	612	CLA	C4A-NA-C1A	3.61	108.33	106.71
24	7	607	CHL	CAC-C3C-C4C	3.61	129.50	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	611	CLA	CMB-C2B-C1B	-3.61	122.91	128.46
28	4	1623	NEX	C31-C30-C29	-3.61	122.15	127.31
25	3	602	CLA	C4A-NA-C1A	3.61	108.33	106.71
34	b	619	BCR	C33-C5-C6	-3.61	120.47	124.53
25	b	616	CLA	CMB-C2B-C3B	3.61	131.43	124.68
29	6	2630	LHG	O7-C7-C8	3.60	119.27	111.50
34	B	618	BCR	C24-C23-C22	-3.60	120.79	126.23
36	C	521	LMG	O7-C10-C11	3.60	119.27	111.50
25	N	612	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
28	S	1623	NEX	C11-C10-C9	-3.60	122.17	127.31
24	2	601	CHL	CAC-C3C-C4C	3.60	129.48	124.81
25	A	410	CLA	C1B-CHB-C4A	-3.60	122.99	130.12
25	p	602	CLA	C4A-NA-C1A	3.60	108.32	106.71
27	r	622	XAT	C15-C14-C13	-3.60	122.17	127.31
25	n	602	CLA	CMB-C2B-C3B	3.60	131.41	124.68
25	y	612	CLA	CMB-C2B-C3B	3.60	131.41	124.68
28	3	1623	NEX	C15-C14-C13	-3.60	122.18	127.31
24	1	601	CHL	C4A-NA-C1A	-3.60	105.09	106.71
25	y	603	CLA	CMB-C2B-C3B	3.60	131.41	124.68
25	r	613	CLA	C1B-CHB-C4A	-3.59	123.00	130.12
25	g	610	CLA	C1B-CHB-C4A	-3.59	123.00	130.12
28	8	1623	NEX	C39-C29-C30	-3.59	117.89	122.92
24	N	601	CHL	CMD-C2D-C3D	-3.59	119.36	127.61
25	G	610	CLA	C1B-CHB-C4A	-3.59	123.01	130.12
28	7	1623	NEX	C35-C34-C33	-3.59	122.19	127.31
25	n	612	CLA	CMB-C2B-C1B	-3.59	122.95	128.46
27	9	1622	XAT	C6-C7-C8	-3.59	118.41	125.99
24	g	608	CHL	CHD-C4C-C3C	-3.59	119.57	124.84
29	0	2630	LHG	O7-C7-C8	3.59	119.23	111.50
24	Y	607	CHL	C1-O2A-CGA	3.59	125.85	116.44
24	q	605	CHL	C1B-CHB-C4A	-3.58	123.02	130.12
25	n	613	CLA	C1B-CHB-C4A	-3.58	123.02	130.12
25	6	614	CLA	CMB-C2B-C3B	3.58	131.38	124.68
28	q	1623	NEX	C31-C30-C29	-3.58	122.20	127.31
25	0	612	CLA	CMB-C2B-C3B	3.58	131.38	124.68
25	S	605	CLA	C1B-CHB-C4A	-3.58	123.03	130.12
25	Y	612	CLA	CMB-C2B-C3B	3.58	131.38	124.68
25	b	604	CLA	C4A-NA-C1A	3.58	108.31	106.71
35	B	623	SQD	O7-S-C6	3.58	111.19	106.94
29	d	409	LHG	O7-C7-C8	3.58	119.21	111.50
24	1	601	CHL	C3B-C4B-NB	3.57	113.83	109.21
24	y	607	CHL	C6-C5-C3	-3.57	104.08	113.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	n	606	CHL	CAC-C3C-C4C	3.57	129.44	124.81
25	b	604	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
27	R	622	XAT	C15-C14-C13	-3.57	122.21	127.31
25	0	611	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
25	1	604	CLA	C1B-CHB-C4A	-3.57	123.05	130.12
25	R	613	CLA	C1B-CHB-C4A	-3.57	123.05	130.12
29	D	409	LHG	O7-C7-C8	3.57	119.19	111.50
27	9	1622	XAT	C26-C27-C28	-3.57	118.45	125.99
24	N	605	CHL	C3B-C4B-NB	3.57	113.82	109.21
27	2	1622	XAT	C6-C7-C8	-3.57	118.45	125.99
25	y	611	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
24	9	601	CHL	CAC-C3C-C4C	3.57	129.44	124.81
24	1	607	CHL	C1B-CHB-C4A	-3.57	123.06	130.12
26	5	1621	LUT	C35-C15-C14	-3.57	116.17	123.47
26	3	1620	LUT	C15-C14-C13	-3.57	122.22	127.31
24	r	606	CHL	CAA-C2A-C3A	-3.56	103.02	112.78
25	0	604	CLA	C1B-CHB-C4A	-3.56	123.06	130.12
25	6	612	CLA	CMB-C2B-C3B	3.56	131.35	124.68
24	Y	609	CHL	C3B-C4B-NB	3.56	113.82	109.21
24	7	601	CHL	C3B-C4B-NB	3.56	113.82	109.21
24	y	606	CHL	CAA-C2A-C3A	-3.56	103.02	112.78
25	C	502	CLA	CMC-C2C-C1C	-3.56	119.61	125.04
24	7	605	CHL	CHD-C4C-C3C	-3.56	119.60	124.84
24	7	601	CHL	CAC-C3C-C4C	3.56	129.43	124.81
24	G	601	CHL	CAC-C3C-C4C	3.56	129.43	124.81
25	6	603	CLA	CMB-C2B-C1B	-3.56	122.99	128.46
24	7	607	CHL	C1B-CHB-C4A	-3.56	123.07	130.12
24	Y	607	CHL	C6-C5-C3	-3.56	104.12	113.45
24	R	606	CHL	CAA-C2A-C3A	-3.56	103.03	112.78
25	B	604	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
25	3	613	CLA	C1B-CHB-C4A	-3.56	123.08	130.12
25	n	610	CLA	C1B-CHB-C4A	-3.55	123.08	130.12
26	3	1621	LUT	C7-C8-C9	-3.55	120.86	126.23
24	G	605	CHL	CAC-C3C-C4C	3.55	129.42	124.81
25	S	604	CLA	CMB-C2B-C3B	3.55	131.33	124.68
25	c	503	CLA	CMB-C2B-C3B	3.55	131.33	124.68
25	R	603	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
25	r	603	CLA	CMB-C2B-C1B	-3.55	123.00	128.46
25	C	508	CLA	C1B-CHB-C4A	-3.55	123.08	130.12
25	G	610	CLA	CMB-C2B-C3B	3.55	131.32	124.68
25	N	610	CLA	C1B-CHB-C4A	-3.55	123.09	130.12
25	c	502	CLA	CMC-C2C-C1C	-3.55	119.64	125.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	b	619	BCR	C24-C23-C22	-3.55	120.88	126.23
25	C	509	CLA	CMB-C2B-C1B	-3.55	123.02	128.46
34	c	517	BCR	C11-C10-C9	-3.54	122.25	127.31
24	Y	606	CHL	CAA-C2A-C3A	-3.54	103.08	112.78
24	y	605	CHL	C3B-C4B-NB	3.54	113.79	109.21
25	s	605	CLA	C1B-CHB-C4A	-3.54	123.10	130.12
25	g	610	CLA	CMB-C2B-C3B	3.54	131.30	124.68
24	y	609	CHL	C3B-C4B-NB	3.54	113.78	109.21
25	N	602	CLA	CMB-C2B-C3B	3.54	131.30	124.68
28	9	1623	NEX	C15-C14-C13	-3.53	122.27	127.31
24	n	601	CHL	C3B-C4B-NB	3.53	113.78	109.21
28	1	1623	NEX	O24-C25-C38	3.53	119.29	115.06
28	3	1623	NEX	O24-C25-C38	3.53	119.29	115.06
25	b	615	CLA	CMB-C2B-C3B	3.53	131.28	124.68
25	r	612	CLA	CMB-C2B-C1B	-3.53	123.04	128.46
25	B	608	CLA	CMB-C2B-C3B	3.53	131.28	124.68
24	0	605	CHL	C3B-C4B-NB	3.53	113.77	109.21
28	9	1623	NEX	C35-C34-C33	-3.53	122.28	127.31
24	n	605	CHL	C3B-C4B-NB	3.52	113.77	109.21
24	q	608	CHL	CAC-C3C-C4C	3.52	129.38	124.81
25	S	604	CLA	C1B-CHB-C4A	-3.52	123.14	130.12
25	1	612	CLA	C4A-NA-C1A	3.52	108.29	106.71
25	s	604	CLA	CMB-C2B-C3B	3.52	131.27	124.68
24	9	605	CHL	CAC-C3C-C4C	3.52	129.38	124.81
25	9	613	CLA	CMB-C2B-C3B	3.52	131.26	124.68
25	B	615	CLA	CMB-C2B-C3B	3.52	131.26	124.68
25	R	612	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
24	g	609	CHL	CMD-C2D-C3D	-3.52	119.52	127.61
34	B	619	BCR	C24-C23-C22	-3.52	120.92	126.23
25	3	614	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
27	0	1622	XAT	C27-C28-C29	-3.52	120.08	125.53
24	N	609	CHL	C1B-CHB-C4A	-3.52	123.16	130.12
25	p	614	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
24	7	606	CHL	CAC-C3C-C4C	3.52	129.37	124.81
25	r	609	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
25	8	614	CLA	CMB-C2B-C1B	-3.51	123.06	128.46
26	r	620	LUT	C18-C5-C6	-3.51	120.58	124.53
25	s	604	CLA	C1B-CHB-C4A	-3.51	123.16	130.12
34	a	411	BCR	C33-C5-C6	-3.51	120.59	124.53
24	n	607	CHL	CHB-C4A-NA	3.51	129.37	124.51
28	N	1623	NEX	C39-C29-C30	-3.51	118.01	122.92
37	C	523	DGD	O6D-C5D-C6D	3.51	113.75	106.67

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	G	609	CHL	CMD-C2D-C3D	-3.51	119.54	127.61
24	2	608	CHL	C3B-C4B-NB	3.51	113.75	109.21
26	Y	1621	LUT	C35-C34-C33	-3.51	122.30	127.31
34	C	517	BCR	C11-C10-C9	-3.51	122.31	127.31
25	6	611	CLA	CMB-C2B-C1B	-3.51	123.08	128.46
26	y	1621	LUT	C35-C34-C33	-3.50	122.31	127.31
24	4	609	CHL	C4A-NA-C1A	3.50	108.28	106.71
25	g	613	CLA	CMB-C2B-C3B	3.50	131.23	124.68
25	4	610	CLA	C1B-CHB-C4A	-3.50	123.18	130.12
27	N	1622	XAT	C4-C3-C2	-3.50	104.02	110.77
24	g	601	CHL	CAC-C3C-C4C	3.50	129.35	124.81
34	b	618	BCR	C7-C8-C9	-3.50	120.95	126.23
25	b	605	CLA	CMB-C2B-C3B	3.50	131.22	124.68
25	8	604	CLA	C1B-CHB-C4A	-3.49	123.20	130.12
24	g	605	CHL	CAC-C3C-C4C	3.49	129.34	124.81
27	0	1622	XAT	C11-C10-C9	-3.49	122.32	127.31
25	n	611	CLA	CMB-C2B-C1B	-3.49	123.10	128.46
34	B	618	BCR	C7-C8-C9	-3.49	120.96	126.23
25	y	604	CLA	CMB-C2B-C3B	3.49	131.20	124.68
24	Y	605	CHL	C3B-C4B-NB	3.49	113.72	109.21
24	0	606	CHL	CHD-C4C-C3C	-3.49	119.72	124.84
24	7	601	CHL	CHD-C4C-C3C	-3.48	119.72	124.84
37	c	523	DGD	O6D-C5D-C6D	3.48	113.70	106.67
25	5	611	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
25	b	612	CLA	C1B-CHB-C4A	-3.48	123.22	130.12
26	1	1620	LUT	C35-C34-C33	-3.48	122.34	127.31
25	r	604	CLA	CMB-C2B-C3B	3.48	131.19	124.68
34	b	618	BCR	C16-C17-C18	-3.48	122.34	127.31
25	5	614	CLA	CMB-C2B-C1B	-3.48	123.11	128.46
27	5	1622	XAT	C6-C7-C8	-3.48	118.63	125.99
34	A	411	BCR	C33-C5-C6	-3.48	120.62	124.53
25	B	612	CLA	C1B-CHB-C4A	-3.48	123.23	130.12
26	R	620	LUT	C18-C5-C6	-3.48	120.62	124.53
25	R	604	CLA	CMB-C2B-C3B	3.48	131.18	124.68
24	n	608	CHL	C3B-C4B-NB	3.48	113.70	109.21
25	S	611	CLA	CMB-C2B-C3B	3.48	131.18	124.68
25	2	604	CLA	C1B-CHB-C4A	-3.47	123.24	130.12
25	Y	604	CLA	CMB-C2B-C3B	3.47	131.18	124.68
26	2	1620	LUT	C35-C15-C14	-3.47	116.36	123.47
25	2	613	CLA	CMB-C2B-C3B	3.47	131.18	124.68
34	B	618	BCR	C16-C17-C18	-3.47	122.35	127.31
25	p	610	CLA	CMB-C2B-C1B	-3.47	123.13	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	3	601	CHL	CHD-C4C-C3C	-3.47	119.74	124.84
24	N	607	CHL	CHB-C4A-NA	3.47	129.31	124.51
25	D	402	CLA	C1B-CHB-C4A	-3.47	123.25	130.12
25	R	611	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
24	4	601	CHL	CHD-C4C-C3C	-3.46	119.75	124.84
25	R	609	CLA	C1B-CHB-C4A	-3.46	123.26	130.12
25	5	602	CLA	C4A-NA-C1A	3.46	108.26	106.71
28	R	623	NEX	C15-C14-C13	-3.46	122.37	127.31
25	5	613	CLA	CMB-C2B-C1B	-3.46	123.14	128.46
24	n	601	CHL	CMD-C2D-C3D	-3.46	119.66	127.61
34	h	101	BCR	C27-C26-C25	-3.46	117.71	122.73
24	7	601	CHL	C4A-NA-C1A	-3.46	105.15	106.71
25	R	609	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
28	8	1623	NEX	O24-C25-C38	3.46	119.20	115.06
25	5	610	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
25	G	613	CLA	CMB-C2B-C3B	3.46	131.15	124.68
27	g	1622	XAT	C24-C23-C22	-3.46	104.10	110.77
28	2	1623	NEX	C35-C34-C33	-3.46	122.38	127.31
25	a	407	CLA	CMB-C2B-C3B	3.46	131.14	124.68
25	S	613	CLA	CMB-C2B-C1B	-3.45	123.15	128.46
25	c	508	CLA	C1B-CHB-C4A	-3.45	123.28	130.12
34	H	101	BCR	C27-C26-C25	-3.45	117.72	122.73
25	9	614	CLA	C1B-CHB-C4A	-3.45	123.28	130.12
26	2	1620	LUT	C7-C8-C9	-3.45	121.02	126.23
24	n	609	CHL	C3B-C4B-NB	3.45	113.67	109.21
27	n	1622	XAT	C4-C3-C2	-3.45	104.11	110.77
25	6	602	CLA	CMB-C2B-C3B	3.45	131.13	124.68
24	r	607	CHL	C3B-C4B-NB	3.45	113.67	109.21
25	c	507	CLA	O2D-CGD-O1D	-3.45	117.10	123.84
25	s	609	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
25	0	614	CLA	CMB-C2B-C3B	3.44	131.12	124.68
37	c	524	DGD	O2G-C1B-C2B	3.44	118.92	111.50
34	B	618	BCR	C20-C21-C22	-3.44	122.40	127.31
25	q	612	CLA	CMB-C2B-C3B	3.44	131.12	124.68
27	G	1622	XAT	C24-C23-C22	-3.44	104.12	110.77
24	p	608	CHL	C3B-C4B-NB	3.44	113.66	109.21
25	r	611	CLA	CMB-C2B-C1B	-3.44	123.17	128.46
24	9	608	CHL	C3B-C4B-NB	3.44	113.66	109.21
25	C	513	CLA	CMB-C2B-C3B	3.44	131.12	124.68
24	7	606	CHL	CHD-C4C-C3C	-3.44	119.78	124.84
25	r	609	CLA	C1B-CHB-C4A	-3.44	123.31	130.12
25	D	402	CLA	CMB-C2B-C3B	3.44	131.11	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	1	1623	NEX	C17-C1-C6	-3.44	107.39	110.47
24	0	601	CHL	C1B-CHB-C4A	-3.44	123.31	130.12
24	2	606	CHL	CAC-C3C-C4C	3.44	129.27	124.81
25	5	610	CLA	C4A-NA-C1A	3.44	108.25	106.71
28	n	1623	NEX	C39-C29-C30	-3.44	118.11	122.92
25	8	613	CLA	C1B-CHB-C4A	-3.44	123.31	130.12
25	b	607	CLA	C1B-CHB-C4A	-3.44	123.31	130.12
27	2	1622	XAT	C27-C28-C29	-3.44	120.20	125.53
24	q	609	CHL	CAC-C3C-C4C	3.44	129.27	124.81
25	d	403	CLA	CMB-C2B-C3B	3.44	131.11	124.68
25	g	604	CLA	C1B-CHB-C4A	-3.44	123.31	130.12
24	g	606	CHL	C3B-C4B-NB	3.44	113.65	109.21
25	s	613	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
25	d	402	CLA	CMB-C2B-C3B	3.43	131.10	124.68
34	a	411	BCR	C24-C23-C22	-3.43	121.05	126.23
24	6	606	CHL	CAC-C3C-C4C	3.43	129.26	124.81
25	A	407	CLA	CMB-C2B-C3B	3.43	131.10	124.68
37	C	524	DGD	C2G-O2G-C1B	-3.43	109.34	117.79
25	N	610	CLA	C4A-NA-C1A	3.43	108.25	106.71
25	N	613	CLA	CHB-C4A-NA	3.43	129.26	124.51
25	D	403	CLA	CMB-C2B-C3B	3.43	131.10	124.68
25	R	602	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
25	N	611	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
25	n	614	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
24	2	606	CHL	CHD-C4C-C3C	-3.43	119.80	124.84
25	C	512	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
25	c	509	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
25	n	613	CLA	CHB-C4A-NA	3.43	129.25	124.51
25	d	402	CLA	C1B-CHB-C4A	-3.43	123.33	130.12
24	p	607	CHL	CHD-C4C-C3C	-3.42	119.81	124.84
27	4	1622	XAT	C35-C34-C33	-3.42	122.42	127.31
34	A	411	BCR	C24-C23-C22	-3.42	121.06	126.23
34	h	101	BCR	C24-C23-C22	-3.42	121.06	126.23
24	p	608	CHL	CAC-C3C-C4C	3.42	129.25	124.81
24	1	609	CHL	C3B-C4B-NB	3.42	113.63	109.21
26	R	620	LUT	C35-C34-C33	-3.42	122.43	127.31
25	c	513	CLA	CMB-C2B-C3B	3.42	131.08	124.68
24	0	609	CHL	CAC-C3C-C4C	3.42	129.25	124.81
25	r	602	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
25	3	613	CLA	CMB-C2B-C3B	3.42	131.07	124.68
25	0	602	CLA	CMB-C2B-C3B	3.42	131.07	124.68
25	B	607	CLA	C1B-CHB-C4A	-3.42	123.35	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	n	603	CLA	CAA-C2A-C3A	-3.42	103.42	112.78
24	G	606	CHL	C3B-C4B-NB	3.42	113.63	109.21
25	2	614	CLA	C4A-NA-C1A	3.42	108.24	106.71
25	S	609	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
25	p	604	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
26	1	1621	LUT	C35-C34-C33	-3.42	122.44	127.31
34	b	618	BCR	C20-C21-C22	-3.42	122.44	127.31
25	2	614	CLA	C1B-CHB-C4A	-3.41	123.36	130.12
25	5	602	CLA	C1B-CHB-C4A	-3.41	123.36	130.12
24	q	609	CHL	C1D-CHD-C4C	-3.41	118.69	126.06
24	R	607	CHL	C3B-C4B-NB	3.41	113.62	109.21
25	S	612	CLA	CMB-C2B-C3B	3.41	131.06	124.68
34	H	101	BCR	C24-C23-C22	-3.41	121.08	126.23
25	G	604	CLA	C1B-CHB-C4A	-3.41	123.36	130.12
34	b	619	BCR	C7-C8-C9	-3.41	121.09	126.23
25	2	614	CLA	CMB-C2B-C1B	-3.41	123.23	128.46
28	8	1623	NEX	C24-C23-C22	-3.41	104.20	110.77
25	C	505	CLA	C4A-NA-C1A	3.41	108.24	106.71
24	1	601	CHL	C1C-C2C-C3C	-3.40	104.41	107.11
27	G	1622	XAT	C4-C3-C2	-3.40	104.20	110.77
25	7	604	CLA	C1B-CHB-C4A	-3.40	123.38	130.12
37	C	524	DGD	O2G-C1B-C2B	3.40	118.83	111.50
25	p	612	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
25	4	612	CLA	CMB-C2B-C3B	3.40	131.04	124.68
37	c	524	DGD	C2G-O2G-C1B	-3.40	109.42	117.79
26	6	1621	LUT	C15-C14-C13	-3.40	122.46	127.31
24	7	607	CHL	CHD-C4C-C3C	-3.40	119.84	124.84
26	r	620	LUT	C35-C34-C33	-3.40	122.46	127.31
24	Y	607	CHL	CAC-C3C-C4C	3.40	129.22	124.81
25	7	614	CLA	CMB-C2B-C1B	-3.40	123.25	128.46
25	9	614	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
25	B	605	CLA	CMB-C2B-C3B	3.39	131.03	124.68
25	c	512	CLA	CMB-C2B-C3B	3.39	131.03	124.68
28	6	1623	NEX	C11-C10-C9	-3.39	122.47	127.31
24	6	605	CHL	C3B-C4B-NB	3.39	113.59	109.21
24	S	607	CHL	C1B-CHB-C4A	-3.39	123.40	130.12
26	n	1620	LUT	C35-C34-C33	-3.39	122.47	127.31
25	0	613	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
27	g	1622	XAT	C15-C14-C13	-3.39	122.47	127.31
28	4	1623	NEX	C26-C27-C28	-3.39	118.83	125.99
25	s	602	CLA	C1B-CHB-C4A	-3.39	123.41	130.12
28	G	1623	NEX	C39-C29-C30	-3.39	118.18	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	B	619	BCR	C7-C8-C9	-3.39	121.12	126.23
25	8	610	CLA	CMB-C2B-C3B	3.39	131.01	124.68
37	c	519	DGD	C3G-O3G-C1D	-3.39	107.12	113.74
25	2	611	CLA	C1B-CHB-C4A	-3.39	123.41	130.12
25	B	603	CLA	C1B-CHB-C4A	-3.39	123.41	130.12
25	0	610	CLA	CMB-C2B-C3B	3.39	131.01	124.68
25	0	610	CLA	C4A-NA-C1A	3.39	108.23	106.71
25	5	613	CLA	CHB-C4A-NA	3.38	129.19	124.51
25	s	612	CLA	CMB-C2B-C3B	3.38	131.01	124.68
27	N	1622	XAT	C15-C35-C34	-3.38	116.54	123.47
24	7	601	CHL	C1C-C2C-C3C	-3.38	104.43	107.11
25	b	603	CLA	C1B-CHB-C4A	-3.38	123.42	130.12
25	N	603	CLA	CAA-C2A-C3A	-3.38	103.52	112.78
24	4	609	CHL	C1D-CHD-C4C	-3.38	118.76	126.06
24	q	601	CHL	CAC-C3C-C4C	3.38	129.20	124.81
28	3	1623	NEX	C24-C23-C22	-3.38	104.25	110.77
24	2	607	CHL	C1B-CHB-C4A	-3.38	123.42	130.12
25	4	614	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
24	s	607	CHL	C1B-CHB-C4A	-3.38	123.43	130.12
25	3	604	CLA	C1B-CHB-C4A	-3.38	123.43	130.12
25	S	602	CLA	C1B-CHB-C4A	-3.38	123.43	130.12
25	4	613	CLA	C1B-CHB-C4A	-3.37	123.44	130.12
25	C	513	CLA	CAA-C2A-C3A	-3.37	103.55	112.78
25	S	613	CLA	C1B-CHB-C4A	-3.37	123.44	130.12
25	s	613	CLA	C1B-CHB-C4A	-3.37	123.44	130.12
28	5	1623	NEX	O24-C25-C38	3.37	119.09	115.06
25	9	614	CLA	C4A-NA-C1A	3.37	108.22	106.71
27	1	1622	XAT	C31-C30-C29	-3.37	122.50	127.31
24	6	607	CHL	CHD-C4C-C3C	-3.37	119.89	124.84
25	5	604	CLA	C1B-CHB-C4A	-3.36	123.45	130.12
26	q	1620	LUT	C31-C30-C29	-3.36	122.51	127.31
25	q	614	CLA	CMB-C2B-C1B	-3.36	123.29	128.46
25	4	614	CLA	C1B-CHB-C4A	-3.36	123.46	130.12
34	C	514	BCR	C20-C21-C22	-3.36	122.51	127.31
24	N	608	CHL	C3B-C4B-NB	3.36	113.56	109.21
25	9	611	CLA	C1B-CHB-C4A	-3.36	123.46	130.12
24	g	601	CHL	CHD-C4C-C3C	-3.36	119.90	124.84
24	0	605	CHL	C1B-CHB-C4A	-3.36	123.46	130.12
25	n	611	CLA	C1B-CHB-C4A	-3.36	123.46	130.12
26	q	1620	LUT	C35-C34-C33	-3.36	122.52	127.31
25	1	614	CLA	CMB-C2B-C1B	-3.36	123.30	128.46
25	4	603	CLA	CHB-C4A-NA	3.36	129.16	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	q	613	CLA	CHB-C4A-NA	3.36	129.16	124.51
24	G	601	CHL	CHD-C4C-C3C	-3.36	119.90	124.84
25	q	613	CLA	C1B-CHB-C4A	-3.36	123.47	130.12
25	9	604	CLA	C1B-CHB-C4A	-3.36	123.47	130.12
25	N	611	CLA	C1B-CHB-C4A	-3.36	123.47	130.12
24	4	601	CHL	CAC-C3C-C4C	3.36	129.16	124.81
34	D	404	BCR	C33-C5-C6	-3.36	120.76	124.53
24	1	601	CHL	CHD-C4C-C3C	-3.36	119.91	124.84
34	c	516	BCR	C20-C21-C22	-3.35	122.52	127.31
24	q	601	CHL	CHD-C4C-C3C	-3.35	119.91	124.84
28	0	1623	NEX	C15-C14-C13	-3.35	122.53	127.31
24	9	606	CHL	CHD-C4C-C3C	-3.35	119.91	124.84
24	r	606	CHL	CHD-C4C-C3C	-3.35	119.91	124.84
24	y	607	CHL	CAC-C3C-C4C	3.35	129.16	124.81
24	R	606	CHL	CHD-C4C-C3C	-3.35	119.92	124.84
24	S	608	CHL	CHD-C4C-C3C	-3.35	119.92	124.84
25	r	601	CLA	CHB-C4A-NA	3.35	129.14	124.51
25	q	610	CLA	C1B-CHB-C4A	-3.35	123.48	130.12
26	N	1620	LUT	C35-C34-C33	-3.35	122.53	127.31
24	N	601	CHL	C1C-C2C-C3C	-3.35	104.46	107.11
25	g	612	CLA	CMB-C2B-C1B	-3.35	123.32	128.46
27	g	1622	XAT	C4-C3-C2	-3.35	104.31	110.77
34	B	620	BCR	C20-C21-C22	-3.35	122.53	127.31
25	2	604	CLA	CMB-C2B-C3B	3.34	130.94	124.68
24	1	607	CHL	CHD-C4C-C3C	-3.34	119.92	124.84
24	N	609	CHL	C3B-C4B-NB	3.34	113.53	109.21
25	s	611	CLA	CMB-C2B-C3B	3.34	130.93	124.68
24	Y	601	CHL	CHD-C4C-C3C	-3.34	119.93	124.84
24	S	606	CHL	C3B-C4B-NB	3.34	113.53	109.21
24	7	609	CHL	C3B-C4B-NB	3.34	113.53	109.21
27	y	1622	XAT	C4-C3-C2	-3.34	104.32	110.77
25	b	617	CLA	CAA-C2A-C3A	-3.34	103.63	112.78
24	3	601	CHL	C1C-C2C-C3C	-3.34	104.46	107.11
24	N	607	CHL	CAC-C3C-C4C	3.34	129.15	124.81
24	s	606	CHL	C3B-C4B-NB	3.34	113.53	109.21
25	G	613	CLA	C1B-CHB-C4A	-3.34	123.50	130.12
25	5	612	CLA	CAA-C2A-C3A	-3.34	103.63	112.78
25	4	610	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
25	y	614	CLA	CMB-C2B-C3B	3.34	130.92	124.68
25	N	604	CLA	C1B-CHB-C4A	-3.34	123.51	130.12
39	D	405	PL9	C7-C8-C9	-3.34	121.24	126.79
27	Y	1622	XAT	C4-C3-C2	-3.34	104.33	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1	1621	LUT	C15-C14-C13	-3.33	122.55	127.31
25	7	604	CLA	C4A-NA-C1A	3.33	108.20	106.71
25	G	611	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
27	R	622	XAT	C24-C23-C22	-3.33	104.33	110.77
25	B	617	CLA	C1B-CHB-C4A	-3.33	123.52	130.12
28	p	1623	NEX	C35-C34-C33	-3.33	122.55	127.31
28	r	623	NEX	C15-C14-C13	-3.33	122.55	127.31
25	g	613	CLA	C1B-CHB-C4A	-3.33	123.52	130.12
25	6	610	CLA	CMB-C2B-C3B	3.33	130.91	124.68
25	N	602	CLA	C4A-NA-C1A	3.33	108.20	106.71
24	n	601	CHL	C1C-C2C-C3C	-3.33	104.47	107.11
28	Y	1623	NEX	C28-C29-C30	3.33	124.05	118.94
24	G	608	CHL	CHD-C4C-C3C	-3.33	119.95	124.84
24	9	608	CHL	CAC-C3C-C4C	3.33	129.13	124.81
24	1	608	CHL	C3B-C4B-NB	3.33	113.51	109.21
26	0	1621	LUT	C15-C14-C13	-3.33	122.56	127.31
25	1	610	CLA	C4A-NA-C1A	3.33	108.20	106.71
34	d	404	BCR	C33-C5-C6	-3.33	120.79	124.53
25	G	612	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
34	C	516	BCR	C20-C21-C22	-3.33	122.56	127.31
25	g	611	CLA	CMB-C2B-C1B	-3.33	123.35	128.46
25	r	603	CLA	CAA-C2A-C3A	-3.33	103.67	112.78
24	5	608	CHL	C3B-C4B-NB	3.33	113.51	109.21
25	7	610	CLA	C4A-NA-C1A	3.32	108.20	106.71
25	b	617	CLA	C1B-CHB-C4A	-3.32	123.54	130.12
25	R	601	CLA	CHB-C4A-NA	3.32	129.10	124.51
25	R	603	CLA	CAA-C2A-C3A	-3.32	103.68	112.78
34	c	514	BCR	C20-C21-C22	-3.32	122.57	127.31
24	3	607	CHL	C3B-C4B-NB	3.32	113.50	109.21
24	3	605	CHL	CAC-C3C-C4C	3.32	129.12	124.81
24	y	609	CHL	CHB-C4A-NA	3.32	129.10	124.51
24	s	601	CHL	C4A-NA-C1A	-3.32	105.22	106.71
27	r	622	XAT	C24-C23-C22	-3.32	104.37	110.77
25	q	602	CLA	C1B-CHB-C4A	-3.32	123.55	130.12
24	2	609	CHL	CAC-C3C-C4C	3.31	129.11	124.81
25	Y	614	CLA	CMB-C2B-C3B	3.31	130.88	124.68
27	q	1622	XAT	C35-C34-C33	-3.31	122.58	127.31
24	g	608	CHL	CAC-C3C-C4C	3.31	129.11	124.81
25	n	604	CLA	C1B-CHB-C4A	-3.31	123.56	130.12
24	8	605	CHL	CAC-C3C-C4C	3.31	129.11	124.81
25	5	604	CLA	CMB-C2B-C1B	-3.31	123.37	128.46
27	p	1622	XAT	C11-C10-C9	-3.31	122.58	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	b	620	BCR	C20-C21-C22	-3.31	122.58	127.31
25	Y	614	CLA	C1B-CHB-C4A	-3.31	123.56	130.12
25	5	611	CLA	C1B-CHB-C4A	-3.31	123.56	130.12
25	B	617	CLA	CAA-C2A-C3A	-3.31	103.72	112.78
24	s	608	CHL	CHD-C4C-C3C	-3.31	119.98	124.84
27	5	1622	XAT	C11-C10-C9	-3.31	122.59	127.31
25	N	614	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
25	c	513	CLA	CAA-C2A-C3A	-3.30	103.74	112.78
25	0	614	CLA	O2D-CGD-O1D	-3.30	117.38	123.84
25	C	509	CLA	CMB-C2B-C3B	3.30	130.85	124.68
25	5	613	CLA	C1B-CHB-C4A	-3.30	123.58	130.12
25	B	610	CLA	C1B-CHB-C4A	-3.30	123.58	130.12
25	y	611	CLA	C1B-CHB-C4A	-3.30	123.59	130.12
27	4	1622	XAT	C4-C3-C2	-3.30	104.41	110.77
25	A	405	CLA	C1B-CHB-C4A	-3.30	123.59	130.12
25	8	610	CLA	C1B-CHB-C4A	-3.30	123.59	130.12
25	6	614	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
25	c	512	CLA	CHB-C4A-NA	3.29	129.07	124.51
25	y	614	CLA	C1B-CHB-C4A	-3.29	123.60	130.12
27	1	1622	XAT	C26-C27-C28	-3.29	119.03	125.99
24	p	601	CHL	CHB-C4A-NA	3.29	129.06	124.51
28	g	1623	NEX	C39-C29-C30	-3.29	118.31	122.92
25	7	614	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
25	Y	611	CLA	C1B-CHB-C4A	-3.29	123.60	130.12
28	y	1623	NEX	C28-C29-C30	3.29	123.99	118.94
24	6	609	CHL	CHD-C4C-C3C	-3.29	120.01	124.84
24	G	608	CHL	CAC-C3C-C4C	3.29	129.08	124.81
28	Y	1623	NEX	C26-C27-C28	-3.29	119.05	125.99
34	B	620	BCR	C16-C17-C18	-3.28	122.62	127.31
24	6	608	CHL	CAC-C3C-C4C	3.28	129.07	124.81
24	g	605	CHL	CHD-C4C-C3C	-3.28	120.01	124.84
25	b	610	CLA	C1B-CHB-C4A	-3.28	123.61	130.12
25	3	610	CLA	CMB-C2B-C3B	3.28	130.82	124.68
25	a	405	CLA	C1B-CHB-C4A	-3.28	123.61	130.12
25	r	610	CLA	CMB-C2B-C3B	3.28	130.82	124.68
28	3	1623	NEX	C11-C10-C9	-3.28	122.63	127.31
29	8	2630	LHG	O7-C7-C8	3.28	118.57	111.50
25	s	612	CLA	CHB-C4A-NA	3.28	129.05	124.51
25	Y	613	CLA	CMB-C2B-C1B	-3.28	123.42	128.46
24	s	601	CHL	CMD-C2D-C3D	-3.28	120.07	127.61
25	p	610	CLA	C1B-CHB-C4A	-3.28	123.62	130.12
24	8	607	CHL	C3B-C4B-NB	3.28	113.45	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	610	CLA	C1B-CHB-C4A	-3.28	123.63	130.12
24	y	601	CHL	CHD-C4C-C3C	-3.28	120.02	124.84
25	0	603	CLA	CMB-C2B-C3B	3.28	130.81	124.68
25	4	610	CLA	C1-C2-C3	-3.28	120.38	126.04
25	3	603	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
28	7	1623	NEX	C2-C1-C6	3.27	112.39	109.21
26	s	1621	LUT	C11-C10-C9	-3.27	122.64	127.31
25	b	616	CLA	C1B-CHB-C4A	-3.27	123.64	130.12
39	d	405	PL9	C7-C8-C9	-3.27	121.34	126.79
25	R	610	CLA	CMB-C2B-C3B	3.27	130.80	124.68
28	2	1623	NEX	C39-C29-C30	-3.27	118.34	122.92
25	d	402	CLA	CAC-C3C-C4C	3.27	129.05	124.81
28	2	1623	NEX	C27-C28-C29	-3.27	120.46	125.53
25	y	613	CLA	CMB-C2B-C1B	-3.27	123.44	128.46
26	8	1620	LUT	C15-C14-C13	-3.27	122.65	127.31
25	6	613	CLA	CMB-C2B-C3B	3.27	130.79	124.68
25	3	603	CLA	CAA-C2A-C3A	-3.27	103.83	112.78
25	1	603	CLA	C1B-CHB-C4A	-3.27	123.65	130.12
24	n	607	CHL	CAC-C3C-C4C	3.27	129.05	124.81
26	9	1621	LUT	C22-C23-C24	-3.27	108.02	111.74
25	S	612	CLA	CHB-C4A-NA	3.27	129.03	124.51
37	C	519	DGD	C3G-O3G-C1D	-3.27	107.36	113.74
25	p	602	CLA	C1B-CHB-C4A	-3.26	123.65	130.12
27	G	1622	XAT	C15-C14-C13	-3.26	122.65	127.31
25	7	603	CLA	C1B-CHB-C4A	-3.26	123.66	130.12
27	9	1622	XAT	C35-C34-C33	-3.26	122.66	127.31
25	n	610	CLA	C4A-NA-C1A	3.26	108.17	106.71
25	8	613	CLA	CMB-C2B-C3B	3.26	130.78	124.68
25	8	603	CLA	CAA-C2A-C3A	-3.26	103.85	112.78
26	S	1621	LUT	C11-C10-C9	-3.26	122.66	127.31
24	G	601	CHL	CHB-C4A-NA	3.26	129.02	124.51
34	b	620	BCR	C16-C17-C18	-3.26	122.66	127.31
25	4	602	CLA	C1B-CHB-C4A	-3.26	123.67	130.12
24	R	608	CHL	C2A-C3A-C4A	-3.26	96.61	101.87
25	Y	610	CLA	C1B-CHB-C4A	-3.26	123.67	130.12
25	6	610	CLA	C1B-CHB-C4A	-3.25	123.67	130.12
25	3	610	CLA	C1B-CHB-C4A	-3.25	123.67	130.12
25	4	612	CLA	CAA-C2A-C3A	-3.25	103.87	112.78
26	4	1621	LUT	C10-C11-C12	-3.25	113.06	123.22
25	c	508	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
25	C	503	CLA	C1B-CHB-C4A	-3.25	123.68	130.12
25	n	602	CLA	C4A-NA-C1A	3.25	108.17	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	R	608	CHL	C3B-C4B-NB	3.25	113.41	109.21
25	3	612	CLA	CMB-C2B-C3B	3.25	130.76	124.68
24	9	607	CHL	CHD-C4C-C3C	-3.25	120.06	124.84
25	B	605	CLA	C1B-CHB-C4A	-3.25	123.68	130.12
25	C	508	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
25	q	603	CLA	CHB-C4A-NA	3.25	129.00	124.51
25	B	616	CLA	C1B-CHB-C4A	-3.25	123.68	130.12
24	0	606	CHL	CMD-C2D-C3D	-3.25	120.14	127.61
25	2	611	CLA	CMB-C2B-C1B	-3.25	123.47	128.46
24	S	608	CHL	C3B-C4B-NB	3.25	113.41	109.21
24	3	609	CHL	C3B-C4B-NB	3.25	113.41	109.21
24	2	607	CHL	CHD-C4C-C3C	-3.25	120.07	124.84
28	y	1623	NEX	C26-C27-C28	-3.24	119.13	125.99
29	3	2630	LHG	O7-C7-C8	3.24	118.49	111.50
26	2	1621	LUT	C22-C23-C24	-3.24	108.05	111.74
25	3	611	CLA	C1B-CHB-C4A	-3.24	123.69	130.12
25	s	609	CLA	C1B-CHB-C4A	-3.24	123.69	130.12
25	S	609	CLA	C1B-CHB-C4A	-3.24	123.70	130.12
25	9	613	CLA	C1B-CHB-C4A	-3.24	123.70	130.12
24	p	607	CHL	C3B-C4B-NB	3.24	113.40	109.21
25	C	512	CLA	CMB-C2B-C3B	3.24	130.74	124.68
28	p	1623	NEX	O24-C25-C38	3.24	118.94	115.06
24	9	606	CHL	CAC-C3C-C4C	3.24	129.01	124.81
25	7	613	CLA	C1B-CHB-C4A	-3.24	123.70	130.12
24	n	605	CHL	CGD-CBD-CAD	-3.24	100.25	110.73
25	D	402	CLA	CAC-C3C-C4C	3.24	129.01	124.81
25	p	612	CLA	CAA-C2A-C3A	-3.24	103.91	112.78
24	5	605	CHL	CHD-C4C-C3C	-3.24	120.08	124.84
25	6	604	CLA	CMB-C2B-C3B	3.24	130.73	124.68
27	n	1622	XAT	C26-C27-C28	-3.24	119.15	125.99
24	s	608	CHL	C3B-C4B-NB	3.24	113.39	109.21
25	4	604	CLA	C1B-CHB-C4A	-3.24	123.71	130.12
24	p	601	CHL	CAC-C3C-C4C	3.23	129.01	124.81
28	7	1623	NEX	C24-C23-C22	-3.23	104.53	110.77
24	g	601	CHL	CHB-C4A-NA	3.23	128.98	124.51
25	7	614	CLA	C1B-CHB-C4A	-3.23	123.72	130.12
24	G	609	CHL	C3B-C4B-NB	3.23	113.39	109.21
24	g	608	CHL	C3B-C4B-NB	3.23	113.39	109.21
27	2	1622	XAT	C35-C34-C33	-3.23	122.70	127.31
28	p	1623	NEX	C31-C30-C29	-3.23	122.70	127.31
34	b	619	BCR	C16-C17-C18	-3.23	122.70	127.31
24	r	608	CHL	C2A-C3A-C4A	-3.23	96.65	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	4	611	CLA	CMB-C2B-C1B	-3.23	123.50	128.46
24	Y	609	CHL	CMB-C2B-C3B	3.23	130.72	124.68
25	n	602	CLA	C1B-CHB-C4A	-3.23	123.72	130.12
34	d	404	BCR	C28-C27-C26	-3.23	108.31	114.08
24	3	609	CHL	CAC-C3C-C4C	3.23	129.00	124.81
27	7	1622	XAT	C36-C21-C26	3.23	118.76	110.05
25	8	611	CLA	C1B-CHB-C4A	-3.23	123.73	130.12
24	r	608	CHL	C3B-C4B-NB	3.23	113.38	109.21
28	r	623	NEX	O24-C25-C38	3.22	118.92	115.06
25	8	603	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
25	b	602	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
24	2	608	CHL	CAC-C3C-C4C	3.22	128.99	124.81
26	p	1620	LUT	C7-C8-C9	-3.22	121.36	126.23
25	g	610	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
25	B	602	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
24	8	609	CHL	C3B-C4B-NB	3.22	113.37	109.21
24	6	605	CHL	CHD-C4C-C3C	-3.22	120.11	124.84
24	g	609	CHL	C3B-C4B-NB	3.22	113.37	109.21
34	D	404	BCR	C28-C27-C26	-3.22	108.33	114.08
28	s	1623	NEX	C17-C1-C6	-3.22	107.59	110.47
26	2	1620	LUT	C11-C10-C9	-3.22	122.72	127.31
25	5	610	CLA	C1B-CHB-C4A	-3.22	123.75	130.12
25	b	605	CLA	C1B-CHB-C4A	-3.22	123.75	130.12
33	A	409	PHO	O2D-CGD-O1D	-3.22	117.55	123.84
29	L	101	LHG	O8-C23-C24	3.21	122.00	111.91
25	G	610	CLA	O2D-CGD-O1D	-3.21	117.55	123.84
25	q	614	CLA	C1B-CHB-C4A	-3.21	123.75	130.12
25	1	614	CLA	O2D-CGD-O1D	-3.21	117.56	123.84
25	3	613	CLA	CHB-C4A-NA	3.21	128.95	124.51
27	G	1622	XAT	C27-C28-C29	-3.21	120.55	125.53
25	2	613	CLA	CHB-C4A-NA	3.21	128.95	124.51
25	y	613	CLA	C1B-CHB-C4A	-3.21	123.76	130.12
25	C	512	CLA	CHB-C4A-NA	3.21	128.95	124.51
27	2	1622	XAT	C26-C27-C28	-3.21	119.20	125.99
24	7	605	CHL	C3B-C4B-NB	3.21	113.36	109.21
24	3	606	CHL	CMD-C2D-C3D	-3.21	120.23	127.61
24	9	607	CHL	C3B-C4B-NB	3.21	113.36	109.21
29	l	101	LHG	O8-C23-C24	3.21	121.97	111.91
25	c	509	CLA	CMB-C2B-C3B	3.21	130.68	124.68
25	c	503	CLA	C1B-CHB-C4A	-3.20	123.77	130.12
24	Y	609	CHL	CHB-C4A-NA	3.20	128.94	124.51
25	7	603	CLA	CMB-C2B-C1B	-3.20	123.54	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	1	603	CLA	CMB-C2B-C1B	-3.20	123.54	128.46
24	G	609	CHL	O2A-CGA-CBA	3.20	121.96	111.91
25	8	612	CLA	CMB-C2B-C3B	3.20	130.67	124.68
25	c	513	CLA	C1B-CHB-C4A	-3.20	123.78	130.12
25	C	507	CLA	CHB-C4A-NA	3.20	128.94	124.51
28	R	623	NEX	O24-C25-C38	3.20	118.89	115.06
28	3	1623	NEX	C35-C34-C33	-3.20	122.74	127.31
24	6	607	CHL	C3B-C4B-NB	3.20	113.35	109.21
33	a	409	PHO	O2D-CGD-O1D	-3.20	117.58	123.84
25	1	614	CLA	C1B-CHB-C4A	-3.20	123.78	130.12
25	Y	613	CLA	C1B-CHB-C4A	-3.20	123.78	130.12
28	q	1623	NEX	C26-C27-C28	-3.20	119.23	125.99
27	5	1622	XAT	C35-C34-C33	-3.20	122.75	127.31
27	8	1622	XAT	C31-C30-C29	-3.20	122.75	127.31
24	9	609	CHL	CAC-C3C-C4C	3.20	128.96	124.81
25	C	513	CLA	C1B-CHB-C4A	-3.20	123.78	130.12
25	1	613	CLA	C1B-CHB-C4A	-3.20	123.79	130.12
24	G	605	CHL	CHD-C4C-C3C	-3.20	120.14	124.84
34	C	514	BCR	C7-C8-C9	-3.20	121.41	126.23
24	6	605	CHL	CAC-C3C-C4C	3.20	128.96	124.81
27	g	1622	XAT	C27-C28-C29	-3.20	120.57	125.53
25	S	611	CLA	C1B-CHB-C4A	-3.20	123.79	130.12
27	p	1622	XAT	C35-C34-C33	-3.20	122.75	127.31
25	R	613	CLA	CMB-C2B-C3B	3.20	130.66	124.68
25	N	610	CLA	CMB-C2B-C3B	3.19	130.66	124.68
25	r	601	CLA	CMB-C2B-C1B	-3.19	123.55	128.46
24	1	607	CHL	OMC-CMC-C2C	-3.19	118.47	125.69
24	9	601	CHL	CMD-C2D-C3D	-3.19	120.27	127.61
24	8	601	CHL	CAC-C3C-C4C	3.19	128.95	124.81
24	6	609	CHL	C3B-C4B-NB	3.19	113.34	109.21
25	2	613	CLA	C1B-CHB-C4A	-3.19	123.79	130.12
24	0	608	CHL	C3B-C4B-NB	3.19	113.34	109.21
25	s	605	CLA	CMB-C2B-C3B	3.19	130.65	124.68
27	5	1622	XAT	C4-C3-C2	-3.19	104.61	110.77
25	d	403	CLA	C1B-CHB-C4A	-3.19	123.80	130.12
24	9	607	CHL	C1B-CHB-C4A	-3.19	123.80	130.12
34	B	618	BCR	C29-C30-C25	3.19	115.39	110.48
24	n	605	CHL	C1B-CHB-C4A	-3.19	123.80	130.12
34	c	514	BCR	C7-C8-C9	-3.19	121.42	126.23
36	c	521	LMG	C7-O1-C1	-3.19	107.51	113.74
27	3	1622	XAT	C35-C34-C33	-3.19	122.76	127.31
34	B	619	BCR	C16-C17-C18	-3.19	122.76	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	607	CHL	C1B-CHB-C4A	-3.19	123.81	130.12
25	D	403	CLA	C1B-CHB-C4A	-3.19	123.81	130.12
25	r	613	CLA	CMB-C2B-C3B	3.19	130.64	124.68
25	8	611	CLA	CMB-C2B-C1B	-3.19	123.57	128.46
25	g	614	CLA	C4A-NA-C1A	3.19	108.14	106.71
34	b	618	BCR	C29-C30-C25	3.18	115.38	110.48
24	2	601	CHL	CMD-C2D-C3D	-3.18	120.29	127.61
25	7	604	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
25	p	611	CLA	C1B-CHB-C4A	-3.18	123.81	130.12
24	p	605	CHL	CMD-C2D-C3D	-3.18	120.29	127.61
25	n	610	CLA	CMB-C2B-C3B	3.18	130.63	124.68
25	R	601	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
28	7	1623	NEX	C26-C27-C28	-3.18	119.27	125.99
25	S	612	CLA	CAA-C2A-C3A	-3.18	104.07	112.78
28	1	1623	NEX	C11-C12-C13	-3.18	117.49	126.42
24	5	607	CHL	C3B-C4B-NB	3.18	113.32	109.21
24	g	609	CHL	O2A-CGA-CBA	3.18	121.88	111.91
29	C	2630	LHG	O7-C7-C8	3.18	118.34	111.50
25	q	604	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
24	N	605	CHL	C1B-CHB-C4A	-3.18	123.83	130.12
24	s	608	CHL	O2A-CGA-CBA	3.17	121.87	111.91
24	8	606	CHL	CMD-C2D-C3D	-3.17	120.31	127.61
24	5	605	CHL	C1B-CHB-C4A	-3.17	123.83	130.12
27	8	1622	XAT	C35-C34-C33	-3.17	122.78	127.31
25	0	613	CLA	C1B-CHB-C4A	-3.17	123.83	130.12
26	0	1621	LUT	C7-C8-C9	-3.17	121.44	126.23
25	n	613	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
25	y	604	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
24	q	601	CHL	C3B-C4B-NB	3.17	113.31	109.21
36	C	521	LMG	C7-O1-C1	-3.17	107.55	113.74
25	N	602	CLA	C1B-CHB-C4A	-3.17	123.84	130.12
25	5	603	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
25	r	616	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
24	n	605	CHL	CMD-C2D-C3D	-3.17	120.33	127.61
25	0	612	CLA	CAA-C2A-C3A	-3.17	104.10	112.78
34	c	517	BCR	C15-C16-C17	-3.17	116.99	123.47
25	q	602	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
25	C	512	CLA	C1B-CHB-C4A	-3.17	123.85	130.12
25	c	509	CLA	CAA-C2A-C3A	-3.17	104.11	112.78
25	Y	604	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
24	y	609	CHL	CMB-C2B-C3B	3.17	130.60	124.68
25	N	612	CLA	CHB-C4A-NA	3.17	128.89	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	0	611	CLA	CMB-C2B-C3B	3.17	130.60	124.68
25	9	611	CLA	CMB-C2B-C1B	-3.16	123.60	128.46
24	s	607	CHL	CAC-C3C-C4C	3.16	128.92	124.81
25	s	610	CLA	CMB-C2B-C3B	3.16	130.60	124.68
25	8	613	CLA	CHB-C4A-NA	3.16	128.89	124.51
26	4	1620	LUT	C15-C14-C13	-3.16	122.80	127.31
25	9	613	CLA	CHB-C4A-NA	3.16	128.88	124.51
24	4	608	CHL	CMB-C2B-C3B	3.16	130.59	124.68
25	1	611	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
25	s	612	CLA	CAA-C2A-C3A	-3.16	104.12	112.78
34	C	515	BCR	C15-C16-C17	-3.16	117.00	123.47
24	6	606	CHL	C3B-C4B-NB	3.16	113.30	109.21
24	G	607	CHL	C3B-C4B-NB	3.16	113.30	109.21
25	N	613	CLA	CMB-C2B-C1B	-3.16	123.61	128.46
24	q	606	CHL	O2A-CGA-CBA	3.16	121.82	111.91
24	1	606	CHL	CAC-C3C-C4C	3.16	128.91	124.81
27	7	1622	XAT	C31-C30-C29	-3.16	122.80	127.31
25	B	617	CLA	CHB-C4A-NA	3.16	128.88	124.51
27	n	1622	XAT	C15-C35-C34	-3.16	117.01	123.47
25	0	610	CLA	C1B-CHB-C4A	-3.16	123.87	130.12
25	y	612	CLA	CAA-C2A-C3A	-3.16	104.14	112.78
25	G	614	CLA	C4A-NA-C1A	3.16	108.12	106.71
24	Y	601	CHL	C3B-C4B-NB	3.16	113.29	109.21
25	5	613	CLA	CMB-C2B-C3B	3.16	130.58	124.68
24	9	607	CHL	CAC-C3C-C4C	3.15	128.90	124.81
25	s	605	CLA	O2D-CGD-O1D	-3.15	117.67	123.84
27	6	1622	XAT	C15-C35-C34	-3.15	117.01	123.47
25	G	611	CLA	C1B-CHB-C4A	-3.15	123.87	130.12
25	c	501	CLA	CMB-C2B-C1B	-3.15	123.62	128.46
25	p	610	CLA	CMB-C2B-C3B	3.15	130.58	124.68
34	c	515	BCR	C15-C16-C17	-3.15	117.02	123.47
24	Y	608	CHL	C3B-C4B-NB	3.15	113.28	109.21
24	S	601	CHL	C4A-NA-C1A	-3.15	105.29	106.71
25	S	610	CLA	CMB-C2B-C3B	3.15	130.57	124.68
24	G	608	CHL	C3B-C4B-NB	3.15	113.28	109.21
25	S	614	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
25	s	614	CLA	O2D-CGD-O1D	-3.15	117.68	123.84
24	g	607	CHL	C3B-C4B-NB	3.15	113.28	109.21
24	3	601	CHL	CAC-C3C-C4C	3.15	128.90	124.81
25	g	612	CLA	CAA-C2A-C3A	-3.15	104.16	112.78
25	Y	612	CLA	CAA-C2A-C3A	-3.15	104.16	112.78
25	G	612	CLA	CAA-C2A-C3A	-3.15	104.16	112.78

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	1	1622	XAT	C36-C21-C26	3.15	118.54	110.05
25	p	612	CLA	CMB-C2B-C3B	3.15	130.56	124.68
25	b	617	CLA	CHB-C4A-NA	3.15	128.86	124.51
24	1	606	CHL	OMC-CMC-C2C	-3.14	118.58	125.69
25	9	604	CLA	CMB-C2B-C3B	3.14	130.56	124.68
25	q	610	CLA	CMB-C2B-C1B	-3.14	123.63	128.46
27	0	1622	XAT	C6-C7-C8	-3.14	119.35	125.99
28	y	1623	NEX	C11-C10-C9	-3.14	122.83	127.31
27	p	1622	XAT	C6-C7-C8	-3.14	119.35	125.99
25	c	507	CLA	CHB-C4A-NA	3.14	128.86	124.51
25	r	610	CLA	C1B-CHB-C4A	-3.14	123.90	130.12
25	3	611	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
25	R	604	CLA	C1B-CHB-C4A	-3.14	123.90	130.12
25	c	512	CLA	C1B-CHB-C4A	-3.14	123.90	130.12
25	c	502	CLA	CHB-C4A-NA	3.14	128.85	124.51
25	6	613	CLA	C1B-CHB-C4A	-3.14	123.90	130.12
25	g	611	CLA	C1B-CHB-C4A	-3.14	123.90	130.12
24	S	608	CHL	O2A-CGA-CBA	3.14	121.76	111.91
25	n	612	CLA	CHB-C4A-NA	3.14	128.85	124.51
25	G	611	CLA	O2D-CGD-O1D	-3.14	117.70	123.84
36	h	102	LMG	O8-C28-C29	3.14	121.75	111.91
25	R	610	CLA	C1B-CHB-C4A	-3.14	123.91	130.12
25	7	611	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
25	4	610	CLA	CMB-C2B-C3B	3.14	130.55	124.68
25	7	602	CLA	CMB-C2B-C3B	3.14	130.55	124.68
34	b	619	BCR	C33-C5-C4	3.14	119.64	113.62
24	8	601	CHL	CHB-C4A-NA	3.13	128.85	124.51
25	3	611	CLA	O2D-CGD-O1D	-3.13	117.71	123.84
26	s	1621	LUT	C18-C5-C6	-3.13	121.01	124.53
24	5	601	CHL	CAC-C3C-C4C	3.13	128.88	124.81
24	S	607	CHL	CAC-C3C-C4C	3.13	128.88	124.81
25	n	614	CLA	C1B-CHB-C4A	-3.13	123.91	130.12
24	5	606	CHL	CHD-C4C-C3C	-3.13	120.24	124.84
24	4	609	CHL	CMB-C2B-C3B	3.13	130.54	124.68
25	C	509	CLA	CAA-C2A-C3A	-3.13	104.21	112.78
24	5	608	CHL	CAC-C3C-C4C	3.13	128.87	124.81
28	G	1623	NEX	C19-C9-C10	-3.13	118.54	122.92
25	c	504	CLA	C1B-CHB-C4A	-3.13	123.92	130.12
34	C	517	BCR	C15-C16-C17	-3.13	117.07	123.47
24	R	606	CHL	O2A-CGA-CBA	3.13	121.72	111.91
26	Y	1621	LUT	C7-C8-C9	-3.13	121.51	126.23
24	n	605	CHL	O2A-CGA-CBA	3.13	121.72	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	7	1623	NEX	C11-C12-C13	-3.13	117.64	126.42
25	q	604	CLA	C1B-CHB-C4A	-3.13	123.93	130.12
24	N	601	CHL	CHB-C4A-NA	3.12	128.83	124.51
27	N	1622	XAT	O24-C25-C38	3.12	118.80	115.06
24	r	606	CHL	O2A-CGA-CBA	3.12	121.71	111.91
25	8	613	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
25	4	604	CLA	CMB-C2B-C1B	-3.12	123.66	128.46
34	B	619	BCR	C33-C5-C4	3.12	119.61	113.62
24	g	609	CHL	CHD-C4C-C3C	-3.12	120.25	124.84
24	0	601	CHL	C3B-C4B-NB	3.12	113.25	109.21
25	C	504	CLA	C1B-CHB-C4A	-3.12	123.94	130.12
25	p	603	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
24	p	606	CHL	C1B-CHB-C4A	-3.12	123.94	130.12
24	N	605	CHL	CGD-CBD-CAD	-3.12	100.63	110.73
24	G	609	CHL	CHD-C4C-C3C	-3.12	120.25	124.84
25	g	611	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
24	p	607	CHL	C4A-NA-C1A	-3.12	105.30	106.71
24	q	609	CHL	CMB-C2B-C3B	3.12	130.51	124.68
36	H	102	LMG	O8-C28-C29	3.12	121.69	111.91
24	S	601	CHL	OMC-CMC-C2C	-3.12	118.64	125.69
25	S	605	CLA	CMB-C2B-C3B	3.12	130.51	124.68
25	s	603	CLA	C1B-CHB-C4A	-3.12	123.94	130.12
26	S	1621	LUT	C18-C5-C6	-3.12	121.03	124.53
25	S	603	CLA	C1B-CHB-C4A	-3.12	123.95	130.12
25	R	616	CLA	CMB-C2B-C1B	-3.12	123.68	128.46
24	8	607	CHL	CMB-C2B-C3B	3.11	130.50	124.68
24	4	606	CHL	O2A-CGA-CBA	3.11	121.68	111.91
25	B	613	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
25	b	613	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
25	9	612	CLA	CHB-C4A-NA	3.11	128.82	124.51
37	c	519	DGD	C2G-O2G-C1B	-3.11	110.13	117.79
24	n	601	CHL	CAC-C3C-C4C	3.11	128.85	124.81
25	r	604	CLA	C1B-CHB-C4A	-3.11	123.95	130.12
24	0	608	CHL	CAC-C3C-C4C	3.11	128.85	124.81
25	n	611	CLA	O2D-CGD-O1D	-3.11	117.76	123.84
25	N	603	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
27	3	1622	XAT	C27-C28-C29	-3.11	120.71	125.53
25	y	603	CLA	CAA-C2A-C3A	-3.11	104.27	112.78
25	g	614	CLA	CMB-C2B-C3B	3.11	130.49	124.68
25	n	603	CLA	CMB-C2B-C1B	-3.11	123.69	128.46
24	2	601	CHL	C1C-C2C-C3C	-3.11	104.65	107.11
24	S	601	CHL	CHD-C4C-C3C	-3.11	120.28	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3	613	CLA	O2D-CGD-O1D	-3.11	117.77	123.84
25	6	611	CLA	C1B-CHB-C4A	-3.10	123.97	130.12
34	h	101	BCR	C20-C21-C22	-3.10	122.88	127.31
25	C	502	CLA	CHB-C4A-NA	3.10	128.81	124.51
27	N	1622	XAT	C18-C5-C4	3.10	117.77	114.28
26	y	1621	LUT	C7-C8-C9	-3.10	121.55	126.23
24	N	607	CHL	CMD-C2D-C3D	-3.10	120.48	127.61
26	3	1621	LUT	C15-C14-C13	-3.10	122.88	127.31
24	2	601	CHL	C1B-CHB-C4A	-3.10	123.97	130.12
25	s	611	CLA	C1B-CHB-C4A	-3.10	123.97	130.12
25	C	507	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
24	7	607	CHL	OMC-CMC-C2C	-3.10	118.67	125.69
25	G	614	CLA	CMB-C2B-C3B	3.10	130.48	124.68
24	R	608	CHL	C4A-NA-C1A	-3.10	105.31	106.71
25	C	501	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
25	p	610	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
25	5	612	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
24	6	608	CHL	O2A-CGA-CBA	3.10	121.63	111.91
25	S	603	CLA	CMB-C2B-C1B	-3.10	123.70	128.46
26	6	1621	LUT	C31-C30-C29	-3.10	122.89	127.31
35	A	412	SQD	O8-S-O7	3.10	118.84	111.27
25	3	612	CLA	C1B-CHB-C4A	-3.09	123.99	130.12
25	s	603	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
25	9	602	CLA	C1B-CHB-C4A	-3.09	123.99	130.12
25	r	610	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
24	8	605	CHL	O2A-CGA-CBA	3.09	121.61	111.91
25	9	614	CLA	O2D-CGD-O1D	-3.09	117.79	123.84
24	8	601	CHL	C1C-C2C-C3C	-3.09	104.66	107.11
24	1	605	CHL	C3B-C4B-NB	3.09	113.20	109.21
34	H	101	BCR	C20-C21-C22	-3.09	122.90	127.31
25	q	611	CLA	C1B-CHB-C4A	-3.09	124.00	130.12
25	n	612	CLA	C1B-CHB-C4A	-3.09	124.00	130.12
26	1	1620	LUT	C21-C26-C27	-3.09	108.80	112.70
25	B	616	CLA	O2D-CGD-O1D	-3.09	117.80	123.84
25	G	612	CLA	C1B-CHB-C4A	-3.09	124.00	130.12
25	N	614	CLA	C1B-CHB-C4A	-3.09	124.01	130.12
25	G	614	CLA	C1B-CHB-C4A	-3.08	124.01	130.12
25	Y	610	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
33	A	408	PHO	CMB-C2B-C3B	3.08	130.45	124.68
25	p	603	CLA	O2D-CGD-O1D	-3.08	117.81	123.84
26	7	1620	LUT	C21-C26-C27	-3.08	108.80	112.70
24	y	601	CHL	C4-C3-C5	3.08	120.46	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	3	1622	XAT	C31-C30-C29	-3.08	122.91	127.31
24	y	601	CHL	C3B-C4B-NB	3.08	113.19	109.21
25	Y	603	CLA	CAA-C2A-C3A	-3.08	104.34	112.78
33	a	408	PHO	CMB-C2B-C3B	3.08	130.44	124.68
25	Y	612	CLA	C1B-CHB-C4A	-3.08	124.02	130.12
26	y	1621	LUT	C22-C23-C24	-3.08	108.23	111.74
37	C	519	DGD	C2G-O2G-C1B	-3.08	110.21	117.79
25	c	509	CLA	CHB-C4A-NA	3.08	128.77	124.51
29	c	2630	LHG	O7-C7-C8	3.08	118.14	111.50
24	3	607	CHL	CMB-C2B-C3B	3.08	130.44	124.68
26	1	1621	LUT	C22-C23-C24	-3.08	108.24	111.74
24	S	601	CHL	CMD-C2D-C3D	-3.08	120.53	127.61
27	0	1622	XAT	C15-C14-C13	-3.08	122.92	127.31
25	b	606	CLA	C1B-CHB-C4A	-3.08	124.02	130.12
25	p	604	CLA	C1B-CHB-C4A	-3.08	124.03	130.12
25	c	513	CLA	O2D-CGD-O1D	-3.08	117.83	123.84
34	B	618	BCR	C27-C26-C25	-3.08	118.27	122.73
26	s	1620	LUT	C35-C34-C33	-3.08	122.92	127.31
25	S	605	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
34	c	514	BCR	C11-C10-C9	-3.07	122.92	127.31
25	b	616	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
24	5	609	CHL	CMD-C2D-C3D	-3.07	120.54	127.61
25	R	610	CLA	O2D-CGD-O1D	-3.07	117.83	123.84
24	y	608	CHL	C3B-C4B-NB	3.07	113.18	109.21
25	4	611	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
25	8	612	CLA	CAA-C2A-C3A	-3.07	104.37	112.78
25	A	406	CLA	C4A-NA-C1A	3.07	108.09	106.71
25	a	406	CLA	C4A-NA-C1A	3.07	108.09	106.71
25	b	608	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
28	0	1623	NEX	C11-C10-C9	-3.07	122.93	127.31
25	p	612	CLA	CHB-C4A-NA	3.07	128.76	124.51
25	6	610	CLA	C4A-NA-C1A	3.07	108.09	106.71
24	2	607	CHL	C3B-C4B-NB	3.07	113.18	109.21
25	8	603	CLA	CHB-C4A-NA	3.07	128.75	124.51
27	5	1622	XAT	C15-C35-C34	-3.07	117.19	123.47
25	0	603	CLA	CHB-C4A-NA	3.07	128.75	124.51
24	G	605	CHL	C1B-CHB-C4A	-3.07	124.04	130.12
25	g	612	CLA	C1B-CHB-C4A	-3.07	124.04	130.12
25	R	603	CLA	CHB-C4A-NA	3.07	128.75	124.51
24	9	609	CHL	CMD-C2D-C3D	-3.07	120.56	127.61
24	Y	601	CHL	C4-C3-C5	3.07	120.43	115.27
25	4	612	CLA	C1B-CHB-C4A	-3.07	124.05	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	N	1622	XAT	C26-C27-C28	-3.07	119.51	125.99
25	0	602	CLA	C4A-NA-C1A	3.07	108.08	106.71
25	B	608	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
34	D	404	BCR	C20-C21-C22	-3.06	122.94	127.31
25	C	509	CLA	CHB-C4A-NA	3.06	128.75	124.51
25	y	612	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
25	3	612	CLA	CAA-C2A-C3A	-3.06	104.39	112.78
35	D	413	SQD	O9-S-C6	3.06	110.58	106.94
24	s	601	CHL	CHD-C4C-C3C	-3.06	120.34	124.84
25	r	611	CLA	O2D-CGD-O1D	-3.06	117.85	123.84
25	1	612	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
24	3	608	CHL	C3B-C4B-NB	3.06	113.17	109.21
34	B	620	BCR	C33-C5-C4	3.06	119.50	113.62
25	5	610	CLA	CMB-C2B-C3B	3.06	130.41	124.68
27	n	1622	XAT	O24-C25-C38	3.06	118.72	115.06
25	3	612	CLA	CHB-C4A-NA	3.06	128.74	124.51
25	b	609	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
25	c	501	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
27	9	1622	XAT	C27-C28-C29	-3.06	120.78	125.53
35	d	413	SQD	O9-S-C6	3.06	110.58	106.94
24	Y	606	CHL	OMC-CMC-C2C	-3.06	118.77	125.69
25	2	603	CLA	CHB-C4A-NA	3.06	128.74	124.51
34	b	619	BCR	C20-C21-C22	-3.06	122.94	127.31
27	0	1622	XAT	C36-C21-C26	3.06	118.30	110.05
24	p	607	CHL	CAC-C3C-C4C	3.06	128.78	124.81
25	5	603	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
24	6	608	CHL	C3B-C4B-NB	3.06	113.16	109.21
25	5	612	CLA	CHB-C4A-NA	3.06	128.74	124.51
25	a	407	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
28	9	1623	NEX	C27-C28-C29	-3.06	120.79	125.53
24	N	605	CHL	CMD-C2D-C3D	-3.06	120.58	127.61
25	r	603	CLA	CHB-C4A-NA	3.06	128.74	124.51
25	0	603	CLA	CAA-C2A-C3A	-3.06	104.41	112.78
35	a	412	SQD	O8-S-O7	3.06	118.74	111.27
25	B	609	CLA	O2D-CGD-O1D	-3.06	117.86	123.84
25	q	611	CLA	CMB-C2B-C1B	-3.06	123.77	128.46
24	y	606	CHL	OMC-CMC-C2C	-3.06	118.78	125.69
34	d	404	BCR	C20-C21-C22	-3.05	122.95	127.31
34	b	618	BCR	C27-C26-C25	-3.05	118.30	122.73
25	g	614	CLA	C1B-CHB-C4A	-3.05	124.07	130.12
25	B	606	CLA	C1B-CHB-C4A	-3.05	124.07	130.12
25	0	611	CLA	C1B-CHB-C4A	-3.05	124.07	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	n	612	CLA	CAA-C2A-C3A	-3.05	104.42	112.78
25	6	603	CLA	CAA-C2A-C3A	-3.05	104.42	112.78
25	2	614	CLA	O2D-CGD-O1D	-3.05	117.87	123.84
25	1	602	CLA	CMB-C2B-C3B	3.05	130.39	124.68
28	8	1623	NEX	C35-C34-C33	-3.05	122.95	127.31
25	6	603	CLA	CMB-C2B-C3B	3.05	130.39	124.68
24	4	608	CHL	CHD-C4C-C3C	-3.05	120.36	124.84
25	r	603	CLA	CMB-C2B-C3B	3.05	130.38	124.68
24	4	606	CHL	CHD-C4C-C3C	-3.05	120.36	124.84
25	n	611	CLA	CMB-C2B-C3B	3.05	130.38	124.68
34	B	619	BCR	C20-C21-C22	-3.05	122.96	127.31
25	A	407	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
27	y	1622	XAT	C35-C34-C33	-3.05	122.96	127.31
26	N	1621	LUT	C18-C5-C6	-3.05	121.11	124.53
24	s	601	CHL	OMC-CMC-C2C	-3.05	118.80	125.69
24	8	608	CHL	C3B-C4B-NB	3.05	113.15	109.21
25	C	513	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
25	N	611	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
25	C	510	CLA	CAA-C2A-C3A	-3.04	104.44	112.78
24	N	609	CHL	CMB-C2B-C3B	3.04	130.37	124.68
34	b	620	BCR	C33-C5-C4	3.04	119.46	113.62
25	c	506	CLA	O2D-CGD-O1D	-3.04	117.89	123.84
25	R	612	CLA	CAA-C2A-C3A	-3.04	104.45	112.78
25	r	612	CLA	CAA-C2A-C3A	-3.04	104.45	112.78
25	7	612	CLA	C1B-CHB-C4A	-3.04	124.09	130.12
27	Y	1622	XAT	C35-C34-C33	-3.04	122.97	127.31
24	n	607	CHL	CMD-C2D-C3D	-3.04	120.62	127.61
25	p	613	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
24	R	606	CHL	CHB-C4A-NA	3.04	128.72	124.51
24	R	606	CHL	C3B-C4B-NB	3.04	113.14	109.21
25	R	603	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
25	6	611	CLA	CMB-C2B-C3B	3.04	130.37	124.68
27	n	1622	XAT	C18-C5-C4	3.04	117.70	114.28
25	R	603	CLA	CMB-C2B-C3B	3.04	130.36	124.68
25	b	612	CLA	O2D-CGD-O1D	-3.04	117.90	123.84
25	9	610	CLA	C4A-NA-C1A	3.04	108.07	106.71
26	2	1621	LUT	C11-C10-C9	-3.04	122.97	127.31
25	5	614	CLA	C1B-CHB-C4A	-3.04	124.10	130.12
26	Y	1621	LUT	C10-C11-C12	-3.04	113.74	123.22
26	p	1621	LUT	C35-C15-C14	-3.04	117.26	123.47
25	n	612	CLA	CMB-C2B-C3B	3.03	130.35	124.68
24	n	601	CHL	CHB-C4A-NA	3.03	128.71	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	4	613	CLA	CHB-C4A-NA	3.03	128.71	124.51
26	y	1621	LUT	C10-C11-C12	-3.03	113.75	123.22
26	n	1621	LUT	C18-C5-C6	-3.03	121.12	124.53
24	r	606	CHL	CHB-C4A-NA	3.03	128.71	124.51
25	r	603	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
25	1	603	CLA	CAA-C2A-C3A	-3.03	104.48	112.78
25	B	605	CLA	CAA-CBA-CGA	-3.03	104.39	113.25
25	N	612	CLA	C1B-CHB-C4A	-3.03	124.11	130.12
25	5	613	CLA	O2D-CGD-O1D	-3.03	117.91	123.84
24	G	601	CHL	C1-C2-C3	-3.03	120.80	126.04
24	3	609	CHL	CHB-C4A-NA	3.03	128.70	124.51
25	2	612	CLA	CMB-C2B-C3B	3.03	130.35	124.68
28	r	623	NEX	C31-C30-C29	-3.03	122.99	127.31
24	r	606	CHL	OMC-CMC-C2C	-3.03	118.84	125.69
25	6	614	CLA	C1B-CHB-C4A	-3.03	124.12	130.12
25	b	613	CLA	C1B-CHB-C4A	-3.03	124.12	130.12
25	c	502	CLA	C1B-CHB-C4A	-3.03	124.12	130.12
34	C	514	BCR	C11-C10-C9	-3.03	122.99	127.31
24	g	605	CHL	C1C-C2C-C3C	-3.03	104.71	107.11
25	2	612	CLA	CHB-C4A-NA	3.02	128.69	124.51
28	r	623	NEX	C39-C29-C30	-3.02	118.69	122.92
25	0	614	CLA	C1B-CHB-C4A	-3.02	124.13	130.12
24	N	605	CHL	O2A-CGA-CBA	3.02	121.39	111.91
25	B	605	CLA	C1-C2-C3	-3.02	120.81	126.04
25	0	604	CLA	CMB-C2B-C3B	3.02	130.33	124.68
25	c	510	CLA	CAA-C2A-C3A	-3.02	104.50	112.78
25	8	614	CLA	C1B-CHB-C4A	-3.02	124.13	130.12
25	q	610	CLA	C1-C2-C3	-3.02	120.82	126.04
25	p	611	CLA	CMB-C2B-C3B	3.02	130.33	124.68
25	5	610	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
25	8	611	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
25	c	511	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
28	q	1623	NEX	C15-C35-C34	-3.02	117.29	123.47
26	0	1621	LUT	C31-C30-C29	-3.02	123.00	127.31
24	r	608	CHL	C4A-NA-C1A	-3.02	105.35	106.71
24	p	606	CHL	CMD-C2D-C3D	-3.02	120.67	127.61
24	7	605	CHL	CAC-C3C-C4C	3.02	128.73	124.81
24	2	605	CHL	C3B-C4B-NB	3.02	113.11	109.21
25	C	501	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
25	C	506	CLA	O2D-CGD-O1D	-3.02	117.94	123.84
25	R	611	CLA	CMB-C2B-C3B	3.02	130.32	124.68
24	n	608	CHL	CHB-C4A-NA	3.02	128.68	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3	602	CLA	C1B-CHB-C4A	-3.02	124.14	130.12
27	1	1622	XAT	C4-C3-C2	-3.02	104.95	110.77
24	2	606	CHL	C3B-C4B-NB	3.02	113.11	109.21
25	N	612	CLA	CMB-C2B-C3B	3.01	130.32	124.68
25	8	612	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
24	s	601	CHL	CMB-C2B-C3B	3.01	130.32	124.68
24	R	606	CHL	OMC-CMC-C2C	-3.01	118.87	125.69
25	R	616	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
25	n	603	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
25	R	611	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
25	3	614	CLA	C1B-CHB-C4A	-3.01	124.15	130.12
25	N	612	CLA	CAA-C2A-C3A	-3.01	104.53	112.78
25	3	603	CLA	CHB-C4A-NA	3.01	128.67	124.51
25	4	602	CLA	O2D-CGD-O1D	-3.01	117.95	123.84
26	8	1621	LUT	C15-C14-C13	-3.01	123.02	127.31
25	r	612	CLA	CHB-C4A-NA	3.01	128.67	124.51
25	r	616	CLA	C1B-CHB-C4A	-3.01	124.16	130.12
27	7	1622	XAT	C4-C3-C2	-3.01	104.96	110.77
26	n	1620	LUT	C21-C26-C27	-3.01	108.90	112.70
24	2	609	CHL	CMB-C2B-C3B	3.01	130.31	124.68
24	3	605	CHL	C4A-NA-C1A	3.01	108.06	106.71
27	Y	1622	XAT	C26-C27-C28	-3.01	119.64	125.99
25	0	613	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
25	N	603	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
25	5	611	CLA	CMB-C2B-C3B	3.00	130.30	124.68
26	S	1620	LUT	C35-C34-C33	-3.00	123.02	127.31
24	Y	607	CHL	CAA-C2A-C3A	-3.00	104.55	112.78
24	p	609	CHL	CMD-C2D-C3D	-3.00	120.70	127.61
25	Y	603	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
24	0	608	CHL	O2A-CGA-CBA	3.00	121.33	111.91
34	c	516	BCR	C10-C11-C12	-3.00	113.85	123.22
25	C	502	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
25	S	614	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
25	B	612	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
34	C	516	BCR	C10-C11-C12	-3.00	113.85	123.22
25	r	601	CLA	CMB-C2B-C3B	3.00	130.29	124.68
25	R	611	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
27	y	1622	XAT	C26-C27-C28	-3.00	119.65	125.99
25	r	609	CLA	CHB-C4A-NA	3.00	128.66	124.51
24	g	601	CHL	C1-C2-C3	-3.00	120.86	126.04
28	3	1623	NEX	C28-C29-C30	3.00	123.54	118.94
25	r	611	CLA	C1B-CHB-C4A	-3.00	124.18	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	r	606	CHL	C3B-C4B-NB	3.00	113.09	109.21
25	b	604	CLA	CMB-C2B-C3B	3.00	130.29	124.68
25	6	612	CLA	CAA-C2A-C3A	-3.00	104.57	112.78
24	6	605	CHL	CMB-C2B-C3B	3.00	130.29	124.68
25	8	612	CLA	CHB-C4A-NA	3.00	128.66	124.51
24	9	605	CHL	C3B-C4B-NB	3.00	113.08	109.21
24	R	607	CHL	CMB-C2B-C3B	3.00	130.28	124.68
25	0	612	CLA	CHB-C4A-NA	2.99	128.65	124.51
29	R	2630	LHG	C5-O7-C7	-2.99	110.42	117.79
24	8	607	CHL	C1-O2A-CGA	2.99	124.30	116.44
25	R	609	CLA	CHB-C4A-NA	2.99	128.65	124.51
28	4	1623	NEX	C15-C35-C34	-2.99	117.34	123.47
24	n	609	CHL	CMB-C2B-C3B	2.99	130.27	124.68
25	B	609	CLA	C1B-CHB-C4A	-2.99	124.19	130.12
25	b	609	CLA	C1B-CHB-C4A	-2.99	124.19	130.12
25	b	605	CLA	CAA-CBA-CGA	-2.99	104.52	113.25
25	7	603	CLA	CAA-C2A-C3A	-2.99	104.59	112.78
24	G	609	CHL	CAC-C3C-C4C	2.99	128.69	124.81
25	p	612	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
24	g	609	CHL	CAC-C3C-C4C	2.99	128.69	124.81
37	C	518	DGD	O1G-C1A-C2A	2.99	121.29	111.91
29	r	2630	LHG	C5-O7-C7	-2.99	110.43	117.79
24	N	601	CHL	C4-C3-C5	2.99	120.30	115.27
25	5	612	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
35	D	413	SQD	C44-O6-C1	-2.99	107.90	113.74
26	G	1621	LUT	C31-C30-C29	-2.99	123.05	127.31
24	g	601	CHL	C1C-C2C-C3C	-2.99	104.74	107.11
25	s	605	CLA	C4A-NA-C1A	2.99	108.05	106.71
24	q	605	CHL	C3B-C4B-NB	2.98	113.07	109.21
34	C	514	BCR	C24-C23-C22	-2.98	121.72	126.23
25	8	602	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
28	R	623	NEX	C31-C30-C29	-2.98	123.05	127.31
25	q	610	CLA	CMB-C2B-C3B	2.98	130.26	124.68
28	S	1623	NEX	C39-C29-C30	-2.98	118.75	122.92
34	b	620	BCR	C15-C14-C13	-2.98	123.05	127.31
27	r	622	XAT	C10-C11-C12	-2.98	113.91	123.22
24	r	607	CHL	O2D-CGD-O1D	-2.98	118.01	123.84
25	s	609	CLA	CMA-C3A-C2A	-2.98	109.14	116.10
25	N	611	CLA	CMB-C2B-C3B	2.98	130.26	124.68
24	r	607	CHL	CMB-C2B-C3B	2.98	130.25	124.68
25	s	614	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
24	5	601	CHL	CMD-C2D-C3D	-2.98	120.76	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	C	511	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
25	9	604	CLA	CHB-C4A-NA	2.98	128.63	124.51
25	0	613	CLA	CMB-C2B-C3B	2.98	130.25	124.68
25	B	613	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
24	7	606	CHL	OMC-CMC-C2C	-2.98	118.95	125.69
25	B	602	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
25	B	604	CLA	CMB-C2B-C3B	2.98	130.25	124.68
25	Y	602	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
24	y	607	CHL	CAA-C2A-C3A	-2.98	104.63	112.78
25	D	403	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
25	b	605	CLA	C1-C2-C3	-2.97	120.90	126.04
24	n	609	CHL	OMC-CMC-C2C	-2.97	118.96	125.69
27	9	1622	XAT	C24-C23-C22	-2.97	105.03	110.77
25	N	614	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
25	R	601	CLA	CMB-C2B-C3B	2.97	130.24	124.68
27	g	1622	XAT	C35-C34-C33	-2.97	123.07	127.31
34	c	516	BCR	C33-C5-C6	-2.97	121.19	124.53
25	4	614	CLA	O2D-CGD-O1D	-2.97	118.03	123.84
26	n	1620	LUT	C15-C14-C13	-2.97	123.07	127.31
24	G	601	CHL	C4-C3-C5	2.97	120.27	115.27
24	8	609	CHL	CAC-C3C-C4C	2.97	128.67	124.81
25	p	614	CLA	CMB-C2B-C3B	2.97	130.24	124.68
24	S	601	CHL	CMB-C2B-C3B	2.97	130.24	124.68
24	Y	606	CHL	C4-C3-C5	2.97	120.27	115.27
24	y	606	CHL	C4-C3-C5	2.97	120.27	115.27
25	0	612	CLA	C1B-CHB-C4A	-2.97	124.23	130.12
25	4	611	CLA	CMB-C2B-C3B	2.97	130.24	124.68
35	d	413	SQD	C44-O6-C1	-2.97	107.94	113.74
24	s	607	CHL	CHD-C4C-C3C	-2.97	120.47	124.84
27	R	622	XAT	C10-C11-C12	-2.97	113.95	123.22
24	G	601	CHL	C4D-CHA-C1A	-2.97	117.64	121.25
27	2	1622	XAT	C24-C23-C22	-2.97	105.04	110.77
28	2	1623	NEX	C15-C14-C13	-2.97	123.07	127.31
25	b	608	CLA	CHB-C4A-NA	2.97	128.62	124.51
27	8	1622	XAT	C27-C28-C29	-2.97	120.93	125.53
25	C	502	CLA	CMC-C2C-C3C	2.97	134.17	126.12
25	R	612	CLA	CHB-C4A-NA	2.96	128.61	124.51
25	G	611	CLA	CMB-C2B-C3B	2.96	130.22	124.68
29	7	2630	LHG	O8-C23-C24	2.96	121.21	111.91
26	5	1620	LUT	C7-C8-C9	-2.96	121.76	126.23
25	y	603	CLA	O2D-CGD-O1D	-2.96	118.04	123.84
27	q	1622	XAT	C4-C3-C2	-2.96	105.05	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	612	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
37	c	518	DGD	O1G-C1A-C2A	2.96	121.20	111.91
25	g	611	CLA	CMB-C2B-C3B	2.96	130.22	124.68
28	R	623	NEX	C39-C29-C30	-2.96	118.78	122.92
34	C	516	BCR	C15-C14-C13	-2.96	123.08	127.31
27	p	1622	XAT	C4-C3-C2	-2.96	105.06	110.77
27	6	1622	XAT	C36-C21-C26	2.96	118.03	110.05
26	s	1621	LUT	C21-C26-C27	-2.96	108.96	112.70
25	y	602	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
24	6	608	CHL	CMB-C2B-C3B	2.96	130.21	124.68
26	p	1620	LUT	C11-C10-C9	-2.96	123.09	127.31
26	7	1621	LUT	C22-C23-C24	-2.95	108.38	111.74
28	s	1623	NEX	C26-C27-C28	-2.95	119.75	125.99
25	y	603	CLA	C1B-CHB-C4A	-2.95	124.27	130.12
24	R	607	CHL	O2D-CGD-O1D	-2.95	118.06	123.84
25	c	502	CLA	CMC-C2C-C3C	2.95	134.14	126.12
25	Y	603	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
35	d	413	SQD	O48-C23-C24	2.95	121.17	111.91
25	d	403	CLA	O2D-CGD-O1D	-2.95	118.06	123.84
34	B	620	BCR	C11-C10-C9	-2.95	123.10	127.31
25	9	614	CLA	CMB-C2B-C3B	2.95	130.20	124.68
24	4	608	CHL	C3B-C4B-NB	2.95	113.03	109.21
25	S	609	CLA	CMA-C3A-C2A	-2.95	109.21	116.10
35	D	413	SQD	O48-C23-C24	2.95	121.17	111.91
34	B	620	BCR	C15-C14-C13	-2.95	123.10	127.31
24	y	607	CHL	C1-C2-C3	-2.95	120.94	126.04
24	R	608	CHL	CAA-C2A-C3A	-2.95	104.70	112.78
34	C	515	BCR	C33-C5-C6	-2.95	121.22	124.53
24	r	608	CHL	CAA-C2A-C3A	-2.95	104.70	112.78
28	S	1623	NEX	C26-C27-C28	-2.95	119.76	125.99
24	7	601	CHL	CHB-C4A-NA	2.95	128.59	124.51
25	7	613	CLA	CHB-C4A-NA	2.95	128.59	124.51
24	G	607	CHL	O2A-CGA-O1A	-2.95	116.15	123.59
26	1	1621	LUT	C7-C8-C9	-2.95	121.78	126.23
25	R	611	CLA	CHB-C4A-NA	2.95	128.59	124.51
25	9	603	CLA	CHB-C4A-NA	2.95	128.59	124.51
25	n	614	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
25	9	611	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
25	9	612	CLA	CMB-C2B-C3B	2.95	130.19	124.68
34	d	404	BCR	C38-C26-C25	-2.94	121.22	124.53
25	q	612	CLA	CAA-C2A-C3A	-2.94	104.71	112.78
24	q	601	CHL	CMB-C2B-C3B	2.94	130.19	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	d	405	PL9	C22-C23-C24	-2.94	120.57	127.66
25	b	605	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
25	5	614	CLA	CMB-C2B-C3B	2.94	130.19	124.68
25	n	604	CLA	CMB-C2B-C3B	2.94	130.19	124.68
25	6	603	CLA	CHB-C4A-NA	2.94	128.58	124.51
25	y	610	CLA	O2D-CGD-O1D	-2.94	118.08	123.84
25	3	603	CLA	CMB-C2B-C3B	2.94	130.18	124.68
28	9	1623	NEX	C39-C29-C30	-2.94	118.80	122.92
24	R	606	CHL	CMD-C2D-C3D	-2.94	120.84	127.61
25	2	602	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
24	3	601	CHL	CHB-C4A-NA	2.94	128.58	124.51
24	r	606	CHL	CMD-C2D-C3D	-2.94	120.85	127.61
25	b	602	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
25	r	611	CLA	CHB-C4A-NA	2.94	128.58	124.51
34	c	515	BCR	C33-C5-C6	-2.94	121.23	124.53
25	1	603	CLA	CHB-C4A-NA	2.94	128.58	124.51
25	C	504	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
25	8	612	CLA	O2D-CGD-O1D	-2.94	118.09	123.84
34	b	618	BCR	C11-C10-C9	-2.94	123.12	127.31
24	9	606	CHL	C3B-C4B-NB	2.94	113.01	109.21
24	p	608	CHL	CHB-C4A-NA	2.94	128.57	124.51
24	n	601	CHL	C4-C3-C5	2.94	120.21	115.27
24	2	606	CHL	O2A-CGA-CBA	2.94	121.12	111.91
24	4	605	CHL	C3B-C4B-NB	2.94	113.00	109.21
25	6	612	CLA	CHB-C4A-NA	2.94	128.57	124.51
25	B	608	CLA	CHB-C4A-NA	2.94	128.57	124.51
39	D	405	PL9	C22-C23-C24	-2.93	120.59	127.66
24	p	607	CHL	C2A-C3A-C4A	-2.93	97.13	101.87
24	7	608	CHL	CHB-C4A-NA	2.93	128.57	124.51
25	q	603	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
26	3	1620	LUT	C31-C30-C29	-2.93	123.12	127.31
24	S	607	CHL	CHD-C4C-C3C	-2.93	120.53	124.84
25	R	616	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
24	Y	607	CHL	O2A-CGA-CBA	2.93	121.11	111.91
25	q	612	CLA	C1B-CHB-C4A	-2.93	124.31	130.12
24	3	605	CHL	O2A-CGA-CBA	2.93	121.11	111.91
29	1	2630	LHG	O8-C23-C24	2.93	121.11	111.91
28	g	1623	NEX	C2-C1-C6	2.93	112.06	109.21
25	2	614	CLA	CMB-C2B-C3B	2.93	130.16	124.68
24	G	601	CHL	C1C-C2C-C3C	-2.93	104.79	107.11
25	Y	614	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
25	b	614	CLA	C1B-CHB-C4A	-2.93	124.32	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	7	1621	LUT	C15-C35-C34	-2.93	117.48	123.47
27	p	1622	XAT	C27-C28-C29	-2.93	120.99	125.53
25	S	605	CLA	C4A-NA-C1A	2.93	108.02	106.71
25	B	614	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
25	c	506	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
34	C	516	BCR	C33-C5-C6	-2.93	121.24	124.53
28	1	1623	NEX	C24-C23-C22	-2.93	105.12	110.77
29	Y	2630	LHG	C5-O7-C7	-2.93	110.59	117.79
24	2	609	CHL	CMD-C2D-C3D	-2.93	120.88	127.61
26	9	1620	LUT	C35-C15-C14	-2.92	117.48	123.47
25	r	611	CLA	CMB-C2B-C3B	2.92	130.15	124.68
24	y	608	CHL	CAC-C3C-C4C	2.92	128.60	124.81
24	5	601	CHL	C1C-C2C-C3C	-2.92	104.79	107.11
24	5	607	CHL	C1C-C2C-C3C	-2.92	104.79	107.11
24	5	607	CHL	C4-C3-C5	2.92	120.19	115.27
24	g	601	CHL	CBC-CAC-C3C	-2.92	104.37	112.43
27	2	1622	XAT	C15-C35-C34	-2.92	117.49	123.47
25	4	614	CLA	CMB-C2B-C3B	2.92	130.15	124.68
24	7	606	CHL	CMD-C2D-C3D	-2.92	120.89	127.61
29	n	2630	LHG	O8-C23-C24	2.92	121.08	111.91
24	G	605	CHL	CAA-C2A-C3A	-2.92	104.78	112.78
24	g	605	CHL	CAA-C2A-C3A	-2.92	104.78	112.78
25	y	614	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
25	4	603	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
25	R	609	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
26	r	620	LUT	C31-C30-C29	-2.92	123.14	127.31
25	B	611	CLA	CMB-C2B-C3B	2.92	130.14	124.68
24	0	605	CHL	CMB-C2B-C3B	2.92	130.14	124.68
25	7	614	CLA	CMB-C2B-C3B	2.92	130.14	124.68
25	G	602	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
25	8	603	CLA	CMB-C2B-C3B	2.92	130.14	124.68
25	8	603	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
24	3	607	CHL	O2A-CGA-CBA	2.92	121.07	111.91
24	Y	608	CHL	O2A-CGA-CBA	2.92	121.06	111.91
24	y	601	CHL	CMD-C2D-C3D	-2.92	120.90	127.61
25	c	513	CLA	CHB-C4A-NA	2.92	128.55	124.51
24	G	601	CHL	C4A-NA-C1A	-2.92	105.39	106.71
25	C	502	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
36	d	412	LMG	O8-C28-C29	2.92	121.06	111.91
26	R	620	LUT	C31-C30-C29	-2.91	123.15	127.31
25	6	613	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
24	Y	608	CHL	CAC-C3C-C4C	2.91	128.59	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	r	616	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
24	0	609	CHL	CHD-C4C-C3C	-2.91	120.56	124.84
24	5	608	CHL	CHB-C4A-NA	2.91	128.54	124.51
34	b	620	BCR	C11-C10-C9	-2.91	123.15	127.31
25	2	603	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
24	1	608	CHL	O2A-CGA-CBA	2.91	121.05	111.91
24	4	609	CHL	O2A-CGA-CBA	2.91	121.05	111.91
25	p	611	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
24	4	601	CHL	C3B-C4B-NB	2.91	112.97	109.21
34	c	516	BCR	C15-C14-C13	-2.91	123.16	127.31
34	D	404	BCR	C38-C26-C25	-2.91	121.26	124.53
24	N	609	CHL	CHD-C4C-C3C	-2.91	120.56	124.84
25	1	611	CLA	CHB-C4A-NA	2.91	128.53	124.51
25	B	605	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
25	s	609	CLA	CAA-C2A-C3A	-2.91	109.31	116.10
25	b	611	CLA	CMB-C2B-C3B	2.91	130.12	124.68
24	3	601	CHL	CMD-C2D-C3D	-2.91	120.93	127.61
25	g	602	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
25	3	612	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
24	q	608	CHL	CMB-C2B-C3B	2.91	130.12	124.68
25	6	603	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
24	s	601	CHL	CAC-C3C-C4C	2.91	128.58	124.81
24	q	609	CHL	CMD-C2D-C3D	-2.91	120.93	127.61
25	C	506	CLA	C1B-CHB-C4A	-2.90	124.36	130.12
25	C	505	CLA	C1-C2-C3	-2.90	121.02	126.04
24	g	605	CHL	C1B-CHB-C4A	-2.90	124.37	130.12
24	g	607	CHL	O2A-CGA-O1A	-2.90	116.26	123.59
25	9	612	CLA	C1B-CHB-C4A	-2.90	124.37	130.12
25	2	603	CLA	CMB-C2B-C1B	-2.90	124.00	128.46
24	G	606	CHL	O2A-CGA-CBA	2.90	121.02	111.91
27	3	1622	XAT	C4-C3-C2	-2.90	105.17	110.77
25	4	612	CLA	CHB-C4A-NA	2.90	128.52	124.51
24	g	607	CHL	OMC-CMC-C2C	-2.90	119.13	125.69
24	p	606	CHL	C1C-C2C-C3C	-2.90	104.81	107.11
25	6	602	CLA	C4A-NA-C1A	2.90	108.01	106.71
25	3	603	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
25	r	613	CLA	CHB-C4A-NA	2.90	128.52	124.51
25	B	605	CLA	CAA-C2A-C3A	-2.90	104.84	112.78
26	6	1621	LUT	C7-C8-C9	-2.90	121.86	126.23
26	9	1620	LUT	C15-C14-C13	-2.90	123.18	127.31
25	1	613	CLA	CHB-C4A-NA	2.90	128.52	124.51
25	p	614	CLA	C1B-CHB-C4A	-2.90	124.38	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	a	405	CLA	O2D-CGD-O1D	-2.90	118.18	123.84
24	1	601	CHL	CHB-C4A-NA	2.90	128.52	124.51
28	5	1623	NEX	C39-C29-C30	-2.90	118.87	122.92
24	n	608	CHL	O2A-CGA-CBA	2.89	120.99	111.91
27	p	1622	XAT	C15-C35-C34	-2.89	117.55	123.47
24	1	606	CHL	CMD-C2D-C3D	-2.89	120.96	127.61
25	q	612	CLA	CHB-C4A-NA	2.89	128.51	124.51
25	c	502	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
24	4	607	CHL	CMD-C2D-C3D	-2.89	120.96	127.61
25	7	612	CLA	CAA-C2A-C3A	-2.89	104.86	112.78
26	y	1620	LUT	C19-C9-C8	2.89	122.64	118.08
24	p	601	CHL	C1C-C2C-C3C	-2.89	104.82	107.11
24	q	605	CHL	CMD-C2D-C3D	-2.89	120.96	127.61
24	g	601	CHL	C4-C3-C5	2.89	120.14	115.27
25	B	607	CLA	CHD-C1D-ND	-2.89	121.80	124.45
25	b	611	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
34	B	618	BCR	C11-C10-C9	-2.89	123.18	127.31
28	4	1623	NEX	O24-C25-C38	2.89	118.52	115.06
24	4	607	CHL	C3B-C4B-NB	2.89	112.95	109.21
26	y	1621	LUT	C16-C1-C6	-2.89	105.61	110.30
26	1	1621	LUT	C15-C35-C34	-2.89	117.55	123.47
24	n	601	CHL	CMB-C2B-C3B	2.89	130.09	124.68
24	1	605	CHL	C1B-CHB-C4A	-2.89	124.39	130.12
25	0	603	CLA	C1B-CHB-C4A	-2.89	124.40	130.12
24	6	606	CHL	CMD-C2D-C3D	-2.89	120.97	127.61
25	q	614	CLA	CMB-C2B-C3B	2.89	130.08	124.68
25	b	605	CLA	CAA-C2A-C3A	-2.89	104.87	112.78
26	N	1620	LUT	C10-C11-C12	-2.89	114.21	123.22
28	1	1623	NEX	C28-C29-C30	2.89	123.37	118.94
24	g	609	CHL	C1C-C2C-C3C	-2.89	104.82	107.11
25	4	610	CLA	CHB-C4A-NA	2.89	128.50	124.51
24	y	601	CHL	C1-C2-C3	-2.89	121.05	126.04
25	b	616	CLA	CHB-C4A-NA	2.88	128.50	124.51
25	r	612	CLA	C1B-CHB-C4A	-2.88	124.40	130.12
24	6	606	CHL	C1C-C2C-C3C	-2.88	104.83	107.11
24	y	608	CHL	O2A-CGA-CBA	2.88	120.96	111.91
25	A	407	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
24	y	609	CHL	CED-O2D-CGD	2.88	122.46	115.94
25	3	614	CLA	CMB-C2B-C3B	2.88	130.07	124.68
39	d	405	PL9	C7-C3-C2	-2.88	119.51	123.30
27	p	1622	XAT	C7-C8-C9	-2.88	121.06	125.53
24	y	605	CHL	CAC-C3C-C4C	2.88	128.55	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	A	405	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
24	g	606	CHL	O2A-CGA-CBA	2.88	120.95	111.91
39	D	405	PL9	C7-C3-C2	-2.88	119.51	123.30
28	0	1623	NEX	C28-C29-C30	2.88	123.36	118.94
24	N	607	CHL	C1-C2-C3	-2.88	121.07	126.04
25	1	614	CLA	CMB-C2B-C3B	2.88	130.06	124.68
25	S	602	CLA	O2D-CGD-O1D	-2.88	118.21	123.84
26	Y	1620	LUT	C19-C9-C8	2.88	122.61	118.08
29	y	2630	LHG	O8-C23-C24	2.88	120.93	111.91
25	8	614	CLA	CMB-C2B-C3B	2.88	130.06	124.68
25	7	611	CLA	CHB-C4A-NA	2.88	128.49	124.51
25	S	609	CLA	CAA-C2A-C3A	-2.88	109.39	116.10
24	N	606	CHL	C3B-C4B-NB	2.88	112.93	109.21
25	4	604	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
28	g	1623	NEX	C35-C34-C33	-2.87	123.21	127.31
28	r	623	NEX	C24-C23-C22	-2.87	105.22	110.77
25	S	602	CLA	CHB-C4A-NA	2.87	128.49	124.51
25	r	609	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
27	7	1622	XAT	C27-C28-C29	-2.87	121.07	125.53
24	G	607	CHL	OMC-CMC-C2C	-2.87	119.19	125.69
25	c	505	CLA	C1-C2-C3	-2.87	121.08	126.04
28	R	623	NEX	C24-C23-C22	-2.87	105.23	110.77
25	n	613	CLA	CMB-C2B-C3B	2.87	130.05	124.68
24	8	605	CHL	OMC-CMC-C2C	-2.87	119.19	125.69
24	2	608	CHL	O2D-CGD-O1D	-2.87	118.22	123.84
24	q	606	CHL	CMB-C2B-C3B	2.87	130.05	124.68
25	N	613	CLA	CMB-C2B-C3B	2.87	130.05	124.68
25	2	604	CLA	CHB-C4A-NA	2.87	128.48	124.51
25	C	506	CLA	CMB-C2B-C3B	2.87	130.05	124.68
34	c	514	BCR	C24-C23-C22	-2.87	121.90	126.23
25	1	611	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
27	0	1622	XAT	C4-C3-C2	-2.87	105.23	110.77
26	N	1620	LUT	C21-C26-C27	-2.87	109.07	112.70
24	G	605	CHL	C1C-C2C-C3C	-2.87	104.84	107.11
24	9	601	CHL	C1C-C2C-C3C	-2.87	104.84	107.11
25	R	613	CLA	CHB-C4A-NA	2.87	128.48	124.51
25	R	612	CLA	CMB-C2B-C3B	2.87	130.04	124.68
25	S	609	CLA	CMB-C2B-C3B	2.87	130.04	124.68
28	p	1623	NEX	C39-C29-C30	-2.87	118.91	122.92
25	r	612	CLA	CMB-C2B-C3B	2.87	130.04	124.68
25	R	612	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
25	N	604	CLA	CMB-C2B-C3B	2.87	130.04	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	r	623	NEX	C4-C3-C2	-2.87	105.24	110.77
24	y	601	CHL	CHB-C4A-NA	2.87	128.47	124.51
24	S	601	CHL	C3B-C4B-NB	2.87	112.92	109.21
25	B	611	CLA	C1B-CHB-C4A	-2.87	124.44	130.12
26	q	1620	LUT	C15-C14-C13	-2.87	123.22	127.31
25	C	507	CLA	C1B-CHB-C4A	-2.86	124.44	130.12
26	g	1621	LUT	C38-C25-C24	-2.86	117.43	123.56
33	a	408	PHO	O1D-CGD-CBD	2.86	129.51	124.74
29	N	2630	LHG	O8-C23-C24	2.86	120.89	111.91
36	D	412	LMG	O8-C28-C29	2.86	120.89	111.91
25	b	606	CLA	CMB-C2B-C1B	-2.86	124.06	128.46
25	9	602	CLA	O2D-CGD-O1D	-2.86	118.24	123.84
33	A	408	PHO	O1D-CGD-CBD	2.86	129.51	124.74
26	Y	1621	LUT	C16-C1-C6	-2.86	105.66	110.30
27	n	1622	XAT	C35-C34-C33	-2.86	123.22	127.31
25	s	609	CLA	CMB-C2B-C3B	2.86	130.03	124.68
24	Y	605	CHL	CAC-C3C-C4C	2.86	128.52	124.81
24	N	601	CHL	CAC-C3C-C4C	2.86	128.52	124.81
35	D	413	SQD	O47-C7-C8	2.86	117.66	111.50
24	G	609	CHL	C1C-C2C-C3C	-2.86	104.84	107.11
25	a	407	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
25	Y	611	CLA	CMB-C2B-C3B	2.86	130.03	124.68
24	4	605	CHL	CMD-C2D-C3D	-2.86	121.04	127.61
25	N	604	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
34	c	515	BCR	C16-C17-C18	-2.86	123.23	127.31
26	G	1621	LUT	C38-C25-C24	-2.86	117.45	123.56
35	d	413	SQD	O47-C7-C8	2.86	117.66	111.50
26	6	1621	LUT	C10-C11-C12	-2.86	114.30	123.22
24	5	607	CHL	O2A-CGA-CBA	2.86	120.87	111.91
25	0	613	CLA	CHB-C4A-NA	2.86	128.46	124.51
25	2	612	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
25	0	602	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
24	N	607	CHL	CMB-C2B-C3B	2.86	130.02	124.68
25	b	611	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
25	9	603	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
28	n	1623	NEX	C11-C10-C9	-2.85	123.24	127.31
24	g	608	CHL	C1C-C2C-C3C	-2.85	104.85	107.11
34	C	516	BCR	C16-C15-C14	-2.85	117.63	123.47
36	s	2631	LMG	O8-C28-C29	2.85	120.86	111.91
26	S	1621	LUT	C21-C26-C27	-2.85	109.09	112.70
24	9	606	CHL	O2A-CGA-CBA	2.85	120.86	111.91
25	b	607	CLA	CHD-C1D-ND	-2.85	121.83	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	B	622	LMG	C8-O7-C10	-2.85	110.77	117.79
25	n	604	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
25	p	613	CLA	CMB-C2B-C1B	-2.85	124.08	128.46
29	q	2630	LHG	O8-C23-C24	2.85	120.86	111.91
24	Y	609	CHL	O2A-CGA-CBA	2.85	120.85	111.91
25	G	612	CLA	CHB-C4A-NA	2.85	128.45	124.51
25	p	611	CLA	CHB-C4A-NA	2.85	128.45	124.51
25	s	604	CLA	CHB-C4A-NA	2.85	128.45	124.51
24	R	608	CHL	O2D-CGD-O1D	-2.85	118.27	123.84
24	7	605	CHL	C1B-CHB-C4A	-2.85	124.47	130.12
25	0	602	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
24	9	608	CHL	CMD-C2D-C3D	-2.85	121.06	127.61
33	A	408	PHO	O2D-CGD-O1D	-2.85	118.27	123.84
33	a	408	PHO	O2D-CGD-O1D	-2.85	118.27	123.84
28	g	1623	NEX	C15-C35-C34	-2.85	117.64	123.47
34	C	516	BCR	C28-C27-C26	-2.85	108.99	114.08
25	B	606	CLA	CMB-C2B-C1B	-2.85	124.09	128.46
24	9	601	CHL	CMB-C2B-C3B	2.85	130.00	124.68
24	9	605	CHL	O2A-CGA-CBA	2.85	120.84	111.91
27	8	1622	XAT	C4-C3-C2	-2.85	105.28	110.77
24	N	601	CHL	CMB-C2B-C3B	2.84	130.00	124.68
25	5	604	CLA	CHB-C4A-NA	2.84	128.44	124.51
24	g	607	CHL	CMB-C2B-C3B	2.84	130.00	124.68
25	S	604	CLA	CHB-C4A-NA	2.84	128.44	124.51
25	6	602	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
25	q	611	CLA	CMB-C2B-C3B	2.84	130.00	124.68
25	c	507	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
25	B	615	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
24	y	609	CHL	O2A-CGA-CBA	2.84	120.82	111.91
24	5	606	CHL	C3B-C4B-NB	2.84	112.88	109.21
25	R	604	CLA	CHB-C4A-NA	2.84	128.44	124.51
34	c	516	BCR	C28-C27-C26	-2.84	109.00	114.08
24	n	605	CHL	CBA-CAA-C2A	-2.84	105.48	113.86
25	g	612	CLA	CHB-C4A-NA	2.84	128.44	124.51
24	G	607	CHL	CMB-C2B-C3B	2.84	129.99	124.68
26	s	1620	LUT	C35-C15-C14	-2.84	117.66	123.47
24	2	607	CHL	CAC-C3C-C4C	2.84	128.49	124.81
24	g	601	CHL	C4D-CHA-C1A	-2.84	117.79	121.25
34	c	516	BCR	C16-C15-C14	-2.84	117.66	123.47
24	N	608	CHL	CHB-C4A-NA	2.84	128.44	124.51
35	B	621	SQD	O48-C23-C24	2.84	120.81	111.91
24	N	608	CHL	O2A-CGA-CBA	2.84	120.81	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	r	608	CHL	O2D-CGD-O1D	-2.84	118.29	123.84
25	B	611	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
25	B	616	CLA	CHB-C4A-NA	2.84	128.44	124.51
24	0	607	CHL	CMB-C2B-C3B	2.84	129.99	124.68
25	7	612	CLA	CHB-C4A-NA	2.84	128.43	124.51
24	q	607	CHL	O2A-CGA-CBA	2.84	120.81	111.91
24	s	601	CHL	C3B-C4B-NB	2.84	112.88	109.21
25	b	615	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
26	Y	1621	LUT	C22-C23-C24	-2.84	108.51	111.74
25	7	603	CLA	CHB-C4A-NA	2.83	128.43	124.51
24	5	609	CHL	C4-C3-C5	2.83	120.04	115.27
24	p	609	CHL	C1C-C2C-C3C	-2.83	104.86	107.11
24	8	609	CHL	CHB-C4A-NA	2.83	128.43	124.51
25	1	612	CLA	CHB-C4A-NA	2.83	128.43	124.51
24	n	609	CHL	CHD-C4C-C3C	-2.83	120.68	124.84
25	N	610	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
24	Y	607	CHL	C1-C2-C3	-2.83	121.14	126.04
35	b	621	SQD	O48-C23-C24	2.83	120.79	111.91
25	y	610	CLA	C4A-NA-C1A	2.83	107.98	106.71
25	r	604	CLA	CHB-C4A-NA	2.83	128.43	124.51
25	6	602	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
24	0	606	CHL	C3B-C4B-NB	2.83	112.87	109.21
24	5	605	CHL	CMB-C2B-C3B	2.83	129.97	124.68
25	c	506	CLA	CMB-C2B-C3B	2.83	129.97	124.68
25	c	504	CLA	CMB-C2B-C1B	-2.83	124.11	128.46
24	q	601	CHL	O2A-CGA-CBA	2.83	120.79	111.91
25	q	614	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
24	1	605	CHL	CAC-C3C-C4C	2.83	128.48	124.81
27	y	1622	XAT	C27-C28-C29	-2.83	121.14	125.53
27	9	1622	XAT	C15-C35-C34	-2.83	117.68	123.47
24	8	608	CHL	CMD-C2D-C3D	-2.83	121.11	127.61
25	C	513	CLA	CHB-C4A-NA	2.83	128.42	124.51
24	n	609	CHL	C4-C3-C5	2.83	120.03	115.27
24	5	609	CHL	O2A-CGA-CBA	2.83	120.77	111.91
24	0	606	CHL	C1C-C2C-C3C	-2.83	104.87	107.11
24	0	608	CHL	CMB-C2B-C3B	2.82	129.96	124.68
26	S	1620	LUT	C35-C15-C14	-2.82	117.69	123.47
25	G	603	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
25	6	611	CLA	CHB-C4A-NA	2.82	128.41	124.51
34	b	620	BCR	C1-C6-C5	-2.82	118.64	122.61
25	3	614	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
28	r	623	NEX	C35-C34-C33	-2.82	123.28	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	c	515	BCR	C20-C21-C22	-2.82	123.28	127.31
24	9	609	CHL	CMB-C2B-C3B	2.82	129.96	124.68
29	9	2630	LHG	O8-C23-C24	2.82	120.76	111.91
26	8	1620	LUT	C31-C30-C29	-2.82	123.29	127.31
24	9	605	CHL	CHD-C4C-C3C	-2.82	120.70	124.84
24	5	609	CHL	C1C-C2C-C3C	-2.82	104.88	107.11
25	y	602	CLA	O2D-CGD-O1D	-2.82	118.33	123.84
24	0	609	CHL	C3B-C4B-NB	2.82	112.85	109.21
36	d	411	LMG	O8-C28-C29	2.82	120.75	111.91
25	s	602	CLA	CHB-C4A-NA	2.82	128.41	124.51
28	q	1623	NEX	O24-C25-C38	2.82	118.43	115.06
25	C	501	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
24	R	606	CHL	CMB-C2B-C3B	2.82	129.95	124.68
25	5	612	CLA	CMB-C2B-C3B	2.82	129.95	124.68
26	Y	1620	LUT	C10-C11-C12	-2.82	114.43	123.22
24	p	609	CHL	C4-C3-C5	2.82	120.01	115.27
25	g	603	CLA	C1B-CHB-C4A	-2.82	124.54	130.12
26	r	620	LUT	C10-C11-C12	-2.82	114.43	123.22
24	N	609	CHL	C4-C3-C5	2.82	120.01	115.27
24	2	605	CHL	CHD-C4C-C3C	-2.82	120.70	124.84
24	5	605	CHL	CMD-C2D-C3D	-2.82	121.14	127.61
24	6	601	CHL	C1C-C2C-C3C	-2.81	104.88	107.11
24	8	601	CHL	CMD-C2D-C3D	-2.81	121.14	127.61
26	R	620	LUT	C10-C11-C12	-2.81	114.44	123.22
24	1	605	CHL	CMB-C2B-C3B	2.81	129.94	124.68
25	y	611	CLA	CMB-C2B-C3B	2.81	129.94	124.68
24	2	608	CHL	C1C-C2C-C3C	-2.81	104.88	107.11
25	2	611	CLA	CMB-C2B-C3B	2.81	129.94	124.68
36	b	622	LMG	C8-O7-C10	-2.81	110.87	117.79
25	G	611	CLA	CHB-C4A-NA	2.81	128.40	124.51
27	6	1622	XAT	C4-C3-C2	-2.81	105.34	110.77
24	3	605	CHL	OMC-CMC-C2C	-2.81	119.33	125.69
25	G	603	CLA	CAA-C2A-C3A	-2.81	105.08	112.78
25	p	604	CLA	CMB-C2B-C3B	2.81	129.94	124.68
26	y	1620	LUT	C10-C11-C12	-2.81	114.45	123.22
24	y	607	CHL	O2A-CGA-CBA	2.81	120.72	111.91
28	8	1623	NEX	C28-C29-C30	2.81	123.25	118.94
27	R	622	XAT	C35-C34-C33	-2.81	123.30	127.31
24	2	605	CHL	O2A-CGA-CBA	2.81	120.72	111.91
25	a	410	CLA	C1-C2-C3	-2.81	121.19	126.04
24	q	601	CHL	CHB-C4A-NA	2.81	128.40	124.51
25	B	614	CLA	CHB-C4A-NA	2.81	128.39	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	0	614	CLA	CHB-C4A-NA	2.81	128.39	124.51
25	G	603	CLA	CHB-C4A-NA	2.81	128.39	124.51
24	p	609	CHL	O2A-CGA-CBA	2.81	120.71	111.91
26	g	1621	LUT	C31-C30-C29	-2.81	123.31	127.31
27	r	622	XAT	C35-C34-C33	-2.81	123.31	127.31
24	1	607	CHL	C3B-C4B-NB	2.81	112.84	109.21
24	7	605	CHL	CMD-C2D-C3D	-2.80	121.16	127.61
24	9	609	CHL	C1B-CHB-C4A	-2.80	124.56	130.12
25	B	603	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
24	p	607	CHL	CMB-C2B-C3B	2.80	129.92	124.68
24	7	609	CHL	C4-C3-C5	2.80	119.98	115.27
24	0	607	CHL	CHB-C4A-NA	2.80	128.39	124.51
25	b	603	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
25	2	604	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
24	G	609	CHL	CMB-C2B-C3B	2.80	129.91	124.68
24	6	609	CHL	C1-C2-C3	-2.80	121.20	126.04
36	S	2631	LMG	O8-C28-C29	2.80	120.69	111.91
24	G	608	CHL	C1C-C2C-C3C	-2.80	104.89	107.11
25	S	613	CLA	CMB-C2B-C3B	2.80	129.91	124.68
25	9	603	CLA	CMB-C2B-C1B	-2.80	124.16	128.46
27	G	1622	XAT	C35-C34-C33	-2.80	123.32	127.31
25	C	507	CLA	CAA-C2A-C3A	-2.80	105.12	112.78
36	D	411	LMG	O8-C28-C29	2.80	120.69	111.91
25	N	604	CLA	CHB-C4A-NA	2.80	128.38	124.51
25	b	615	CLA	CHB-C4A-NA	2.80	128.38	124.51
24	0	601	CHL	O2A-CGA-CBA	2.80	120.69	111.91
26	s	1620	LUT	C38-C25-C24	-2.80	117.58	123.56
28	s	1623	NEX	C39-C29-C30	-2.80	119.01	122.92
25	5	603	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
28	r	623	NEX	C15-C35-C34	-2.80	117.75	123.47
25	y	611	CLA	CHB-C4A-NA	2.80	128.38	124.51
24	8	606	CHL	CMB-C2B-C3B	2.80	129.91	124.68
25	s	609	CLA	O2D-CGD-O1D	-2.80	118.37	123.84
24	3	607	CHL	CAA-C2A-C3A	-2.80	105.12	112.78
25	g	612	CLA	CMB-C2B-C3B	2.79	129.91	124.68
24	n	607	CHL	CMB-C2B-C3B	2.79	129.91	124.68
24	8	605	CHL	C4A-NA-C1A	2.79	107.96	106.71
25	p	603	CLA	C1B-CHB-C4A	-2.79	124.58	130.12
24	2	608	CHL	CMD-C2D-C3D	-2.79	121.19	127.61
25	s	613	CLA	CMB-C2B-C3B	2.79	129.90	124.68
24	1	606	CHL	CMB-C2B-C3B	2.79	129.90	124.68
25	6	611	CLA	O2D-CGD-O1D	-2.79	118.38	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	4	606	CHL	CMB-C2B-C3B	2.79	129.90	124.68
28	n	1623	NEX	C26-C27-C28	-2.79	120.09	125.99
24	p	607	CHL	C1B-CHB-C4A	-2.79	124.59	130.12
24	2	607	CHL	O2A-CGA-CBA	2.79	120.66	111.91
25	G	612	CLA	CMB-C2B-C3B	2.79	129.90	124.68
25	c	501	CLA	C1B-CHB-C4A	-2.79	124.60	130.12
29	c	2630	LHG	C5-O7-C7	-2.79	110.93	117.79
25	Y	603	CLA	CHB-C4A-NA	2.79	128.37	124.51
25	Y	602	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
24	r	606	CHL	CMB-C2B-C3B	2.79	129.89	124.68
25	g	603	CLA	CAA-C2A-C3A	-2.79	105.15	112.78
28	q	1623	NEX	C2-C1-C6	2.79	111.92	109.21
34	C	515	BCR	C16-C17-C18	-2.79	123.33	127.31
24	l	609	CHL	C4-C3-C5	2.79	119.96	115.27
25	p	610	CLA	CHB-C4A-NA	2.78	128.36	124.51
25	q	604	CLA	CHB-C4A-NA	2.78	128.36	124.51
25	A	410	CLA	C1-C2-C3	-2.78	121.23	126.04
24	9	607	CHL	CMD-C2D-C3D	-2.78	121.21	127.61
39	d	405	PL9	C12-C13-C14	-2.78	120.96	127.66
25	a	405	CLA	CBA-CAA-C2A	-2.78	105.65	113.86
24	7	605	CHL	CMB-C2B-C3B	2.78	129.88	124.68
27	Y	1622	XAT	C27-C28-C29	-2.78	121.22	125.53
36	c	521	LMG	O8-C28-C29	2.78	120.63	111.91
25	l	611	CLA	CMB-C2B-C3B	2.78	129.88	124.68
24	6	609	CHL	C1B-CHB-C4A	-2.78	124.61	130.12
24	Y	601	CHL	CMD-C2D-C3D	-2.78	121.22	127.61
26	S	1620	LUT	C38-C25-C24	-2.78	117.61	123.56
25	3	610	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
25	8	610	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
25	g	611	CLA	CHB-C4A-NA	2.78	128.35	124.51
24	9	607	CHL	O2A-CGA-CBA	2.78	120.63	111.91
24	8	608	CHL	CMB-C2B-C3B	2.78	129.88	124.68
25	C	509	CLA	C1B-CHB-C4A	-2.78	124.62	130.12
25	Y	613	CLA	CMB-C2B-C3B	2.78	129.87	124.68
25	2	613	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
25	8	614	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
25	g	603	CLA	CHB-C4A-NA	2.77	128.35	124.51
25	y	613	CLA	CMB-C2B-C3B	2.77	129.87	124.68
25	5	604	CLA	CMB-C2B-C3B	2.77	129.87	124.68
25	5	612	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
25	b	614	CLA	CHB-C4A-NA	2.77	128.34	124.51
26	s	1620	LUT	C10-C11-C12	-2.77	114.57	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	4	603	CLA	CAA-C2A-C3A	-2.77	105.19	112.78
25	A	405	CLA	CBA-CAA-C2A	-2.77	105.68	113.86
25	B	610	CLA	CHB-C4A-NA	2.77	128.34	124.51
25	G	613	CLA	CHB-C4A-NA	2.77	128.34	124.51
25	5	603	CLA	CHB-C4A-NA	2.77	128.34	124.51
25	5	614	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
25	0	611	CLA	O2D-CGD-O1D	-2.77	118.42	123.84
34	B	620	BCR	C1-C6-C5	-2.77	118.71	122.61
25	S	609	CLA	O2D-CGD-O1D	-2.77	118.43	123.84
25	R	602	CLA	CMB-C2B-C3B	2.77	129.86	124.68
25	B	611	CLA	CHB-C4A-NA	2.77	128.34	124.51
24	2	601	CHL	C4A-NA-C1A	-2.77	105.46	106.71
24	1	606	CHL	O2A-CGA-CBA	2.77	120.59	111.91
24	4	607	CHL	CHD-C4C-C3C	-2.76	120.78	124.84
36	C	521	LMG	O8-C28-C29	2.76	120.58	111.91
29	3	2630	LHG	O8-C23-C24	2.76	120.58	111.91
28	G	1623	NEX	C15-C35-C34	-2.76	117.81	123.47
28	N	1623	NEX	C26-C27-C28	-2.76	120.15	125.99
25	7	602	CLA	C1B-CHB-C4A	-2.76	124.64	130.12
25	7	611	CLA	CMB-C2B-C3B	2.76	129.85	124.68
25	0	611	CLA	CHB-C4A-NA	2.76	128.33	124.51
25	c	509	CLA	C1B-CHB-C4A	-2.76	124.64	130.12
24	n	606	CHL	C3B-C4B-NB	2.76	112.78	109.21
25	4	604	CLA	CHB-C4A-NA	2.76	128.33	124.51
25	p	603	CLA	CHB-C4A-NA	2.76	128.33	124.51
25	g	613	CLA	CHB-C4A-NA	2.76	128.33	124.51
24	S	601	CHL	CAC-C3C-C4C	2.76	128.39	124.81
25	9	604	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
25	Y	611	CLA	CHB-C4A-NA	2.76	128.32	124.51
25	n	614	CLA	CMB-C2B-C3B	2.76	129.84	124.68
25	p	612	CLA	O2D-CGD-O1D	-2.76	118.45	123.84
25	c	503	CLA	CAA-CBA-CGA	-2.76	105.20	113.25
25	S	603	CLA	CHB-C4A-NA	2.76	128.32	124.51
24	5	605	CHL	O2D-CGD-O1D	-2.76	118.45	123.84
24	4	601	CHL	CMB-C2B-C3B	2.75	129.83	124.68
25	2	602	CLA	O2D-CGD-O1D	-2.75	118.45	123.84
27	5	1622	XAT	C31-C30-C29	-2.75	123.38	127.31
25	C	503	CLA	CAA-CBA-CGA	-2.75	105.21	113.25
24	G	608	CHL	CMD-C2D-C3D	-2.75	121.28	127.61
26	7	1620	LUT	C10-C11-C12	-2.75	114.63	123.22
26	4	1621	LUT	C18-C5-C6	-2.75	121.44	124.53
26	S	1620	LUT	C10-C11-C12	-2.75	114.63	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3	611	CLA	CHB-C4A-NA	2.75	128.32	124.51
24	Y	607	CHL	CMD-C2D-C3D	-2.75	121.28	127.61
25	s	602	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
26	n	1621	LUT	C38-C25-C24	-2.75	117.68	123.56
25	8	611	CLA	CMB-C2B-C3B	2.75	129.82	124.68
25	b	611	CLA	CHB-C4A-NA	2.75	128.31	124.51
24	y	607	CHL	CMD-C2D-C3D	-2.75	121.29	127.61
25	7	611	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
29	c	2630	LHG	O8-C23-C24	2.75	120.53	111.91
27	Y	1622	XAT	C15-C35-C34	-2.75	117.84	123.47
25	G	603	CLA	CMB-C2B-C1B	-2.75	124.24	128.46
25	b	610	CLA	CHB-C4A-NA	2.75	128.31	124.51
24	3	606	CHL	CMB-C2B-C3B	2.75	129.82	124.68
24	g	601	CHL	C4A-NA-C1A	-2.75	105.47	106.71
24	3	608	CHL	CMB-C2B-C3B	2.75	129.82	124.68
25	B	607	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
26	4	1621	LUT	C38-C25-C24	-2.75	117.68	123.56
34	C	515	BCR	C20-C21-C22	-2.75	123.39	127.31
24	1	609	CHL	O2A-CGA-CBA	2.74	120.52	111.91
34	H	101	BCR	C29-C30-C25	2.74	114.70	110.48
24	p	605	CHL	CHD-C4C-C3C	-2.74	120.81	124.84
25	n	610	CLA	O2D-CGD-O1D	-2.74	118.47	123.84
25	1	603	CLA	CMB-C2B-C3B	2.74	129.81	124.68
25	r	609	CLA	CMB-C2B-C3B	2.74	129.81	124.68
24	9	609	CHL	C4-C3-C5	2.74	119.88	115.27
25	C	510	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
25	g	603	CLA	CMB-C2B-C1B	-2.74	124.25	128.46
24	9	608	CHL	C1C-C2C-C3C	-2.74	104.94	107.11
28	9	1623	NEX	C31-C30-C29	-2.74	123.40	127.31
24	q	607	CHL	CMD-C2D-C3D	-2.74	121.31	127.61
24	3	608	CHL	CMD-C2D-C3D	-2.74	121.31	127.61
25	q	604	CLA	CMB-C2B-C3B	2.74	129.80	124.68
34	b	620	BCR	C28-C27-C26	-2.74	109.19	114.08
25	n	604	CLA	CHB-C4A-NA	2.74	128.30	124.51
26	5	1621	LUT	C7-C8-C9	-2.74	122.10	126.23
26	0	1621	LUT	C18-C5-C6	-2.74	121.45	124.53
25	c	510	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
25	b	614	CLA	O2D-CGD-O1D	-2.74	118.49	123.84
24	0	609	CHL	CMD-C2D-C3D	-2.74	121.32	127.61
28	6	1623	NEX	C28-C29-C30	2.74	123.14	118.94
24	9	601	CHL	O2A-CGA-CBA	2.74	120.50	111.91
24	n	607	CHL	O2A-CGA-CBA	2.74	120.50	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	7	614	CLA	CHB-C4A-NA	2.74	128.29	124.51
25	q	611	CLA	CHB-C4A-NA	2.74	128.29	124.51
24	7	607	CHL	CMB-C2B-C3B	2.74	129.80	124.68
24	N	605	CHL	CBA-CAA-C2A	-2.73	105.79	113.86
24	g	609	CHL	CMB-C2B-C3B	2.73	129.79	124.68
24	y	609	CHL	C1C-C2C-C3C	-2.73	104.94	107.11
26	8	1620	LUT	C35-C15-C14	-2.73	117.87	123.47
24	2	609	CHL	CHD-C4C-C3C	-2.73	120.82	124.84
28	7	1623	NEX	C4-C3-C2	-2.73	105.49	110.77
24	0	601	CHL	CAC-C3C-C4C	2.73	128.36	124.81
28	0	1623	NEX	C30-C31-C32	-2.73	114.69	123.22
29	C	2630	LHG	O8-C23-C24	2.73	120.48	111.91
26	6	1621	LUT	C38-C25-C24	-2.73	117.72	123.56
25	9	613	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
29	D	410	LHG	O8-C23-C24	2.73	120.47	111.91
24	N	601	CHL	CGD-CBD-CAD	-2.73	101.89	110.73
24	7	609	CHL	O2A-CGA-CBA	2.73	120.47	111.91
25	6	614	CLA	CHB-C4A-NA	2.73	128.29	124.51
25	8	611	CLA	CHB-C4A-NA	2.73	128.29	124.51
24	8	607	CHL	O2A-CGA-CBA	2.73	120.47	111.91
24	5	605	CHL	C3B-C4B-NB	2.73	112.74	109.21
24	7	608	CHL	O2A-CGA-CBA	2.73	120.47	111.91
25	4	612	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
26	q	1621	LUT	C18-C5-C6	-2.73	121.46	124.53
25	y	612	CLA	C1-C2-C3	-2.73	121.32	126.04
25	C	501	CLA	CHB-C4A-NA	2.73	128.28	124.51
27	y	1622	XAT	C15-C35-C34	-2.73	117.89	123.47
39	D	405	PL9	C12-C13-C14	-2.73	121.09	127.66
25	p	613	CLA	CHB-C4A-NA	2.73	128.28	124.51
25	y	603	CLA	CHB-C4A-NA	2.73	128.28	124.51
24	7	606	CHL	O2A-CGA-CBA	2.73	120.47	111.91
26	3	1621	LUT	C30-C31-C32	-2.73	114.71	123.22
25	s	603	CLA	CMB-C2B-C3B	2.73	129.78	124.68
25	B	615	CLA	CHB-C4A-NA	2.73	128.28	124.51
25	2	611	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
27	8	1622	XAT	C15-C35-C34	-2.73	117.89	123.47
25	a	410	CLA	CHB-C4A-NA	2.73	128.28	124.51
26	r	620	LUT	C2-C3-C4	2.73	114.03	110.30
24	2	609	CHL	C1C-C2C-C3C	-2.73	104.95	107.11
25	C	512	CLA	CAA-C2A-C3A	-2.72	105.32	112.78
25	r	602	CLA	CMB-C2B-C3B	2.72	129.78	124.68
24	s	606	CHL	C4A-NA-C1A	-2.72	105.48	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	q	607	CHL	CMB-C2B-C3B	2.72	129.78	124.68
25	R	609	CLA	CMB-C2B-C3B	2.72	129.78	124.68
24	4	608	CHL	CMD-C2D-C3D	-2.72	121.35	127.61
24	6	609	CHL	CMD-C2D-C3D	-2.72	121.35	127.61
24	q	609	CHL	CHD-C1D-C2D	2.72	131.19	125.48
24	5	607	CHL	CMB-C2B-C3B	2.72	129.77	124.68
25	3	611	CLA	CMB-C2B-C3B	2.72	129.77	124.68
26	6	1621	LUT	C2-C3-C4	-2.72	106.58	110.30
24	2	609	CHL	C4-C3-C5	2.72	119.85	115.27
25	b	607	CLA	O2D-CGD-O1D	-2.72	118.52	123.84
28	g	1623	NEX	C4-C3-C2	-2.72	105.52	110.77
34	h	101	BCR	C29-C30-C25	2.72	114.67	110.48
24	q	605	CHL	O2A-CGA-CBA	2.72	120.44	111.91
26	9	1620	LUT	C11-C10-C9	-2.72	123.43	127.31
24	7	606	CHL	C3B-C4B-NB	2.72	112.73	109.21
25	S	603	CLA	CMB-C2B-C3B	2.72	129.77	124.68
26	1	1620	LUT	C10-C11-C12	-2.72	114.73	123.22
26	R	620	LUT	C2-C3-C4	2.72	114.03	110.30
24	p	605	CHL	C3B-C4B-NB	2.72	112.72	109.21
24	Y	608	CHL	C1C-C2C-C3C	-2.72	104.96	107.11
29	d	410	LHG	O8-C23-C24	2.72	120.44	111.91
27	y	1622	XAT	C36-C21-C26	2.72	117.38	110.05
24	Y	601	CHL	CHB-C4A-NA	2.72	128.27	124.51
34	c	515	BCR	C11-C10-C9	-2.72	123.43	127.31
25	9	611	CLA	CMB-C2B-C3B	2.72	129.76	124.68
25	s	603	CLA	CHB-C4A-NA	2.72	128.27	124.51
26	7	1620	LUT	C7-C8-C9	-2.72	122.13	126.23
24	9	605	CHL	CMB-C2B-C3B	2.72	129.76	124.68
24	6	601	CHL	CAC-C3C-C4C	2.72	128.33	124.81
24	8	605	CHL	CHD-C4C-C3C	-2.72	120.85	124.84
25	1	602	CLA	C1B-CHB-C4A	-2.71	124.74	130.12
28	6	1623	NEX	C30-C31-C32	-2.71	114.75	123.22
25	g	604	CLA	CHB-C4A-NA	2.71	128.26	124.51
24	p	605	CHL	O2D-CGD-O1D	-2.71	118.53	123.84
25	5	611	CLA	CHB-C4A-NA	2.71	128.26	124.51
25	5	611	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
37	C	520	DGD	O1G-C1A-C2A	2.71	120.42	111.91
37	c	520	DGD	O1G-C1A-C2A	2.71	120.42	111.91
24	9	607	CHL	C1C-C2C-C3C	-2.71	104.96	107.11
28	R	623	NEX	C35-C34-C33	-2.71	123.44	127.31
25	A	410	CLA	CHB-C4A-NA	2.71	128.26	124.51
26	2	1621	LUT	C31-C30-C29	-2.71	123.44	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Y	1622	XAT	C36-C21-C26	2.71	117.36	110.05
26	N	1620	LUT	C15-C14-C13	-2.71	123.44	127.31
24	4	605	CHL	C1C-C2C-C3C	-2.71	104.96	107.11
26	s	1621	LUT	C16-C1-C6	-2.71	105.91	110.30
25	n	603	CLA	CHB-C4A-NA	2.71	128.26	124.51
26	5	1620	LUT	C36-C21-C26	2.71	113.65	109.55
25	d	403	CLA	CHB-C4A-NA	2.71	128.26	124.51
29	y	2630	LHG	C5-O7-C7	-2.71	111.12	117.79
24	5	607	CHL	C2A-C3A-C4A	-2.71	97.50	101.87
34	B	620	BCR	C28-C27-C26	-2.71	109.24	114.08
26	G	1620	LUT	C10-C11-C12	-2.71	114.77	123.22
25	B	613	CLA	C2A-C1A-CHA	2.71	128.59	123.86
25	c	501	CLA	CHB-C4A-NA	2.71	128.25	124.51
24	0	605	CHL	CAC-C3C-C4C	2.71	128.32	124.81
24	p	605	CHL	CAC-C3C-C4C	2.71	128.32	124.81
25	g	602	CLA	CHB-C4A-NA	2.71	128.25	124.51
24	S	607	CHL	C3B-C4B-NB	2.70	112.71	109.21
26	1	1620	LUT	C7-C8-C9	-2.70	122.15	126.23
25	q	610	CLA	CHB-C4A-NA	2.70	128.25	124.51
26	g	1620	LUT	C10-C11-C12	-2.70	114.78	123.22
24	5	605	CHL	C4-C3-C5	2.70	119.82	115.27
24	Y	606	CHL	CMD-C2D-C3D	-2.70	121.39	127.61
25	b	613	CLA	C2A-C1A-CHA	2.70	128.59	123.86
25	D	403	CLA	CHB-C4A-NA	2.70	128.25	124.51
25	B	614	CLA	O2D-CGD-O1D	-2.70	118.55	123.84
28	R	623	NEX	C15-C35-C34	-2.70	117.94	123.47
29	Y	2630	LHG	O8-C23-C24	2.70	120.39	111.91
24	4	605	CHL	O2A-CGA-CBA	2.70	120.39	111.91
25	4	610	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
25	B	604	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
24	2	605	CHL	CMB-C2B-C3B	2.70	129.73	124.68
25	N	603	CLA	CHB-C4A-NA	2.70	128.25	124.51
25	6	610	CLA	O2D-CGD-O1D	-2.70	118.56	123.84
24	2	609	CHL	CHB-C4A-NA	2.70	128.24	124.51
25	G	604	CLA	CHB-C4A-NA	2.70	128.24	124.51
24	2	601	CHL	CMB-C2B-C3B	2.70	129.73	124.68
25	b	602	CLA	CMB-C2B-C3B	2.70	129.73	124.68
26	n	1621	LUT	C19-C9-C8	2.70	122.33	118.08
24	y	608	CHL	CHB-C4A-NA	2.70	128.24	124.51
25	7	603	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
24	y	606	CHL	CMD-C2D-C3D	-2.70	121.41	127.61
25	B	602	CLA	CMB-C2B-C3B	2.70	129.72	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	6	1620	LUT	C3-C4-C5	-2.70	106.48	111.85
25	G	602	CLA	CHB-C4A-NA	2.69	128.24	124.51
25	R	602	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
24	1	601	CHL	CMB-C2B-C3B	2.69	129.72	124.68
24	9	601	CHL	C11-C10-C8	-2.69	107.21	115.92
25	n	612	CLA	O2D-CGD-O1D	-2.69	118.57	123.84
24	7	607	CHL	C3B-C4B-NB	2.69	112.69	109.21
26	S	1621	LUT	C16-C1-C6	-2.69	105.93	110.30
24	1	607	CHL	C4-C3-C5	2.69	119.80	115.27
25	b	604	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
36	A	413	LMG	O8-C28-C29	2.69	120.35	111.91
25	7	603	CLA	CMB-C2B-C3B	2.69	129.71	124.68
26	4	1620	LUT	C31-C30-C29	-2.69	123.47	127.31
24	G	607	CHL	CAA-C2A-C3A	-2.69	105.41	112.78
26	6	1620	LUT	C1-C2-C3	2.69	119.72	113.64
25	r	603	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
26	q	1621	LUT	C19-C9-C8	2.69	122.31	118.08
25	1	614	CLA	CHB-C4A-NA	2.69	128.23	124.51
36	a	413	LMG	O8-C28-C29	2.69	120.35	111.91
24	4	601	CHL	O2A-CGA-CBA	2.69	120.35	111.91
25	c	512	CLA	CAA-C2A-C3A	-2.69	105.42	112.78
26	N	1621	LUT	C38-C25-C24	-2.69	117.81	123.56
26	8	1621	LUT	C30-C31-C32	-2.69	114.83	123.22
26	0	1621	LUT	C38-C25-C24	-2.69	117.81	123.56
24	0	608	CHL	CMD-C2D-C3D	-2.69	121.43	127.61
24	7	601	CHL	C2A-C1A-CHA	-2.69	119.16	123.86
25	4	603	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
24	6	609	CHL	CMB-C2B-C3B	2.69	129.70	124.68
24	2	607	CHL	C1C-C2C-C3C	-2.69	104.98	107.11
24	Y	609	CHL	C1C-C2C-C3C	-2.69	104.98	107.11
35	a	412	SQD	O48-C23-C24	2.69	120.33	111.91
24	G	607	CHL	CHB-C4A-NA	2.69	128.22	124.51
26	q	1620	LUT	C38-C25-C24	-2.69	117.81	123.56
24	N	606	CHL	CMD-C2D-C3D	-2.68	121.44	127.61
24	p	609	CHL	CMB-C2B-C3B	2.68	129.70	124.68
29	8	2630	LHG	O8-C23-C24	2.68	120.33	111.91
24	p	606	CHL	C3B-C4B-NB	2.68	112.68	109.21
26	2	1621	LUT	C18-C5-C6	-2.68	121.52	124.53
25	0	604	CLA	CHB-C4A-NA	2.68	128.22	124.51
25	G	614	CLA	O2D-CGD-O1D	-2.68	118.59	123.84
24	7	607	CHL	C4D-CHA-C1A	-2.68	117.98	121.25
24	s	607	CHL	C3B-C4B-NB	2.68	112.68	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	612	CLA	C1-C2-C3	-2.68	121.41	126.04
29	C	2630	LHG	C5-O7-C7	-2.68	111.19	117.79
24	9	609	CHL	C1C-C2C-C3C	-2.68	104.99	107.11
25	r	602	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
25	l	603	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
27	6	1622	XAT	C31-C32-C33	-2.68	118.89	126.42
35	A	412	SQD	O48-C23-C24	2.68	120.32	111.91
24	p	608	CHL	CMD-C2D-C3D	-2.68	121.45	127.61
28	8	1623	NEX	C17-C1-C6	-2.68	108.08	110.47
25	Y	610	CLA	C4A-NA-C1A	2.68	107.91	106.71
24	n	609	CHL	CMD-C2D-C3D	-2.68	121.45	127.61
24	5	601	CHL	CMB-C2B-C3B	2.68	129.69	124.68
26	s	1621	LUT	C38-C25-C24	-2.68	117.83	123.56
24	y	606	CHL	CAC-C3C-C4C	2.68	128.28	124.81
24	l	607	CHL	C4D-CHA-C1A	-2.68	117.99	121.25
24	9	605	CHL	CAA-C2A-C3A	-2.68	105.45	112.78
26	S	1621	LUT	C38-C25-C24	-2.68	117.83	123.56
24	l	608	CHL	CMB-C2B-C3B	2.68	129.68	124.68
26	y	1621	LUT	C3-C4-C5	-2.67	106.53	111.85
26	y	1620	LUT	C15-C14-C13	-2.67	123.50	127.31
25	4	611	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
24	0	607	CHL	O2A-CGA-CBA	2.67	120.30	111.91
25	0	603	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
25	9	612	CLA	O2D-CGD-O1D	-2.67	118.61	123.84
25	C	504	CLA	CHB-C4A-NA	2.67	128.21	124.51
26	l	1621	LUT	C18-C5-C4	2.67	119.30	114.36
28	S	1623	NEX	O24-C25-C38	2.67	118.26	115.06
24	4	607	CHL	O2A-CGA-CBA	2.67	120.29	111.91
25	R	603	CLA	O2D-CGD-O1D	-2.67	118.62	123.84
25	g	610	CLA	CHB-C4A-NA	2.67	128.20	124.51
28	s	1623	NEX	O24-C25-C38	2.67	118.25	115.06
24	8	605	CHL	CMD-C2D-C3D	-2.67	121.48	127.61
25	R	613	CLA	O2D-CGD-O1D	-2.67	118.63	123.84
24	q	606	CHL	CHD-C4C-C3C	-2.66	120.92	124.84
25	6	613	CLA	CHB-C4A-NA	2.66	128.20	124.51
25	q	612	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
26	q	1621	LUT	C10-C11-C12	-2.66	114.90	123.22
24	8	609	CHL	C1C-C2C-C3C	-2.66	105.00	107.11
25	C	511	CLA	C1B-CHB-C4A	-2.66	124.84	130.12
34	b	619	BCR	C29-C30-C25	2.66	114.58	110.48
24	S	606	CHL	C4A-NA-C1A	-2.66	105.51	106.71
26	R	620	LUT	C7-C8-C9	-2.66	122.21	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	s	601	CHL	C1B-CHB-C4A	-2.66	124.84	130.12
25	1	604	CLA	O2D-CGD-O1D	-2.66	118.63	123.84
24	r	608	CHL	CMB-C2B-C3B	2.66	129.66	124.68
24	5	606	CHL	CMD-C2D-C3D	-2.66	121.49	127.61
25	2	612	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
27	0	1622	XAT	C7-C8-C9	-2.66	121.40	125.53
24	g	607	CHL	CMD-C2D-C3D	-2.66	121.49	127.61
24	7	601	CHL	C4-C3-C5	2.66	119.75	115.27
34	C	515	BCR	C11-C10-C9	-2.66	123.51	127.31
24	Y	606	CHL	CAC-C3C-C4C	2.66	128.26	124.81
24	2	605	CHL	CAA-C2A-C3A	-2.66	105.50	112.78
26	S	1620	LUT	C30-C31-C32	-2.66	114.92	123.22
24	0	607	CHL	O2D-CGD-O1D	-2.66	118.64	123.84
24	1	607	CHL	CMB-C2B-C3B	2.66	129.65	124.68
27	p	1622	XAT	C26-C27-C28	-2.66	120.37	125.99
24	1	607	CHL	O2A-CGA-CBA	2.66	120.25	111.91
28	y	1623	NEX	C17-C1-C6	-2.66	108.09	110.47
24	N	608	CHL	CMD-C2D-C3D	-2.66	121.50	127.61
26	Y	1621	LUT	C3-C4-C5	-2.66	106.56	111.85
35	D	413	SQD	O6-C1-C2	2.66	112.45	108.30
24	7	606	CHL	CMB-C2B-C3B	2.66	129.65	124.68
24	p	607	CHL	C4D-CHA-C1A	-2.65	118.02	121.25
25	g	602	CLA	C1-C2-C3	-2.65	121.45	126.04
24	y	608	CHL	C1C-C2C-C3C	-2.65	105.01	107.11
24	n	605	CHL	CMB-C2B-C3B	2.65	129.64	124.68
24	6	601	CHL	O2A-CGA-CBA	2.65	120.23	111.91
24	S	601	CHL	C1B-CHB-C4A	-2.65	124.86	130.12
24	2	606	CHL	CMD-C2D-C3D	-2.65	121.51	127.61
25	q	602	CLA	CHB-C4A-NA	2.65	128.18	124.51
28	R	623	NEX	C4-C3-C2	-2.65	105.65	110.77
25	C	508	CLA	CHB-C4A-NA	2.65	128.18	124.51
24	Y	606	CHL	C3B-C4B-NB	2.65	112.64	109.21
24	2	601	CHL	CHD-C4C-C3C	-2.65	120.94	124.84
25	q	604	CLA	O2D-CGD-CBD	2.65	115.98	111.27
25	A	406	CLA	CHB-C4A-NA	2.65	128.18	124.51
25	a	406	CLA	CHB-C4A-NA	2.65	128.18	124.51
24	p	601	CHL	CMD-C2D-C3D	-2.65	121.52	127.61
25	B	608	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
25	g	614	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
24	n	601	CHL	O2A-CGA-CBA	2.65	120.22	111.91
26	3	1620	LUT	C35-C15-C14	-2.65	118.05	123.47
24	7	607	CHL	O2A-CGA-CBA	2.65	120.22	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	G	610	CLA	CHB-C4A-NA	2.65	128.18	124.51
24	n	609	CHL	O1D-CGD-CBD	-2.65	119.06	124.48
25	y	613	CLA	CHB-C4A-NA	2.65	128.18	124.51
26	9	1621	LUT	C18-C5-C6	-2.65	121.55	124.53
29	Y	2630	LHG	C9-C8-C7	-2.65	103.99	113.62
24	4	609	CHL	CMD-C2D-C3D	-2.65	121.52	127.61
24	5	608	CHL	CMD-C2D-C3D	-2.65	121.52	127.61
25	C	507	CLA	C7-C6-C5	-2.65	106.17	113.36
26	0	1620	LUT	C38-C25-C24	-2.65	117.89	123.56
26	R	620	LUT	C16-C1-C6	-2.65	106.00	110.30
28	5	1623	NEX	C31-C30-C29	-2.65	123.53	127.31
26	s	1621	LUT	C35-C15-C14	-2.65	118.05	123.47
25	5	603	CLA	CAA-C2A-C3A	-2.65	105.53	112.78
24	Y	601	CHL	O1D-CGD-CBD	-2.65	119.07	124.48
25	6	603	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
25	q	610	CLA	O2D-CGD-O1D	-2.65	118.66	123.84
24	n	606	CHL	CMD-C2D-C3D	-2.65	121.52	127.61
28	Y	1623	NEX	C11-C10-C9	-2.65	123.53	127.31
24	9	608	CHL	CMB-C2B-C3B	2.65	129.63	124.68
26	0	1621	LUT	C16-C1-C6	-2.65	106.01	110.30
26	q	1621	LUT	C3-C4-C5	-2.65	106.58	111.85
29	p	2630	LHG	O8-C23-C24	2.65	120.21	111.91
25	c	511	CLA	C1B-CHB-C4A	-2.65	124.88	130.12
24	g	609	CHL	C4-C3-C5	2.65	119.72	115.27
24	6	601	CHL	CMB-C2B-C3B	2.65	129.63	124.68
24	g	607	CHL	CHB-C4A-NA	2.65	128.17	124.51
25	Y	612	CLA	CHB-C4A-NA	2.65	128.17	124.51
25	c	504	CLA	CHB-C4A-NA	2.65	128.17	124.51
24	G	601	CHL	C2A-C1A-CHA	-2.65	119.23	123.86
26	p	1620	LUT	C38-C25-C24	-2.64	117.90	123.56
25	s	610	CLA	C4A-NA-C1A	2.64	107.89	106.71
24	5	608	CHL	CMB-C2B-C3B	2.64	129.62	124.68
24	q	601	CHL	C1C-C2C-C3C	-2.64	105.02	107.11
24	G	609	CHL	C4-C3-C5	2.64	119.72	115.27
34	B	619	BCR	C29-C30-C25	2.64	114.55	110.48
24	3	605	CHL	CHD-C4C-C3C	-2.64	120.95	124.84
25	r	616	CLA	CMB-C2B-C3B	2.64	129.62	124.68
26	q	1620	LUT	C1-C2-C3	2.64	119.61	113.64
29	S	2630	LHG	O8-C23-C24	2.64	120.20	111.91
28	4	1623	NEX	C11-C12-C13	-2.64	118.99	126.42
25	b	607	CLA	CHB-C4A-NA	2.64	128.16	124.51
24	q	607	CHL	C3B-C4B-NB	2.64	112.62	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	7	608	CHL	CMB-C2B-C3B	2.64	129.62	124.68
25	0	612	CLA	O2D-CGD-O1D	-2.64	118.67	123.84
24	7	609	CHL	C1C-C2C-C3C	-2.64	105.02	107.11
25	R	616	CLA	CHB-C4A-NA	2.64	128.16	124.51
35	d	413	SQD	O6-C1-C2	2.64	112.43	108.30
26	4	1620	LUT	C38-C25-C24	-2.64	117.91	123.56
24	s	606	CHL	CBA-CAA-C2A	-2.64	108.45	114.02
29	2	2630	LHG	O8-C23-C24	2.64	120.19	111.91
26	Y	1620	LUT	C15-C14-C13	-2.64	123.55	127.31
24	g	601	CHL	C2A-C1A-CHA	-2.64	119.25	123.86
25	a	407	CLA	CHB-C4A-NA	2.64	128.16	124.51
24	0	609	CHL	CMB-C2B-C3B	2.64	129.61	124.68
24	n	609	CHL	C1C-C2C-C3C	-2.64	105.02	107.11
25	S	612	CLA	O2D-CGD-O1D	-2.64	118.69	123.84
34	b	619	BCR	C15-C16-C17	-2.64	118.08	123.47
26	s	1620	LUT	C30-C31-C32	-2.63	115.00	123.22
24	p	605	CHL	CMB-C2B-C3B	2.63	129.61	124.68
24	G	606	CHL	CMD-C2D-C3D	-2.63	121.55	127.61
24	3	609	CHL	C1C-C2C-C3C	-2.63	105.02	107.11
25	b	608	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
28	g	1623	NEX	C31-C30-C29	-2.63	123.55	127.31
24	3	609	CHL	O2A-CGA-CBA	2.63	120.17	111.91
26	3	1621	LUT	C10-C11-C12	-2.63	115.00	123.22
26	5	1620	LUT	C10-C11-C12	-2.63	115.00	123.22
25	r	613	CLA	O2D-CGD-O1D	-2.63	118.69	123.84
26	y	1620	LUT	C30-C31-C32	-2.63	115.00	123.22
24	1	605	CHL	CMD-C2D-C3D	-2.63	121.56	127.61
25	n	614	CLA	CHB-C4A-NA	2.63	128.15	124.51
24	y	601	CHL	O1D-CGD-CBD	-2.63	119.10	124.48
24	Y	601	CHL	C11-C10-C8	-2.63	107.42	115.92
24	q	601	CHL	C4A-NA-C1A	-2.63	105.52	106.71
27	3	1622	XAT	C15-C35-C34	-2.63	118.09	123.47
24	R	608	CHL	CMB-C2B-C3B	2.63	129.60	124.68
25	g	604	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
28	G	1623	NEX	C35-C34-C33	-2.63	123.56	127.31
25	4	604	CLA	CMB-C2B-C3B	2.63	129.59	124.68
28	Y	1623	NEX	C30-C31-C32	-2.63	115.02	123.22
26	r	620	LUT	C15-C35-C34	-2.63	118.09	123.47
33	a	409	PHO	CMC-C2C-C3C	2.63	129.90	124.94
24	2	608	CHL	CMB-C2B-C3B	2.63	129.59	124.68
24	p	608	CHL	C1C-C2C-C3C	-2.63	105.03	107.11
24	N	607	CHL	O2A-CGA-CBA	2.63	120.15	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	r	620	LUT	C16-C1-C6	-2.63	106.04	110.30
26	Y	1620	LUT	C30-C31-C32	-2.63	115.02	123.22
25	N	612	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
24	n	606	CHL	CHB-C4A-NA	2.63	128.14	124.51
25	q	614	CLA	CHB-C4A-NA	2.63	128.14	124.51
24	g	608	CHL	CMD-C2D-C3D	-2.63	121.57	127.61
26	G	1621	LUT	C22-C23-C24	-2.63	108.75	111.74
24	0	601	CHL	C6-C5-C3	-2.63	106.57	113.45
24	N	609	CHL	CMD-C2D-C3D	-2.63	121.57	127.61
24	n	608	CHL	CMD-C2D-C3D	-2.63	121.58	127.61
24	9	606	CHL	C1C-C2C-C3C	-2.62	105.03	107.11
26	1	1621	LUT	C10-C11-C12	-2.62	115.03	123.22
24	2	605	CHL	CMD-C2D-C3D	-2.62	121.58	127.61
24	7	601	CHL	CMB-C2B-C3B	2.62	129.59	124.68
26	R	620	LUT	C15-C35-C34	-2.62	118.10	123.47
34	B	618	BCR	C3-C4-C5	-2.62	109.39	114.08
28	4	1623	NEX	C2-C1-C6	2.62	111.76	109.21
25	A	407	CLA	CHB-C4A-NA	2.62	128.14	124.51
24	3	605	CHL	CMD-C2D-C3D	-2.62	121.58	127.61
25	B	616	CLA	CAA-C2A-C3A	-2.62	105.60	112.78
25	y	612	CLA	CHB-C4A-NA	2.62	128.14	124.51
24	n	609	CHL	O2A-CGA-CBA	2.62	120.14	111.91
26	7	1621	LUT	C10-C11-C12	-2.62	115.03	123.22
28	y	1623	NEX	C30-C31-C32	-2.62	115.03	123.22
24	N	606	CHL	CHB-C4A-NA	2.62	128.14	124.51
25	c	503	CLA	CHB-C4A-NA	2.62	128.14	124.51
24	y	606	CHL	C3B-C4B-NB	2.62	112.60	109.21
37	C	523	DGD	O1G-C1A-C2A	2.62	120.13	111.91
37	c	523	DGD	O1G-C1A-C2A	2.62	120.13	111.91
24	g	607	CHL	CAA-C2A-C3A	-2.62	105.60	112.78
25	G	602	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
25	9	610	CLA	O2D-CGD-O1D	-2.62	118.72	123.84
25	5	603	CLA	CMB-C2B-C3B	2.62	129.58	124.68
24	6	608	CHL	CMD-C2D-C3D	-2.62	121.59	127.61
25	2	614	CLA	CHD-C1D-ND	-2.62	122.05	124.45
25	S	604	CLA	CHD-C1D-ND	-2.62	122.05	124.45
25	C	503	CLA	CHB-C4A-NA	2.62	128.13	124.51
26	3	1620	LUT	C21-C26-C27	-2.62	109.39	112.70
25	N	614	CLA	CMB-C2B-C3B	2.62	129.57	124.68
25	r	616	CLA	CHB-C4A-NA	2.62	128.13	124.51
26	4	1621	LUT	C35-C34-C33	-2.62	123.58	127.31
24	Y	608	CHL	CHB-C4A-NA	2.62	128.13	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	613	CLA	CHB-C4A-NA	2.62	128.13	124.51
24	N	609	CHL	O2A-CGA-CBA	2.61	120.11	111.91
25	s	604	CLA	CHD-C1D-ND	-2.61	122.05	124.45
25	7	604	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
24	7	607	CHL	C4-C3-C5	2.61	119.67	115.27
25	b	617	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
25	0	611	CLA	C1-C2-C3	-2.61	121.52	126.04
26	r	620	LUT	C7-C8-C9	-2.61	122.29	126.23
25	B	607	CLA	CHB-C4A-NA	2.61	128.12	124.51
25	c	508	CLA	CHB-C4A-NA	2.61	128.12	124.51
25	p	604	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
24	9	605	CHL	CMD-C2D-C3D	-2.61	121.60	127.61
34	B	619	BCR	C15-C16-C17	-2.61	118.12	123.47
25	p	613	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
24	y	609	CHL	C4-C3-C5	2.61	119.66	115.27
25	N	614	CLA	CHB-C4A-NA	2.61	128.12	124.51
26	0	1621	LUT	C10-C11-C12	-2.61	115.07	123.22
25	b	608	CLA	C7-C6-C5	-2.61	106.27	113.36
24	2	607	CHL	CMB-C2B-C3B	2.61	129.56	124.68
25	c	504	CLA	C4-C3-C5	2.61	119.66	115.27
25	b	603	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
25	R	616	CLA	CMB-C2B-C3B	2.61	129.56	124.68
24	5	607	CHL	C4D-CHA-C1A	-2.61	118.08	121.25
28	4	1623	NEX	C17-C1-C6	-2.61	108.14	110.47
29	4	2630	LHG	O8-C23-C24	2.61	120.09	111.91
24	1	601	CHL	C2A-C1A-CHA	-2.61	119.30	123.86
25	9	614	CLA	CHD-C1D-ND	-2.61	122.06	124.45
25	c	507	CLA	CAA-C2A-C3A	-2.61	105.64	112.78
24	g	606	CHL	CMD-C2D-C3D	-2.61	121.62	127.61
25	C	504	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
25	g	602	CLA	O2D-CGD-O1D	-2.61	118.74	123.84
25	B	605	CLA	O2A-CGA-O1A	-2.61	117.02	123.59
24	p	608	CHL	CMB-C2B-C3B	2.61	129.55	124.68
24	4	607	CHL	CMB-C2B-C3B	2.61	129.55	124.68
25	G	602	CLA	C1-C2-C3	-2.60	121.54	126.04
25	c	507	CLA	C7-C6-C5	-2.60	106.28	113.36
24	9	605	CHL	C1C-C2C-C3C	-2.60	105.05	107.11
24	S	606	CHL	CBA-CAA-C2A	-2.60	108.52	114.02
28	n	1623	NEX	C24-C23-C22	-2.60	105.75	110.77
26	2	1621	LUT	C7-C8-C9	-2.60	122.30	126.23
24	5	607	CHL	C4A-NA-C1A	-2.60	105.54	106.71
24	1	609	CHL	C1C-C2C-C3C	-2.60	105.05	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	c	506	CLA	CHB-C4A-NA	2.60	128.11	124.51
33	A	409	PHO	CMC-C2C-C3C	2.60	129.85	124.94
24	S	608	CHL	CMB-C2B-C3B	2.60	129.54	124.68
25	p	614	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
24	0	601	CHL	C1-C2-C3	-2.60	121.55	126.04
28	N	1623	NEX	C24-C23-C22	-2.60	105.75	110.77
34	b	618	BCR	C3-C4-C5	-2.60	109.44	114.08
28	Y	1623	NEX	C5-C4-C3	-2.60	108.67	111.75
24	s	608	CHL	CMB-C2B-C3B	2.60	129.54	124.68
24	0	606	CHL	CMB-C2B-C3B	2.60	129.54	124.68
28	s	1623	NEX	C15-C35-C34	-2.60	118.15	123.47
25	n	613	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
25	0	610	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
25	b	616	CLA	CAA-C2A-C3A	-2.60	105.67	112.78
24	3	607	CHL	C1-O2A-CGA	2.60	123.26	116.44
25	B	617	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
25	4	611	CLA	CHB-C4A-NA	2.60	128.10	124.51
34	b	619	BCR	C8-C7-C6	-2.60	119.91	127.20
26	5	1621	LUT	C3-C4-C5	-2.60	106.68	111.85
25	p	603	CLA	CMB-C2B-C3B	2.60	129.53	124.68
25	r	610	CLA	CHB-C4A-NA	2.60	128.10	124.51
24	8	609	CHL	CMB-C2B-C3B	2.59	129.53	124.68
25	b	605	CLA	O2A-CGA-O1A	-2.59	117.04	123.59
25	2	610	CLA	CHB-C4A-NA	2.59	128.10	124.51
24	n	601	CHL	CGD-CBD-CAD	-2.59	102.33	110.73
27	5	1622	XAT	C7-C8-C9	-2.59	121.51	125.53
29	s	2630	LHG	O8-C23-C24	2.59	120.05	111.91
24	7	607	CHL	C1-C2-C3	-2.59	121.56	126.04
24	0	606	CHL	O2A-CGA-CBA	2.59	120.04	111.91
24	3	606	CHL	O2D-CGD-O1D	-2.59	118.77	123.84
26	S	1621	LUT	C35-C15-C14	-2.59	118.17	123.47
28	N	1623	NEX	C16-C1-C6	2.59	112.79	110.47
25	1	612	CLA	O2D-CGD-O1D	-2.59	118.77	123.84
24	Y	605	CHL	CMB-C2B-C3B	2.59	129.52	124.68
26	3	1620	LUT	C10-C11-C12	-2.59	115.14	123.22
34	A	411	BCR	C11-C10-C9	-2.59	123.62	127.31
34	a	411	BCR	C11-C10-C9	-2.59	123.62	127.31
28	1	1623	NEX	C5-C4-C3	-2.59	108.68	111.75
24	N	601	CHL	O2A-CGA-CBA	2.59	120.03	111.91
34	B	619	BCR	C8-C7-C6	-2.59	119.94	127.20
24	n	601	CHL	CBC-CAC-C3C	-2.59	105.30	112.43
24	q	601	CHL	CMD-C2D-C3D	-2.59	121.67	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	c	519	DGD	O3G-C1D-C2D	2.59	112.34	108.30
25	8	604	CLA	O2D-CGD-O1D	-2.58	118.78	123.84
25	C	504	CLA	C4-C3-C5	2.58	119.62	115.27
25	R	610	CLA	CHB-C4A-NA	2.58	128.09	124.51
24	0	609	CHL	C1-C2-C3	-2.58	121.57	126.04
25	c	501	CLA	CMB-C2B-C3B	2.58	129.51	124.68
34	c	516	BCR	C7-C8-C9	-2.58	122.33	126.23
24	G	601	CHL	CBC-CAC-C3C	-2.58	105.31	112.43
25	4	603	CLA	C2A-C1A-CHA	2.58	128.38	123.86
25	c	504	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
26	n	1620	LUT	C20-C13-C12	2.58	122.15	118.08
24	5	601	CHL	C4-C3-C5	2.58	119.61	115.27
24	3	609	CHL	CMB-C2B-C3B	2.58	129.51	124.68
25	G	604	CLA	O2D-CGD-O1D	-2.58	118.79	123.84
28	1	1623	NEX	C26-C27-C28	-2.58	120.53	125.99
24	y	605	CHL	CMB-C2B-C3B	2.58	129.51	124.68
24	6	607	CHL	O2A-CGA-CBA	2.58	120.01	111.91
24	q	609	CHL	C3A-C2A-C1A	-2.58	97.47	101.34
25	8	603	CLA	O2D-CGD-O1D	-2.58	118.80	123.84
25	B	609	CLA	CHB-C4A-NA	2.58	128.08	124.51
25	b	609	CLA	CHB-C4A-NA	2.58	128.08	124.51
26	N	1621	LUT	C19-C9-C8	2.58	122.14	118.08
26	4	1620	LUT	C18-C5-C6	-2.58	121.63	124.53
34	D	404	BCR	C38-C26-C27	2.58	118.56	113.62
24	1	609	CHL	CMD-C2D-C3D	-2.58	121.69	127.61
24	y	605	CHL	CHB-C4A-NA	2.57	128.07	124.51
25	C	506	CLA	CHB-C4A-NA	2.57	128.07	124.51
34	d	404	BCR	C38-C26-C27	2.57	118.56	113.62
24	q	601	CHL	C7-C6-C5	-2.57	106.37	113.36
26	n	1620	LUT	C38-C25-C24	-2.57	118.05	123.56
25	1	612	CLA	CAA-C2A-C3A	-2.57	105.73	112.78
25	9	611	CLA	CHB-C4A-NA	2.57	128.07	124.51
24	3	607	CHL	CMD-C2D-C3D	-2.57	121.70	127.61
24	3	608	CHL	C1B-CHB-C4A	-2.57	125.02	130.12
24	G	608	CHL	CMB-C2B-C3B	2.57	129.49	124.68
25	q	603	CLA	O2D-CGD-O1D	-2.57	118.81	123.84
25	B	603	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
26	q	1621	LUT	C38-C25-C24	-2.57	118.06	123.56
25	6	612	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
25	C	510	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
24	1	606	CHL	C3B-C4B-NB	2.57	112.53	109.21
26	6	1620	LUT	C38-C25-C24	-2.57	118.06	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	r	612	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
26	n	1620	LUT	C10-C11-C12	-2.57	115.21	123.22
34	C	515	BCR	C21-C20-C19	-2.57	115.21	123.22
25	g	610	CLA	CAA-CBA-CGA	-2.57	105.75	113.25
25	7	604	CLA	CHB-C4A-NA	2.57	128.06	124.51
25	p	603	CLA	CAA-C2A-C3A	-2.57	105.75	112.78
26	s	1621	LUT	C18-C5-C4	2.57	119.11	114.36
24	q	605	CHL	CMB-C2B-C3B	2.57	129.48	124.68
25	1	610	CLA	O2D-CGD-O1D	-2.57	118.82	123.84
25	B	612	CLA	CAC-C3C-C4C	2.56	128.14	124.81
24	s	607	CHL	CMB-C2B-C3B	2.56	129.48	124.68
25	a	405	CLA	CHB-C4A-NA	2.56	128.06	124.51
24	1	609	CHL	CMB-C2B-C3B	2.56	129.47	124.68
26	6	1620	LUT	C10-C11-C12	-2.56	115.22	123.22
34	b	618	BCR	C15-C16-C17	-2.56	118.22	123.47
25	7	604	CLA	CMB-C2B-C3B	2.56	129.47	124.68
24	5	606	CHL	C1B-CHB-C4A	-2.56	125.04	130.12
24	y	607	CHL	C3B-C4B-NB	2.56	112.52	109.21
24	5	609	CHL	CMB-C2B-C3B	2.56	129.47	124.68
24	7	609	CHL	CMB-C2B-C3B	2.56	129.47	124.68
28	3	1623	NEX	C17-C1-C6	-2.56	108.18	110.47
24	2	605	CHL	C1C-C2C-C3C	-2.56	105.08	107.11
24	6	606	CHL	O2A-CGA-CBA	2.56	119.94	111.91
24	G	605	CHL	CMD-C2D-C3D	-2.56	121.72	127.61
25	n	602	CLA	O2D-CGD-O1D	-2.56	118.83	123.84
24	4	609	CHL	CHD-C1D-C2D	2.56	130.85	125.48
24	q	605	CHL	C1C-C2C-C3C	-2.56	105.08	107.11
25	B	608	CLA	C7-C6-C5	-2.56	106.41	113.36
26	Y	1620	LUT	C11-C10-C9	-2.56	123.66	127.31
24	Y	605	CHL	CHB-C4A-NA	2.56	128.05	124.51
25	s	612	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
25	C	507	CLA	C2A-C1A-CHA	2.56	128.33	123.86
25	b	612	CLA	CAC-C3C-C4C	2.56	128.13	124.81
29	l	101	LHG	C5-O7-C7	-2.56	111.49	117.79
24	p	601	CHL	CMB-C2B-C3B	2.56	129.46	124.68
25	N	602	CLA	C1-C2-C3	-2.56	121.62	126.04
24	q	606	CHL	CMD-C2D-C3D	-2.56	121.73	127.61
25	3	603	CLA	O2D-CGD-O1D	-2.56	118.84	123.84
26	4	1621	LUT	C15-C14-C13	-2.56	123.66	127.31
26	p	1621	LUT	C15-C14-C13	-2.56	123.66	127.31
25	c	511	CLA	CHB-C4A-NA	2.56	128.05	124.51
24	Y	609	CHL	C4-C3-C5	2.56	119.57	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	5	1620	LUT	C15-C35-C34	-2.56	118.24	123.47
28	5	1623	NEX	C17-C1-C6	-2.56	108.19	110.47
28	G	1623	NEX	C4-C3-C2	-2.55	105.84	110.77
29	4	2630	LHG	C5-O7-C7	-2.55	111.50	117.79
25	R	612	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
28	6	1623	NEX	C15-C35-C34	-2.55	118.24	123.47
25	c	510	CLA	O2D-CGD-O1D	-2.55	118.84	123.84
34	B	618	BCR	C15-C16-C17	-2.55	118.24	123.47
25	s	611	CLA	CHB-C4A-NA	2.55	128.04	124.51
24	n	607	CHL	C3B-C4B-NB	2.55	112.51	109.21
24	8	609	CHL	O1D-CGD-CBD	-2.55	119.26	124.48
37	C	519	DGD	O1G-C1A-C2A	2.55	119.92	111.91
26	s	1621	LUT	C15-C14-C13	-2.55	123.67	127.31
24	8	601	CHL	CMB-C2B-C3B	2.55	129.45	124.68
34	a	411	BCR	C38-C26-C25	-2.55	121.66	124.53
25	5	614	CLA	CHB-C4A-NA	2.55	128.04	124.51
24	y	607	CHL	CMB-C2B-C3B	2.55	129.45	124.68
25	G	610	CLA	CAA-CBA-CGA	-2.55	105.80	113.25
24	9	609	CHL	O2A-CGA-CBA	2.55	119.91	111.91
24	2	605	CHL	C4D-CHA-C1A	-2.55	118.15	121.25
29	s	2630	LHG	C5-O7-C7	-2.55	111.51	117.79
28	S	1623	NEX	C24-C23-C22	-2.55	105.85	110.77
24	8	607	CHL	C1C-C2C-C3C	-2.55	105.09	107.11
26	4	1621	LUT	C3-C4-C5	-2.55	106.78	111.85
25	A	405	CLA	CHB-C4A-NA	2.55	128.04	124.51
25	c	502	CLA	CHC-C1C-NC	2.55	128.07	124.20
24	N	606	CHL	C1C-C2C-C3C	-2.55	105.09	107.11
25	C	511	CLA	CHB-C4A-NA	2.55	128.03	124.51
25	s	613	CLA	O2D-CGD-O1D	-2.55	118.86	123.84
26	N	1620	LUT	C38-C25-C24	-2.55	118.11	123.56
24	Y	607	CHL	O1D-CGD-CBD	-2.55	119.28	124.48
25	N	603	CLA	CMB-C2B-C3B	2.55	129.44	124.68
26	1	1620	LUT	C18-C5-C6	-2.55	121.67	124.53
24	Y	607	CHL	C3B-C4B-NB	2.54	112.50	109.21
37	C	518	DGD	C2G-O2G-C1B	-2.54	111.53	117.79
24	g	606	CHL	C4A-NA-C1A	-2.54	105.56	106.71
26	S	1621	LUT	C18-C5-C4	2.54	119.07	114.36
27	0	1622	XAT	C15-C35-C34	-2.54	118.26	123.47
24	0	606	CHL	C6-C7-C8	-2.54	107.69	115.92
24	6	606	CHL	CMB-C2B-C3B	2.54	129.44	124.68
24	8	607	CHL	CMD-C2D-C3D	-2.54	121.76	127.61
24	N	601	CHL	O2D-CGD-O1D	-2.54	118.86	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	4	1621	LUT	C20-C13-C12	2.54	122.08	118.08
24	0	609	CHL	C4-C3-C5	2.54	119.55	115.27
24	3	609	CHL	O1D-CGD-CBD	-2.54	119.28	124.48
25	7	612	CLA	O2D-CGD-O1D	-2.54	118.87	123.84
25	B	612	CLA	C1-C2-C3	-2.54	121.65	126.04
24	p	607	CHL	C1C-C2C-C3C	-2.54	105.10	107.11
24	n	601	CHL	O2D-CGD-O1D	-2.54	118.87	123.84
25	2	603	CLA	CAA-C2A-C3A	-2.54	105.83	112.78
24	2	607	CHL	CMD-C2D-C3D	-2.54	121.78	127.61
27	n	1622	XAT	C10-C11-C12	-2.54	115.30	123.22
37	c	519	DGD	O1G-C1A-C2A	2.54	119.87	111.91
34	A	411	BCR	C28-C27-C26	-2.54	109.55	114.08
25	r	613	CLA	CHD-C1D-ND	-2.53	122.12	124.45
24	S	607	CHL	CMB-C2B-C3B	2.53	129.42	124.68
25	N	613	CLA	O2D-CGD-O1D	-2.53	118.88	123.84
34	c	514	BCR	C16-C15-C14	-2.53	118.28	123.47
25	S	610	CLA	C4A-NA-C1A	2.53	107.84	106.71
24	p	607	CHL	O2A-CGA-CBA	2.53	119.86	111.91
37	C	519	DGD	O3G-C1D-C2D	2.53	112.26	108.30
24	y	601	CHL	C1-O2A-CGA	2.53	123.09	116.44
29	0	2630	LHG	O8-C23-C24	2.53	119.85	111.91
25	C	509	CLA	C2A-C1A-CHA	2.53	128.28	123.86
24	Y	607	CHL	CMB-C2B-C3B	2.53	129.41	124.68
25	R	613	CLA	CHD-C1D-ND	-2.53	122.13	124.45
25	n	603	CLA	CMB-C2B-C3B	2.53	129.41	124.68
26	5	1621	LUT	C38-C25-C24	-2.53	118.15	123.56
24	5	608	CHL	O2A-CGA-CBA	2.53	119.84	111.91
24	g	605	CHL	CMD-C2D-C3D	-2.53	121.80	127.61
25	p	602	CLA	CHB-C4A-NA	2.53	128.01	124.51
24	q	601	CHL	O2D-CGD-O1D	-2.53	118.90	123.84
26	g	1621	LUT	C3-C4-C5	-2.53	106.82	111.85
24	9	607	CHL	CMB-C2B-C3B	2.53	129.40	124.68
34	A	411	BCR	C38-C26-C25	-2.53	121.69	124.53
26	6	1620	LUT	C8-C7-C6	-2.53	120.11	127.20
25	3	614	CLA	CHB-C4A-NA	2.53	128.00	124.51
24	g	605	CHL	O2D-CGD-O1D	-2.53	118.90	123.84
25	3	604	CLA	O2D-CGD-O1D	-2.53	118.90	123.84
25	r	613	CLA	C4-C3-C5	2.52	119.52	115.27
25	C	502	CLA	CHC-C1C-NC	2.52	128.03	124.20
24	0	601	CHL	CMB-C2B-C3B	2.52	129.40	124.68
26	S	1621	LUT	C15-C14-C13	-2.52	123.71	127.31
27	N	1622	XAT	C24-C23-C22	-2.52	105.90	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	4	614	CLA	CHB-C4A-NA	2.52	128.00	124.51
28	5	1623	NEX	C30-C31-C32	-2.52	115.35	123.22
37	c	524	DGD	O1G-C1A-C2A	2.52	119.82	111.91
24	9	605	CHL	C4D-CHA-C1A	-2.52	118.18	121.25
25	D	402	CLA	CBA-CAA-C2A	-2.52	106.42	113.86
25	s	602	CLA	O2D-CGD-CBD	2.52	115.75	111.27
24	n	605	CHL	C4-C3-C5	2.52	119.51	115.27
24	g	601	CHL	OMC-CMC-C2C	-2.52	119.99	125.69
27	2	1622	XAT	C31-C32-C33	-2.52	119.34	126.42
37	c	518	DGD	C2G-O2G-C1B	-2.52	111.59	117.79
26	y	1620	LUT	C11-C10-C9	-2.52	123.72	127.31
25	N	602	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
25	7	610	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
24	3	607	CHL	C1C-C2C-C3C	-2.52	105.12	107.11
34	a	411	BCR	C28-C27-C26	-2.52	109.58	114.08
25	9	602	CLA	C4-C3-C5	2.52	119.50	115.27
25	S	613	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
24	6	606	CHL	C6-C7-C8	-2.52	107.79	115.92
25	R	602	CLA	O2D-CGD-CBD	2.51	115.74	111.27
28	s	1623	NEX	C31-C32-C33	-2.51	119.35	126.42
25	c	505	CLA	O2D-CGD-O1D	-2.51	118.92	123.84
25	C	501	CLA	CMB-C2B-C3B	2.51	129.38	124.68
24	G	605	CHL	O2D-CGD-O1D	-2.51	118.92	123.84
27	8	1622	XAT	C10-C11-C12	-2.51	115.38	123.22
27	n	1622	XAT	C24-C23-C22	-2.51	105.92	110.77
28	n	1623	NEX	C16-C1-C6	2.51	112.72	110.47
25	C	503	CLA	O2D-CGD-O1D	-2.51	118.93	123.84
25	1	604	CLA	CHB-C4A-NA	2.51	127.98	124.51
25	Y	614	CLA	CHB-C4A-NA	2.51	127.98	124.51
25	y	614	CLA	CHB-C4A-NA	2.51	127.98	124.51
34	c	515	BCR	C21-C20-C19	-2.51	115.38	123.22
24	p	608	CHL	O2A-CGA-CBA	2.51	119.79	111.91
25	b	612	CLA	C1-C2-C3	-2.51	121.70	126.04
29	D	408	LHG	O8-C23-C24	2.51	119.78	111.91
24	N	609	CHL	O1D-CGD-CBD	-2.51	119.35	124.48
24	6	605	CHL	CMD-C2D-C3D	-2.51	121.84	127.61
24	s	608	CHL	O2A-CGA-O1A	-2.51	117.26	123.59
24	y	607	CHL	O1D-CGD-CBD	-2.51	119.35	124.48
29	d	408	LHG	O8-C23-C24	2.51	119.78	111.91
25	9	602	CLA	CHB-C4A-NA	2.51	127.98	124.51
26	6	1620	LUT	C18-C5-C6	-2.51	121.71	124.53
24	0	608	CHL	C1C-C2C-C3C	-2.51	105.12	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	9	606	CHL	C1B-CHB-C4A	-2.51	125.15	130.12
29	S	2630	LHG	C5-O7-C7	-2.51	111.62	117.79
28	1	1623	NEX	C4-C3-C2	-2.51	105.93	110.77
24	G	601	CHL	CGD-CBD-CAD	-2.51	102.62	110.73
24	6	607	CHL	CMB-C2B-C3B	2.51	129.37	124.68
26	8	1621	LUT	C10-C11-C12	-2.51	115.40	123.22
25	Y	612	CLA	O2D-CGD-O1D	-2.51	118.94	123.84
28	q	1623	NEX	C11-C12-C13	-2.50	119.38	126.42
25	7	613	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
26	7	1620	LUT	C38-C25-C24	-2.50	118.20	123.56
34	C	514	BCR	C16-C15-C14	-2.50	118.34	123.47
24	9	609	CHL	CHD-C4C-C3C	-2.50	121.16	124.84
25	d	402	CLA	CBA-CAA-C2A	-2.50	106.47	113.86
24	n	605	CHL	C1-C2-C3	-2.50	121.71	126.04
24	n	601	CHL	C2A-C1A-CHA	-2.50	119.48	123.86
25	n	611	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	5	604	CLA	O2D-CGD-O1D	-2.50	118.94	123.84
27	n	1622	XAT	C40-C33-C32	2.50	122.02	118.08
37	C	524	DGD	O1G-C1A-C2A	2.50	119.76	111.91
28	G	1623	NEX	C31-C30-C29	-2.50	123.74	127.31
24	G	605	CHL	CMB-C2B-C3B	2.50	129.36	124.68
25	c	509	CLA	C2A-C1A-CHA	2.50	128.23	123.86
24	4	601	CHL	C1B-CHB-C4A	-2.50	125.17	130.12
25	1	612	CLA	O2A-CGA-O1A	-2.50	117.28	123.59
25	G	603	CLA	O2D-CGD-O1D	-2.50	118.95	123.84
24	8	608	CHL	C1B-CHB-C4A	-2.50	125.17	130.12
26	8	1620	LUT	C11-C10-C9	-2.50	123.74	127.31
24	1	607	CHL	O2D-CGD-O1D	-2.50	118.95	123.84
24	5	608	CHL	C1C-C2C-C3C	-2.50	105.13	107.11
24	y	607	CHL	C11-C10-C8	-2.50	107.84	115.92
25	0	613	CLA	CHD-C1D-ND	-2.50	122.16	124.45
24	r	607	CHL	C4D-CHA-C1A	-2.50	118.21	121.25
24	g	601	CHL	CGD-CBD-CAD	-2.50	102.65	110.73
28	2	1623	NEX	C28-C29-C30	2.50	122.77	118.94
25	5	602	CLA	CHB-C4A-NA	2.50	127.96	124.51
25	3	602	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
25	C	505	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
25	q	611	CLA	O2D-CGD-O1D	-2.50	118.96	123.84
24	N	605	CHL	O1D-CGD-CBD	-2.49	119.38	124.48
25	1	602	CLA	O2D-CGD-O1D	-2.49	118.96	123.84
34	A	411	BCR	C10-C11-C12	-2.49	115.43	123.22
34	a	411	BCR	C10-C11-C12	-2.49	115.43	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	s	1620	LUT	C3-C4-C5	-2.49	106.88	111.85
25	S	611	CLA	CHB-C4A-NA	2.49	127.96	124.51
25	N	610	CLA	C1-C2-C3	-2.49	121.73	126.04
25	c	511	CLA	O2D-CGD-CBD	2.49	115.70	111.27
25	r	602	CLA	O2D-CGD-CBD	2.49	115.70	111.27
25	0	604	CLA	CHD-C1D-ND	-2.49	122.16	124.45
28	s	1623	NEX	C24-C23-C22	-2.49	105.96	110.77
25	2	611	CLA	CHB-C4A-NA	2.49	127.96	124.51
26	9	1621	LUT	C11-C10-C9	-2.49	123.75	127.31
25	y	612	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
26	1	1621	LUT	C2-C3-C4	2.49	113.71	110.30
26	3	1620	LUT	C18-C5-C6	-2.49	121.73	124.53
24	8	606	CHL	C3B-C4B-NB	2.49	112.43	109.21
26	2	1621	LUT	C1-C2-C3	2.49	119.27	113.64
24	S	608	CHL	O2A-CGA-O1A	-2.49	117.31	123.59
24	9	601	CHL	CAA-CBA-CGA	-2.49	105.98	113.25
24	G	601	CHL	O2A-CGA-CBA	2.49	119.72	111.91
24	R	607	CHL	C4D-CHA-C1A	-2.49	118.22	121.25
24	p	607	CHL	C1-C2-C3	-2.49	121.74	126.04
34	a	411	BCR	C21-C20-C19	-2.49	115.45	123.22
24	2	609	CHL	O2A-CGA-CBA	2.49	119.72	111.91
34	H	101	BCR	C38-C26-C27	2.49	118.40	113.62
26	1	1620	LUT	C38-C25-C24	-2.49	118.23	123.56
24	2	606	CHL	C1C-C2C-C3C	-2.49	105.14	107.11
24	q	606	CHL	CED-O2D-CGD	2.49	121.56	115.94
26	y	1621	LUT	C38-C25-C24	-2.49	118.24	123.56
25	7	602	CLA	O2D-CGD-O1D	-2.49	118.97	123.84
27	g	1622	XAT	C15-C35-C34	-2.49	118.38	123.47
25	8	614	CLA	CHB-C4A-NA	2.49	127.95	124.51
26	2	1620	LUT	C38-C25-C24	-2.49	118.24	123.56
25	A	406	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
25	a	406	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
25	a	410	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
28	q	1623	NEX	C27-C28-C29	-2.49	121.67	125.53
25	g	603	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
24	r	608	CHL	O2A-CGA-CBA	2.49	119.71	111.91
25	1	613	CLA	O2D-CGD-O1D	-2.49	118.98	123.84
24	6	609	CHL	O2A-CGA-CBA	2.49	119.71	111.91
26	Y	1621	LUT	C38-C25-C24	-2.49	118.24	123.56
25	D	403	CLA	CHD-C1D-ND	-2.49	122.17	124.45
26	5	1620	LUT	C22-C23-C24	-2.48	108.91	111.74
26	9	1620	LUT	C38-C25-C24	-2.48	118.25	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	9	603	CLA	CAA-C2A-C3A	-2.48	105.98	112.78
26	0	1620	LUT	C35-C15-C14	-2.48	118.39	123.47
25	C	504	CLA	CMB-C2B-C3B	2.48	129.32	124.68
24	5	609	CHL	C1B-CHB-C4A	-2.48	125.20	130.12
24	p	601	CHL	O2A-CGA-CBA	2.48	119.70	111.91
27	N	1622	XAT	C10-C11-C12	-2.48	115.47	123.22
24	g	605	CHL	CMB-C2B-C3B	2.48	129.32	124.68
24	R	608	CHL	O2A-CGA-CBA	2.48	119.70	111.91
26	1	1621	LUT	C38-C25-C24	-2.48	118.25	123.56
26	y	1621	LUT	C15-C35-C34	-2.48	118.39	123.47
34	C	516	BCR	C7-C8-C9	-2.48	122.49	126.23
25	n	610	CLA	C1-C2-C3	-2.48	121.75	126.04
26	7	1621	LUT	C38-C25-C24	-2.48	118.25	123.56
24	N	607	CHL	C3B-C4B-NB	2.48	112.42	109.21
24	2	601	CHL	C4-C3-C5	2.48	119.44	115.27
24	8	609	CHL	C4A-NA-C1A	-2.48	105.59	106.71
24	4	605	CHL	CMB-C2B-C3B	2.48	129.31	124.68
24	S	606	CHL	O2D-CGD-O1D	-2.48	119.00	123.84
25	c	507	CLA	C2A-C1A-CHA	2.48	128.19	123.86
26	3	1621	LUT	C38-C25-C24	-2.47	118.27	123.56
24	9	606	CHL	CMB-C2B-C3B	2.47	129.31	124.68
28	S	1623	NEX	C2-C1-C6	2.47	111.61	109.21
25	s	614	CLA	O2A-CGA-O1A	-2.47	117.35	123.59
24	g	605	CHL	O2A-CGA-CBA	2.47	119.67	111.91
24	0	601	CHL	C6-C7-C8	-2.47	107.93	115.92
24	n	607	CHL	C1-O2A-CGA	2.47	122.93	116.44
25	A	410	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
26	1	1621	LUT	C1-C2-C3	2.47	119.22	113.64
24	s	606	CHL	O2D-CGD-O1D	-2.47	119.01	123.84
25	s	613	CLA	CHB-C4A-NA	2.47	127.93	124.51
24	5	605	CHL	CAC-C3C-C4C	2.47	128.01	124.81
24	N	601	CHL	C2A-C1A-CHA	-2.47	119.54	123.86
26	S	1620	LUT	C3-C4-C5	-2.47	106.94	111.85
36	a	413	LMG	C7-O1-C1	-2.47	108.92	113.74
24	g	606	CHL	CMB-C2B-C3B	2.47	129.29	124.68
24	4	606	CHL	CMD-C2D-C3D	-2.47	121.94	127.61
25	s	611	CLA	O2D-CGD-O1D	-2.47	119.01	123.84
28	S	1623	NEX	C31-C32-C33	-2.47	119.49	126.42
24	y	601	CHL	C11-C10-C8	-2.47	107.95	115.92
24	7	601	CHL	O1D-CGD-CBD	-2.47	119.44	124.48
25	R	610	CLA	C1-C2-C3	-2.47	121.78	126.04
26	4	1620	LUT	C1-C2-C3	2.47	119.21	113.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	7	1623	NEX	C19-C9-C10	-2.47	119.47	122.92
34	h	101	BCR	C38-C26-C27	2.46	118.35	113.62
25	S	603	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
25	8	602	CLA	O2D-CGD-O1D	-2.46	119.02	123.84
24	5	601	CHL	O1D-CGD-CBD	-2.46	119.44	124.48
34	A	411	BCR	C21-C20-C19	-2.46	115.53	123.22
25	y	610	CLA	O2A-CGA-O1A	-2.46	117.38	123.59
29	G	2630	LHG	C6-C5-C4	-2.46	105.96	111.79
26	Y	1621	LUT	C15-C35-C34	-2.46	118.43	123.47
26	n	1620	LUT	C31-C30-C29	-2.46	123.80	127.31
24	8	606	CHL	CHD-C4C-C3C	-2.46	121.22	124.84
28	r	623	NEX	C30-C31-C32	-2.46	115.54	123.22
26	N	1620	LUT	C35-C15-C14	-2.46	118.44	123.47
25	R	613	CLA	C4-C3-C5	2.46	119.41	115.27
24	G	606	CHL	CMB-C2B-C3B	2.46	129.28	124.68
28	n	1623	NEX	O4-C5-C18	-2.46	105.02	109.39
26	8	1621	LUT	C38-C25-C24	-2.46	118.30	123.56
24	Y	601	CHL	C1-C2-C3	-2.46	121.79	126.04
24	9	606	CHL	CMD-C2D-C3D	-2.46	121.96	127.61
24	4	601	CHL	C4-C3-C5	2.46	119.41	115.27
26	6	1620	LUT	C19-C9-C8	2.46	121.95	118.08
24	7	609	CHL	CMD-C2D-C3D	-2.46	121.96	127.61
24	G	605	CHL	O2A-CGA-CBA	2.46	119.62	111.91
24	7	607	CHL	O2D-CGD-O1D	-2.46	119.03	123.84
24	8	606	CHL	O2D-CGD-O1D	-2.46	119.03	123.84
24	4	601	CHL	C1C-C2C-C3C	-2.46	105.17	107.11
25	C	511	CLA	O2D-CGD-CBD	2.45	115.63	111.27
26	9	1621	LUT	C38-C25-C24	-2.45	118.31	123.56
25	r	610	CLA	C1-C2-C3	-2.45	121.80	126.04
26	p	1621	LUT	C31-C30-C29	-2.45	123.81	127.31
25	4	613	CLA	O2D-CGD-O1D	-2.45	119.04	123.84
25	S	614	CLA	O2A-CGA-O1A	-2.45	117.40	123.59
25	2	603	CLA	CMB-C2B-C3B	2.45	129.27	124.68
24	5	601	CHL	C11-C10-C8	-2.45	107.99	115.92
24	Y	606	CHL	CMB-C2B-C3B	2.45	129.26	124.68
25	8	604	CLA	CHB-C4A-NA	2.45	127.90	124.51
24	n	601	CHL	C11-C10-C8	-2.45	108.00	115.92
26	p	1621	LUT	C38-C25-C24	-2.45	118.32	123.56
25	r	601	CLA	CHA-C1A-NA	-2.45	120.79	126.40
26	9	1621	LUT	C31-C30-C29	-2.45	123.81	127.31
24	4	601	CHL	O1D-CGD-CBD	-2.45	119.47	124.48
25	s	610	CLA	O2A-CGA-O1A	-2.45	117.41	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	0	604	CLA	O2D-CGD-O1D	-2.45	119.05	123.84
24	q	605	CHL	CHD-C4C-C3C	-2.45	121.24	124.84
24	7	601	CHL	CGD-CBD-CAD	-2.45	102.81	110.73
24	N	605	CHL	C1-C2-C3	-2.45	121.81	126.04
24	R	607	CHL	C4-C3-C5	2.45	119.39	115.27
24	0	605	CHL	CMD-C2D-C3D	-2.44	121.99	127.61
29	g	2630	LHG	C6-C5-C4	-2.44	106.01	111.79
24	y	608	CHL	CMD-C2D-C3D	-2.44	121.99	127.61
25	c	503	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
24	g	609	CHL	C1B-CHB-C4A	-2.44	125.28	130.12
25	Y	610	CLA	O2A-CGA-O1A	-2.44	117.43	123.59
25	D	402	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
25	S	613	CLA	CHB-C4A-NA	2.44	127.89	124.51
24	6	609	CHL	OMC-CMC-C2C	-2.44	120.17	125.69
25	d	403	CLA	CHD-C1D-ND	-2.44	122.21	124.45
34	C	517	BCR	C1-C6-C5	-2.44	119.18	122.61
25	9	610	CLA	CHB-C4A-NA	2.44	127.89	124.51
24	5	601	CHL	CHB-C4A-NA	2.44	127.88	124.51
24	8	607	CHL	C4-C3-C5	2.44	119.37	115.27
25	C	507	CLA	O2D-CGD-CBD	2.44	115.60	111.27
25	S	611	CLA	O2D-CGD-O1D	-2.44	119.07	123.84
24	G	609	CHL	C1B-CHB-C4A	-2.44	125.29	130.12
26	y	1620	LUT	C38-C25-C24	-2.44	118.34	123.56
26	1	1621	LUT	C11-C10-C9	-2.44	123.83	127.31
26	4	1620	LUT	C3-C4-C5	-2.44	107.00	111.85
34	d	404	BCR	C35-C13-C12	2.44	121.92	118.08
24	5	606	CHL	C1C-C2C-C3C	-2.44	105.18	107.11
24	7	605	CHL	C1C-C2C-C3C	-2.44	105.18	107.11
25	p	602	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
24	0	609	CHL	O2A-CGA-CBA	2.44	119.55	111.91
24	0	609	CHL	O1D-CGD-CBD	-2.44	119.50	124.48
34	D	404	BCR	C35-C13-C12	2.44	121.91	118.08
25	d	402	CLA	O2D-CGD-O1D	-2.44	119.08	123.84
25	R	601	CLA	CHA-C1A-NA	-2.43	120.82	126.40
26	9	1621	LUT	C7-C8-C9	-2.43	122.56	126.23
26	6	1621	LUT	C16-C1-C6	-2.43	106.35	110.30
24	7	607	CHL	CMD-C2D-C3D	-2.43	122.01	127.61
25	S	610	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
25	s	603	CLA	O2D-CGD-O1D	-2.43	119.08	123.84
26	4	1620	LUT	C16-C1-C6	-2.43	106.35	110.30
26	9	1621	LUT	C18-C5-C4	2.43	118.86	114.36
24	Y	608	CHL	CMD-C2D-C3D	-2.43	122.02	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	R	623	NEX	C30-C31-C32	-2.43	115.63	123.22
25	y	610	CLA	CHB-C4A-NA	2.43	127.87	124.51
26	3	1620	LUT	C11-C10-C9	-2.43	123.84	127.31
39	d	405	PL9	O1-C4-C3	-2.43	118.04	120.72
25	N	611	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	p	604	CLA	CHB-C4A-NA	2.43	127.87	124.51
24	q	607	CHL	CHD-C4C-C3C	-2.43	121.27	124.84
26	1	1621	LUT	C18-C5-C6	-2.43	121.80	124.53
24	1	607	CHL	CMD-C2D-C3D	-2.43	122.03	127.61
24	1	601	CHL	O1D-CGD-CBD	-2.43	119.52	124.48
24	N	601	CHL	C1-C2-C3	-2.43	121.84	126.04
26	5	1620	LUT	C11-C10-C9	-2.43	123.85	127.31
25	G	613	CLA	O2D-CGD-O1D	-2.43	119.09	123.84
24	y	606	CHL	CMB-C2B-C3B	2.43	129.22	124.68
24	p	601	CHL	C4-C3-C5	2.43	119.35	115.27
34	H	101	BCR	C2-C3-C4	-2.43	105.96	111.38
27	3	1622	XAT	C10-C11-C12	-2.43	115.65	123.22
34	c	514	BCR	C21-C20-C19	-2.43	115.65	123.22
25	c	507	CLA	O2D-CGD-CBD	2.42	115.58	111.27
24	6	607	CHL	OMC-CMC-C2C	-2.42	120.20	125.69
28	G	1623	NEX	C5-C4-C3	-2.42	108.88	111.75
24	G	601	CHL	C4D-C3D-CAD	2.42	110.95	108.10
26	8	1620	LUT	C21-C26-C27	-2.42	109.64	112.70
25	0	611	CLA	CHD-C1D-ND	-2.42	122.23	124.45
25	Y	610	CLA	CHB-C4A-NA	2.42	127.86	124.51
28	3	1623	NEX	C2-C1-C6	2.42	111.57	109.21
24	n	607	CHL	C4-C3-C5	2.42	119.35	115.27
29	g	2630	LHG	C5-O7-C7	-2.42	111.83	117.79
24	1	607	CHL	C1-C2-C3	-2.42	121.85	126.04
25	q	613	CLA	O2D-CGD-O1D	-2.42	119.10	123.84
25	p	614	CLA	CHD-C1D-ND	-2.42	122.23	124.45
27	3	1622	XAT	C11-C10-C9	-2.42	123.86	127.31
24	6	609	CHL	C4-C3-C5	2.42	119.34	115.27
28	0	1623	NEX	C15-C35-C34	-2.42	118.52	123.47
24	g	601	CHL	O1D-CGD-CBD	-2.42	119.54	124.48
24	8	609	CHL	O2A-CGA-CBA	2.42	119.49	111.91
24	5	606	CHL	CMB-C2B-C3B	2.42	129.20	124.68
24	5	607	CHL	C1B-CHB-C4A	-2.42	125.33	130.12
26	8	1621	LUT	C3-C4-C5	-2.42	107.04	111.85
34	H	101	BCR	C30-C25-C26	-2.42	119.21	122.61
24	s	606	CHL	CMD-C2D-C3D	-2.42	122.06	127.61
36	A	413	LMG	C7-O1-C1	-2.42	109.02	113.74

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	n	602	CLA	C1-C2-C3	-2.41	121.87	126.04
24	s	608	CHL	CMD-C2D-C3D	-2.41	122.06	127.61
25	b	611	CLA	CAA-CBA-CGA	-2.41	106.20	113.25
29	6	2630	LHG	O8-C23-C24	2.41	119.48	111.91
25	3	604	CLA	CHB-C4A-NA	2.41	127.85	124.51
25	G	611	CLA	O2D-CGD-CBD	2.41	115.56	111.27
25	q	602	CLA	CHD-C1D-ND	-2.41	122.24	124.45
34	b	618	BCR	C33-C5-C6	-2.41	121.82	124.53
28	4	1623	NEX	C39-C29-C30	-2.41	119.54	122.92
28	1	1623	NEX	C30-C31-C32	-2.41	115.69	123.22
25	3	610	CLA	CHB-C4A-NA	2.41	127.84	124.51
25	b	606	CLA	CHB-C4A-NA	2.41	127.84	124.51
24	S	608	CHL	CMD-C2D-C3D	-2.41	122.08	127.61
24	7	608	CHL	CMD-C2D-C3D	-2.41	122.08	127.61
25	9	603	CLA	O2D-CGD-O1D	-2.41	119.13	123.84
26	8	1620	LUT	C10-C11-C12	-2.41	115.71	123.22
34	C	514	BCR	C21-C20-C19	-2.41	115.71	123.22
28	8	1623	NEX	C4-C3-C2	-2.41	106.13	110.77
25	p	613	CLA	CMB-C2B-C3B	2.41	129.18	124.68
36	a	413	LMG	C8-O7-C10	-2.41	111.87	117.79
28	9	1623	NEX	O24-C25-C38	2.41	117.94	115.06
25	B	611	CLA	CAA-CBA-CGA	-2.40	106.23	113.25
24	9	608	CHL	C1B-CHB-C4A	-2.40	125.36	130.12
34	h	101	BCR	C2-C3-C4	-2.40	106.01	111.38
29	5	2630	LHG	O8-C23-C24	2.40	119.45	111.91
34	c	517	BCR	C1-C6-C5	-2.40	119.23	122.61
24	1	601	CHL	CGD-CBD-CAD	-2.40	102.96	110.73
24	6	605	CHL	C1C-C2C-C3C	-2.40	105.21	107.11
25	G	612	CLA	O2D-CGD-O1D	-2.40	119.14	123.84
34	B	618	BCR	C38-C26-C27	2.40	118.23	113.62
29	G	2630	LHG	C5-O7-C7	-2.40	111.88	117.79
24	3	608	CHL	C1C-C2C-C3C	-2.40	105.21	107.11
24	0	605	CHL	C1C-C2C-C3C	-2.40	105.21	107.11
24	8	608	CHL	O2A-CGA-CBA	2.40	119.44	111.91
27	N	1622	XAT	C5-C4-C3	-2.40	108.00	112.75
24	N	606	CHL	CAA-C2A-C3A	-2.40	106.21	112.78
25	S	610	CLA	O2D-CGD-O1D	-2.40	119.15	123.84
25	c	505	CLA	CHB-C4A-NA	2.40	127.83	124.51
26	4	1620	LUT	C11-C10-C9	-2.40	123.89	127.31
24	3	608	CHL	O2A-CGA-CBA	2.40	119.43	111.91
26	7	1620	LUT	C18-C5-C6	-2.40	121.83	124.53
28	g	1623	NEX	C24-C23-C22	-2.40	106.14	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	n	606	CHL	CAA-C2A-C3A	-2.40	106.21	112.78
24	3	607	CHL	C4-C3-C5	2.40	119.30	115.27
24	4	605	CHL	CHD-C4C-C3C	-2.40	121.32	124.84
24	p	605	CHL	O1D-CGD-CBD	-2.40	119.58	124.48
29	L	101	LHG	C5-O7-C7	-2.40	111.89	117.79
24	S	606	CHL	CMD-C2D-C3D	-2.40	122.10	127.61
25	g	612	CLA	O2D-CGD-O1D	-2.40	119.16	123.84
24	n	605	CHL	CAA-C2A-C3A	-2.40	106.22	112.78
27	n	1622	XAT	C5-C4-C3	-2.39	108.01	112.75
24	r	606	CHL	C4-C3-C5	2.39	119.30	115.27
24	8	608	CHL	C1C-C2C-C3C	-2.39	105.21	107.11
36	A	413	LMG	C8-O7-C10	-2.39	111.90	117.79
24	y	605	CHL	OMC-CMC-C2C	-2.39	120.28	125.69
25	Y	611	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
24	N	605	CHL	CMB-C2B-C3B	2.39	129.16	124.68
24	y	608	CHL	CMB-C2B-C3B	2.39	129.16	124.68
25	2	603	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
34	d	404	BCR	C33-C5-C4	2.39	118.21	113.62
24	p	607	CHL	CMD-C2D-C3D	-2.39	122.11	127.61
28	S	1623	NEX	C15-C35-C34	-2.39	118.58	123.47
25	b	602	CLA	CHB-C4A-NA	2.39	127.82	124.51
26	Y	1620	LUT	C21-C26-C27	-2.39	109.68	112.70
25	b	616	CLA	C2A-C1A-CHA	2.39	128.03	123.86
25	8	614	CLA	CHD-C1D-ND	-2.39	122.26	124.45
24	n	606	CHL	C1C-C2C-C3C	-2.39	105.22	107.11
24	y	601	CHL	C1C-C2C-C3C	-2.39	105.22	107.11
26	5	1620	LUT	C38-C25-C24	-2.39	118.45	123.56
24	S	607	CHL	CMD-C2D-C3D	-2.39	122.13	127.61
24	5	605	CHL	O2A-CGA-CBA	2.39	119.39	111.91
24	n	601	CHL	C1-C2-C3	-2.39	121.92	126.04
28	S	1623	NEX	C11-C12-C13	-2.38	119.72	126.42
24	N	605	CHL	C4-C3-C5	2.38	119.28	115.27
24	g	601	CHL	O2A-CGA-CBA	2.38	119.39	111.91
34	b	618	BCR	C38-C26-C27	2.38	118.19	113.62
24	Y	605	CHL	OMC-CMC-C2C	-2.38	120.30	125.69
27	9	1622	XAT	C31-C32-C33	-2.38	119.73	126.42
34	B	619	BCR	C3-C4-C5	-2.38	109.83	114.08
26	4	1621	LUT	C19-C9-C8	2.38	121.83	118.08
25	B	602	CLA	CHB-C4A-NA	2.38	127.80	124.51
25	y	611	CLA	O2D-CGD-O1D	-2.38	119.19	123.84
24	0	601	CHL	C1C-C2C-C3C	-2.38	105.23	107.11
34	b	619	BCR	C3-C4-C5	-2.38	109.83	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	G	601	CHL	OMC-CMC-C2C	-2.38	120.31	125.69
28	y	1623	NEX	C2-C1-C6	2.38	111.52	109.21
24	R	606	CHL	C4-C3-C5	2.38	119.27	115.27
24	6	607	CHL	O2D-CGD-O1D	-2.38	119.19	123.84
28	G	1623	NEX	C24-C23-C22	-2.38	106.18	110.77
24	Y	608	CHL	CMB-C2B-C3B	2.38	129.12	124.68
24	r	606	CHL	O1D-CGD-CBD	-2.38	119.62	124.48
24	q	608	CHL	C3B-C4B-NB	2.38	112.28	109.21
25	s	610	CLA	O2D-CGD-CBD	2.38	115.49	111.27
28	Y	1623	NEX	C11-C12-C13	-2.38	119.74	126.42
34	B	618	BCR	C33-C5-C6	-2.38	121.86	124.53
25	R	602	CLA	C1B-CHB-C4A	-2.37	125.41	130.12
25	g	611	CLA	O2D-CGD-CBD	2.37	115.49	111.27
24	6	601	CHL	C6-C5-C3	-2.37	107.23	113.45
27	G	1622	XAT	C15-C35-C34	-2.37	118.61	123.47
25	4	602	CLA	CHB-C4A-NA	2.37	127.79	124.51
25	Y	602	CLA	CHB-C4A-NA	2.37	127.79	124.51
25	B	616	CLA	CAC-C3C-C4C	2.37	127.89	124.81
26	Y	1620	LUT	C38-C25-C24	-2.37	118.48	123.56
25	4	612	CLA	C2A-C1A-CHA	2.37	128.01	123.86
25	S	612	CLA	C2A-C1A-CHA	2.37	128.01	123.86
28	R	623	NEX	C17-C1-C6	-2.37	108.35	110.47
27	0	1622	XAT	C26-C27-C28	-2.37	120.98	125.99
27	3	1622	XAT	C31-C32-C33	-2.37	119.75	126.42
25	r	602	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
34	h	101	BCR	C30-C25-C26	-2.37	119.27	122.61
25	C	505	CLA	CHB-C4A-NA	2.37	127.79	124.51
24	p	605	CHL	C1C-C2C-C3C	-2.37	105.23	107.11
24	3	605	CHL	CED-O2D-CGD	2.37	121.30	115.94
25	B	616	CLA	C2A-C1A-CHA	2.37	128.00	123.86
25	8	610	CLA	CHB-C4A-NA	2.37	127.79	124.51
26	S	1621	LUT	C1-C2-C3	2.37	118.99	113.64
24	2	601	CHL	C11-C10-C8	-2.37	108.26	115.92
34	D	404	BCR	C33-C5-C4	2.37	118.17	113.62
39	D	405	PL9	O1-C4-C3	-2.37	118.11	120.72
24	g	608	CHL	CMB-C2B-C3B	2.37	129.11	124.68
25	c	504	CLA	CMB-C2B-C3B	2.37	129.11	124.68
24	9	601	CHL	C1-C2-C3	-2.37	121.95	126.04
29	n	2630	LHG	C5-O7-C7	-2.37	111.96	117.79
24	3	606	CHL	C3B-C4B-NB	2.37	112.27	109.21
29	7	2630	LHG	C5-O7-C7	-2.37	111.97	117.79
26	2	1620	LUT	C21-C26-C27	-2.37	109.71	112.70

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	8	1622	XAT	C11-C10-C9	-2.36	123.94	127.31
26	S	1620	LUT	C8-C7-C6	-2.36	120.56	127.20
26	s	1621	LUT	C1-C2-C3	2.36	118.98	113.64
24	y	606	CHL	O2A-CGA-CBA	2.36	119.33	111.91
25	b	606	CLA	CMB-C2B-C3B	2.36	129.10	124.68
28	9	1623	NEX	C11-C12-C13	-2.36	119.78	126.42
25	1	610	CLA	CHB-C4A-NA	2.36	127.78	124.51
24	N	601	CHL	C11-C10-C8	-2.36	108.28	115.92
25	3	612	CLA	C2A-C1A-CHA	2.36	127.99	123.86
24	6	607	CHL	C11-C10-C8	-2.36	108.28	115.92
24	p	605	CHL	C4D-CHA-C1A	-2.36	118.38	121.25
28	Y	1623	NEX	C19-C9-C10	-2.36	119.61	122.92
25	5	610	CLA	CHB-C4A-NA	2.36	127.78	124.51
24	Y	606	CHL	O2A-CGA-CBA	2.36	119.32	111.91
29	G	2630	LHG	O8-C23-C24	2.36	119.31	111.91
26	y	1620	LUT	C16-C1-C6	-2.36	106.47	110.30
28	r	623	NEX	C40-C33-C32	2.36	121.80	118.08
24	8	605	CHL	CMB-C2B-C3B	2.36	129.09	124.68
25	B	606	CLA	CMB-C2B-C3B	2.36	129.09	124.68
25	B	606	CLA	CHB-C4A-NA	2.36	127.77	124.51
24	r	606	CHL	O2A-CGA-O1A	-2.36	117.64	123.59
26	6	1620	LUT	C35-C15-C14	-2.36	118.64	123.47
24	3	605	CHL	CMB-C2B-C3B	2.36	129.09	124.68
25	s	612	CLA	C2A-C1A-CHA	2.36	127.98	123.86
29	N	2630	LHG	C5-O7-C7	-2.36	111.99	117.79
24	R	606	CHL	O2A-CGA-O1A	-2.36	117.64	123.59
26	9	1621	LUT	C36-C21-C26	2.36	113.12	109.55
25	1	610	CLA	O2A-CGA-O1A	-2.36	117.64	123.59
24	R	606	CHL	O1D-CGD-CBD	-2.36	119.66	124.48
28	4	1623	NEX	C35-C34-C33	-2.36	123.95	127.31
28	7	1623	NEX	C28-C29-C30	2.36	122.56	118.94
24	R	608	CHL	CMD-C2D-C3D	-2.36	122.19	127.61
24	p	601	CHL	O1D-CGD-CBD	-2.36	119.66	124.48
25	s	609	CLA	C1D-ND-C4D	-2.36	104.66	106.33
24	G	601	CHL	O1D-CGD-CBD	-2.36	119.66	124.48
29	g	2630	LHG	O8-C23-C24	2.36	119.30	111.91
24	N	605	CHL	CAA-C2A-C3A	-2.36	106.33	112.78
24	2	601	CHL	C11-C12-C13	-2.36	108.31	115.92
24	y	605	CHL	C1C-C2C-C3C	-2.36	105.25	107.11
24	q	605	CHL	CED-O2D-CGD	2.36	121.26	115.94
35	A	412	SQD	C45-O47-C7	-2.35	111.99	117.79
26	R	620	LUT	C11-C10-C9	-2.35	123.95	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	N	1623	NEX	C30-C31-C32	-2.35	115.87	123.22
26	q	1621	LUT	C15-C35-C34	-2.35	118.66	123.47
35	b	623	SQD	C45-O47-C7	-2.35	112.00	117.79
24	6	609	CHL	C1C-C2C-C3C	-2.35	105.25	107.11
35	a	412	SQD	C45-O47-C7	-2.35	112.00	117.79
24	8	605	CHL	CED-O2D-CGD	2.35	121.25	115.94
26	0	1620	LUT	C18-C5-C6	-2.35	121.89	124.53
24	n	601	CHL	C4D-CHA-C1A	-2.35	118.39	121.25
29	y	2630	LHG	C9-C8-C7	-2.35	105.07	113.62
25	5	602	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
25	5	612	CLA	C2A-C1A-CHA	2.35	127.97	123.86
24	q	601	CHL	C1-C2-C3	-2.35	121.98	126.04
28	p	1623	NEX	C11-C12-C13	-2.35	119.81	126.42
28	2	1623	NEX	C11-C12-C13	-2.35	119.81	126.42
25	c	509	CLA	O2D-CGD-O1D	-2.35	119.24	123.84
24	s	607	CHL	CMD-C2D-C3D	-2.35	122.21	127.61
25	9	612	CLA	CAA-C2A-C3A	-2.35	106.34	112.78
24	9	601	CHL	C11-C12-C13	-2.35	108.33	115.92
26	9	1621	LUT	C1-C2-C3	2.35	118.95	113.64
26	R	620	LUT	C8-C7-C6	-2.35	120.60	127.20
25	9	603	CLA	CMB-C2B-C3B	2.35	129.07	124.68
24	y	605	CHL	C1B-CHB-C4A	-2.35	125.47	130.12
26	g	1621	LUT	C8-C7-C6	-2.35	120.61	127.20
24	r	608	CHL	CMD-C2D-C3D	-2.35	122.21	127.61
27	6	1622	XAT	C28-C29-C30	2.35	122.54	118.94
26	s	1620	LUT	C8-C7-C6	-2.35	120.61	127.20
34	B	620	BCR	C29-C28-C27	-2.35	106.13	111.38
28	R	623	NEX	C40-C33-C32	2.35	121.77	118.08
24	6	601	CHL	C1-C2-C3	-2.35	121.99	126.04
25	n	603	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
24	Y	601	CHL	C1C-C2C-C3C	-2.35	105.25	107.11
24	Y	606	CHL	CHB-C4A-NA	2.34	127.75	124.51
35	b	621	SQD	O8-S-C6	2.34	109.48	105.74
24	1	605	CHL	C1C-C2C-C3C	-2.34	105.25	107.11
25	B	616	CLA	O2D-CGD-CBD	2.34	115.43	111.27
25	b	616	CLA	CAC-C3C-C4C	2.34	127.85	124.81
25	B	607	CLA	O2D-CGD-CBD	2.34	115.43	111.27
25	b	607	CLA	O2D-CGD-CBD	2.34	115.43	111.27
24	9	605	CHL	O2D-CGD-O1D	-2.34	119.26	123.84
24	8	601	CHL	O2A-CGA-CBA	2.34	119.26	111.91
33	A	409	PHO	O1D-CGD-CBD	2.34	128.64	124.74
28	9	1623	NEX	C24-C23-C22	-2.34	106.25	110.77

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	8	603	CLA	C2A-C1A-CHA	2.34	127.95	123.86
25	3	614	CLA	CHD-C1D-ND	-2.34	122.30	124.45
24	0	608	CHL	CHB-C4A-NA	2.34	127.75	124.51
24	r	607	CHL	OMC-CMC-C2C	-2.34	120.39	125.69
27	g	1622	XAT	C10-C11-C12	-2.34	115.92	123.22
25	2	604	CLA	CHD-C1D-ND	-2.34	122.30	124.45
24	3	606	CHL	CHD-C4C-C3C	-2.34	121.40	124.84
36	H	102	LMG	C6-C5-C4	-2.34	107.53	113.00
24	7	608	CHL	OMC-CMC-C2C	-2.34	120.40	125.69
24	q	609	CHL	C2A-C3A-C4A	-2.34	98.09	101.87
26	r	620	LUT	C8-C7-C6	-2.34	120.64	127.20
25	s	610	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
34	h	101	BCR	C16-C15-C14	-2.34	118.69	123.47
25	s	604	CLA	O2A-CGA-O1A	-2.34	117.69	123.59
28	s	1623	NEX	C11-C12-C13	-2.34	119.85	126.42
25	C	509	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
26	N	1620	LUT	C8-C7-C6	-2.34	120.64	127.20
24	2	605	CHL	O2D-CGD-O1D	-2.34	119.27	123.84
24	Y	609	CHL	C1-C2-C3	-2.34	122.00	126.04
24	N	601	CHL	O1D-CGD-CBD	-2.34	119.71	124.48
25	1	602	CLA	CHB-C4A-NA	2.34	127.74	124.51
25	S	604	CLA	O2A-CGA-O1A	-2.33	117.70	123.59
24	N	606	CHL	CMB-C2B-C3B	2.33	129.04	124.68
25	6	604	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
25	S	610	CLA	CHB-C4A-NA	2.33	127.74	124.51
25	s	610	CLA	CHB-C4A-NA	2.33	127.74	124.51
25	N	603	CLA	O2D-CGD-O1D	-2.33	119.28	123.84
25	y	602	CLA	CHB-C4A-NA	2.33	127.74	124.51
25	q	603	CLA	CAA-C2A-C3A	-2.33	106.39	112.78
35	B	621	SQD	O8-S-C6	2.33	109.46	105.74
25	7	604	CLA	CAC-C3C-C2C	-2.33	123.54	127.53
34	H	101	BCR	C16-C15-C14	-2.33	118.70	123.47
24	q	601	CHL	C4-C3-C5	2.33	119.19	115.27
24	G	606	CHL	C1C-C2C-C3C	-2.33	105.26	107.11
24	3	609	CHL	OMC-CMC-C2C	-2.33	120.42	125.69
26	p	1620	LUT	C36-C21-C26	2.33	113.08	109.55
25	Y	603	CLA	O2D-CGD-CBD	2.33	115.41	111.27
26	3	1620	LUT	C30-C31-C32	-2.33	115.94	123.22
34	C	517	BCR	C10-C11-C12	-2.33	115.95	123.22
26	2	1621	LUT	C38-C25-C24	-2.33	118.58	123.56
27	4	1622	XAT	C7-C8-C9	-2.33	121.92	125.53
25	C	507	CLA	CHA-C1A-NA	-2.33	121.07	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	y	601	CHL	O2D-CGD-O1D	-2.33	119.29	123.84
24	R	607	CHL	OMC-CMC-C2C	-2.33	120.42	125.69
25	b	616	CLA	O2D-CGD-CBD	2.33	115.40	111.27
25	6	604	CLA	CHB-C4A-NA	2.33	127.73	124.51
25	c	513	CLA	O2A-CGA-O1A	-2.33	117.72	123.59
25	n	614	CLA	CHD-C1D-ND	-2.33	122.32	124.45
28	7	1623	NEX	C15-C35-C34	-2.33	118.71	123.47
26	r	620	LUT	C11-C10-C9	-2.32	123.99	127.31
34	b	620	BCR	C29-C28-C27	-2.32	106.18	111.38
25	y	603	CLA	O2D-CGD-CBD	2.32	115.40	111.27
33	a	409	PHO	O1D-CGD-CBD	2.32	128.61	124.74
26	S	1621	LUT	C31-C30-C29	-2.32	124.00	127.31
24	4	601	CHL	C1-O2A-CGA	2.32	122.54	116.44
24	N	606	CHL	C2A-C1A-CHA	-2.32	119.80	123.86
26	Y	1620	LUT	C7-C8-C9	-2.32	122.73	126.23
26	4	1620	LUT	C31-C32-C33	-2.32	119.90	126.42
24	2	607	CHL	O2D-CGD-O1D	-2.32	119.30	123.84
25	R	601	CLA	CAA-C2A-C1A	2.32	119.57	111.97
24	2	601	CHL	C1-C2-C3	-2.32	122.03	126.04
24	n	606	CHL	C2A-C1A-CHA	-2.32	119.81	123.86
25	c	510	CLA	CHB-C4A-NA	2.32	127.72	124.51
24	r	607	CHL	C4-C3-C5	2.32	119.17	115.27
34	c	517	BCR	C10-C11-C12	-2.32	115.99	123.22
24	s	606	CHL	OMC-CMC-C2C	-2.32	120.45	125.69
24	5	601	CHL	C1-O2A-CGA	2.32	122.52	116.44
27	N	1622	XAT	C7-C8-C9	-2.32	121.94	125.53
29	D	409	LHG	O8-C23-C24	2.32	119.18	111.91
24	n	607	CHL	O1D-CGD-CBD	-2.32	119.75	124.48
24	q	609	CHL	O2A-CGA-CBA	2.32	119.17	111.91
24	Y	605	CHL	C1C-C2C-C3C	-2.31	105.28	107.11
39	D	405	PL9	C32-C33-C34	-2.31	122.09	127.66
39	d	405	PL9	C32-C33-C34	-2.31	122.09	127.66
28	n	1623	NEX	C30-C31-C32	-2.31	115.99	123.22
25	7	610	CLA	O2A-CGA-O1A	-2.31	117.75	123.59
26	q	1620	LUT	C19-C9-C8	2.31	121.72	118.08
25	R	604	CLA	O2D-CGD-O1D	-2.31	119.31	123.84
24	6	601	CHL	CHB-C4A-NA	2.31	127.71	124.51
26	G	1621	LUT	C8-C7-C6	-2.31	120.71	127.20
24	1	608	CHL	CMD-C2D-C3D	-2.31	122.30	127.61
26	s	1621	LUT	C31-C30-C29	-2.31	124.01	127.31
26	Y	1620	LUT	C2-C3-C4	-2.31	107.14	110.30
26	7	1620	LUT	C30-C31-C32	-2.31	116.01	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	G	606	CHL	CHB-C4A-NA	2.31	127.71	124.51
25	c	512	CLA	O2D-CGD-O1D	-2.31	119.32	123.84
29	r	2630	LHG	O8-C23-C24	2.31	119.15	111.91
36	C	521	LMG	C8-O7-C10	-2.31	112.11	117.79
25	9	614	CLA	CHB-C4A-NA	2.31	127.70	124.51
25	r	610	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
25	8	612	CLA	C2A-C1A-CHA	2.31	127.89	123.86
25	p	604	CLA	CHD-C1D-ND	-2.31	122.33	124.45
24	1	608	CHL	CHB-C4A-NA	2.31	127.70	124.51
24	7	605	CHL	O2D-CGD-O1D	-2.31	119.33	123.84
25	R	610	CLA	O2A-CGA-O1A	-2.31	117.77	123.59
26	1	1620	LUT	C30-C31-C32	-2.31	116.02	123.22
25	d	403	CLA	O2D-CGD-CBD	2.31	115.36	111.27
29	R	2630	LHG	O8-C23-C24	2.31	119.14	111.91
25	C	510	CLA	CHB-C4A-NA	2.31	127.70	124.51
24	7	609	CHL	O1D-CGD-CBD	-2.31	119.77	124.48
24	3	601	CHL	CMB-C2B-C3B	2.31	128.99	124.68
24	y	609	CHL	C1-C2-C3	-2.30	122.06	126.04
25	C	512	CLA	O2D-CGD-O1D	-2.30	119.33	123.84
24	6	601	CHL	C2A-C1A-CHA	-2.30	119.83	123.86
25	7	610	CLA	CHB-C4A-NA	2.30	127.70	124.51
24	Y	609	CHL	CMD-C2D-C3D	-2.30	122.31	127.61
36	c	521	LMG	C8-O7-C10	-2.30	112.12	117.79
25	2	612	CLA	CAA-C2A-C3A	-2.30	106.47	112.78
24	r	607	CHL	CMD-C2D-C3D	-2.30	122.32	127.61
25	S	609	CLA	C1D-ND-C4D	-2.30	104.70	106.33
24	4	601	CHL	O2D-CGD-O1D	-2.30	119.34	123.84
26	Y	1620	LUT	C16-C1-C6	-2.30	106.57	110.30
24	5	605	CHL	C1C-C2C-C3C	-2.30	105.29	107.11
24	N	601	CHL	C4D-CHA-C1A	-2.30	118.45	121.25
26	6	1620	LUT	C39-C29-C28	2.30	121.70	118.08
39	d	405	PL9	C36-C37-C38	-2.30	104.32	111.88
24	6	606	CHL	O2D-CGD-O1D	-2.30	119.34	123.84
24	9	601	CHL	C4-C3-C5	2.30	119.14	115.27
26	5	1620	LUT	C8-C9-C10	-2.30	115.41	118.94
39	D	405	PL9	C36-C37-C38	-2.30	104.32	111.88
28	5	1623	NEX	C11-C12-C13	-2.30	119.95	126.42
24	p	609	CHL	CHD-C4C-C3C	-2.30	121.46	124.84
24	R	606	CHL	C4A-NA-C1A	-2.30	105.67	106.71
28	G	1623	NEX	C11-C12-C13	-2.30	119.96	126.42
24	S	606	CHL	OMC-CMC-C2C	-2.30	120.49	125.69
24	6	607	CHL	CMD-C2D-C3D	-2.30	122.33	127.61

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	7	606	CHL	C1C-C2C-C3C	-2.30	105.29	107.11
25	R	616	CLA	CHD-C1D-ND	-2.30	122.34	124.45
25	N	610	CLA	CHB-C4A-NA	2.30	127.69	124.51
25	2	603	CLA	C2A-C1A-CHA	2.30	127.88	123.86
25	2	610	CLA	O2D-CGD-O1D	-2.30	119.35	123.84
26	5	1621	LUT	C20-C13-C12	2.30	121.70	118.08
24	S	601	CHL	O2A-CGA-CBA	2.30	121.41	114.03
24	y	606	CHL	CHB-C4A-NA	2.30	127.69	124.51
26	n	1620	LUT	C35-C15-C14	-2.30	118.77	123.47
28	5	1623	NEX	C35-C15-C14	-2.30	118.77	123.47
24	5	605	CHL	O1D-CGD-CBD	-2.30	119.79	124.48
24	r	606	CHL	C4A-NA-C1A	-2.30	105.67	106.71
25	r	616	CLA	CHD-C1D-ND	-2.29	122.34	124.45
29	q	2630	LHG	C5-O7-C7	-2.29	112.14	117.79
25	6	610	CLA	CHB-C4A-NA	2.29	127.68	124.51
37	c	520	DGD	C2G-O2G-C1B	-2.29	112.15	117.79
24	Y	605	CHL	C1B-CHB-C4A	-2.29	125.58	130.12
24	R	607	CHL	CMD-C2D-C3D	-2.29	122.34	127.61
24	n	601	CHL	O1D-CGD-CBD	-2.29	119.79	124.48
27	y	1622	XAT	C18-C5-C4	2.29	116.86	114.28
24	n	608	CHL	C1C-C2C-C3C	-2.29	105.30	107.11
25	2	614	CLA	CHB-C4A-NA	2.29	127.68	124.51
26	p	1621	LUT	C7-C8-C9	-2.29	122.78	126.23
25	7	602	CLA	CHB-C4A-NA	2.29	127.68	124.51
24	1	601	CHL	C4-C3-C5	2.29	119.12	115.27
34	c	514	BCR	C10-C11-C12	-2.29	116.07	123.22
24	p	606	CHL	CED-O2D-CGD	2.29	121.11	115.94
24	5	609	CHL	O2D-CGD-O1D	-2.29	119.36	123.84
24	1	609	CHL	CHB-C4A-NA	2.29	127.68	124.51
25	3	602	CLA	CHB-C4A-NA	2.29	127.68	124.51
24	4	607	CHL	OMC-CMC-C2C	-2.29	120.51	125.69
25	r	604	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
24	0	606	CHL	O2D-CGD-O1D	-2.29	119.37	123.84
24	g	606	CHL	C1C-C2C-C3C	-2.29	105.30	107.11
24	3	601	CHL	O1D-CGD-CBD	-2.29	119.81	124.48
24	G	607	CHL	CMD-C2D-C3D	-2.29	122.35	127.61
24	4	608	CHL	O1D-CGD-CBD	-2.29	119.81	124.48
27	7	1622	XAT	O4-C5-C6	-2.29	57.07	58.96
28	6	1623	NEX	C24-C23-C22	-2.29	106.36	110.77
34	C	514	BCR	C33-C5-C6	-2.29	121.96	124.53
34	B	620	BCR	C21-C20-C19	-2.29	116.08	123.22
24	6	609	CHL	O1D-CGD-CBD	-2.29	119.81	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	606	CHL	CHB-C4A-NA	2.29	127.67	124.51
25	b	610	CLA	O2D-CGD-O1D	-2.28	119.37	123.84
27	n	1622	XAT	C7-C8-C9	-2.28	121.98	125.53
24	N	607	CHL	C6-C5-C3	-2.28	107.47	113.45
24	5	605	CHL	C4D-CHA-C1A	-2.28	118.47	121.25
24	q	609	CHL	C1-O2A-CGA	2.28	122.44	116.44
27	8	1622	XAT	C31-C32-C33	-2.28	120.00	126.42
26	2	1621	LUT	C18-C5-C4	2.28	118.58	114.36
29	d	409	LHG	O8-C23-C24	2.28	119.07	111.91
28	q	1623	NEX	C17-C1-C6	-2.28	108.43	110.47
25	B	610	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
25	r	601	CLA	CAA-C2A-C1A	2.28	119.45	111.97
26	4	1620	LUT	C21-C26-C27	-2.28	109.82	112.70
25	2	602	CLA	CHB-C4A-NA	2.28	127.67	124.51
24	p	606	CHL	C4D-CHA-C1A	-2.28	118.47	121.25
25	q	604	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
25	S	610	CLA	O2D-CGD-CBD	2.28	115.32	111.27
35	B	623	SQD	C45-O47-C7	-2.28	112.18	117.79
25	D	403	CLA	O2D-CGD-CBD	2.28	115.32	111.27
25	1	611	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
25	7	611	CLA	O2D-CGD-O1D	-2.28	119.39	123.84
24	5	601	CHL	O2A-CGA-CBA	2.28	119.05	111.91
24	4	605	CHL	C1D-CHD-C4C	-2.28	121.15	126.06
25	c	507	CLA	CHA-C1A-NA	-2.28	121.19	126.40
24	q	605	CHL	C1D-CHD-C4C	-2.28	121.15	126.06
36	B	622	LMG	O8-C28-C29	2.28	119.05	111.91
24	2	606	CHL	CMB-C2B-C3B	2.28	128.94	124.68
25	C	502	CLA	C16-C15-C13	-2.28	108.56	115.92
24	0	601	CHL	O2A-CGA-O1A	-2.27	117.85	123.59
35	d	413	SQD	O48-C23-O10	-2.27	117.85	123.59
24	1	605	CHL	O2D-CGD-O1D	-2.27	119.39	123.84
37	C	520	DGD	C2G-O2G-C1B	-2.27	112.19	117.79
27	Y	1622	XAT	C18-C5-C4	2.27	116.84	114.28
25	s	605	CLA	CHB-C4A-NA	2.27	127.66	124.51
25	S	612	CLA	CHA-C1A-NA	-2.27	121.19	126.40
28	q	1623	NEX	C39-C29-C30	-2.27	119.74	122.92
25	p	614	CLA	CHB-C4A-NA	2.27	127.65	124.51
25	c	510	CLA	C6-C7-C8	-2.27	108.58	115.92
25	n	610	CLA	CHB-C4A-NA	2.27	127.65	124.51
27	G	1622	XAT	C10-C11-C12	-2.27	116.13	123.22
36	b	622	LMG	O8-C28-C29	2.27	119.03	111.91
28	g	1623	NEX	C19-C9-C10	-2.27	119.74	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	5	607	CHL	CMD-C2D-C3D	-2.27	122.39	127.61
28	q	1623	NEX	C4-C3-C2	-2.27	106.39	110.77
25	r	602	CLA	CHB-C4A-NA	2.27	127.65	124.51
25	s	612	CLA	CHA-C1A-NA	-2.27	121.20	126.40
24	s	601	CHL	O2A-CGA-CBA	2.27	121.32	114.03
28	N	1623	NEX	C19-C9-C10	-2.27	119.75	122.92
24	3	601	CHL	O2A-CGA-CBA	2.27	119.03	111.91
28	p	1623	NEX	C35-C15-C14	-2.27	118.83	123.47
24	0	605	CHL	OMC-CMC-C2C	-2.27	120.56	125.69
25	b	603	CLA	CHB-C4A-NA	2.27	127.65	124.51
25	c	503	CLA	C4-C3-C5	2.27	119.08	115.27
24	N	607	CHL	C4D-C3D-CAD	2.27	110.77	108.10
28	2	1623	NEX	C24-C23-C22	-2.26	106.40	110.77
24	n	607	CHL	C1C-C2C-C3C	-2.26	105.32	107.11
25	S	605	CLA	CHB-C4A-NA	2.26	127.64	124.51
26	Y	1620	LUT	C3-C4-C5	-2.26	107.34	111.85
28	N	1623	NEX	C28-C29-C30	2.26	122.42	118.94
24	y	601	CHL	CMB-C2B-C3B	2.26	128.91	124.68
24	6	608	CHL	CHB-C4A-NA	2.26	127.64	124.51
25	6	611	CLA	CHD-C1D-ND	-2.26	122.37	124.45
28	g	1623	NEX	C5-C4-C3	-2.26	109.07	111.75
24	5	605	CHL	C1-O2A-CGA	2.26	122.38	116.44
35	D	413	SQD	O48-C23-O10	-2.26	117.88	123.59
24	5	601	CHL	C6-C5-C3	2.26	119.39	113.45
24	4	606	CHL	O2A-CGA-O1A	-2.26	117.88	123.59
25	C	510	CLA	C6-C7-C8	-2.26	108.61	115.92
24	s	608	CHL	C1B-CHB-C4A	-2.26	125.64	130.12
36	d	412	LMG	C8-O7-C10	-2.26	112.22	117.79
25	8	604	CLA	CHD-C1D-ND	-2.26	122.38	124.45
26	3	1621	LUT	C16-C1-C6	-2.26	106.63	110.30
25	0	610	CLA	CHB-C4A-NA	2.26	127.64	124.51
26	0	1621	LUT	C3-C4-C5	-2.26	107.35	111.85
25	n	602	CLA	CHB-C4A-NA	2.26	127.64	124.51
29	p	2630	LHG	C5-O7-C7	-2.26	112.23	117.79
24	q	609	CHL	O1D-CGD-CBD	-2.26	119.86	124.48
25	c	502	CLA	CHC-C1C-C2C	-2.26	120.47	126.72
36	d	411	LMG	C8-O7-C10	-2.26	112.23	117.79
24	9	607	CHL	O2D-CGD-O1D	-2.26	119.42	123.84
27	1	1622	XAT	O4-C5-C6	-2.26	57.09	58.96
24	q	606	CHL	O2A-CGA-O1A	-2.26	117.90	123.59
36	D	412	LMG	C8-O7-C10	-2.26	112.23	117.79
27	5	1622	XAT	C25-C24-C23	2.26	117.21	112.75

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	B	623	SQD	O48-C23-C24	2.26	118.98	111.91
25	N	602	CLA	CHB-C4A-NA	2.25	127.63	124.51
25	C	513	CLA	O2A-CGA-O1A	-2.25	117.90	123.59
24	n	606	CHL	CMB-C2B-C3B	2.25	128.90	124.68
24	Y	605	CHL	CMD-C2D-C3D	-2.25	122.43	127.61
24	y	605	CHL	CMD-C2D-C3D	-2.25	122.43	127.61
24	2	606	CHL	O2A-CGA-O1A	-2.25	117.91	123.59
25	y	612	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
26	9	1620	LUT	C18-C5-C6	-2.25	122.00	124.53
35	b	623	SQD	O48-C23-C24	2.25	118.97	111.91
34	b	620	BCR	C21-C20-C19	-2.25	116.19	123.22
24	n	606	CHL	O1D-CGD-CBD	-2.25	119.88	124.48
26	5	1620	LUT	C8-C7-C6	-2.25	120.88	127.20
24	n	601	CHL	C4A-NA-C1A	-2.25	105.69	106.71
25	Y	612	CLA	O2A-CGA-O1A	-2.25	117.91	123.59
25	3	603	CLA	C2A-C1A-CHA	2.25	127.80	123.86
26	9	1620	LUT	C21-C26-C27	-2.25	109.86	112.70
24	q	608	CHL	CMD-C2D-C3D	-2.25	122.44	127.61
24	8	609	CHL	C4-C3-C5	2.25	119.06	115.27
26	N	1621	LUT	C1-C2-C3	2.25	118.72	113.64
24	G	606	CHL	C4A-NA-C1A	-2.25	105.69	106.71
24	Y	607	CHL	C1C-C2C-C3C	-2.25	105.33	107.11
26	n	1621	LUT	C1-C2-C3	2.25	118.72	113.64
29	5	2630	LHG	C5-O7-C7	-2.25	112.26	117.79
24	2	608	CHL	C1B-CHB-C4A	-2.25	125.67	130.12
25	B	614	CLA	CAA-C2A-C3A	-2.25	106.62	112.78
24	q	601	CHL	C1B-CHB-C4A	-2.25	125.67	130.12
25	S	609	CLA	CHB-C4A-NA	2.25	127.62	124.51
25	1	613	CLA	CAA-CBA-CGA	-2.25	106.69	113.25
25	R	602	CLA	CHB-C4A-NA	2.25	127.62	124.51
29	1	2630	LHG	C5-O7-C7	-2.25	112.26	117.79
34	c	517	BCR	C16-C17-C18	-2.25	124.11	127.31
25	r	601	CLA	O2D-CGD-O1D	-2.24	119.45	123.84
25	Y	604	CLA	CHB-C4A-NA	2.24	127.62	124.51
25	b	609	CLA	O2D-CGD-CBD	2.24	115.26	111.27
24	8	609	CHL	C2A-C1A-CHA	-2.24	119.94	123.86
24	g	606	CHL	CHB-C4A-NA	2.24	127.61	124.51
28	g	1623	NEX	C5-C6-C1	2.24	121.92	119.70
34	H	101	BCR	C3-C4-C5	-2.24	110.07	114.08
24	G	607	CHL	O2D-CGD-O1D	-2.24	119.45	123.84
25	C	502	CLA	CHC-C1C-C2C	-2.24	120.52	126.72
25	q	603	CLA	C2A-C1A-CHA	2.24	127.78	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	R	608	CHL	C11-C10-C8	-2.24	108.68	115.92
24	6	601	CHL	CMD-C2D-C3D	-2.24	122.46	127.61
24	7	607	CHL	C1-O2A-CGA	2.24	122.32	116.44
25	7	610	CLA	C1-C2-C3	-2.24	122.17	126.04
24	Y	605	CHL	O2D-CGD-O1D	-2.24	119.46	123.84
27	3	1622	XAT	O4-C5-C6	-2.24	57.11	58.96
25	N	614	CLA	CHD-C1D-ND	-2.24	122.40	124.45
24	N	608	CHL	C1C-C2C-C3C	-2.24	105.34	107.11
24	0	607	CHL	C1C-C2C-C3C	-2.24	105.34	107.11
25	B	609	CLA	O2D-CGD-CBD	2.24	115.25	111.27
25	q	612	CLA	C2A-C1A-CHA	2.24	127.77	123.86
34	c	516	BCR	C34-C9-C8	2.24	121.60	118.08
34	h	101	BCR	C3-C4-C5	-2.24	110.08	114.08
24	0	608	CHL	O2D-CGD-O1D	-2.24	119.46	123.84
24	p	609	CHL	O2D-CGD-O1D	-2.24	119.46	123.84
24	Y	607	CHL	O2A-C1-C2	2.24	114.52	108.64
25	c	502	CLA	C16-C15-C13	-2.24	108.69	115.92
24	7	609	CHL	CHB-C4A-NA	2.24	127.61	124.51
24	y	607	CHL	C1C-C2C-C3C	-2.24	105.34	107.11
36	D	411	LMG	C8-O7-C10	-2.24	112.28	117.79
24	N	608	CHL	CMB-C2B-C3B	2.24	128.86	124.68
25	y	604	CLA	CHD-C1D-ND	-2.24	122.40	124.45
26	9	1620	LUT	C31-C30-C29	-2.24	124.12	127.31
25	b	614	CLA	CAA-C2A-C3A	-2.24	106.66	112.78
24	Y	609	CHL	CAC-C3C-C4C	2.24	127.71	124.81
25	3	604	CLA	CHD-C1D-ND	-2.24	122.40	124.45
26	s	1621	LUT	C39-C29-C28	2.23	121.60	118.08
24	g	609	CHL	O1D-CGD-CBD	-2.23	119.91	124.48
28	p	1623	NEX	C24-C23-C22	-2.23	106.46	110.77
26	8	1620	LUT	C18-C5-C6	-2.23	122.02	124.53
25	R	604	CLA	CHD-C1D-ND	-2.23	122.40	124.45
26	S	1621	LUT	C39-C29-C28	2.23	121.60	118.08
27	0	1622	XAT	C35-C34-C33	-2.23	124.12	127.31
26	9	1620	LUT	C20-C13-C14	-2.23	119.80	122.92
24	N	606	CHL	O1D-CGD-CBD	-2.23	119.92	124.48
25	C	511	CLA	CAA-CBA-CGA	-2.23	106.73	113.25
28	4	1623	NEX	C24-C23-C22	-2.23	106.46	110.77
24	r	608	CHL	C11-C10-C8	-2.23	108.70	115.92
24	n	609	CHL	CAA-C2A-C3A	-2.23	106.67	112.78
24	0	609	CHL	CED-O2D-CGD	2.23	120.98	115.94
26	q	1620	LUT	C15-C35-C34	-2.23	118.90	123.47
25	S	602	CLA	O2D-CGD-CBD	2.23	115.23	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	N	601	CHL	C4D-C3D-CAD	2.23	110.72	108.10
24	G	606	CHL	C2A-C1A-CHA	-2.23	119.96	123.86
34	d	404	BCR	C23-C24-C25	-2.23	120.94	127.20
24	2	601	CHL	OMC-CMC-C2C	-2.23	120.65	125.69
26	4	1620	LUT	C7-C8-C9	-2.23	122.87	126.23
24	r	606	CHL	CAA-CBA-CGA	-2.23	106.75	113.25
25	8	602	CLA	CHB-C4A-NA	2.23	127.59	124.51
34	C	514	BCR	C10-C11-C12	-2.23	116.27	123.22
24	y	605	CHL	O2D-CGD-O1D	-2.23	119.49	123.84
25	y	602	CLA	CAA-CBA-CGA	-2.23	106.75	113.25
27	Y	1622	XAT	C10-C11-C12	-2.23	116.27	123.22
25	y	613	CLA	C2D-C1D-ND	-2.23	108.46	110.10
34	b	620	BCR	C39-C30-C25	-2.23	106.69	110.30
24	n	608	CHL	CMB-C2B-C3B	2.22	128.84	124.68
36	h	102	LMG	O8-C28-O10	-2.22	117.98	123.59
24	G	606	CHL	CED-O2D-CGD	2.22	120.96	115.94
24	2	601	CHL	O2A-CGA-CBA	2.22	118.88	111.91
34	C	516	BCR	C34-C9-C8	2.22	121.58	118.08
24	6	608	CHL	O2D-CGD-O1D	-2.22	119.49	123.84
26	0	1620	LUT	C39-C29-C28	2.22	121.58	118.08
25	b	603	CLA	C2A-C1A-CHA	2.22	127.74	123.86
27	G	1622	XAT	C11-C10-C9	-2.22	124.14	127.31
24	N	609	CHL	CAA-C2A-C3A	-2.22	106.70	112.78
26	n	1621	LUT	C30-C31-C32	-2.22	116.29	123.22
36	H	102	LMG	O8-C28-O10	-2.22	117.99	123.59
24	s	608	CHL	O2D-CGD-O1D	-2.22	119.50	123.84
25	9	602	CLA	CHD-C1D-ND	-2.22	122.42	124.45
24	g	606	CHL	CED-O2D-CGD	2.22	120.95	115.94
24	r	607	CHL	C7-C6-C5	-2.22	107.33	113.36
24	1	601	CHL	O2A-CGA-CBA	2.22	118.87	111.91
24	8	606	CHL	C1C-C2C-C3C	-2.22	105.35	107.11
25	S	614	CLA	CHB-C4A-NA	2.22	127.58	124.51
34	D	404	BCR	C23-C24-C25	-2.22	120.97	127.20
26	0	1620	LUT	C19-C9-C8	2.22	121.57	118.08
25	g	603	CLA	CMB-C2B-C3B	2.22	128.83	124.68
34	b	619	BCR	C39-C30-C25	-2.22	106.70	110.30
28	4	1623	NEX	C27-C28-C29	-2.22	122.09	125.53
24	8	607	CHL	CAA-C2A-C3A	-2.22	106.71	112.78
24	1	606	CHL	C4-C3-C5	2.22	119.00	115.27
25	G	610	CLA	CHD-C1D-ND	-2.22	122.42	124.45
24	N	607	CHL	C1C-C2C-C3C	-2.22	105.36	107.11
24	7	601	CHL	C4D-CHA-C1A	-2.22	118.55	121.25

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	7	1623	NEX	C30-C31-C32	-2.22	116.30	123.22
33	a	409	PHO	O2D-CGD-CBD	2.22	113.80	111.00
24	S	601	CHL	O2A-CGA-O1A	-2.22	117.78	123.30
24	5	606	CHL	C4D-CHA-C1A	-2.21	118.55	121.25
27	2	1622	XAT	C7-C8-C9	-2.21	122.09	125.53
33	A	409	PHO	O2D-CGD-CBD	2.21	113.80	111.00
28	y	1623	NEX	C5-C4-C3	-2.21	109.12	111.75
24	q	601	CHL	C1-O2A-CGA	2.21	122.25	116.44
24	G	608	CHL	C4D-CHA-C1A	-2.21	118.56	121.25
26	q	1620	LUT	C10-C11-C12	-2.21	116.31	123.22
25	G	603	CLA	CMB-C2B-C3B	2.21	128.82	124.68
25	Y	604	CLA	CHD-C1D-ND	-2.21	122.42	124.45
26	G	1620	LUT	C8-C7-C6	-2.21	120.99	127.20
24	R	606	CHL	CAA-CBA-CGA	-2.21	106.79	113.25
26	p	1621	LUT	C36-C21-C26	2.21	112.89	109.55
26	Y	1621	LUT	C31-C30-C29	-2.21	124.16	127.31
26	p	1621	LUT	C16-C1-C6	-2.21	106.71	110.30
28	4	1623	NEX	C4-C3-C2	-2.21	106.50	110.77
25	s	609	CLA	CHB-C4A-NA	2.21	127.57	124.51
25	1	604	CLA	CMB-C2B-C1B	-2.21	125.07	128.46
27	0	1622	XAT	C31-C32-C33	-2.21	120.21	126.42
26	r	620	LUT	C38-C25-C24	-2.21	118.83	123.56
24	5	609	CHL	O1D-CGD-CBD	-2.21	119.97	124.48
37	c	518	DGD	O3G-C3G-C2G	-2.21	105.57	110.90
26	n	1620	LUT	C7-C8-C9	-2.21	122.90	126.23
34	C	517	BCR	C33-C5-C6	-2.21	122.05	124.53
26	q	1620	LUT	C21-C26-C27	-2.21	109.91	112.70
24	N	607	CHL	O1D-CGD-CBD	-2.21	119.97	124.48
28	g	1623	NEX	C20-C13-C14	-2.21	119.83	122.92
25	n	602	CLA	CAA-CBA-CGA	-2.21	106.81	113.25
24	y	606	CHL	O1D-CGD-CBD	-2.21	119.97	124.48
25	y	604	CLA	CHB-C4A-NA	2.21	127.56	124.51
34	B	619	BCR	C39-C30-C25	-2.21	106.72	110.30
26	8	1620	LUT	C30-C31-C32	-2.21	116.33	123.22
25	6	611	CLA	C1-C2-C3	-2.21	122.23	126.04
26	y	1620	LUT	C7-C8-C9	-2.20	122.90	126.23
25	n	603	CLA	CBC-CAC-C3C	-2.20	106.36	112.43
25	R	601	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
24	8	605	CHL	O2A-CGA-O1A	-2.20	118.03	123.59
24	Y	606	CHL	O1D-CGD-CBD	-2.20	119.97	124.48
24	q	601	CHL	O1D-CGD-CBD	-2.20	119.98	124.48
26	7	1621	LUT	C31-C30-C29	-2.20	124.17	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	2	1623	NEX	C31-C30-C29	-2.20	124.17	127.31
25	g	610	CLA	CHD-C1D-ND	-2.20	122.43	124.45
24	5	601	CHL	C4D-CHA-C1A	-2.20	118.57	121.25
24	3	601	CHL	O2D-CGD-O1D	-2.20	119.53	123.84
24	8	601	CHL	O2D-CGD-O1D	-2.20	119.53	123.84
25	4	604	CLA	O2A-CGA-O1A	-2.20	118.03	123.59
28	2	1623	NEX	O24-C25-C38	2.20	117.69	115.06
25	s	614	CLA	CHB-C4A-NA	2.20	127.56	124.51
27	q	1622	XAT	C24-C23-C22	-2.20	106.52	110.77
25	g	613	CLA	O2D-CGD-O1D	-2.20	119.53	123.84
26	5	1621	LUT	C36-C21-C26	2.20	112.88	109.55
34	b	620	BCR	C34-C9-C10	-2.20	119.84	122.92
37	C	518	DGD	O1G-C1A-O1A	-2.20	118.04	123.59
34	B	620	BCR	C39-C30-C25	-2.20	106.73	110.30
27	G	1622	XAT	C30-C31-C32	-2.20	116.36	123.22
37	C	518	DGD	O3G-C3G-C2G	-2.20	105.60	110.90
24	S	608	CHL	C1B-CHB-C4A	-2.20	125.77	130.12
27	9	1622	XAT	C4-C3-C2	-2.20	106.53	110.77
24	0	607	CHL	CMD-C2D-C3D	-2.20	122.56	127.61
24	2	606	CHL	C1B-CHB-C4A	-2.20	125.77	130.12
26	y	1621	LUT	C31-C30-C29	-2.20	124.18	127.31
24	4	601	CHL	CMD-C2D-C3D	-2.20	122.56	127.61
24	5	605	CHL	C7-C6-C5	-2.20	107.40	113.36
28	q	1623	NEX	C24-C23-C22	-2.20	106.53	110.77
24	n	605	CHL	O1D-CGD-CBD	-2.19	119.99	124.48
39	d	405	PL9	C42-C43-C44	-2.19	122.38	127.66
26	3	1621	LUT	C35-C15-C14	-2.19	118.98	123.47
24	g	605	CHL	C4D-CHA-C1A	-2.19	118.58	121.25
25	r	604	CLA	CHD-C1D-ND	-2.19	122.44	124.45
26	1	1621	LUT	C16-C1-C6	-2.19	106.74	110.30
34	c	514	BCR	C33-C5-C6	-2.19	122.06	124.53
25	y	614	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
24	s	608	CHL	C4D-CHA-C1A	-2.19	118.58	121.25
25	B	603	CLA	CHB-C4A-NA	2.19	127.54	124.51
26	s	1621	LUT	C30-C31-C32	-2.19	116.38	123.22
24	Y	601	CHL	CMB-C2B-C3B	2.19	128.78	124.68
24	8	601	CHL	C4-C3-C5	2.19	118.96	115.27
25	R	602	CLA	CAA-CBA-CGA	-2.19	106.85	113.25
37	c	519	DGD	O1G-C1A-O1A	-2.19	118.06	123.59
24	p	609	CHL	O1D-CGD-CBD	-2.19	120.00	124.48
28	G	1623	NEX	C5-C6-C1	2.19	121.87	119.70
24	r	608	CHL	CHB-C4A-NA	2.19	127.54	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
34	h	101	BCR	C8-C9-C10	2.19	122.30	118.94
24	6	605	CHL	O1D-CGD-CBD	-2.19	120.00	124.48
26	8	1620	LUT	C38-C25-C24	-2.19	118.87	123.56
24	g	601	CHL	CMB-C2B-C3B	2.19	128.77	124.68
26	5	1621	LUT	C31-C30-C29	-2.19	124.19	127.31
25	Y	614	CLA	O2A-CGA-O1A	-2.19	118.07	123.59
24	4	607	CHL	C2A-C3A-C4A	-2.19	98.33	101.87
24	n	601	CHL	C4D-C3D-CAD	2.19	110.67	108.10
24	q	608	CHL	OMC-CMC-C2C	-2.19	120.74	125.69
26	3	1620	LUT	C19-C9-C8	2.19	121.52	118.08
34	C	517	BCR	C36-C18-C19	2.19	121.52	118.08
24	r	608	CHL	C1C-C2C-C3C	-2.19	105.38	107.11
27	y	1622	XAT	C10-C11-C12	-2.19	116.39	123.22
24	S	608	CHL	O2D-CGD-O1D	-2.19	119.56	123.84
24	8	606	CHL	O1D-CGD-CBD	-2.19	120.01	124.48
24	q	607	CHL	OMC-CMC-C2C	-2.19	120.74	125.69
26	R	620	LUT	C38-C25-C24	-2.19	118.88	123.56
24	G	601	CHL	CMB-C2B-C3B	2.19	128.77	124.68
24	2	607	CHL	C4A-NA-C1A	2.19	107.69	106.71
24	4	605	CHL	C4A-NA-C1A	2.19	107.69	106.71
26	q	1620	LUT	C18-C5-C6	-2.19	122.07	124.53
40	f	101	HEM	CMB-C2B-C1B	-2.19	121.71	125.04
27	R	622	XAT	O24-C25-C26	-2.19	57.15	58.96
34	c	517	BCR	C36-C18-C19	2.18	121.52	118.08
25	C	511	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
25	r	602	CLA	CAA-CBA-CGA	-2.18	106.87	113.25
24	y	609	CHL	O1D-CGD-CBD	-2.18	120.02	124.48
26	Y	1620	LUT	C35-C15-C14	-2.18	119.00	123.47
24	s	601	CHL	O2A-CGA-O1A	-2.18	117.86	123.30
26	y	1620	LUT	C21-C26-C27	-2.18	109.94	112.70
25	Y	602	CLA	CAA-CBA-CGA	-2.18	106.87	113.25
24	1	607	CHL	C1-O2A-CGA	2.18	122.17	116.44
26	9	1620	LUT	C16-C1-C6	-2.18	106.76	110.30
24	9	609	CHL	CAA-CBA-CGA	-2.18	106.87	113.25
37	C	519	DGD	O1G-C1A-O1A	-2.18	118.08	123.59
25	5	613	CLA	CHD-C1D-ND	-2.18	122.45	124.45
24	6	601	CHL	C11-C10-C8	-2.18	108.87	115.92
24	1	609	CHL	O2D-CGD-O1D	-2.18	119.58	123.84
24	3	606	CHL	O1D-CGD-CBD	-2.18	120.02	124.48
26	q	1620	LUT	C8-C7-C6	-2.18	121.08	127.20
25	G	610	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
25	5	604	CLA	CHD-C1D-ND	-2.18	122.45	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	D	405	PL9	C42-C43-C44	-2.18	122.41	127.66
24	g	607	CHL	C1B-CHB-C4A	-2.18	125.80	130.12
25	S	604	CLA	O2D-CGD-O1D	-2.18	119.58	123.84
25	p	614	CLA	O2A-CGA-O1A	-2.18	118.09	123.59
25	G	603	CLA	CAA-CBA-CGA	-2.18	106.89	113.25
25	B	604	CLA	CHB-C4A-NA	2.18	127.53	124.51
26	N	1620	LUT	C31-C30-C29	-2.18	124.20	127.31
27	8	1622	XAT	O4-C5-C6	-2.18	57.16	58.96
25	b	616	CLA	C11-C12-C13	-2.18	108.88	115.92
25	5	602	CLA	CHD-C1D-ND	-2.18	122.45	124.45
26	5	1621	LUT	C10-C11-C12	-2.18	116.42	123.22
29	y	2630	LHG	O8-C23-O10	-2.18	118.10	123.59
24	y	609	CHL	CMD-C2D-C3D	-2.18	122.61	127.61
40	F	101	HEM	CBA-CAA-C2A	-2.18	108.91	112.62
26	g	1620	LUT	C8-C7-C6	-2.18	121.09	127.20
26	3	1620	LUT	C38-C25-C24	-2.18	118.90	123.56
24	y	609	CHL	CAC-C3C-C4C	2.18	127.63	124.81
26	n	1621	LUT	C10-C11-C12	-2.18	116.43	123.22
25	y	614	CLA	CHD-C1D-ND	-2.18	122.45	124.45
24	4	605	CHL	O2D-CGD-O1D	-2.17	119.59	123.84
27	7	1622	XAT	O24-C25-C26	-2.17	57.16	58.96
28	n	1623	NEX	C28-C29-C30	2.17	122.28	118.94
24	q	609	CHL	C1C-C2C-C3C	-2.17	105.39	107.11
25	B	603	CLA	C2A-C1A-CHA	2.17	127.66	123.86
26	N	1621	LUT	C30-C31-C32	-2.17	116.43	123.22
24	S	608	CHL	C4D-CHA-C1A	-2.17	118.60	121.25
26	2	1620	LUT	C16-C1-C6	-2.17	106.77	110.30
27	g	1622	XAT	C30-C31-C32	-2.17	116.44	123.22
24	9	606	CHL	O2A-CGA-O1A	-2.17	118.11	123.59
25	s	604	CLA	O2D-CGD-O1D	-2.17	119.59	123.84
25	8	611	CLA	CHD-C1D-ND	-2.17	122.46	124.45
26	G	1621	LUT	C3-C4-C5	-2.17	107.53	111.85
26	y	1620	LUT	C35-C15-C14	-2.17	119.03	123.47
25	B	605	CLA	CHB-C4A-NA	2.17	127.51	124.51
26	S	1621	LUT	C30-C31-C32	-2.17	116.44	123.22
37	C	524	DGD	C6D-C5D-C4D	-2.17	107.56	112.09
24	0	605	CHL	O1D-CGD-CBD	-2.17	120.05	124.48
25	b	604	CLA	CHB-C4A-NA	2.17	127.51	124.51
27	p	1622	XAT	C31-C30-C29	-2.17	124.22	127.31
28	q	1623	NEX	C35-C34-C33	-2.17	124.22	127.31
25	g	610	CLA	O2A-CGA-O1A	-2.17	118.12	123.59
25	b	612	CLA	CHB-C4A-NA	2.17	127.51	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	p	605	CHL	O2A-CGA-CBA	2.17	118.71	111.91
26	2	1620	LUT	C18-C5-C6	-2.17	122.09	124.53
24	Y	609	CHL	O1D-CGD-CBD	-2.17	120.05	124.48
34	a	411	BCR	C20-C21-C22	-2.17	124.22	127.31
26	5	1620	LUT	C35-C15-C14	-2.17	119.03	123.47
25	S	605	CLA	C1-C2-C3	-2.17	123.25	126.75
25	b	606	CLA	O2D-CGD-O1D	-2.17	119.60	123.84
25	3	613	CLA	CHD-C1D-ND	-2.17	122.46	124.45
24	5	609	CHL	CHD-C4C-C3C	-2.17	121.66	124.84
26	7	1621	LUT	C36-C21-C26	2.17	112.83	109.55
34	c	517	BCR	C33-C5-C6	-2.16	122.10	124.53
37	c	518	DGD	O1G-C1A-O1A	-2.16	118.13	123.59
26	6	1620	LUT	C30-C31-C32	-2.16	116.46	123.22
24	R	608	CHL	CHB-C4A-NA	2.16	127.50	124.51
33	a	408	PHO	C1B-NB-C4B	2.16	111.53	107.09
27	8	1622	XAT	C24-C23-C22	-2.16	106.59	110.77
28	y	1623	NEX	C11-C12-C13	-2.16	120.34	126.42
25	7	613	CLA	CAA-CBA-CGA	-2.16	106.93	113.25
25	g	603	CLA	CAA-CBA-CGA	-2.16	106.93	113.25
24	g	606	CHL	C2A-C1A-CHA	-2.16	120.08	123.86
25	B	606	CLA	O2D-CGD-O1D	-2.16	119.61	123.84
28	9	1623	NEX	C26-C27-C28	-2.16	121.42	125.99
27	6	1622	XAT	C39-C29-C30	-2.16	119.89	122.92
24	p	606	CHL	CMB-C2B-C3B	2.16	128.72	124.68
25	B	612	CLA	CHB-C4A-NA	2.16	127.50	124.51
25	b	605	CLA	CHB-C4A-NA	2.16	127.50	124.51
28	p	1623	NEX	C30-C31-C32	-2.16	116.47	123.22
24	3	606	CHL	C4D-CHA-C1A	-2.16	118.62	121.25
24	N	609	CHL	C1D-CHD-C4C	-2.16	121.40	126.06
26	0	1620	LUT	C10-C11-C12	-2.16	116.48	123.22
24	1	608	CHL	C1B-CHB-C4A	-2.16	125.84	130.12
24	6	605	CHL	OMC-CMC-C2C	-2.16	120.81	125.69
24	4	609	CHL	C4-C3-C5	2.16	118.90	115.27
27	9	1622	XAT	C7-C8-C9	-2.16	122.18	125.53
25	g	604	CLA	CHD-C1D-ND	-2.16	122.47	124.45
34	C	517	BCR	C16-C17-C18	-2.16	124.23	127.31
24	p	606	CHL	CHD-C4C-C3C	-2.16	121.67	124.84
34	h	101	BCR	C37-C22-C21	-2.16	119.90	122.92
25	g	614	CLA	CHD-C1D-ND	-2.16	122.47	124.45
28	G	1623	NEX	C28-C29-C30	2.16	122.25	118.94
24	R	608	CHL	C1C-C2C-C3C	-2.16	105.40	107.11
25	2	611	CLA	O2A-CGA-O1A	-2.16	117.92	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	B	616	CLA	C11-C12-C13	-2.16	108.95	115.92
33	A	408	PHO	OBD-CAD-CBD	-2.16	122.66	125.82
26	3	1621	LUT	C39-C29-C28	2.16	121.47	118.08
25	9	611	CLA	O2A-CGA-O1A	-2.15	117.93	123.30
28	g	1623	NEX	C26-C27-C28	-2.15	121.44	125.99
25	0	603	CLA	CHD-C1D-ND	-2.15	122.47	124.45
26	8	1621	LUT	C16-C1-C6	-2.15	106.81	110.30
24	n	609	CHL	CBC-CAC-C3C	-2.15	106.50	112.43
26	4	1620	LUT	C8-C7-C6	-2.15	121.16	127.20
26	G	1621	LUT	C35-C15-C14	-2.15	119.06	123.47
26	y	1621	LUT	C21-C26-C27	-2.15	109.98	112.70
25	C	505	CLA	C7-C6-C5	-2.15	107.52	113.36
24	g	607	CHL	O2D-CGD-O1D	-2.15	119.63	123.84
26	4	1621	LUT	C15-C35-C34	-2.15	119.07	123.47
25	c	505	CLA	C7-C6-C5	-2.15	107.52	113.36
24	y	609	CHL	C2A-C1A-CHA	-2.15	120.10	123.86
24	3	605	CHL	C1-C2-C3	-2.15	122.33	126.04
24	y	601	CHL	C3A-C2A-C1A	-2.15	98.12	101.34
24	p	609	CHL	C1B-CHB-C4A	-2.15	125.86	130.12
24	n	609	CHL	C1D-CHD-C4C	-2.15	121.42	126.06
33	A	408	PHO	C1B-NB-C4B	2.15	111.50	107.09
24	3	601	CHL	C4-C3-C5	2.15	118.88	115.27
34	b	620	BCR	C38-C26-C25	-2.15	122.12	124.53
25	3	611	CLA	CHD-C1D-ND	-2.15	122.48	124.45
27	y	1622	XAT	C19-C9-C8	2.15	121.46	118.08
24	1	608	CHL	OMC-CMC-C2C	-2.14	120.84	125.69
27	2	1622	XAT	C4-C3-C2	-2.14	106.63	110.77
24	G	605	CHL	C4D-CHA-C1A	-2.14	118.64	121.25
24	n	607	CHL	C4D-CHA-C1A	-2.14	118.64	121.25
25	b	607	CLA	CAA-CBA-CGA	-2.14	106.99	113.25
24	g	608	CHL	C4D-CHA-C1A	-2.14	118.64	121.25
24	G	607	CHL	C1C-C2C-C3C	-2.14	105.41	107.11
25	N	602	CLA	CAA-CBA-CGA	-2.14	106.99	113.25
24	Y	609	CHL	C2A-C1A-CHA	-2.14	120.11	123.86
25	Y	614	CLA	CHD-C1D-ND	-2.14	122.48	124.45
25	0	610	CLA	CHD-C1D-ND	-2.14	122.48	124.45
25	5	614	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
24	7	601	CHL	O2A-CGA-CBA	2.14	118.63	111.91
26	p	1620	LUT	C10-C11-C12	-2.14	116.53	123.22
26	N	1621	LUT	C10-C11-C12	-2.14	116.54	123.22
27	1	1622	XAT	C40-C33-C34	-2.14	119.92	122.92
37	c	524	DGD	C6D-C5D-C4D	-2.14	107.62	112.09

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	6	601	CHL	C11-C12-C13	-2.14	109.00	115.92
36	S	2631	LMG	C8-O7-C10	-2.14	112.52	117.79
24	p	609	CHL	CHB-C4A-NA	2.14	127.47	124.51
24	5	607	CHL	O2D-CGD-O1D	-2.14	119.66	123.84
25	9	604	CLA	CHD-C1D-ND	-2.14	122.49	124.45
26	G	1621	LUT	C19-C9-C8	2.14	121.44	118.08
26	5	1621	LUT	C18-C5-C6	-2.14	122.13	124.53
34	a	411	BCR	C33-C5-C4	2.14	117.72	113.62
24	G	609	CHL	O1D-CGD-CBD	-2.14	120.11	124.48
24	N	609	CHL	CHB-C4A-NA	2.14	127.47	124.51
40	F	101	HEM	CBD-CAD-C3D	-2.14	106.69	112.63
33	a	408	PHO	OBD-CAD-CBD	-2.13	122.69	125.82
24	1	601	CHL	C4D-CHA-C1A	-2.13	118.65	121.25
40	F	101	HEM	CMB-C2B-C1B	-2.13	121.79	125.04
25	2	602	CLA	C1-C2-C3	-2.13	122.35	126.04
25	b	605	CLA	O2D-CGD-CBD	2.13	115.06	111.27
25	Y	613	CLA	C2D-C1D-ND	-2.13	108.53	110.10
24	4	605	CHL	CED-O2D-CGD	2.13	120.76	115.94
34	H	101	BCR	C37-C22-C21	-2.13	119.93	122.92
27	r	622	XAT	O24-C25-C26	-2.13	57.19	58.96
24	G	607	CHL	C1B-CHB-C4A	-2.13	125.89	130.12
24	8	608	CHL	C4D-C3D-CAD	2.13	110.61	108.10
24	8	609	CHL	O2D-CGD-O1D	-2.13	119.67	123.84
24	N	607	CHL	C4D-CHA-C1A	-2.13	118.65	121.25
25	B	617	CLA	C2A-C1A-CHA	2.13	127.59	123.86
33	a	408	PHO	C16-C15-C13	-2.13	109.03	115.92
24	1	609	CHL	O1D-CGD-CBD	-2.13	120.12	124.48
24	6	601	CHL	O2A-CGA-O1A	-2.13	118.21	123.59
24	n	609	CHL	CHB-C4A-NA	2.13	127.46	124.51
26	Y	1621	LUT	C21-C26-C27	-2.13	110.01	112.70
24	8	607	CHL	CAC-C3C-C4C	2.13	127.58	124.81
28	g	1623	NEX	C17-C1-C6	-2.13	108.56	110.47
26	0	1620	LUT	C8-C7-C6	-2.13	121.22	127.20
24	g	601	CHL	C4D-C3D-CAD	2.13	110.61	108.10
25	p	613	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
24	9	601	CHL	CHD-C4C-C3C	-2.13	121.71	124.84
27	N	1622	XAT	C40-C33-C32	2.13	121.43	118.08
25	B	605	CLA	O2D-CGD-CBD	2.13	115.05	111.27
25	p	610	CLA	O2A-CGA-O1A	-2.13	118.22	123.59
25	7	612	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
24	9	609	CHL	O2D-CGD-O1D	-2.13	119.68	123.84
28	Y	1623	NEX	O24-C25-C26	-2.12	57.20	58.96

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	608	CHL	C2A-C1A-CHA	-2.12	120.14	123.86
26	p	1620	LUT	C15-C35-C34	-2.12	119.12	123.47
33	A	408	PHO	C16-C15-C13	-2.12	109.05	115.92
27	1	1622	XAT	O24-C25-C26	-2.12	57.20	58.96
24	6	605	CHL	C4D-CHA-C1A	-2.12	118.66	121.25
24	p	601	CHL	C2A-C1A-CHA	-2.12	120.15	123.86
26	0	1621	LUT	C18-C5-C4	2.12	118.29	114.36
24	y	608	CHL	C2A-C1A-CHA	-2.12	120.15	123.86
34	D	404	BCR	C30-C25-C26	-2.12	119.62	122.61
34	C	515	BCR	C36-C18-C19	2.12	121.42	118.08
25	G	611	CLA	O2A-CGA-O1A	-2.12	118.01	123.30
24	1	606	CHL	CAA-C2A-C3A	-2.12	106.97	112.78
28	7	1623	NEX	C17-C1-C6	-2.12	108.57	110.47
24	p	605	CHL	C1-O2A-CGA	2.12	122.01	116.44
26	G	1620	LUT	C2-C3-C4	2.12	113.21	110.30
25	C	508	CLA	CHD-C4C-NC	2.12	127.54	124.20
34	C	517	BCR	C33-C5-C4	2.12	117.69	113.62
25	B	607	CLA	CAA-CBA-CGA	-2.12	107.06	113.25
34	A	411	BCR	C33-C5-C4	2.12	117.69	113.62
24	4	606	CHL	CED-O2D-CGD	2.12	120.73	115.94
25	g	611	CLA	O2A-CGA-O1A	-2.12	118.02	123.30
26	Y	1621	LUT	C30-C31-C32	-2.12	116.61	123.22
24	6	606	CHL	O1D-CGD-CBD	-2.12	120.15	124.48
24	3	608	CHL	O2D-CGD-O1D	-2.12	119.70	123.84
24	8	608	CHL	O2D-CGD-O1D	-2.12	119.70	123.84
25	c	508	CLA	CHD-C4C-NC	2.12	127.54	124.20
25	7	613	CLA	C2D-C1D-ND	-2.12	108.54	110.10
24	S	601	CHL	CED-O2D-CGD	2.12	120.72	115.94
26	r	620	LUT	C30-C31-C32	-2.12	116.61	123.22
26	y	1620	LUT	C3-C4-C5	-2.12	107.64	111.85
34	B	620	BCR	C38-C26-C25	-2.12	122.15	124.53
24	1	607	CHL	CAA-CBA-CGA	-2.12	107.07	113.25
25	A	410	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
25	b	617	CLA	C2A-C1A-CHA	2.12	127.56	123.86
26	9	1620	LUT	C20-C13-C12	2.12	121.41	118.08
27	G	1622	XAT	C40-C33-C32	2.12	121.41	118.08
27	Y	1622	XAT	C19-C9-C8	2.12	121.41	118.08
28	r	623	NEX	C35-C15-C14	-2.12	119.14	123.47
24	s	601	CHL	CED-O2D-CGD	2.12	120.72	115.94
24	5	605	CHL	C2A-C1A-CHA	-2.11	120.16	123.86
25	b	603	CLA	O2D-CGD-CBD	2.11	115.03	111.27
34	B	620	BCR	C16-C15-C14	-2.11	119.14	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	3	609	CHL	O2D-CGD-O1D	-2.11	119.70	123.84
34	H	101	BCR	C8-C9-C10	2.11	122.18	118.94
25	8	603	CLA	CHA-C1A-NA	-2.11	121.56	126.40
24	7	607	CHL	C2A-C3A-C4A	-2.11	98.46	101.87
28	y	1623	NEX	O24-C25-C26	-2.11	57.21	58.96
25	9	603	CLA	C2A-C1A-CHA	2.11	127.55	123.86
25	a	410	CLA	O2A-CGA-O1A	-2.11	118.26	123.59
36	h	102	LMG	O7-C10-O9	-2.11	118.60	123.70
24	Y	601	CHL	CGD-CBD-CAD	-2.11	103.89	110.73
24	6	605	CHL	CAA-C2A-C3A	-2.11	107.00	112.78
25	8	613	CLA	CHD-C1D-ND	-2.11	122.51	124.45
24	8	605	CHL	C1-C2-C3	-2.11	122.39	126.04
25	7	602	CLA	C4-C3-C5	2.11	118.82	115.27
24	S	606	CHL	O1D-CGD-CBD	-2.11	120.17	124.48
24	p	605	CHL	C2A-C1A-CHA	-2.11	120.17	123.86
24	S	606	CHL	CHB-C4A-NA	2.11	127.43	124.51
27	3	1622	XAT	C24-C23-C22	-2.11	106.70	110.77
25	4	602	CLA	CHD-C1D-ND	-2.11	122.52	124.45
34	B	620	BCR	C34-C9-C10	-2.11	119.97	122.92
26	8	1620	LUT	C19-C9-C8	2.11	121.40	118.08
24	7	606	CHL	O1D-CGD-CBD	-2.11	120.17	124.48
34	d	404	BCR	C30-C25-C26	-2.11	119.64	122.61
25	6	614	CLA	O2D-CGD-CBD	2.11	115.01	111.27
24	q	605	CHL	O1D-CGD-CBD	-2.11	120.17	124.48
26	9	1620	LUT	C39-C29-C28	2.11	121.40	118.08
36	d	412	LMG	O8-C28-O10	-2.11	118.27	123.59
24	2	607	CHL	O1D-CGD-CBD	-2.11	120.17	124.48
36	s	2631	LMG	C8-O7-C10	-2.11	112.60	117.79
33	a	409	PHO	O2A-CGA-O1A	-2.11	118.28	123.59
24	6	608	CHL	C1C-C2C-C3C	-2.11	105.44	107.11
24	p	601	CHL	O2D-CGD-O1D	-2.11	119.72	123.84
28	s	1623	NEX	C20-C13-C14	-2.10	119.97	122.92
24	6	605	CHL	CAA-C2A-C1A	2.10	118.87	111.97
25	c	501	CLA	O2D-CGD-CBD	2.10	115.00	111.27
25	N	603	CLA	CBC-CAC-C3C	-2.10	106.64	112.43
25	b	617	CLA	O2A-CGA-O1A	-2.10	118.29	123.59
25	B	613	CLA	CHA-C1A-NA	-2.10	121.58	126.40
33	A	409	PHO	O2A-CGA-O1A	-2.10	118.29	123.59
24	n	607	CHL	C1-C2-C3	-2.10	122.41	126.04
24	3	609	CHL	C4-C3-C5	2.10	118.81	115.27
24	8	606	CHL	C4D-CHA-C1A	-2.10	118.69	121.25
24	N	605	CHL	O2D-CGD-O1D	-2.10	119.73	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	601	CHL	O2A-CGA-CBA	2.10	118.50	111.91
26	R	620	LUT	C30-C31-C32	-2.10	116.66	123.22
26	8	1621	LUT	C35-C15-C14	-2.10	119.17	123.47
25	B	606	CLA	C1-C2-C3	-2.10	122.41	126.04
25	B	603	CLA	O2D-CGD-CBD	2.10	115.00	111.27
28	5	1623	NEX	C16-C1-C6	2.10	112.35	110.47
24	G	606	CHL	C4D-CHA-C1A	-2.10	118.69	121.25
24	0	609	CHL	C1D-CHD-C4C	-2.10	121.53	126.06
24	n	605	CHL	CBC-CAC-C3C	-2.10	106.64	112.43
36	H	102	LMG	O7-C10-O9	-2.10	118.63	123.70
27	7	1622	XAT	C35-C15-C14	-2.10	119.17	123.47
34	A	411	BCR	C20-C21-C22	-2.10	124.31	127.31
24	7	606	CHL	C4-C3-C5	2.10	118.80	115.27
26	7	1621	LUT	C3-C4-C5	-2.10	107.67	111.85
35	b	621	SQD	C44-O6-C1	-2.10	109.64	113.74
24	g	601	CHL	CAA-CBA-CGA	-2.10	107.12	113.25
26	y	1621	LUT	C30-C31-C32	-2.10	116.67	123.22
25	g	604	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
26	Y	1620	LUT	C20-C13-C12	2.10	121.38	118.08
24	3	607	CHL	C1-C2-C3	-2.10	122.42	126.04
26	n	1620	LUT	C8-C7-C6	-2.10	121.32	127.20
28	7	1623	NEX	C5-C4-C3	-2.10	109.26	111.75
25	1	610	CLA	C1-C2-C3	-2.10	122.42	126.04
25	5	610	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
28	0	1623	NEX	C16-C1-C6	2.10	112.35	110.47
26	p	1621	LUT	C10-C11-C12	-2.10	116.68	123.22
25	5	614	CLA	CHD-C1D-ND	-2.09	122.53	124.45
24	0	606	CHL	C4D-CHA-C1A	-2.09	118.70	121.25
25	N	610	CLA	O2A-CGA-O1A	-2.09	118.31	123.59
34	c	517	BCR	C33-C5-C4	2.09	117.64	113.62
25	0	613	CLA	CAA-CBA-CGA	-2.09	107.14	113.25
33	a	408	PHO	CMA-C3A-C4A	-2.09	109.79	114.38
24	s	606	CHL	O1D-CGD-CBD	-2.09	120.20	124.48
27	4	1622	XAT	C24-C23-C22	-2.09	106.73	110.77
25	y	613	CLA	CAC-C3C-C4C	2.09	127.53	124.81
24	3	601	CHL	C1-O2A-CGA	2.09	121.93	116.44
36	D	412	LMG	O8-C28-O10	-2.09	118.31	123.59
25	3	603	CLA	CHA-C1A-NA	-2.09	121.61	126.40
24	8	601	CHL	O1D-CGD-CBD	-2.09	120.20	124.48
26	3	1621	LUT	C3-C4-C5	-2.09	107.69	111.85
24	6	601	CHL	CED-O2D-CGD	2.09	120.67	115.94
24	2	606	CHL	O1D-CGD-CBD	-2.09	120.21	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	1	607	CHL	C1C-C2C-C3C	-2.09	105.45	107.11
24	n	607	CHL	C2A-C1A-CHA	-2.09	120.20	123.86
26	s	1620	LUT	C15-C14-C13	-2.09	124.33	127.31
24	Y	601	CHL	O2D-CGD-O1D	-2.09	119.75	123.84
24	7	601	CHL	O2D-CGD-O1D	-2.09	119.75	123.84
25	9	612	CLA	C2A-C1A-CHA	2.09	127.51	123.86
24	4	608	CHL	OMC-CMC-C2C	-2.09	120.96	125.69
25	S	605	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
25	C	511	CLA	CHD-C1D-ND	-2.09	122.53	124.45
27	1	1622	XAT	C40-C33-C32	2.09	121.37	118.08
25	0	613	CLA	O2A-CGA-O1A	-2.09	118.32	123.59
26	5	1621	LUT	C16-C1-C6	-2.09	106.91	110.30
26	8	1621	LUT	C39-C29-C28	2.09	121.36	118.08
25	b	613	CLA	CHA-C1A-NA	-2.09	121.62	126.40
26	6	1620	LUT	C40-C33-C32	2.09	121.36	118.08
34	c	515	BCR	C36-C18-C19	2.09	121.36	118.08
25	b	607	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
35	B	621	SQD	C44-O6-C1	-2.09	109.66	113.74
29	Y	2630	LHG	O8-C23-O10	-2.09	118.33	123.59
34	b	620	BCR	C16-C15-C14	-2.09	119.20	123.47
24	8	609	CHL	OMC-CMC-C2C	-2.09	120.97	125.69
24	9	601	CHL	OMC-CMC-C2C	-2.09	120.97	125.69
25	6	612	CLA	C2A-C1A-CHA	2.09	127.50	123.86
25	B	607	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
26	y	1620	LUT	C2-C3-C4	-2.08	107.45	110.30
26	4	1620	LUT	C18-C5-C4	2.08	118.22	114.36
26	S	1620	LUT	C40-C33-C32	2.08	121.36	118.08
24	1	607	CHL	C2A-C3A-C4A	-2.08	98.50	101.87
25	B	617	CLA	O2A-CGA-O1A	-2.08	118.33	123.59
24	4	607	CHL	CED-O2D-CGD	2.08	120.65	115.94
25	p	602	CLA	CHD-C1D-ND	-2.08	122.54	124.45
33	A	408	PHO	CMA-C3A-C4A	-2.08	109.81	114.38
28	1	1623	NEX	C2-C1-C6	2.08	111.24	109.21
24	3	608	CHL	C4D-CHA-C1A	-2.08	118.71	121.25
25	9	610	CLA	C1-C2-C3	-2.08	122.44	126.04
24	8	605	CHL	C3B-C4B-NB	2.08	111.90	109.21
24	S	608	CHL	C1C-C2C-C3C	-2.08	105.46	107.11
27	r	622	XAT	C31-C30-C29	-2.08	124.34	127.31
24	3	607	CHL	CED-O2D-CGD	2.08	120.64	115.94
24	8	607	CHL	C4D-CHA-C1A	-2.08	118.72	121.25
24	0	605	CHL	CAA-C2A-C1A	2.08	118.80	111.97
25	1	604	CLA	CAC-C3C-C4C	2.08	127.51	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	3	1623	NEX	C16-C1-C6	2.08	112.33	110.47
24	0	606	CHL	CHB-C4A-NA	2.08	127.39	124.51
24	s	606	CHL	CHB-C4A-NA	2.08	127.39	124.51
25	b	606	CLA	C1-C2-C3	-2.08	122.44	126.04
24	5	606	CHL	CED-O2D-CGD	2.08	120.64	115.94
26	Y	1621	LUT	C36-C21-C26	2.08	112.70	109.55
25	6	610	CLA	C1-C2-C3	-2.08	122.45	126.04
25	n	610	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
26	2	1620	LUT	C30-C31-C32	-2.08	116.73	123.22
26	0	1620	LUT	C11-C10-C9	-2.08	124.34	127.31
24	4	606	CHL	C4D-CHA-C1A	-2.08	118.72	121.25
25	y	603	CLA	CBA-CAA-C2A	-2.08	107.73	113.86
25	8	610	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
26	1	1621	LUT	C36-C21-C26	2.08	112.69	109.55
26	G	1621	LUT	C16-C1-C6	-2.08	106.93	110.30
24	g	607	CHL	C1C-C2C-C3C	-2.08	105.47	107.11
26	6	1621	LUT	C35-C15-C14	-2.08	119.22	123.47
24	q	607	CHL	CAA-C2A-C3A	-2.08	107.09	112.78
25	7	602	CLA	CHD-C1D-ND	-2.08	122.55	124.45
29	d	408	LHG	C5-O7-C7	-2.08	112.68	117.79
24	9	606	CHL	CED-O2D-CGD	2.08	120.63	115.94
24	s	607	CHL	C1C-C2C-C3C	-2.08	105.47	107.11
25	0	612	CLA	C2A-C1A-CHA	2.07	127.49	123.86
26	2	1620	LUT	C39-C29-C28	2.07	121.35	118.08
26	n	1621	LUT	C35-C15-C14	-2.07	119.22	123.47
25	9	613	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
27	2	1622	XAT	O4-C5-C6	-2.07	57.24	58.96
24	4	609	CHL	CAA-CBA-CGA	-2.07	107.19	113.25
24	1	606	CHL	CBC-CAC-C3C	-2.07	106.71	112.43
24	p	605	CHL	OMC-CMC-C2C	-2.07	121.00	125.69
24	y	607	CHL	C16-C15-C13	-2.07	109.22	115.92
24	7	606	CHL	CAA-C2A-C3A	-2.07	107.10	112.78
25	N	613	CLA	CAC-C3C-C4C	2.07	127.50	124.81
24	g	606	CHL	C4D-CHA-C1A	-2.07	118.73	121.25
26	7	1621	LUT	C18-C5-C6	-2.07	122.20	124.53
25	R	601	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
24	Y	609	CHL	C1B-CHB-C4A	-2.07	126.02	130.12
26	q	1621	LUT	C36-C21-C26	2.07	112.68	109.55
24	n	605	CHL	CHB-C4A-NA	2.07	127.37	124.51
39	d	405	PL9	C41-C39-C38	-2.07	116.93	121.12
24	2	609	CHL	O2D-CGD-O1D	-2.07	119.79	123.84
35	b	623	SQD	O6-C44-C45	-2.07	105.91	110.90

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	7	2630	LHG	O8-C23-O10	-2.07	118.37	123.59
24	8	608	CHL	OMC-CMC-C2C	-2.07	121.01	125.69
24	G	608	CHL	O1D-CGD-CBD	-2.07	120.25	124.48
25	3	610	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
33	A	408	PHO	O2A-CGA-O1A	-2.07	118.37	123.59
26	y	1620	LUT	C8-C7-C6	-2.07	121.39	127.20
25	3	613	CLA	O2A-CGA-O1A	-2.07	118.37	123.59
28	n	1623	NEX	O24-C25-C26	-2.07	57.25	58.96
26	y	1620	LUT	C20-C13-C12	2.07	121.33	118.08
24	p	607	CHL	O2D-CGD-O1D	-2.07	119.80	123.84
24	4	606	CHL	C3B-C4B-NB	2.07	111.88	109.21
25	c	505	CLA	C2D-C1D-ND	-2.07	108.58	110.10
29	4	2630	LHG	O7-C7-O9	-2.07	118.71	123.70
24	N	607	CHL	C4-C3-C5	2.07	118.75	115.27
25	0	610	CLA	C1-C2-C3	-2.06	122.47	126.04
27	g	1622	XAT	C40-C33-C32	2.06	121.33	118.08
25	5	604	CLA	O2A-CGA-O1A	-2.06	118.38	123.59
27	q	1622	XAT	O4-C5-C6	-2.06	57.25	58.96
25	p	612	CLA	C2A-C1A-CHA	2.06	127.47	123.86
25	9	602	CLA	C6-C7-C8	-2.06	109.25	115.92
39	D	405	PL9	C41-C39-C38	-2.06	116.94	121.12
25	G	614	CLA	CHD-C1D-ND	-2.06	122.56	124.45
37	c	524	DGD	O5D-C1E-C2E	2.06	111.52	108.30
25	Y	603	CLA	CBA-CAA-C2A	-2.06	107.77	113.86
28	G	1623	NEX	C26-C27-C28	-2.06	121.63	125.99
34	b	619	BCR	C35-C13-C14	-2.06	120.03	122.92
24	Y	608	CHL	O2D-CGD-O1D	-2.06	119.81	123.84
33	a	408	PHO	O2A-CGA-O1A	-2.06	118.39	123.59
24	s	607	CHL	OMC-CMC-C2C	-2.06	121.03	125.69
24	1	601	CHL	O2D-CGD-O1D	-2.06	119.81	123.84
34	C	515	BCR	C38-C26-C25	-2.06	122.21	124.53
34	B	620	BCR	C3-C4-C5	-2.06	110.40	114.08
28	p	1623	NEX	O24-C25-C26	-2.06	57.25	58.96
25	B	616	CLA	C2C-C1C-NC	2.06	111.90	109.97
34	B	620	BCR	C15-C16-C17	-2.06	119.25	123.47
34	b	620	BCR	C3-C4-C5	-2.06	110.40	114.08
34	B	619	BCR	C35-C13-C14	-2.06	120.04	122.92
26	3	1621	LUT	C2-C3-C4	-2.06	107.48	110.30
27	R	622	XAT	C31-C30-C29	-2.06	124.37	127.31
25	C	501	CLA	C7-C6-C5	-2.06	107.77	113.36
24	g	601	CHL	O2D-CGD-O1D	-2.06	119.81	123.84
24	R	607	CHL	C7-C6-C5	-2.06	107.77	113.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	602	CLA	CAA-CBA-CGA	-2.06	107.24	113.25
38	d	401	BCT	O3-C-O1	-2.06	114.21	119.55
26	Y	1620	LUT	C8-C9-C10	-2.06	115.78	118.94
28	5	1623	NEX	O24-C25-C26	-2.06	57.25	58.96
26	S	1620	LUT	C15-C14-C13	-2.06	124.37	127.31
26	y	1620	LUT	C8-C9-C10	-2.06	115.78	118.94
25	Y	613	CLA	CAC-C3C-C4C	2.06	127.48	124.81
24	Y	601	CHL	C3A-C2A-C1A	-2.06	98.26	101.34
26	s	1620	LUT	C40-C33-C32	2.06	121.32	118.08
25	n	612	CLA	CHA-C1A-NA	-2.06	121.69	126.40
25	c	502	CLA	O1D-CGD-CBD	2.06	128.69	124.48
34	b	620	BCR	C10-C11-C12	-2.06	116.80	123.22
25	9	610	CLA	C1D-ND-C4D	-2.06	104.88	106.33
24	p	601	CHL	C11-C12-C13	-2.06	109.28	115.92
25	c	511	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
26	7	1621	LUT	C19-C9-C8	2.05	121.31	118.08
34	c	516	BCR	C30-C25-C26	-2.05	119.72	122.61
24	s	608	CHL	C1C-C2C-C3C	-2.05	105.48	107.11
34	b	620	BCR	C15-C16-C17	-2.05	119.27	123.47
25	b	604	CLA	CAA-CBA-CGA	-2.05	107.25	113.25
24	N	609	CHL	CBC-CAC-C3C	-2.05	106.77	112.43
24	S	607	CHL	OMC-CMC-C2C	-2.05	121.05	125.69
24	y	609	CHL	C6-C7-C8	-2.05	109.28	115.92
25	p	604	CLA	C4-C3-C5	2.05	118.72	115.27
34	B	620	BCR	C10-C11-C12	-2.05	116.81	123.22
28	g	1623	NEX	C28-C29-C30	2.05	122.09	118.94
25	2	613	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
25	r	601	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
26	3	1620	LUT	C8-C7-C6	-2.05	121.44	127.20
33	A	409	PHO	CMA-C3A-C4A	-2.05	109.88	114.38
25	c	507	CLA	O2A-CGA-O1A	-2.05	118.42	123.59
27	q	1622	XAT	O24-C25-C26	-2.05	57.26	58.96
24	2	608	CHL	CHB-C4A-NA	2.05	127.35	124.51
36	S	2631	LMG	C6-C5-C4	-2.05	108.20	113.00
29	L	101	LHG	O8-C23-O10	-2.05	118.42	123.59
24	N	607	CHL	C2A-C1A-CHA	-2.05	120.28	123.86
28	N	1623	NEX	O24-C25-C26	-2.05	57.26	58.96
26	q	1620	LUT	C3-C4-C5	-2.05	107.77	111.85
24	9	601	CHL	C2A-C3A-C4A	-2.05	98.56	101.87
37	C	518	DGD	C3G-C2G-C1G	-2.05	106.94	111.79
26	s	1620	LUT	C19-C9-C8	2.05	121.30	118.08
25	C	508	CLA	O1D-CGD-CBD	2.05	128.67	124.48

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	g	608	CHL	O1D-CGD-CBD	-2.05	120.30	124.48
38	D	401	BCT	O3-C-O1	-2.05	114.24	119.55
26	l	1621	LUT	C30-C31-C32	-2.05	116.83	123.22
27	n	1622	XAT	C31-C32-C33	-2.05	120.67	126.42
25	G	604	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
25	r	612	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
26	y	1621	LUT	C36-C21-C26	2.04	112.64	109.55
34	C	516	BCR	C30-C25-C26	-2.04	119.73	122.61
26	0	1620	LUT	C31-C30-C29	-2.04	124.39	127.31
28	p	1623	NEX	C19-C9-C10	-2.04	120.06	122.92
25	c	501	CLA	C7-C6-C5	-2.04	107.81	113.36
25	S	614	CLA	CHD-C1D-ND	-2.04	122.58	124.45
25	N	613	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
24	s	607	CHL	O2D-CGD-O1D	-2.04	119.84	123.84
37	c	518	DGD	C3G-C2G-C1G	-2.04	106.96	111.79
25	A	406	CLA	CHD-C1D-ND	-2.04	122.58	124.45
25	a	406	CLA	CHD-C1D-ND	-2.04	122.58	124.45
24	s	606	CHL	CMB-C2B-C3B	2.04	128.50	124.68
24	n	607	CHL	C4D-C3D-CAD	2.04	110.50	108.10
25	8	613	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
27	l	1622	XAT	C35-C15-C14	-2.04	119.29	123.47
24	4	601	CHL	CHB-C4A-NA	2.04	127.33	124.51
26	l	1620	LUT	C16-C1-C6	-2.04	106.99	110.30
25	C	501	CLA	O2D-CGD-CBD	2.04	114.89	111.27
26	g	1620	LUT	C31-C30-C29	-2.04	124.40	127.31
24	N	608	CHL	O2A-CGA-O1A	-2.04	118.44	123.59
28	g	1623	NEX	C11-C12-C13	-2.04	120.69	126.42
26	S	1620	LUT	C20-C13-C12	2.04	121.29	118.08
25	2	603	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
26	y	1621	LUT	C18-C5-C6	-2.04	122.24	124.53
25	G	604	CLA	CHD-C1D-ND	-2.04	122.58	124.45
26	N	1621	LUT	C35-C15-C14	-2.04	119.30	123.47
24	g	607	CHL	CGD-CBD-CAD	-2.04	104.13	110.73
26	Y	1621	LUT	C18-C5-C6	-2.04	122.24	124.53
26	y	1620	LUT	C22-C23-C24	-2.04	109.42	111.74
25	a	406	CLA	C1-C2-C3	-2.04	122.52	126.04
24	r	608	CHL	O1D-CGD-CBD	-2.04	120.31	124.48
25	D	402	CLA	C4-C3-C5	2.04	118.70	115.27
24	y	609	CHL	C1B-CHB-C4A	-2.04	126.08	130.12
24	3	609	CHL	C4A-NA-C1A	-2.04	105.79	106.71
24	n	605	CHL	O2A-CGA-O1A	-2.04	118.45	123.59
25	4	603	CLA	CHA-C1A-NA	-2.04	121.73	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	7	604	CLA	CHD-C1D-ND	-2.04	122.58	124.45
25	g	602	CLA	C6-C7-C8	-2.04	109.34	115.92
25	3	611	CLA	O2D-CGD-CBD	2.04	114.89	111.27
27	q	1622	XAT	C18-C5-C4	2.04	116.57	114.28
26	G	1620	LUT	C31-C30-C29	-2.04	124.40	127.31
24	g	605	CHL	O1D-CGD-CBD	-2.04	120.32	124.48
25	6	610	CLA	CHD-C1D-ND	-2.04	122.58	124.45
24	p	601	CHL	C1-C2-C3	-2.04	122.52	126.04
36	s	2631	LMG	C6-C5-C4	-2.04	108.24	113.00
24	2	605	CHL	CED-O2D-CGD	2.04	120.54	115.94
26	1	1621	LUT	C31-C30-C29	-2.03	124.41	127.31
25	2	610	CLA	C1-C2-C3	-2.03	122.53	126.04
25	6	612	CLA	CHA-C1A-NA	-2.03	121.74	126.40
29	1	2630	LHG	C6-C5-C4	-2.03	106.98	111.79
24	R	608	CHL	O1D-CGD-CBD	-2.03	120.32	124.48
29	D	408	LHG	C5-O7-C7	-2.03	112.79	117.79
24	7	601	CHL	C1-C2-C3	-2.03	122.53	126.04
25	s	614	CLA	CHD-C1D-ND	-2.03	122.59	124.45
26	9	1621	LUT	C15-C35-C34	-2.03	119.31	123.47
24	1	608	CHL	C4D-CHA-C1A	-2.03	118.78	121.25
25	C	509	CLA	C11-C10-C8	-2.03	109.35	115.92
26	q	1621	LUT	C8-C9-C10	-2.03	115.82	118.94
26	q	1620	LUT	C31-C32-C33	-2.03	120.71	126.42
24	Y	609	CHL	O2D-CGD-O1D	-2.03	119.87	123.84
25	B	604	CLA	CAA-CBA-CGA	-2.03	107.32	113.25
36	h	102	LMG	C4-C3-C2	2.03	114.37	110.82
27	4	1622	XAT	O24-C25-C26	-2.03	57.28	58.96
24	0	601	CHL	C2A-C3A-C4A	-2.03	98.59	101.87
25	C	506	CLA	O2A-CGA-O1A	-2.03	118.47	123.59
25	4	612	CLA	CHA-C1A-NA	-2.03	121.75	126.40
24	8	608	CHL	C4D-CHA-C1A	-2.03	118.78	121.25
24	6	609	CHL	CED-O2D-CGD	2.03	120.53	115.94
33	a	409	PHO	CMA-C3A-C4A	-2.03	109.93	114.38
26	Y	1620	LUT	C8-C7-C6	-2.03	121.50	127.20
26	g	1620	LUT	C2-C3-C4	2.03	113.08	110.30
26	4	1621	LUT	C36-C21-C26	2.03	112.62	109.55
27	r	622	XAT	C15-C35-C34	-2.03	119.32	123.47
25	G	614	CLA	CHB-C4A-NA	2.03	127.32	124.51
25	C	502	CLA	O1D-CGD-CBD	2.03	128.63	124.48
25	c	511	CLA	CHD-C1D-ND	-2.03	122.59	124.45
26	4	1620	LUT	C10-C11-C12	-2.03	116.89	123.22
24	6	608	CHL	O2A-CGA-O1A	-2.03	118.48	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	b	616	CLA	C2C-C1C-NC	2.03	111.87	109.97
24	3	608	CHL	C4D-C3D-CAD	2.03	110.48	108.10
24	Y	609	CHL	C6-C7-C8	-2.03	109.37	115.92
25	C	509	CLA	C11-C12-C13	-2.03	109.37	115.92
25	3	611	CLA	O2A-CGA-O1A	-2.03	118.48	123.59
24	S	607	CHL	C1C-C2C-C3C	-2.03	105.51	107.11
27	y	1622	XAT	O24-C25-C26	-2.03	57.28	58.96
27	6	1622	XAT	O24-C25-C26	-2.03	57.28	58.96
24	S	607	CHL	O2D-CGD-O1D	-2.03	119.88	123.84
24	7	607	CHL	CAA-CBA-CGA	-2.03	107.33	113.25
25	b	616	CLA	CHA-C1A-NA	-2.03	121.76	126.40
25	B	616	CLA	CHA-C1A-NA	-2.02	121.76	126.40
28	4	1623	NEX	C5-C6-C1	2.02	121.70	119.70
25	c	508	CLA	O1D-CGD-CBD	2.02	128.63	124.48
24	7	606	CHL	O2D-CGD-O1D	-2.02	119.88	123.84
29	l	101	LHG	O8-C23-O10	-2.02	118.48	123.59
33	A	408	PHO	CMC-C2C-C3C	2.02	128.76	124.94
34	c	515	BCR	C38-C26-C27	2.02	117.50	113.62
37	C	524	DGD	O5D-C1E-C2E	2.02	111.46	108.30
25	n	613	CLA	O2A-CGA-O1A	-2.02	118.49	123.59
24	n	605	CHL	CAC-C3C-C4C	2.02	127.44	124.81
24	l	609	CHL	C1-C2-C3	-2.02	122.54	126.04
25	q	610	CLA	CHD-C1D-ND	-2.02	122.59	124.45
25	a	410	CLA	CHC-C1C-NC	2.02	127.27	124.20
24	s	601	CHL	O2D-CGD-O1D	-2.02	119.88	123.84
24	y	605	CHL	O1D-CGD-CBD	-2.02	120.35	124.48
37	C	520	DGD	O1G-C1A-O1A	-2.02	118.49	123.59
37	c	520	DGD	O1G-C1A-O1A	-2.02	118.49	123.59
28	4	1623	NEX	C38-C25-C24	2.02	116.56	114.28
27	3	1622	XAT	O24-C25-C26	-2.02	57.28	58.96
25	A	406	CLA	C1-C2-C3	-2.02	122.55	126.04
24	9	606	CHL	O1D-CGD-CBD	-2.02	120.35	124.48
24	7	607	CHL	C4D-C3D-CAD	2.02	110.48	108.10
27	G	1622	XAT	O4-C5-C6	-2.02	57.29	58.96
24	G	609	CHL	C2A-C1A-CHA	-2.02	120.33	123.86
26	2	1621	LUT	C39-C29-C28	2.02	121.26	118.08
25	c	509	CLA	C11-C10-C8	-2.02	109.39	115.92
25	1	604	CLA	C1-C2-C3	-2.02	122.55	126.04
24	3	605	CHL	C3B-C4B-NB	2.02	111.82	109.21
24	0	605	CHL	CED-O2D-CGD	2.02	120.50	115.94
25	y	610	CLA	O1D-CGD-CBD	2.02	128.61	124.48
24	9	608	CHL	CHB-C4A-NA	2.02	127.30	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	9	605	CHL	CED-O2D-CGD	2.02	120.50	115.94
24	3	607	CHL	C4D-C3D-CAD	2.02	110.47	108.10
25	g	614	CLA	O2A-CGA-O1A	-2.02	118.50	123.59
24	N	609	CHL	C1-C2-C3	-2.02	122.55	126.04
27	5	1622	XAT	O24-C25-C26	-2.02	57.29	58.96
25	n	612	CLA	C2A-C1A-CHA	2.02	127.39	123.86
34	h	101	BCR	C2-C1-C6	2.02	113.59	110.48
28	s	1623	NEX	O24-C25-C26	-2.02	57.29	58.96
24	3	601	CHL	CBC-CAC-C3C	-2.02	106.87	112.43
28	q	1623	NEX	C38-C25-C24	2.02	116.55	114.28
24	4	601	CHL	C7-C6-C5	-2.02	107.88	113.36
24	7	605	CHL	OMC-CMC-C2C	-2.02	121.13	125.69
26	S	1620	LUT	C19-C9-C8	2.02	121.25	118.08
26	4	1621	LUT	C30-C31-C32	-2.02	116.93	123.22
25	4	614	CLA	CHD-C1D-ND	-2.02	122.60	124.45
27	R	622	XAT	C15-C35-C34	-2.01	119.35	123.47
24	3	605	CHL	O2A-CGA-O1A	-2.01	118.51	123.59
25	s	613	CLA	CHA-C1A-NA	-2.01	121.79	126.40
27	p	1622	XAT	C11-C12-C13	-2.01	120.76	126.42
26	G	1621	LUT	C10-C11-C12	-2.01	116.93	123.22
24	n	609	CHL	C1-C2-C3	-2.01	122.56	126.04
25	6	613	CLA	C1-C2-C3	-2.01	122.56	126.04
25	g	614	CLA	CHB-C4A-NA	2.01	127.30	124.51
24	g	606	CHL	O1D-CGD-CBD	-2.01	120.37	124.48
24	G	609	CHL	O2A-CGA-O1A	-2.01	118.51	123.59
28	p	1623	NEX	C17-C1-C6	-2.01	108.67	110.47
24	8	601	CHL	C4D-CHA-C1A	-2.01	118.80	121.25
37	C	523	DGD	O1G-C1A-O1A	-2.01	118.51	123.59
27	g	1622	XAT	O4-C5-C6	-2.01	57.29	58.96
27	Y	1622	XAT	O24-C25-C26	-2.01	57.29	58.96
35	B	623	SQD	O6-C44-C45	-2.01	106.05	110.90
25	Y	610	CLA	C11-C10-C8	-2.01	109.42	115.92
24	0	605	CHL	C4D-CHA-C1A	-2.01	118.80	121.25
28	7	1623	NEX	O24-C25-C26	-2.01	57.29	58.96
25	7	614	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
24	2	608	CHL	C4D-CHA-C1A	-2.01	118.80	121.25
24	6	601	CHL	C4D-CHA-C1A	-2.01	118.80	121.25
29	q	2630	LHG	O7-C7-O9	-2.01	118.84	123.70
27	5	1622	XAT	C26-C27-C28	-2.01	121.74	125.99
25	s	605	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
29	1	2630	LHG	O8-C23-O10	-2.01	118.52	123.59
39	D	405	PL9	C20-C19-C21	2.01	118.65	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
24	Y	607	CHL	CGD-CBD-CAD	-2.01	104.22	110.73
33	a	408	PHO	CMC-C2C-C3C	2.01	128.73	124.94
24	l	606	CHL	O1D-CGD-CBD	-2.01	120.37	124.48
27	r	622	XAT	C19-C9-C8	2.01	121.24	118.08
25	R	612	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
24	S	607	CHL	O1D-CGD-CBD	-2.01	120.37	124.48
25	S	613	CLA	CHA-C1A-NA	-2.01	121.80	126.40
24	3	609	CHL	C1D-CHD-C4C	-2.01	121.72	126.06
25	c	509	CLA	C11-C12-C13	-2.01	109.43	115.92
24	Y	605	CHL	O1D-CGD-CBD	-2.01	120.37	124.48
24	S	606	CHL	CMB-C2B-C3B	2.01	128.44	124.68
24	G	606	CHL	O2A-CGA-O1A	-2.01	118.52	123.59
25	3	614	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
25	R	616	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
25	c	506	CLA	O2A-CGA-O1A	-2.01	118.52	123.59
25	q	612	CLA	CHA-C1A-NA	-2.01	121.80	126.40
24	9	607	CHL	O1D-CGD-CBD	-2.01	120.38	124.48
24	l	601	CHL	C4D-C3D-CAD	2.01	110.46	108.10
25	R	616	CLA	O2D-CGD-CBD	2.01	114.83	111.27
25	0	614	CLA	O2D-CGD-CBD	2.01	114.83	111.27
25	r	616	CLA	O2D-CGD-CBD	2.01	114.83	111.27
26	9	1621	LUT	C30-C31-C32	-2.01	116.96	123.22
24	7	606	CHL	CBC-CAC-C3C	-2.01	106.90	112.43
27	9	1622	XAT	O4-C5-C6	-2.01	57.30	58.96
24	S	601	CHL	O2D-CGD-O1D	-2.00	119.92	123.84
24	y	608	CHL	O2D-CGD-O1D	-2.00	119.92	123.84
25	G	614	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
24	8	607	CHL	C4D-C3D-CAD	2.00	110.46	108.10
25	0	602	CLA	CHB-C4A-NA	2.00	127.28	124.51
25	9	603	CLA	O2A-CGA-O1A	-2.00	118.53	123.59
24	g	609	CHL	C2A-C1A-CHA	-2.00	120.35	123.86
28	r	623	NEX	C2-C1-C6	2.00	111.16	109.21
24	8	607	CHL	CED-O2D-CGD	2.00	120.47	115.94
24	5	605	CHL	C11-C12-C13	-2.00	109.44	115.92
25	D	402	CLA	CHB-C4A-NA	2.00	127.28	124.51
24	S	601	CHL	O1D-CGD-CBD	-2.00	120.38	124.48
34	B	619	BCR	C11-C12-C13	-2.00	120.79	126.42
25	B	611	CLA	CHC-C1C-NC	2.00	127.24	124.20
26	8	1620	LUT	C8-C7-C6	-2.00	121.58	127.20
25	2	604	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
25	A	410	CLA	CHC-C1C-NC	2.00	127.24	124.20
26	s	1620	LUT	C20-C13-C12	2.00	121.23	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	8	611	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
25	8	614	CLA	O2A-CGA-O1A	-2.00	118.54	123.59
25	b	616	CLA	C3A-C2A-C1A	2.00	104.34	101.34
25	G	602	CLA	C6-C7-C8	-2.00	109.45	115.92
28	2	1623	NEX	C16-C1-C6	2.00	112.26	110.47
25	S	603	CLA	CHD-C1D-ND	-2.00	122.61	124.45
25	B	616	CLA	C3A-C2A-C1A	2.00	104.34	101.34
33	A	409	PHO	C1B-NB-C4B	2.00	111.20	107.09
28	S	1623	NEX	C28-C29-C30	2.00	122.01	118.94
26	g	1621	LUT	C1-C2-C3	2.00	118.16	113.64
25	C	502	CLA	C11-C12-C13	-2.00	109.45	115.92
24	1	605	CHL	OMC-CMC-C2C	-2.00	121.16	125.69
25	4	612	CLA	O2D-CGD-CBD	2.00	114.82	111.27

All (591) chirality outliers are listed below:

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

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Mol	Chain	Res	Type	Atom
24	2	606	CHL	NC
24	2	606	CHL	NA
24	2	607	CHL	ND
24	2	607	CHL	NC
24	2	607	CHL	NA
24	2	608	CHL	ND
24	2	608	CHL	NC
24	2	608	CHL	NA
24	2	609	CHL	ND
24	2	609	CHL	NC
24	2	609	CHL	NA
24	3	601	CHL	ND
24	3	601	CHL	NC
24	3	601	CHL	NA
24	3	605	CHL	ND
24	3	605	CHL	NC
24	3	605	CHL	NA
24	3	606	CHL	ND
24	3	606	CHL	NC
24	3	606	CHL	NA
24	3	607	CHL	ND
24	3	607	CHL	NC
24	3	607	CHL	NA
24	3	608	CHL	ND
24	3	608	CHL	NC
24	3	608	CHL	NA
24	3	609	CHL	ND
24	3	609	CHL	NC
24	3	609	CHL	NA
24	4	601	CHL	ND
24	4	601	CHL	NC
24	4	601	CHL	NA
24	4	605	CHL	ND
24	4	605	CHL	NC
24	4	605	CHL	NA
24	4	606	CHL	ND
24	4	606	CHL	NC
24	4	606	CHL	NA
24	4	607	CHL	ND
24	4	607	CHL	NC
24	4	607	CHL	NA
24	4	608	CHL	ND

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Mol	Chain	Res	Type	Atom
24	4	608	CHL	NC
24	4	608	CHL	NA
24	4	609	CHL	ND
24	4	609	CHL	NC
24	4	609	CHL	NA
24	5	601	CHL	ND
24	5	601	CHL	NC
24	5	601	CHL	NA
24	5	605	CHL	ND
24	5	605	CHL	NC
24	5	605	CHL	NA
24	5	606	CHL	ND
24	5	606	CHL	NC
24	5	606	CHL	NA
24	5	607	CHL	ND
24	5	607	CHL	NC
24	5	607	CHL	NA
24	5	608	CHL	ND
24	5	608	CHL	NC
24	5	608	CHL	NA
24	5	609	CHL	ND
24	5	609	CHL	NC
24	5	609	CHL	NA
24	6	601	CHL	ND
24	6	601	CHL	NC
24	6	601	CHL	NA
24	6	605	CHL	ND
24	6	605	CHL	NC
24	6	605	CHL	NA
24	6	606	CHL	ND
24	6	606	CHL	NC
24	6	606	CHL	NA
24	6	607	CHL	ND
24	6	607	CHL	NC
24	6	607	CHL	NA
24	6	608	CHL	ND
24	6	608	CHL	NC
24	6	608	CHL	NA
24	6	609	CHL	ND
24	6	609	CHL	NC
24	6	609	CHL	NA
24	G	601	CHL	ND

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

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Mol	Chain	Res	Type	Atom
24	R	608	CHL	NC
24	R	608	CHL	NA
24	S	601	CHL	ND
24	S	601	CHL	NC
24	S	601	CHL	NA
24	S	606	CHL	ND
24	S	606	CHL	NC
24	S	606	CHL	NA
24	S	607	CHL	ND
24	S	607	CHL	NC
24	S	607	CHL	NA
24	S	608	CHL	ND
24	S	608	CHL	NC
24	S	608	CHL	NA
24	Y	601	CHL	ND
24	Y	601	CHL	NC
24	Y	601	CHL	NA
24	Y	605	CHL	ND
24	Y	605	CHL	NC
24	Y	605	CHL	NA
24	Y	606	CHL	ND
24	Y	606	CHL	NC
24	Y	606	CHL	NA
24	Y	607	CHL	ND
24	Y	607	CHL	NC
24	Y	607	CHL	NA
24	Y	608	CHL	ND
24	Y	608	CHL	NC
24	Y	608	CHL	NA
24	Y	609	CHL	ND
24	Y	609	CHL	NC
24	Y	609	CHL	NA
24	0	601	CHL	ND
24	0	601	CHL	NC
24	0	601	CHL	NA
24	0	605	CHL	ND
24	0	605	CHL	NC
24	0	605	CHL	NA
24	0	606	CHL	ND
24	0	606	CHL	NC
24	0	606	CHL	NA
24	0	607	CHL	ND

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Mol	Chain	Res	Type	Atom
24	0	607	CHL	NC
24	0	607	CHL	NA
24	0	608	CHL	ND
24	0	608	CHL	NC
24	0	608	CHL	NA
24	0	609	CHL	ND
24	0	609	CHL	NC
24	0	609	CHL	NA
24	7	601	CHL	ND
24	7	601	CHL	NC
24	7	601	CHL	NA
24	7	605	CHL	ND
24	7	605	CHL	NC
24	7	605	CHL	NA
24	7	606	CHL	ND
24	7	606	CHL	NC
24	7	606	CHL	NA
24	7	607	CHL	ND
24	7	607	CHL	NC
24	7	607	CHL	NA
24	7	608	CHL	ND
24	7	608	CHL	NC
24	7	608	CHL	NA
24	7	609	CHL	ND
24	7	609	CHL	NC
24	7	609	CHL	NA
24	8	601	CHL	ND
24	8	601	CHL	NC
24	8	601	CHL	NA
24	8	605	CHL	ND
24	8	605	CHL	NC
24	8	605	CHL	NA
24	8	606	CHL	ND
24	8	606	CHL	NC
24	8	606	CHL	NA
24	8	607	CHL	ND
24	8	607	CHL	NC
24	8	607	CHL	NA
24	8	608	CHL	ND
24	8	608	CHL	NC
24	8	608	CHL	NA
24	8	609	CHL	ND

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Mol	Chain	Res	Type	Atom
24	8	609	CHL	NC
24	8	609	CHL	NA
24	9	601	CHL	ND
24	9	601	CHL	NC
24	9	601	CHL	NA
24	9	605	CHL	ND
24	9	605	CHL	NC
24	9	605	CHL	NA
24	9	606	CHL	ND
24	9	606	CHL	NC
24	9	606	CHL	NA
24	9	607	CHL	ND
24	9	607	CHL	NC
24	9	607	CHL	NA
24	9	608	CHL	ND
24	9	608	CHL	NC
24	9	608	CHL	NA
24	9	609	CHL	ND
24	9	609	CHL	NC
24	9	609	CHL	NA
24	p	601	CHL	ND
24	p	601	CHL	NC
24	p	601	CHL	NA
24	p	605	CHL	ND
24	p	605	CHL	NC
24	p	605	CHL	NA
24	p	606	CHL	ND
24	p	606	CHL	NC
24	p	606	CHL	NA
24	p	607	CHL	ND
24	p	607	CHL	NC
24	p	607	CHL	NA
24	p	608	CHL	ND
24	p	608	CHL	NC
24	p	608	CHL	NA
24	p	609	CHL	ND
24	p	609	CHL	NC
24	p	609	CHL	NA
24	q	601	CHL	ND
24	q	601	CHL	NC
24	q	601	CHL	NA
24	q	605	CHL	ND

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Mol	Chain	Res	Type	Atom
24	q	605	CHL	NC
24	q	605	CHL	NA
24	q	606	CHL	ND
24	q	606	CHL	NC
24	q	606	CHL	NA
24	q	607	CHL	ND
24	q	607	CHL	NC
24	q	607	CHL	NA
24	q	608	CHL	ND
24	q	608	CHL	NC
24	q	608	CHL	NA
24	q	609	CHL	ND
24	q	609	CHL	NC
24	q	609	CHL	NA
24	g	601	CHL	ND
24	g	601	CHL	NC
24	g	601	CHL	NA
24	g	605	CHL	ND
24	g	605	CHL	NC
24	g	605	CHL	NA
24	g	606	CHL	ND
24	g	606	CHL	NC
24	g	606	CHL	NA
24	g	607	CHL	ND
24	g	607	CHL	NC
24	g	607	CHL	NA
24	g	608	CHL	ND
24	g	608	CHL	NC
24	g	608	CHL	NA
24	g	609	CHL	ND
24	g	609	CHL	NC
24	g	609	CHL	NA
24	n	601	CHL	ND
24	n	601	CHL	NC
24	n	601	CHL	NA
24	n	605	CHL	ND
24	n	605	CHL	NC
24	n	605	CHL	NA
24	n	606	CHL	ND
24	n	606	CHL	NC
24	n	606	CHL	NA
24	n	607	CHL	ND

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

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Mol	Chain	Res	Type	Atom
24	r	607	CHL	NC
24	r	607	CHL	NA
24	r	608	CHL	ND
24	r	608	CHL	NC
24	r	608	CHL	NA
25	1	602	CLA	ND
25	1	603	CLA	ND
25	1	604	CLA	ND
25	1	610	CLA	ND
25	1	611	CLA	ND
25	1	612	CLA	ND
25	1	614	CLA	ND
25	2	603	CLA	ND
25	2	604	CLA	ND
25	2	610	CLA	ND
25	2	611	CLA	ND
25	2	612	CLA	ND
25	2	613	CLA	ND
25	3	602	CLA	ND
25	3	603	CLA	ND
25	3	604	CLA	ND
25	3	610	CLA	ND
25	3	611	CLA	ND
25	3	612	CLA	ND
25	3	614	CLA	ND
25	4	602	CLA	ND
25	4	603	CLA	ND
25	4	604	CLA	ND
25	4	610	CLA	ND
25	4	611	CLA	ND
25	4	612	CLA	ND
25	4	613	CLA	ND
25	4	614	CLA	ND
25	5	602	CLA	ND
25	5	603	CLA	ND
25	5	604	CLA	ND
25	5	610	CLA	ND
25	5	611	CLA	ND
25	5	612	CLA	ND
25	5	613	CLA	ND
25	6	602	CLA	ND
25	6	603	CLA	ND

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Mol	Chain	Res	Type	Atom
25	6	610	CLA	ND
25	6	611	CLA	ND
25	6	612	CLA	ND
25	6	614	CLA	ND
25	A	405	CLA	ND
25	A	406	CLA	ND
25	A	407	CLA	ND
25	A	410	CLA	ND
25	B	602	CLA	ND
25	B	603	CLA	ND
25	B	604	CLA	ND
25	B	605	CLA	ND
25	B	606	CLA	ND
25	B	608	CLA	ND
25	B	609	CLA	ND
25	B	610	CLA	ND
25	B	611	CLA	ND
25	B	612	CLA	ND
25	B	613	CLA	ND
25	B	614	CLA	ND
25	B	615	CLA	ND
25	B	616	CLA	ND
25	B	617	CLA	ND
25	C	501	CLA	ND
25	C	502	CLA	ND
25	C	503	CLA	ND
25	C	504	CLA	ND
25	C	505	CLA	ND
25	C	506	CLA	ND
25	C	507	CLA	ND
25	C	508	CLA	ND
25	C	509	CLA	ND
25	C	510	CLA	ND
25	C	512	CLA	ND
25	C	513	CLA	ND
25	D	402	CLA	ND
25	D	403	CLA	ND
25	G	602	CLA	ND
25	G	603	CLA	ND
25	G	604	CLA	ND
25	G	610	CLA	ND
25	G	611	CLA	ND

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Mol	Chain	Res	Type	Atom
25	G	612	CLA	ND
25	G	613	CLA	ND
25	G	614	CLA	ND
25	N	602	CLA	ND
25	N	603	CLA	ND
25	N	604	CLA	ND
25	N	610	CLA	ND
25	N	611	CLA	ND
25	N	612	CLA	ND
25	N	613	CLA	ND
25	N	614	CLA	ND
25	R	601	CLA	ND
25	R	602	CLA	ND
25	R	603	CLA	ND
25	R	604	CLA	ND
25	R	609	CLA	ND
25	R	610	CLA	ND
25	R	611	CLA	ND
25	R	612	CLA	ND
25	S	603	CLA	ND
25	S	604	CLA	ND
25	S	605	CLA	ND
25	S	609	CLA	ND
25	S	610	CLA	ND
25	S	611	CLA	ND
25	S	612	CLA	ND
25	S	614	CLA	ND
25	Y	602	CLA	ND
25	Y	603	CLA	ND
25	Y	610	CLA	ND
25	Y	611	CLA	ND
25	Y	612	CLA	ND
25	Y	614	CLA	ND
25	0	602	CLA	ND
25	0	603	CLA	ND
25	0	604	CLA	ND
25	0	610	CLA	ND
25	0	611	CLA	ND
25	0	612	CLA	ND
25	0	614	CLA	ND
25	7	602	CLA	ND
25	7	603	CLA	ND

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Mol	Chain	Res	Type	Atom
25	7	604	CLA	ND
25	7	610	CLA	ND
25	7	611	CLA	ND
25	7	612	CLA	ND
25	7	614	CLA	ND
25	8	602	CLA	ND
25	8	603	CLA	ND
25	8	604	CLA	ND
25	8	610	CLA	ND
25	8	611	CLA	ND
25	8	612	CLA	ND
25	8	614	CLA	ND
25	9	602	CLA	ND
25	9	603	CLA	ND
25	9	604	CLA	ND
25	9	610	CLA	ND
25	9	611	CLA	ND
25	9	612	CLA	ND
25	9	613	CLA	ND
25	p	602	CLA	ND
25	p	603	CLA	ND
25	p	604	CLA	ND
25	p	610	CLA	ND
25	p	611	CLA	ND
25	p	612	CLA	ND
25	p	613	CLA	ND
25	q	602	CLA	ND
25	q	603	CLA	ND
25	q	610	CLA	ND
25	q	611	CLA	ND
25	q	612	CLA	ND
25	q	613	CLA	ND
25	q	614	CLA	ND
25	a	405	CLA	ND
25	a	406	CLA	ND
25	a	407	CLA	ND
25	a	410	CLA	ND
25	b	602	CLA	ND
25	b	603	CLA	ND
25	b	604	CLA	ND
25	b	605	CLA	ND
25	b	606	CLA	ND

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Mol	Chain	Res	Type	Atom
25	b	608	CLA	ND
25	b	609	CLA	ND
25	b	610	CLA	ND
25	b	611	CLA	ND
25	b	612	CLA	ND
25	b	613	CLA	ND
25	b	614	CLA	ND
25	b	615	CLA	ND
25	b	616	CLA	ND
25	b	617	CLA	ND
25	c	501	CLA	ND
25	c	502	CLA	ND
25	c	503	CLA	ND
25	c	504	CLA	ND
25	c	505	CLA	ND
25	c	506	CLA	ND
25	c	507	CLA	ND
25	c	508	CLA	ND
25	c	509	CLA	ND
25	c	510	CLA	ND
25	c	512	CLA	ND
25	c	513	CLA	ND
25	d	402	CLA	ND
25	d	403	CLA	ND
25	g	602	CLA	ND
25	g	603	CLA	ND
25	g	604	CLA	ND
25	g	610	CLA	ND
25	g	611	CLA	ND
25	g	612	CLA	ND
25	g	613	CLA	ND
25	g	614	CLA	ND
25	n	602	CLA	ND
25	n	603	CLA	ND
25	n	604	CLA	ND
25	n	610	CLA	ND
25	n	611	CLA	ND
25	n	612	CLA	ND
25	n	613	CLA	ND
25	n	614	CLA	ND
25	s	603	CLA	ND
25	s	604	CLA	ND

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Mol	Chain	Res	Type	Atom
25	s	605	CLA	ND
25	s	609	CLA	ND
25	s	610	CLA	ND
25	s	611	CLA	ND
25	s	612	CLA	ND
25	s	614	CLA	ND
25	y	602	CLA	ND
25	y	603	CLA	ND
25	y	610	CLA	ND
25	y	611	CLA	ND
25	y	612	CLA	ND
25	y	614	CLA	ND
25	r	601	CLA	ND
25	r	602	CLA	ND
25	r	603	CLA	ND
25	r	604	CLA	ND
25	r	609	CLA	ND
25	r	610	CLA	ND
25	r	611	CLA	ND
25	r	612	CLA	ND

All (5618) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
24	1	605	CHL	C1C-C2C-CMC-OMC
24	1	605	CHL	C3C-C2C-CMC-OMC
24	1	606	CHL	C1A-C2A-CAA-CBA
24	1	606	CHL	C1C-C2C-CMC-OMC
24	1	606	CHL	C3C-C2C-CMC-OMC
24	1	607	CHL	C1C-C2C-CMC-OMC
24	1	607	CHL	C3C-C2C-CMC-OMC
24	1	608	CHL	C1A-C2A-CAA-CBA
24	1	608	CHL	C1C-C2C-CMC-OMC
24	1	608	CHL	C3C-C2C-CMC-OMC
24	1	609	CHL	C1C-C2C-CMC-OMC
24	1	609	CHL	C3C-C2C-CMC-OMC
24	2	601	CHL	C3A-C2A-CAA-CBA
24	2	601	CHL	C1C-C2C-CMC-OMC
24	2	601	CHL	C3C-C2C-CMC-OMC
24	2	601	CHL	C2-C3-C5-C6
24	2	601	CHL	C4-C3-C5-C6
24	2	605	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	2	605	CHL	C3A-C2A-CAA-CBA
24	2	605	CHL	C1C-C2C-CMC-OMC
24	2	605	CHL	C3C-C2C-CMC-OMC
24	2	606	CHL	C1C-C2C-CMC-OMC
24	2	606	CHL	C3C-C2C-CMC-OMC
24	2	607	CHL	C1C-C2C-CMC-OMC
24	2	607	CHL	C3C-C2C-CMC-OMC
24	2	609	CHL	C1C-C2C-CMC-OMC
24	2	609	CHL	C3C-C2C-CMC-OMC
24	3	601	CHL	CHA-CBD-CGD-O1D
24	3	601	CHL	CHA-CBD-CGD-O2D
24	3	601	CHL	C6-C7-C8-C9
24	3	605	CHL	C1C-C2C-CMC-OMC
24	3	605	CHL	C3C-C2C-CMC-OMC
24	3	606	CHL	C1A-C2A-CAA-CBA
24	3	607	CHL	C11-C12-C13-C14
24	3	608	CHL	C1C-C2C-CMC-OMC
24	3	608	CHL	C3C-C2C-CMC-OMC
24	3	609	CHL	C1A-C2A-CAA-CBA
24	3	609	CHL	C1C-C2C-CMC-OMC
24	3	609	CHL	C3C-C2C-CMC-OMC
24	4	601	CHL	C1A-C2A-CAA-CBA
24	4	605	CHL	C1A-C2A-CAA-CBA
24	4	607	CHL	C1A-C2A-CAA-CBA
24	4	607	CHL	C3A-C2A-CAA-CBA
24	4	607	CHL	C1C-C2C-CMC-OMC
24	4	607	CHL	C3C-C2C-CMC-OMC
24	4	608	CHL	C1C-C2C-CMC-OMC
24	4	608	CHL	C3C-C2C-CMC-OMC
24	4	609	CHL	C3C-C2C-CMC-OMC
24	4	609	CHL	C11-C10-C8-C9
24	5	601	CHL	C3C-C2C-CMC-OMC
24	5	605	CHL	C3C-C2C-CMC-OMC
24	5	605	CHL	CHA-CBD-CGD-O1D
24	5	605	CHL	CHA-CBD-CGD-O2D
24	5	606	CHL	CBD-CGD-O2D-CED
24	5	607	CHL	C1A-C2A-CAA-CBA
24	5	607	CHL	C3C-C2C-CMC-OMC
24	5	607	CHL	C11-C12-C13-C14
24	5	608	CHL	C3C-C2C-CMC-OMC
24	5	609	CHL	C1C-C2C-CMC-OMC
24	5	609	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
24	6	601	CHL	C3C-C2C-CMC-OMC
24	6	605	CHL	C1C-C2C-CMC-OMC
24	6	605	CHL	C3C-C2C-CMC-OMC
24	6	606	CHL	C1A-C2A-CAA-CBA
24	6	607	CHL	C1A-C2A-CAA-CBA
24	6	607	CHL	C3A-C2A-CAA-CBA
24	6	607	CHL	C1C-C2C-CMC-OMC
24	6	607	CHL	C3C-C2C-CMC-OMC
24	6	607	CHL	CBD-CGD-O2D-CED
24	6	607	CHL	C6-C7-C8-C9
24	6	608	CHL	C3C-C2C-CMC-OMC
24	6	609	CHL	C1C-C2C-CMC-OMC
24	6	609	CHL	C3C-C2C-CMC-OMC
24	6	609	CHL	CBD-CGD-O2D-CED
24	G	601	CHL	C1A-C2A-CAA-CBA
24	G	601	CHL	C3A-C2A-CAA-CBA
24	G	601	CHL	C1C-C2C-CMC-OMC
24	G	601	CHL	C3C-C2C-CMC-OMC
24	G	601	CHL	C2-C3-C5-C6
24	G	601	CHL	C4-C3-C5-C6
24	G	605	CHL	C3A-C2A-CAA-CBA
24	G	605	CHL	C2A-CAA-CBA-CGA
24	G	605	CHL	C1C-C2C-CMC-OMC
24	G	605	CHL	C3C-C2C-CMC-OMC
24	G	607	CHL	C1A-C2A-CAA-CBA
24	G	607	CHL	C1C-C2C-CMC-OMC
24	G	607	CHL	C3C-C2C-CMC-OMC
24	G	608	CHL	C3C-C2C-CMC-OMC
24	G	609	CHL	C1C-C2C-CMC-OMC
24	G	609	CHL	C3C-C2C-CMC-OMC
24	N	605	CHL	C1C-C2C-CMC-OMC
24	N	605	CHL	C3C-C2C-CMC-OMC
24	N	605	CHL	C11-C12-C13-C14
24	N	605	CHL	C12-C13-C15-C16
24	N	608	CHL	C1C-C2C-CMC-OMC
24	N	608	CHL	C3C-C2C-CMC-OMC
24	N	609	CHL	C1C-C2C-CMC-OMC
24	N	609	CHL	C3C-C2C-CMC-OMC
24	R	606	CHL	C1C-C2C-CMC-OMC
24	R	606	CHL	C3C-C2C-CMC-OMC
24	R	607	CHL	C1C-C2C-CMC-OMC
24	R	607	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
24	R	607	CHL	CHA-CBD-CGD-O1D
24	R	607	CHL	CHA-CBD-CGD-O2D
24	R	607	CHL	CAD-CBD-CGD-O1D
24	R	607	CHL	C4-C3-C5-C6
24	S	601	CHL	C1C-C2C-CMC-OMC
24	S	601	CHL	C3C-C2C-CMC-OMC
24	S	601	CHL	CHA-CBD-CGD-O1D
24	S	601	CHL	CHA-CBD-CGD-O2D
24	S	606	CHL	C1C-C2C-CMC-OMC
24	S	606	CHL	C3C-C2C-CMC-OMC
24	S	607	CHL	C1C-C2C-CMC-OMC
24	S	607	CHL	C3C-C2C-CMC-OMC
24	S	608	CHL	C3C-C2C-CMC-OMC
24	S	608	CHL	CHA-CBD-CGD-O1D
24	S	608	CHL	CHA-CBD-CGD-O2D
24	S	608	CHL	CAD-CBD-CGD-O1D
24	S	608	CHL	CAD-CBD-CGD-O2D
24	S	608	CHL	CBD-CGD-O2D-CED
24	Y	605	CHL	C1C-C2C-CMC-OMC
24	Y	605	CHL	C3C-C2C-CMC-OMC
24	Y	606	CHL	C1A-C2A-CAA-CBA
24	Y	606	CHL	C1C-C2C-CMC-OMC
24	Y	607	CHL	C3C-C2C-CMC-OMC
24	Y	607	CHL	CHA-CBD-CGD-O1D
24	0	601	CHL	C3C-C2C-CMC-OMC
24	0	605	CHL	C1C-C2C-CMC-OMC
24	0	605	CHL	C3C-C2C-CMC-OMC
24	0	606	CHL	C1A-C2A-CAA-CBA
24	0	606	CHL	C14-C13-C15-C16
24	0	607	CHL	C1A-C2A-CAA-CBA
24	0	607	CHL	C1C-C2C-CMC-OMC
24	0	607	CHL	C3C-C2C-CMC-OMC
24	0	607	CHL	C14-C13-C15-C16
24	7	605	CHL	C1C-C2C-CMC-OMC
24	7	605	CHL	C3C-C2C-CMC-OMC
24	7	606	CHL	C1C-C2C-CMC-OMC
24	7	607	CHL	C1C-C2C-CMC-OMC
24	7	607	CHL	C3C-C2C-CMC-OMC
24	7	608	CHL	C1C-C2C-CMC-OMC
24	7	608	CHL	C3C-C2C-CMC-OMC
24	7	608	CHL	CBD-CGD-O2D-CED
24	8	601	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	8	601	CHL	CHA-CBD-CGD-O2D
24	8	605	CHL	C1C-C2C-CMC-OMC
24	8	605	CHL	C3C-C2C-CMC-OMC
24	8	606	CHL	C1A-C2A-CAA-CBA
24	8	608	CHL	C1C-C2C-CMC-OMC
24	8	608	CHL	C3C-C2C-CMC-OMC
24	8	609	CHL	C1A-C2A-CAA-CBA
24	8	609	CHL	C1C-C2C-CMC-OMC
24	8	609	CHL	C3C-C2C-CMC-OMC
24	9	601	CHL	C3A-C2A-CAA-CBA
24	9	601	CHL	C1C-C2C-CMC-OMC
24	9	601	CHL	C3C-C2C-CMC-OMC
24	9	605	CHL	C1A-C2A-CAA-CBA
24	9	605	CHL	C3A-C2A-CAA-CBA
24	9	605	CHL	C1C-C2C-CMC-OMC
24	9	605	CHL	C3C-C2C-CMC-OMC
24	9	606	CHL	C1C-C2C-CMC-OMC
24	9	606	CHL	C3C-C2C-CMC-OMC
24	9	607	CHL	C1C-C2C-CMC-OMC
24	9	607	CHL	C3C-C2C-CMC-OMC
24	p	605	CHL	C1C-C2C-CMC-OMC
24	p	605	CHL	C3C-C2C-CMC-OMC
24	p	605	CHL	CHA-CBD-CGD-O1D
24	p	605	CHL	CHA-CBD-CGD-O2D
24	p	605	CHL	C14-C13-C15-C16
24	p	607	CHL	C1A-C2A-CAA-CBA
24	p	607	CHL	C3C-C2C-CMC-OMC
24	p	608	CHL	C1C-C2C-CMC-OMC
24	p	608	CHL	C3C-C2C-CMC-OMC
24	p	609	CHL	C1C-C2C-CMC-OMC
24	p	609	CHL	C3C-C2C-CMC-OMC
24	q	605	CHL	C1C-C2C-CMC-OMC
24	q	605	CHL	C3C-C2C-CMC-OMC
24	q	606	CHL	C1A-C2A-CAA-CBA
24	q	606	CHL	C3A-C2A-CAA-CBA
24	q	607	CHL	C1C-C2C-CMC-OMC
24	q	607	CHL	C3C-C2C-CMC-OMC
24	q	608	CHL	C1C-C2C-CMC-OMC
24	q	608	CHL	C3C-C2C-CMC-OMC
24	g	601	CHL	C1A-C2A-CAA-CBA
24	g	601	CHL	C3A-C2A-CAA-CBA
24	g	601	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
24	g	601	CHL	C3C-C2C-CMC-OMC
24	g	601	CHL	C2-C3-C5-C6
24	g	601	CHL	C4-C3-C5-C6
24	g	605	CHL	C3A-C2A-CAA-CBA
24	g	605	CHL	C2A-CAA-CBA-CGA
24	g	605	CHL	C1C-C2C-CMC-OMC
24	g	605	CHL	C3C-C2C-CMC-OMC
24	g	607	CHL	C1A-C2A-CAA-CBA
24	g	607	CHL	C1C-C2C-CMC-OMC
24	g	607	CHL	C3C-C2C-CMC-OMC
24	g	609	CHL	C1C-C2C-CMC-OMC
24	g	609	CHL	C3C-C2C-CMC-OMC
24	n	605	CHL	C1C-C2C-CMC-OMC
24	n	605	CHL	C3C-C2C-CMC-OMC
24	n	608	CHL	C1C-C2C-CMC-OMC
24	n	608	CHL	C3C-C2C-CMC-OMC
24	n	609	CHL	C1C-C2C-CMC-OMC
24	n	609	CHL	C3C-C2C-CMC-OMC
24	s	601	CHL	C1C-C2C-CMC-OMC
24	s	601	CHL	C3C-C2C-CMC-OMC
24	s	601	CHL	CHA-CBD-CGD-O1D
24	s	601	CHL	CHA-CBD-CGD-O2D
24	s	606	CHL	C1C-C2C-CMC-OMC
24	s	606	CHL	C3C-C2C-CMC-OMC
24	s	607	CHL	C1C-C2C-CMC-OMC
24	s	607	CHL	C3C-C2C-CMC-OMC
24	s	608	CHL	C3C-C2C-CMC-OMC
24	s	608	CHL	CHA-CBD-CGD-O1D
24	s	608	CHL	CHA-CBD-CGD-O2D
24	s	608	CHL	CAD-CBD-CGD-O1D
24	s	608	CHL	CAD-CBD-CGD-O2D
24	s	608	CHL	CBD-CGD-O2D-CED
24	y	605	CHL	C1C-C2C-CMC-OMC
24	y	605	CHL	C3C-C2C-CMC-OMC
24	y	606	CHL	C1A-C2A-CAA-CBA
24	y	606	CHL	C1C-C2C-CMC-OMC
24	y	607	CHL	C3C-C2C-CMC-OMC
24	y	607	CHL	CHA-CBD-CGD-O1D
24	r	606	CHL	C1C-C2C-CMC-OMC
24	r	606	CHL	C3C-C2C-CMC-OMC
24	r	607	CHL	C1C-C2C-CMC-OMC
24	r	607	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
24	r	607	CHL	CHA-CBD-CGD-O1D
24	r	607	CHL	CHA-CBD-CGD-O2D
24	r	607	CHL	CAD-CBD-CGD-O1D
24	r	607	CHL	C4-C3-C5-C6
25	1	602	CLA	C2-C3-C5-C6
25	1	602	CLA	C4-C3-C5-C6
25	1	604	CLA	CBD-CGD-O2D-CED
25	1	614	CLA	C3A-C2A-CAA-CBA
25	1	614	CLA	CHA-CBD-CGD-O1D
25	1	614	CLA	CHA-CBD-CGD-O2D
25	1	614	CLA	CAD-CBD-CGD-O1D
25	1	614	CLA	CAD-CBD-CGD-O2D
25	1	614	CLA	CBD-CGD-O2D-CED
25	2	604	CLA	C1A-C2A-CAA-CBA
25	2	604	CLA	C3A-C2A-CAA-CBA
25	2	604	CLA	CBD-CGD-O2D-CED
25	2	611	CLA	C1A-C2A-CAA-CBA
25	2	611	CLA	C3A-C2A-CAA-CBA
25	2	611	CLA	CHA-CBD-CGD-O1D
25	2	612	CLA	CBD-CGD-O2D-CED
25	2	613	CLA	CHA-CBD-CGD-O1D
25	2	613	CLA	CHA-CBD-CGD-O2D
25	2	613	CLA	CBD-CGD-O2D-CED
25	3	604	CLA	C3A-C2A-CAA-CBA
25	3	604	CLA	CBD-CGD-O2D-CED
25	3	604	CLA	C2-C3-C5-C6
25	3	604	CLA	C4-C3-C5-C6
25	3	611	CLA	CHA-CBD-CGD-O1D
25	3	611	CLA	CAD-CBD-CGD-O1D
25	3	611	CLA	CAD-CBD-CGD-O2D
25	3	612	CLA	C1A-C2A-CAA-CBA
25	3	613	CLA	C1A-C2A-CAA-CBA
25	3	614	CLA	CBD-CGD-O2D-CED
25	4	603	CLA	CBD-CGD-O2D-CED
25	4	604	CLA	C1A-C2A-CAA-CBA
25	4	604	CLA	C3A-C2A-CAA-CBA
25	4	604	CLA	CHA-CBD-CGD-O1D
25	4	604	CLA	CHA-CBD-CGD-O2D
25	4	604	CLA	CAD-CBD-CGD-O1D
25	4	611	CLA	CBD-CGD-O2D-CED
25	4	613	CLA	CBD-CGD-O2D-CED
25	4	614	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	4	614	CLA	CBD-CGD-O2D-CED
25	5	602	CLA	CBD-CGD-O2D-CED
25	5	603	CLA	CHA-CBD-CGD-O2D
25	5	604	CLA	C3A-C2A-CAA-CBA
25	5	604	CLA	CBD-CGD-O2D-CED
25	5	611	CLA	C2A-CAA-CBA-CGA
25	5	611	CLA	CHA-CBD-CGD-O1D
25	5	611	CLA	CHA-CBD-CGD-O2D
25	6	604	CLA	CHA-CBD-CGD-O1D
25	6	604	CLA	CHA-CBD-CGD-O2D
25	6	613	CLA	C1A-C2A-CAA-CBA
25	6	613	CLA	CHA-CBD-CGD-O1D
25	6	613	CLA	CHA-CBD-CGD-O2D
25	6	614	CLA	CHA-CBD-CGD-O1D
25	6	614	CLA	CHA-CBD-CGD-O2D
25	6	614	CLA	CAD-CBD-CGD-O1D
25	6	614	CLA	CBD-CGD-O2D-CED
25	A	405	CLA	CBD-CGD-O2D-CED
25	A	406	CLA	CHA-CBD-CGD-O1D
25	A	406	CLA	CHA-CBD-CGD-O2D
25	A	407	CLA	CHA-CBD-CGD-O1D
25	A	407	CLA	CHA-CBD-CGD-O2D
25	B	603	CLA	C1A-C2A-CAA-CBA
25	B	605	CLA	C1A-C2A-CAA-CBA
25	B	606	CLA	C14-C13-C15-C16
25	B	609	CLA	CBD-CGD-O2D-CED
25	B	613	CLA	C1A-C2A-CAA-CBA
25	B	613	CLA	C3A-C2A-CAA-CBA
25	B	615	CLA	CHA-CBD-CGD-O1D
25	B	615	CLA	CHA-CBD-CGD-O2D
25	B	615	CLA	CAD-CBD-CGD-O1D
25	B	616	CLA	CHA-CBD-CGD-O1D
25	B	616	CLA	CHA-CBD-CGD-O2D
25	B	617	CLA	O1A-CGA-O2A-C1
25	C	501	CLA	CHA-CBD-CGD-O1D
25	C	501	CLA	CHA-CBD-CGD-O2D
25	C	501	CLA	CAD-CBD-CGD-O1D
25	C	502	CLA	CHA-CBD-CGD-O1D
25	C	502	CLA	CHA-CBD-CGD-O2D
25	C	502	CLA	CAD-CBD-CGD-O1D
25	C	502	CLA	CBD-CGD-O2D-CED
25	C	504	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	C	504	CLA	CHA-CBD-CGD-O2D
25	C	504	CLA	CAD-CBD-CGD-O1D
25	C	504	CLA	CAD-CBD-CGD-O2D
25	C	506	CLA	CHA-CBD-CGD-O1D
25	C	506	CLA	CHA-CBD-CGD-O2D
25	C	506	CLA	CAD-CBD-CGD-O1D
25	C	506	CLA	CBD-CGD-O2D-CED
25	C	507	CLA	CHA-CBD-CGD-O1D
25	C	507	CLA	CHA-CBD-CGD-O2D
25	C	513	CLA	CBD-CGD-O2D-CED
25	D	402	CLA	C2-C3-C5-C6
25	D	402	CLA	C4-C3-C5-C6
25	D	403	CLA	C1A-C2A-CAA-CBA
25	D	403	CLA	C3A-C2A-CAA-CBA
25	D	403	CLA	CBD-CGD-O2D-CED
25	G	603	CLA	C1A-C2A-CAA-CBA
25	G	603	CLA	C3A-C2A-CAA-CBA
25	G	604	CLA	C1A-C2A-CAA-CBA
25	G	604	CLA	C3A-C2A-CAA-CBA
25	G	604	CLA	CHA-CBD-CGD-O1D
25	G	604	CLA	CHA-CBD-CGD-O2D
25	G	604	CLA	CAD-CBD-CGD-O1D
25	G	611	CLA	CHA-CBD-CGD-O1D
25	G	611	CLA	CHA-CBD-CGD-O2D
25	G	613	CLA	CHA-CBD-CGD-O1D
25	G	613	CLA	CHA-CBD-CGD-O2D
25	N	603	CLA	C1A-C2A-CAA-CBA
25	N	604	CLA	C1A-C2A-CAA-CBA
25	N	604	CLA	C3A-C2A-CAA-CBA
25	N	611	CLA	C1A-C2A-CAA-CBA
25	N	611	CLA	CAD-CBD-CGD-O1D
25	N	611	CLA	CAD-CBD-CGD-O2D
25	N	611	CLA	CBD-CGD-O2D-CED
25	N	612	CLA	CBD-CGD-O2D-CED
25	R	601	CLA	CBD-CGD-O2D-CED
25	R	604	CLA	C1A-C2A-CAA-CBA
25	R	610	CLA	CBD-CGD-O2D-CED
25	R	611	CLA	C1A-C2A-CAA-CBA
25	R	611	CLA	C3A-C2A-CAA-CBA
25	R	613	CLA	C1A-C2A-CAA-CBA
25	R	613	CLA	C3A-C2A-CAA-CBA
25	R	613	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	R	613	CLA	CHA-CBD-CGD-O2D
25	R	613	CLA	CBD-CGD-O2D-CED
25	R	613	CLA	C2-C3-C5-C6
25	R	613	CLA	C4-C3-C5-C6
25	R	616	CLA	C1A-C2A-CAA-CBA
25	R	616	CLA	C3A-C2A-CAA-CBA
25	S	603	CLA	CHA-CBD-CGD-O1D
25	S	603	CLA	CHA-CBD-CGD-O2D
25	S	604	CLA	CBD-CGD-O2D-CED
25	S	605	CLA	C1A-C2A-CAA-CBA
25	S	605	CLA	CHA-CBD-CGD-O1D
25	S	605	CLA	CHA-CBD-CGD-O2D
25	S	610	CLA	CHA-CBD-CGD-O1D
25	S	610	CLA	CHA-CBD-CGD-O2D
25	S	612	CLA	CBD-CGD-O2D-CED
25	S	613	CLA	CBD-CGD-O2D-CED
25	S	613	CLA	O1D-CGD-O2D-CED
25	S	614	CLA	CBD-CGD-O2D-CED
25	S	614	CLA	O1D-CGD-O2D-CED
25	Y	603	CLA	CHA-CBD-CGD-O1D
25	Y	603	CLA	CHA-CBD-CGD-O2D
25	Y	614	CLA	CHA-CBD-CGD-O1D
25	Y	614	CLA	CHA-CBD-CGD-O2D
25	0	604	CLA	CHA-CBD-CGD-O1D
25	0	604	CLA	CHA-CBD-CGD-O2D
25	0	604	CLA	CBD-CGD-O2D-CED
25	0	613	CLA	CHA-CBD-CGD-O1D
25	0	613	CLA	CHA-CBD-CGD-O2D
25	0	614	CLA	CHA-CBD-CGD-O1D
25	0	614	CLA	CHA-CBD-CGD-O2D
25	0	614	CLA	CAD-CBD-CGD-O1D
25	0	614	CLA	CBD-CGD-O2D-CED
25	7	602	CLA	C2-C3-C5-C6
25	7	602	CLA	C4-C3-C5-C6
25	7	604	CLA	CHA-CBD-CGD-O1D
25	7	611	CLA	C1A-C2A-CAA-CBA
25	7	611	CLA	C3A-C2A-CAA-CBA
25	7	613	CLA	CHA-CBD-CGD-O1D
25	7	613	CLA	CHA-CBD-CGD-O2D
25	7	614	CLA	C3A-C2A-CAA-CBA
25	7	614	CLA	CHA-CBD-CGD-O1D
25	7	614	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	7	614	CLA	CAD-CBD-CGD-O1D
25	7	614	CLA	CAD-CBD-CGD-O2D
25	7	614	CLA	CBD-CGD-O2D-CED
25	8	604	CLA	C3A-C2A-CAA-CBA
25	8	604	CLA	CBD-CGD-O2D-CED
25	8	611	CLA	CHA-CBD-CGD-O1D
25	8	611	CLA	CHA-CBD-CGD-O2D
25	8	611	CLA	CAD-CBD-CGD-O1D
25	8	611	CLA	CAD-CBD-CGD-O2D
25	8	612	CLA	C1A-C2A-CAA-CBA
25	8	613	CLA	C1A-C2A-CAA-CBA
25	8	614	CLA	CBD-CGD-O2D-CED
25	9	602	CLA	C2-C3-C5-C6
25	9	602	CLA	C4-C3-C5-C6
25	9	604	CLA	C1A-C2A-CAA-CBA
25	9	604	CLA	C3A-C2A-CAA-CBA
25	9	611	CLA	C1A-C2A-CAA-CBA
25	9	611	CLA	C3A-C2A-CAA-CBA
25	9	611	CLA	CHA-CBD-CGD-O1D
25	9	611	CLA	CHA-CBD-CGD-O2D
25	9	612	CLA	CBD-CGD-O2D-CED
25	9	613	CLA	CHA-CBD-CGD-O1D
25	9	613	CLA	CHA-CBD-CGD-O2D
25	p	602	CLA	CBD-CGD-O2D-CED
25	p	603	CLA	CHA-CBD-CGD-O1D
25	p	603	CLA	CHA-CBD-CGD-O2D
25	p	604	CLA	C3A-C2A-CAA-CBA
25	p	611	CLA	CHA-CBD-CGD-O1D
25	p	611	CLA	CHA-CBD-CGD-O2D
25	p	613	CLA	CHA-CBD-CGD-O1D
25	p	613	CLA	CHA-CBD-CGD-O2D
25	p	614	CLA	CBD-CGD-O2D-CED
25	q	602	CLA	CBD-CGD-O2D-CED
25	q	604	CLA	C3A-C2A-CAA-CBA
25	q	604	CLA	CAD-CBD-CGD-O1D
25	q	604	CLA	CAD-CBD-CGD-O2D
25	q	611	CLA	CBD-CGD-O2D-CED
25	q	614	CLA	CBD-CGD-O2D-CED
25	a	405	CLA	CBD-CGD-O2D-CED
25	a	406	CLA	CHA-CBD-CGD-O1D
25	a	406	CLA	CHA-CBD-CGD-O2D
25	a	407	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	a	407	CLA	CHA-CBD-CGD-O2D
25	b	603	CLA	C1A-C2A-CAA-CBA
25	b	605	CLA	C1A-C2A-CAA-CBA
25	b	605	CLA	CHA-CBD-CGD-O1D
25	b	606	CLA	C14-C13-C15-C16
25	b	609	CLA	CBD-CGD-O2D-CED
25	b	613	CLA	C1A-C2A-CAA-CBA
25	b	613	CLA	C3A-C2A-CAA-CBA
25	b	615	CLA	CHA-CBD-CGD-O1D
25	b	615	CLA	CHA-CBD-CGD-O2D
25	b	615	CLA	CAD-CBD-CGD-O1D
25	b	616	CLA	CHA-CBD-CGD-O1D
25	b	616	CLA	CHA-CBD-CGD-O2D
25	b	617	CLA	O1A-CGA-O2A-C1
25	c	501	CLA	CHA-CBD-CGD-O1D
25	c	501	CLA	CHA-CBD-CGD-O2D
25	c	501	CLA	CAD-CBD-CGD-O1D
25	c	502	CLA	CHA-CBD-CGD-O1D
25	c	502	CLA	CHA-CBD-CGD-O2D
25	c	502	CLA	CAD-CBD-CGD-O1D
25	c	502	CLA	CBD-CGD-O2D-CED
25	c	503	CLA	C1A-C2A-CAA-CBA
25	c	503	CLA	C2-C3-C5-C6
25	c	503	CLA	C4-C3-C5-C6
25	c	504	CLA	CHA-CBD-CGD-O1D
25	c	504	CLA	CHA-CBD-CGD-O2D
25	c	504	CLA	CAD-CBD-CGD-O1D
25	c	504	CLA	CAD-CBD-CGD-O2D
25	c	506	CLA	CHA-CBD-CGD-O1D
25	c	506	CLA	CHA-CBD-CGD-O2D
25	c	506	CLA	CAD-CBD-CGD-O1D
25	c	506	CLA	CAD-CBD-CGD-O2D
25	c	506	CLA	CBD-CGD-O2D-CED
25	c	507	CLA	CHA-CBD-CGD-O1D
25	c	507	CLA	CHA-CBD-CGD-O2D
25	c	511	CLA	CHA-CBD-CGD-O1D
25	c	511	CLA	CHA-CBD-CGD-O2D
25	c	513	CLA	CBD-CGD-O2D-CED
25	c	513	CLA	C4-C3-C5-C6
25	d	402	CLA	C2-C3-C5-C6
25	d	402	CLA	C4-C3-C5-C6
25	d	403	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	d	403	CLA	C3A-C2A-CAA-CBA
25	d	403	CLA	CBD-CGD-O2D-CED
25	g	603	CLA	C1A-C2A-CAA-CBA
25	g	603	CLA	C3A-C2A-CAA-CBA
25	g	604	CLA	C1A-C2A-CAA-CBA
25	g	604	CLA	C3A-C2A-CAA-CBA
25	g	604	CLA	CHA-CBD-CGD-O1D
25	g	604	CLA	CHA-CBD-CGD-O2D
25	g	604	CLA	CAD-CBD-CGD-O1D
25	g	611	CLA	CHA-CBD-CGD-O1D
25	g	611	CLA	CHA-CBD-CGD-O2D
25	n	603	CLA	C1A-C2A-CAA-CBA
25	n	604	CLA	C1A-C2A-CAA-CBA
25	n	604	CLA	C3A-C2A-CAA-CBA
25	n	611	CLA	CAD-CBD-CGD-O1D
25	n	611	CLA	CAD-CBD-CGD-O2D
25	n	611	CLA	CBD-CGD-O2D-CED
25	n	612	CLA	CBD-CGD-O2D-CED
25	s	603	CLA	CHA-CBD-CGD-O1D
25	s	603	CLA	CHA-CBD-CGD-O2D
25	s	604	CLA	CBD-CGD-O2D-CED
25	s	605	CLA	C1A-C2A-CAA-CBA
25	s	605	CLA	CHA-CBD-CGD-O1D
25	s	605	CLA	CHA-CBD-CGD-O2D
25	s	610	CLA	CHA-CBD-CGD-O1D
25	s	610	CLA	CHA-CBD-CGD-O2D
25	s	612	CLA	CBD-CGD-O2D-CED
25	s	613	CLA	CBD-CGD-O2D-CED
25	s	613	CLA	O1D-CGD-O2D-CED
25	s	614	CLA	CBD-CGD-O2D-CED
25	s	614	CLA	O1D-CGD-O2D-CED
25	y	603	CLA	CHA-CBD-CGD-O1D
25	y	603	CLA	CHA-CBD-CGD-O2D
25	y	614	CLA	CHA-CBD-CGD-O1D
25	y	614	CLA	CHA-CBD-CGD-O2D
25	r	601	CLA	C3A-C2A-CAA-CBA
25	r	601	CLA	CBD-CGD-O2D-CED
25	r	604	CLA	C1A-C2A-CAA-CBA
25	r	610	CLA	CBD-CGD-O2D-CED
25	r	611	CLA	C1A-C2A-CAA-CBA
25	r	611	CLA	C3A-C2A-CAA-CBA
25	r	613	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	r	613	CLA	C3A-C2A-CAA-CBA
25	r	613	CLA	CHA-CBD-CGD-O1D
25	r	613	CLA	CHA-CBD-CGD-O2D
25	r	613	CLA	CBD-CGD-O2D-CED
25	r	613	CLA	C2-C3-C5-C6
25	r	613	CLA	C4-C3-C5-C6
25	r	616	CLA	C1A-C2A-CAA-CBA
25	r	616	CLA	C3A-C2A-CAA-CBA
26	2	1621	LUT	C7-C8-C9-C10
26	2	1621	LUT	C7-C8-C9-C19
26	3	1620	LUT	C27-C28-C29-C39
26	4	1620	LUT	C31-C32-C33-C34
26	4	1620	LUT	C31-C32-C33-C40
26	4	1621	LUT	C11-C12-C13-C20
26	6	1620	LUT	C1-C6-C7-C8
26	N	1620	LUT	C1-C6-C7-C8
26	N	1621	LUT	C1-C6-C7-C8
26	9	1621	LUT	C7-C8-C9-C10
26	9	1621	LUT	C7-C8-C9-C19
26	p	1621	LUT	C1-C6-C7-C8
26	p	1621	LUT	C27-C28-C29-C39
26	q	1620	LUT	C1-C6-C7-C8
26	n	1620	LUT	C1-C6-C7-C8
26	n	1621	LUT	C1-C6-C7-C8
27	1	1622	XAT	C31-C32-C33-C40
27	2	1622	XAT	C31-C32-C33-C34
27	2	1622	XAT	C31-C32-C33-C40
27	6	1622	XAT	C31-C32-C33-C34
27	6	1622	XAT	C31-C32-C33-C40
27	7	1622	XAT	C31-C32-C33-C40
27	9	1622	XAT	C31-C32-C33-C34
27	9	1622	XAT	C31-C32-C33-C40
28	1	1623	NEX	C11-C12-C13-C14
28	1	1623	NEX	C11-C12-C13-C20
28	S	1623	NEX	C11-C12-C13-C14
28	S	1623	NEX	C11-C12-C13-C20
28	Y	1623	NEX	C31-C32-C33-C34
28	Y	1623	NEX	C31-C32-C33-C40
28	7	1623	NEX	C11-C12-C13-C14
28	7	1623	NEX	C11-C12-C13-C20
28	s	1623	NEX	C11-C12-C13-C14
28	s	1623	NEX	C11-C12-C13-C20

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Mol	Chain	Res	Type	Atoms
28	y	1623	NEX	C31-C32-C33-C34
28	y	1623	NEX	C31-C32-C33-C40
29	1	2630	LHG	C4-O6-P-O3
29	2	2630	LHG	C1-C2-C3-O3
29	2	2630	LHG	C4-O6-P-O5
29	3	2630	LHG	C4-O6-P-O3
29	3	2630	LHG	C4-O6-P-O4
29	3	2630	LHG	C4-O6-P-O5
29	4	2630	LHG	C4-O6-P-O3
29	4	2630	LHG	C4-O6-P-O4
29	4	2630	LHG	C4-O6-P-O5
29	5	2630	LHG	O1-C1-C2-C3
29	5	2630	LHG	C4-O6-P-O4
29	6	2630	LHG	O1-C1-C2-C3
29	6	2630	LHG	C4-O6-P-O5
29	C	2630	LHG	O1-C1-C2-C3
29	D	408	LHG	C3-O3-P-O5
29	D	408	LHG	C4-O6-P-O4
29	D	409	LHG	C4-O6-P-O3
29	D	410	LHG	C3-O3-P-O4
29	D	410	LHG	C3-O3-P-O5
29	D	410	LHG	C3-O3-P-O6
29	L	101	LHG	C3-O3-P-O5
29	L	101	LHG	C4-O6-P-O3
29	L	101	LHG	C4-O6-P-O4
29	L	101	LHG	C4-O6-P-O5
29	N	2630	LHG	C3-O3-P-O4
29	N	2630	LHG	C4-O6-P-O4
29	N	2630	LHG	C4-O6-P-O5
29	N	2630	LHG	O7-C5-C6-O8
29	R	2630	LHG	C3-O3-P-O4
29	R	2630	LHG	C4-O6-P-O5
29	Y	2630	LHG	C1-C2-C3-O3
29	Y	2630	LHG	C4-O6-P-O3
29	Y	2630	LHG	C4-O6-P-O4
29	Y	2630	LHG	C4-O6-P-O5
29	0	2630	LHG	C4-O6-P-O4
29	0	2630	LHG	C4-O6-P-O5
29	7	2630	LHG	C4-O6-P-O3
29	8	2630	LHG	C4-O6-P-O3
29	8	2630	LHG	C4-O6-P-O4
29	8	2630	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
29	9	2630	LHG	C1-C2-C3-O3
29	9	2630	LHG	C3-O3-P-O6
29	9	2630	LHG	C4-O6-P-O5
29	p	2630	LHG	O1-C1-C2-C3
29	p	2630	LHG	C4-O6-P-O4
29	q	2630	LHG	C3-O3-P-O5
29	c	2630	LHG	C4-O6-P-O3
29	d	408	LHG	C3-O3-P-O5
29	d	408	LHG	C4-O6-P-O4
29	d	409	LHG	C4-O6-P-O3
29	d	410	LHG	C3-O3-P-O4
29	d	410	LHG	C3-O3-P-O5
29	d	410	LHG	C3-O3-P-O6
29	l	101	LHG	C3-O3-P-O5
29	l	101	LHG	C4-O6-P-O5
29	n	2630	LHG	C3-O3-P-O4
29	n	2630	LHG	C4-O6-P-O4
29	n	2630	LHG	C4-O6-P-O5
29	n	2630	LHG	O7-C5-C6-O8
29	s	2630	LHG	O1-C1-C2-C3
29	y	2630	LHG	C1-C2-C3-O3
29	y	2630	LHG	C4-O6-P-O3
29	y	2630	LHG	C4-O6-P-O4
29	y	2630	LHG	C4-O6-P-O5
29	r	2630	LHG	C3-O3-P-O4
29	r	2630	LHG	C4-O6-P-O5
34	B	620	BCR	C7-C8-C9-C34
34	C	516	BCR	C7-C8-C9-C10
34	C	516	BCR	C7-C8-C9-C34
34	C	516	BCR	C21-C22-C23-C24
34	C	516	BCR	C37-C22-C23-C24
34	H	101	BCR	C7-C8-C9-C10
34	H	101	BCR	C7-C8-C9-C34
34	H	101	BCR	C23-C24-C25-C30
34	b	620	BCR	C7-C8-C9-C34
34	c	516	BCR	C7-C8-C9-C10
34	c	516	BCR	C7-C8-C9-C34
34	c	516	BCR	C21-C22-C23-C24
34	c	516	BCR	C37-C22-C23-C24
34	h	101	BCR	C7-C8-C9-C10
34	h	101	BCR	C7-C8-C9-C34
34	h	101	BCR	C23-C24-C25-C30

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Mol	Chain	Res	Type	Atoms
35	A	412	SQD	O5-C5-C6-S
35	A	412	SQD	C5-C6-S-O8
35	A	412	SQD	C5-C6-S-O9
35	B	621	SQD	C2-C1-O6-C44
35	B	621	SQD	C8-C7-O47-C45
35	a	412	SQD	O5-C5-C6-S
35	a	412	SQD	C5-C6-S-O8
35	a	412	SQD	C5-C6-S-O9
35	b	621	SQD	C2-C1-O6-C44
35	b	621	SQD	C8-C7-O47-C45
36	S	2631	LMG	O7-C8-C9-O8
36	s	2631	LMG	O7-C8-C9-O8
37	C	519	DGD	C2E-C1E-O5D-C6D
37	C	519	DGD	O6E-C1E-O5D-C6D
37	c	519	DGD	C2E-C1E-O5D-C6D
37	c	519	DGD	O6E-C1E-O5D-C6D
39	D	405	PL9	C7-C8-C9-C10
39	D	405	PL9	C22-C23-C24-C26
39	D	405	PL9	C37-C38-C39-C40
39	d	405	PL9	C7-C8-C9-C10
39	d	405	PL9	C22-C23-C24-C26
39	d	405	PL9	C37-C38-C39-C40
39	d	405	PL9	C42-C43-C44-C45
24	6	609	CHL	O1D-CGD-O2D-CED
24	0	609	CHL	O1D-CGD-O2D-CED
25	6	604	CLA	O1D-CGD-O2D-CED
25	A	405	CLA	O1D-CGD-O2D-CED
25	G	612	CLA	O1D-CGD-O2D-CED
25	R	613	CLA	O1D-CGD-O2D-CED
25	S	603	CLA	O1D-CGD-O2D-CED
25	0	604	CLA	O1D-CGD-O2D-CED
25	a	405	CLA	O1D-CGD-O2D-CED
25	g	612	CLA	O1D-CGD-O2D-CED
25	s	603	CLA	O1D-CGD-O2D-CED
25	r	613	CLA	O1D-CGD-O2D-CED
24	4	607	CHL	O1D-CGD-O2D-CED
24	G	608	CHL	O1D-CGD-O2D-CED
24	q	607	CHL	O1D-CGD-O2D-CED
24	g	608	CHL	O1D-CGD-O2D-CED
25	5	612	CLA	O1D-CGD-O2D-CED
25	6	613	CLA	O1D-CGD-O2D-CED
25	C	503	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	N	612	CLA	O1D-CGD-O2D-CED
25	p	612	CLA	O1D-CGD-O2D-CED
25	q	604	CLA	O1D-CGD-O2D-CED
25	c	503	CLA	O1D-CGD-O2D-CED
25	n	612	CLA	O1D-CGD-O2D-CED
24	1	607	CHL	CBD-CGD-O2D-CED
24	1	608	CHL	CBD-CGD-O2D-CED
24	1	609	CHL	CBD-CGD-O2D-CED
24	2	601	CHL	CBD-CGD-O2D-CED
24	3	608	CHL	CBD-CGD-O2D-CED
24	4	607	CHL	CBD-CGD-O2D-CED
24	4	608	CHL	CBD-CGD-O2D-CED
24	4	609	CHL	CBD-CGD-O2D-CED
24	5	608	CHL	CBD-CGD-O2D-CED
24	6	606	CHL	CBD-CGD-O2D-CED
24	6	608	CHL	CBD-CGD-O2D-CED
24	G	606	CHL	CBD-CGD-O2D-CED
24	G	608	CHL	CBD-CGD-O2D-CED
24	N	606	CHL	CBD-CGD-O2D-CED
24	N	608	CHL	CBD-CGD-O2D-CED
24	Y	607	CHL	CBD-CGD-O2D-CED
24	0	606	CHL	CBD-CGD-O2D-CED
24	0	608	CHL	CBD-CGD-O2D-CED
24	0	609	CHL	CBD-CGD-O2D-CED
24	7	607	CHL	CBD-CGD-O2D-CED
24	8	608	CHL	CBD-CGD-O2D-CED
24	9	601	CHL	CBD-CGD-O2D-CED
24	9	608	CHL	CBD-CGD-O2D-CED
24	p	608	CHL	CBD-CGD-O2D-CED
24	q	607	CHL	CBD-CGD-O2D-CED
24	q	608	CHL	CBD-CGD-O2D-CED
24	g	606	CHL	CBD-CGD-O2D-CED
24	g	607	CHL	CBD-CGD-O2D-CED
24	g	608	CHL	CBD-CGD-O2D-CED
24	n	606	CHL	CBD-CGD-O2D-CED
24	n	608	CHL	CBD-CGD-O2D-CED
24	y	607	CHL	CBD-CGD-O2D-CED
25	2	603	CLA	CBD-CGD-O2D-CED
25	2	611	CLA	CBD-CGD-O2D-CED
25	3	602	CLA	CBD-CGD-O2D-CED
25	3	603	CLA	CBD-CGD-O2D-CED
25	3	612	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	4	602	CLA	CBD-CGD-O2D-CED
25	5	603	CLA	CBD-CGD-O2D-CED
25	5	612	CLA	CBD-CGD-O2D-CED
25	6	604	CLA	CBD-CGD-O2D-CED
25	6	611	CLA	CBD-CGD-O2D-CED
25	6	613	CLA	CBD-CGD-O2D-CED
25	B	602	CLA	CBD-CGD-O2D-CED
25	B	603	CLA	CBD-CGD-O2D-CED
25	B	606	CLA	CBD-CGD-O2D-CED
25	B	608	CLA	CBD-CGD-O2D-CED
25	B	612	CLA	CBD-CGD-O2D-CED
25	B	614	CLA	CBD-CGD-O2D-CED
25	B	616	CLA	CBD-CGD-O2D-CED
25	C	503	CLA	CBD-CGD-O2D-CED
25	C	508	CLA	CBD-CGD-O2D-CED
25	G	612	CLA	CBD-CGD-O2D-CED
25	N	614	CLA	CBD-CGD-O2D-CED
25	R	603	CLA	CBD-CGD-O2D-CED
25	R	612	CLA	CBD-CGD-O2D-CED
25	S	603	CLA	CBD-CGD-O2D-CED
25	S	605	CLA	CBD-CGD-O2D-CED
25	S	610	CLA	CBD-CGD-O2D-CED
25	Y	614	CLA	CBD-CGD-O2D-CED
25	0	611	CLA	CBD-CGD-O2D-CED
25	8	602	CLA	CBD-CGD-O2D-CED
25	8	612	CLA	CBD-CGD-O2D-CED
25	9	603	CLA	CBD-CGD-O2D-CED
25	9	604	CLA	CBD-CGD-O2D-CED
25	9	611	CLA	CBD-CGD-O2D-CED
25	9	613	CLA	CBD-CGD-O2D-CED
25	p	603	CLA	CBD-CGD-O2D-CED
25	p	612	CLA	CBD-CGD-O2D-CED
25	q	603	CLA	CBD-CGD-O2D-CED
25	q	604	CLA	CBD-CGD-O2D-CED
25	q	613	CLA	CBD-CGD-O2D-CED
25	b	602	CLA	CBD-CGD-O2D-CED
25	b	603	CLA	CBD-CGD-O2D-CED
25	b	606	CLA	CBD-CGD-O2D-CED
25	b	608	CLA	CBD-CGD-O2D-CED
25	b	612	CLA	CBD-CGD-O2D-CED
25	b	614	CLA	CBD-CGD-O2D-CED
25	b	616	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	c	503	CLA	CBD-CGD-O2D-CED
25	c	508	CLA	CBD-CGD-O2D-CED
25	g	612	CLA	CBD-CGD-O2D-CED
25	n	614	CLA	CBD-CGD-O2D-CED
25	s	603	CLA	CBD-CGD-O2D-CED
25	s	605	CLA	CBD-CGD-O2D-CED
25	s	610	CLA	CBD-CGD-O2D-CED
25	y	614	CLA	CBD-CGD-O2D-CED
25	r	603	CLA	CBD-CGD-O2D-CED
25	r	612	CLA	CBD-CGD-O2D-CED
25	C	505	CLA	O1A-CGA-O2A-C1
25	S	614	CLA	O1A-CGA-O2A-C1
25	c	505	CLA	O1A-CGA-O2A-C1
25	s	614	CLA	O1A-CGA-O2A-C1
29	C	2630	LHG	O10-C23-O8-C6
29	c	2630	LHG	O10-C23-O8-C6
24	1	608	CHL	O1D-CGD-O2D-CED
24	5	608	CHL	O1D-CGD-O2D-CED
24	6	607	CHL	O1D-CGD-O2D-CED
24	9	601	CHL	O1D-CGD-O2D-CED
25	1	614	CLA	O1D-CGD-O2D-CED
25	3	604	CLA	O1D-CGD-O2D-CED
25	3	612	CLA	O1D-CGD-O2D-CED
25	4	603	CLA	O1D-CGD-O2D-CED
25	5	602	CLA	O1D-CGD-O2D-CED
25	6	611	CLA	O1D-CGD-O2D-CED
25	B	606	CLA	O1D-CGD-O2D-CED
25	B	608	CLA	O1D-CGD-O2D-CED
25	R	612	CLA	O1D-CGD-O2D-CED
25	0	611	CLA	O1D-CGD-O2D-CED
25	7	614	CLA	O1D-CGD-O2D-CED
25	8	604	CLA	O1D-CGD-O2D-CED
25	p	602	CLA	O1D-CGD-O2D-CED
25	b	606	CLA	O1D-CGD-O2D-CED
25	b	608	CLA	O1D-CGD-O2D-CED
25	r	612	CLA	O1D-CGD-O2D-CED
24	2	601	CHL	O1D-CGD-O2D-CED
24	4	608	CHL	O1D-CGD-O2D-CED
24	7	608	CHL	O1D-CGD-O2D-CED
24	9	608	CHL	O1D-CGD-O2D-CED
24	p	608	CHL	O1D-CGD-O2D-CED
25	1	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	2	604	CLA	O1D-CGD-O2D-CED
25	4	611	CLA	O1D-CGD-O2D-CED
25	4	614	CLA	O1D-CGD-O2D-CED
25	6	614	CLA	O1D-CGD-O2D-CED
25	C	502	CLA	O1D-CGD-O2D-CED
25	C	506	CLA	O1D-CGD-O2D-CED
25	0	614	CLA	O1D-CGD-O2D-CED
25	8	612	CLA	O1D-CGD-O2D-CED
25	p	614	CLA	O1D-CGD-O2D-CED
25	q	611	CLA	O1D-CGD-O2D-CED
25	c	502	CLA	O1D-CGD-O2D-CED
25	c	506	CLA	O1D-CGD-O2D-CED
25	d	403	CLA	O1D-CGD-O2D-CED
25	S	614	CLA	CBA-CGA-O2A-C1
25	s	614	CLA	CBA-CGA-O2A-C1
29	C	2630	LHG	C24-C23-O8-C6
24	1	605	CHL	CBD-CGD-O2D-CED
24	4	606	CHL	CBD-CGD-O2D-CED
24	0	607	CHL	CBD-CGD-O2D-CED
24	7	605	CHL	CBD-CGD-O2D-CED
24	9	606	CHL	CBD-CGD-O2D-CED
24	p	607	CHL	CBD-CGD-O2D-CED
24	p	609	CHL	CBD-CGD-O2D-CED
24	q	606	CHL	CBD-CGD-O2D-CED
24	q	609	CHL	CBD-CGD-O2D-CED
25	1	612	CLA	CBD-CGD-O2D-CED
25	6	602	CLA	CBD-CGD-O2D-CED
25	B	605	CLA	CBD-CGD-O2D-CED
25	B	615	CLA	CBD-CGD-O2D-CED
25	G	603	CLA	CBD-CGD-O2D-CED
25	Y	603	CLA	CBD-CGD-O2D-CED
25	Y	604	CLA	CBD-CGD-O2D-CED
25	Y	612	CLA	CBD-CGD-O2D-CED
25	0	602	CLA	CBD-CGD-O2D-CED
25	8	603	CLA	CBD-CGD-O2D-CED
25	b	605	CLA	CBD-CGD-O2D-CED
25	b	615	CLA	CBD-CGD-O2D-CED
25	c	507	CLA	CBD-CGD-O2D-CED
25	g	603	CLA	CBD-CGD-O2D-CED
25	y	603	CLA	CBD-CGD-O2D-CED
25	y	604	CLA	CBD-CGD-O2D-CED
25	y	612	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	N	605	CHL	O1A-CGA-O2A-C1
24	n	605	CHL	O1A-CGA-O2A-C1
25	1	614	CLA	O1A-CGA-O2A-C1
25	R	611	CLA	O1A-CGA-O2A-C1
25	R	612	CLA	O1A-CGA-O2A-C1
25	S	613	CLA	O1A-CGA-O2A-C1
25	0	611	CLA	O1A-CGA-O2A-C1
25	7	614	CLA	O1A-CGA-O2A-C1
25	q	613	CLA	O1A-CGA-O2A-C1
25	s	605	CLA	O1A-CGA-O2A-C1
25	s	613	CLA	O1A-CGA-O2A-C1
25	r	611	CLA	O1A-CGA-O2A-C1
25	r	612	CLA	O1A-CGA-O2A-C1
24	S	608	CHL	O1D-CGD-O2D-CED
24	s	608	CHL	O1D-CGD-O2D-CED
25	4	613	CLA	O1D-CGD-O2D-CED
25	5	604	CLA	O1D-CGD-O2D-CED
25	B	609	CLA	O1D-CGD-O2D-CED
25	D	403	CLA	O1D-CGD-O2D-CED
25	N	611	CLA	O1D-CGD-O2D-CED
25	R	601	CLA	O1D-CGD-O2D-CED
25	R	610	CLA	O1D-CGD-O2D-CED
25	S	604	CLA	O1D-CGD-O2D-CED
25	b	609	CLA	O1D-CGD-O2D-CED
25	n	611	CLA	O1D-CGD-O2D-CED
25	s	604	CLA	O1D-CGD-O2D-CED
25	s	612	CLA	O1D-CGD-O2D-CED
25	r	601	CLA	O1D-CGD-O2D-CED
25	r	610	CLA	O1D-CGD-O2D-CED
24	5	606	CHL	O1D-CGD-O2D-CED
25	2	612	CLA	O1D-CGD-O2D-CED
25	2	613	CLA	O1D-CGD-O2D-CED
25	3	614	CLA	O1D-CGD-O2D-CED
25	S	612	CLA	O1D-CGD-O2D-CED
25	9	612	CLA	O1D-CGD-O2D-CED
25	q	602	CLA	O1D-CGD-O2D-CED
25	c	513	CLA	O1D-CGD-O2D-CED
24	2	606	CHL	CBD-CGD-O2D-CED
24	5	609	CHL	CBD-CGD-O2D-CED
24	R	607	CHL	CBD-CGD-O2D-CED
24	Y	606	CHL	CBD-CGD-O2D-CED
24	Y	608	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	y	606	CHL	CBD-CGD-O2D-CED
24	y	608	CHL	CBD-CGD-O2D-CED
25	2	614	CLA	CBD-CGD-O2D-CED
25	4	604	CLA	CBD-CGD-O2D-CED
25	5	614	CLA	CBD-CGD-O2D-CED
25	G	614	CLA	CBD-CGD-O2D-CED
25	R	611	CLA	CBD-CGD-O2D-CED
25	9	614	CLA	CBD-CGD-O2D-CED
25	c	511	CLA	CBD-CGD-O2D-CED
25	r	611	CLA	CBD-CGD-O2D-CED
33	A	408	PHO	CBD-CGD-O2D-CED
33	a	408	PHO	CBD-CGD-O2D-CED
24	q	608	CHL	O1D-CGD-O2D-CED
25	B	616	CLA	O1D-CGD-O2D-CED
25	C	513	CLA	O1D-CGD-O2D-CED
25	8	614	CLA	O1D-CGD-O2D-CED
25	q	614	CLA	O1D-CGD-O2D-CED
25	n	614	CLA	O1D-CGD-O2D-CED
35	B	621	SQD	O49-C7-O47-C45
35	b	621	SQD	O49-C7-O47-C45
25	S	611	CLA	O1A-CGA-O2A-C1
25	N	614	CLA	O1D-CGD-O2D-CED
24	2	601	CHL	C3-C5-C6-C7
24	3	607	CHL	C3-C5-C6-C7
24	4	601	CHL	C3-C5-C6-C7
24	5	607	CHL	C3-C5-C6-C7
24	6	601	CHL	C3-C5-C6-C7
24	G	601	CHL	C3-C5-C6-C7
24	p	605	CHL	C3-C5-C6-C7
25	1	602	CLA	C3-C5-C6-C7
25	1	604	CLA	C3-C5-C6-C7
25	2	603	CLA	C3-C5-C6-C7
25	3	603	CLA	C3-C5-C6-C7
25	6	602	CLA	C3-C5-C6-C7
25	B	609	CLA	C3-C5-C6-C7
25	B	615	CLA	C3-C5-C6-C7
25	B	617	CLA	C3-C5-C6-C7
25	C	509	CLA	C3-C5-C6-C7
25	N	613	CLA	C3-C5-C6-C7
25	R	603	CLA	C3-C5-C6-C7
25	R	613	CLA	C3-C5-C6-C7
25	Y	612	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	0	602	CLA	C3-C5-C6-C7
25	7	602	CLA	C3-C5-C6-C7
25	9	603	CLA	C3-C5-C6-C7
25	b	609	CLA	C3-C5-C6-C7
25	b	615	CLA	C3-C5-C6-C7
25	b	617	CLA	C3-C5-C6-C7
25	c	509	CLA	C3-C5-C6-C7
25	n	613	CLA	C3-C5-C6-C7
25	y	612	CLA	C3-C5-C6-C7
25	r	603	CLA	C3-C5-C6-C7
25	r	613	CLA	C3-C5-C6-C7
25	3	614	CLA	CBA-CGA-O2A-C1
25	B	617	CLA	CBA-CGA-O2A-C1
25	C	505	CLA	CBA-CGA-O2A-C1
25	G	614	CLA	CBA-CGA-O2A-C1
25	R	611	CLA	CBA-CGA-O2A-C1
25	R	612	CLA	CBA-CGA-O2A-C1
25	R	616	CLA	CBA-CGA-O2A-C1
25	8	614	CLA	CBA-CGA-O2A-C1
25	b	617	CLA	CBA-CGA-O2A-C1
25	c	505	CLA	CBA-CGA-O2A-C1
25	g	614	CLA	CBA-CGA-O2A-C1
25	s	605	CLA	CBA-CGA-O2A-C1
25	r	611	CLA	CBA-CGA-O2A-C1
25	r	612	CLA	CBA-CGA-O2A-C1
25	r	616	CLA	CBA-CGA-O2A-C1
29	c	2630	LHG	C24-C23-O8-C6
24	g	606	CHL	O1D-CGD-O2D-CED
25	2	611	CLA	O1D-CGD-O2D-CED
25	B	602	CLA	O1D-CGD-O2D-CED
25	b	602	CLA	O1D-CGD-O2D-CED
25	b	616	CLA	O1D-CGD-O2D-CED
24	2	608	CHL	CBD-CGD-O2D-CED
24	R	606	CHL	CBD-CGD-O2D-CED
24	7	609	CHL	CBD-CGD-O2D-CED
24	r	606	CHL	CBD-CGD-O2D-CED
24	r	607	CHL	CBD-CGD-O2D-CED
25	5	613	CLA	CBD-CGD-O2D-CED
25	p	604	CLA	CBD-CGD-O2D-CED
25	g	614	CLA	CBD-CGD-O2D-CED
25	C	510	CLA	O1A-CGA-O2A-C1
25	c	510	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	s	611	CLA	O1A-CGA-O2A-C1
25	8	602	CLA	O1D-CGD-O2D-CED
24	5	607	CHL	C4-C3-C5-C6
25	8	604	CLA	C4-C3-C5-C6
24	R	607	CHL	C2-C3-C5-C6
24	r	607	CHL	C2-C3-C5-C6
25	8	604	CLA	C2-C3-C5-C6
25	c	513	CLA	C2-C3-C5-C6
39	d	405	PL9	C12-C11-C9-C8
24	3	609	CHL	CBD-CGD-O2D-CED
25	C	511	CLA	CBD-CGD-O2D-CED
25	N	604	CLA	CBD-CGD-O2D-CED
25	7	604	CLA	CBD-CGD-O2D-CED
25	n	604	CLA	CBD-CGD-O2D-CED
24	1	601	CHL	C2A-CAA-CBA-CGA
24	1	605	CHL	C2A-CAA-CBA-CGA
24	1	607	CHL	C2A-CAA-CBA-CGA
24	2	601	CHL	C2A-CAA-CBA-CGA
24	2	607	CHL	C2A-CAA-CBA-CGA
24	Y	605	CHL	C2A-CAA-CBA-CGA
24	7	601	CHL	C2A-CAA-CBA-CGA
24	7	605	CHL	C2A-CAA-CBA-CGA
24	7	607	CHL	C2A-CAA-CBA-CGA
24	9	601	CHL	C2A-CAA-CBA-CGA
24	9	607	CHL	C2A-CAA-CBA-CGA
24	n	608	CHL	C2A-CAA-CBA-CGA
24	y	605	CHL	C2A-CAA-CBA-CGA
25	3	611	CLA	C2A-CAA-CBA-CGA
25	B	607	CLA	C2A-CAA-CBA-CGA
25	B	611	CLA	C2A-CAA-CBA-CGA
25	C	513	CLA	C2A-CAA-CBA-CGA
25	R	613	CLA	C2A-CAA-CBA-CGA
25	S	613	CLA	C2A-CAA-CBA-CGA
25	7	604	CLA	C2A-CAA-CBA-CGA
25	8	611	CLA	C2A-CAA-CBA-CGA
25	q	613	CLA	C2A-CAA-CBA-CGA
25	b	607	CLA	C2A-CAA-CBA-CGA
25	b	611	CLA	C2A-CAA-CBA-CGA
25	c	513	CLA	C2A-CAA-CBA-CGA
25	s	613	CLA	C2A-CAA-CBA-CGA
25	r	613	CLA	C2A-CAA-CBA-CGA
25	Y	611	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	g	613	CLA	O1A-CGA-O2A-C1
25	y	611	CLA	O1A-CGA-O2A-C1
25	3	602	CLA	O1D-CGD-O2D-CED
25	Y	614	CLA	O1D-CGD-O2D-CED
25	y	614	CLA	O1D-CGD-O2D-CED
24	5	605	CHL	C3-C5-C6-C7
24	6	607	CHL	C3-C5-C6-C7
24	9	601	CHL	C3-C5-C6-C7
24	g	601	CHL	C3-C5-C6-C7
25	5	602	CLA	C3-C5-C6-C7
25	C	508	CLA	C3-C5-C6-C7
25	G	613	CLA	C3-C5-C6-C7
25	0	613	CLA	C3-C5-C6-C7
25	7	604	CLA	C3-C5-C6-C7
25	c	508	CLA	C3-C5-C6-C7
25	g	613	CLA	C3-C5-C6-C7
25	q	612	CLA	C2A-CAA-CBA-CGA
24	N	605	CHL	CBA-CGA-O2A-C1
24	R	607	CHL	CBA-CGA-O2A-C1
24	n	605	CHL	CBA-CGA-O2A-C1
24	r	607	CHL	CBA-CGA-O2A-C1
25	l	614	CLA	CBA-CGA-O2A-C1
25	C	512	CLA	CBA-CGA-O2A-C1
25	G	613	CLA	CBA-CGA-O2A-C1
25	S	605	CLA	CBA-CGA-O2A-C1
25	S	611	CLA	CBA-CGA-O2A-C1
25	S	613	CLA	CBA-CGA-O2A-C1
25	Y	612	CLA	CBA-CGA-O2A-C1
25	0	611	CLA	CBA-CGA-O2A-C1
25	7	614	CLA	CBA-CGA-O2A-C1
25	p	614	CLA	CBA-CGA-O2A-C1
25	q	613	CLA	CBA-CGA-O2A-C1
25	c	513	CLA	CBA-CGA-O2A-C1
25	g	613	CLA	CBA-CGA-O2A-C1
25	s	611	CLA	CBA-CGA-O2A-C1
25	s	613	CLA	CBA-CGA-O2A-C1
25	y	612	CLA	CBA-CGA-O2A-C1
24	1	607	CHL	O1D-CGD-O2D-CED
24	N	606	CHL	O1D-CGD-O2D-CED
24	7	607	CHL	O1D-CGD-O2D-CED
25	S	605	CLA	O1D-CGD-O2D-CED
25	9	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
39	D	405	PL9	C22-C23-C24-C25
39	D	405	PL9	C42-C43-C44-C45
39	d	405	PL9	C22-C23-C24-C25
24	1	606	CHL	CBD-CGD-O2D-CED
24	5	607	CHL	CBD-CGD-O2D-CED
24	8	609	CHL	CBD-CGD-O2D-CED
25	B	611	CLA	CBD-CGD-O2D-CED
25	7	612	CLA	CBD-CGD-O2D-CED
25	b	611	CLA	CBD-CGD-O2D-CED
24	3	608	CHL	O1D-CGD-O2D-CED
24	4	609	CHL	O1D-CGD-O2D-CED
24	G	606	CHL	O1D-CGD-O2D-CED
24	0	606	CHL	O1D-CGD-O2D-CED
24	n	608	CHL	O1D-CGD-O2D-CED
25	9	611	CLA	O1D-CGD-O2D-CED
25	9	613	CLA	O1D-CGD-O2D-CED
39	D	405	PL9	C7-C8-C9-C11
39	d	405	PL9	C7-C8-C9-C11
25	A	405	CLA	O1A-CGA-O2A-C1
25	G	613	CLA	O1A-CGA-O2A-C1
25	G	614	CLA	O1A-CGA-O2A-C1
25	S	605	CLA	O1A-CGA-O2A-C1
25	a	405	CLA	O1A-CGA-O2A-C1
24	8	608	CHL	O1D-CGD-O2D-CED
25	q	603	CLA	O1D-CGD-O2D-CED
24	2	609	CHL	CBD-CGD-O2D-CED
24	3	607	CHL	CBD-CGD-O2D-CED
24	5	601	CHL	CBD-CGD-O2D-CED
24	G	609	CHL	CBD-CGD-O2D-CED
24	S	606	CHL	CBD-CGD-O2D-CED
24	Y	605	CHL	CBD-CGD-O2D-CED
24	8	607	CHL	CBD-CGD-O2D-CED
24	g	609	CHL	CBD-CGD-O2D-CED
24	s	606	CHL	CBD-CGD-O2D-CED
24	y	605	CHL	CBD-CGD-O2D-CED
25	3	610	CLA	CBD-CGD-O2D-CED
25	C	512	CLA	CBD-CGD-O2D-CED
25	G	613	CLA	CBD-CGD-O2D-CED
25	0	613	CLA	CBD-CGD-O2D-CED
25	8	613	CLA	CBD-CGD-O2D-CED
25	q	612	CLA	CBD-CGD-O2D-CED
25	c	512	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	y	610	CLA	CBD-CGD-O2D-CED
24	n	606	CHL	O1D-CGD-O2D-CED
25	5	603	CLA	O1D-CGD-O2D-CED
25	C	508	CLA	O1D-CGD-O2D-CED
25	R	603	CLA	O1D-CGD-O2D-CED
25	p	603	CLA	O1D-CGD-O2D-CED
25	c	508	CLA	O1D-CGD-O2D-CED
25	s	605	CLA	O1D-CGD-O2D-CED
29	Y	2630	LHG	O2-C2-C3-O3
29	y	2630	LHG	O2-C2-C3-O3
24	Y	606	CHL	C3-C5-C6-C7
24	0	601	CHL	C3-C5-C6-C7
24	0	607	CHL	C3-C5-C6-C7
24	y	606	CHL	C3-C5-C6-C7
25	6	612	CLA	C3-C5-C6-C7
25	C	504	CLA	C3-C5-C6-C7
25	0	612	CLA	C3-C5-C6-C7
25	8	603	CLA	C3-C5-C6-C7
25	c	504	CLA	C3-C5-C6-C7
24	1	607	CHL	CBA-CGA-O2A-C1
25	5	614	CLA	CBA-CGA-O2A-C1
25	6	611	CLA	CBA-CGA-O2A-C1
25	S	602	CLA	CBA-CGA-O2A-C1
25	Y	611	CLA	CBA-CGA-O2A-C1
25	c	512	CLA	CBA-CGA-O2A-C1
25	s	602	CLA	CBA-CGA-O2A-C1
25	y	611	CLA	CBA-CGA-O2A-C1
25	3	614	CLA	O1A-CGA-O2A-C1
25	6	611	CLA	O1A-CGA-O2A-C1
25	R	616	CLA	O1A-CGA-O2A-C1
25	8	614	CLA	O1A-CGA-O2A-C1
25	g	614	CLA	O1A-CGA-O2A-C1
25	r	616	CLA	O1A-CGA-O2A-C1
24	Y	607	CHL	O1D-CGD-O2D-CED
24	g	607	CHL	O1D-CGD-O2D-CED
25	4	602	CLA	O1D-CGD-O2D-CED
25	B	603	CLA	O1D-CGD-O2D-CED
25	B	612	CLA	O1D-CGD-O2D-CED
25	B	614	CLA	O1D-CGD-O2D-CED
25	b	612	CLA	O1D-CGD-O2D-CED
25	b	614	CLA	O1D-CGD-O2D-CED
25	r	603	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	y	607	CHL	O1D-CGD-O2D-CED
25	s	610	CLA	O1D-CGD-O2D-CED
24	4	601	CHL	CBD-CGD-O2D-CED
24	N	609	CHL	CBD-CGD-O2D-CED
24	S	601	CHL	CBD-CGD-O2D-CED
24	S	607	CHL	CBD-CGD-O2D-CED
24	Y	609	CHL	CBD-CGD-O2D-CED
24	0	605	CHL	CBD-CGD-O2D-CED
24	n	609	CHL	CBD-CGD-O2D-CED
24	s	601	CHL	CBD-CGD-O2D-CED
24	s	607	CHL	CBD-CGD-O2D-CED
25	5	611	CLA	CBD-CGD-O2D-CED
25	C	501	CLA	CBD-CGD-O2D-CED
25	Y	610	CLA	CBD-CGD-O2D-CED
25	8	610	CLA	CBD-CGD-O2D-CED
25	g	611	CLA	CBD-CGD-O2D-CED
36	h	102	LMG	O6-C5-C6-O5
25	b	603	CLA	O1D-CGD-O2D-CED
24	r	607	CHL	O1A-CGA-O2A-C1
24	6	606	CHL	O1D-CGD-O2D-CED
24	6	608	CHL	O1D-CGD-O2D-CED
25	2	603	CLA	O1D-CGD-O2D-CED
25	S	610	CLA	O1D-CGD-O2D-CED
25	q	613	CLA	O1D-CGD-O2D-CED
24	7	606	CHL	CBD-CGD-O2D-CED
25	G	611	CLA	CBD-CGD-O2D-CED
25	p	610	CLA	CBD-CGD-O2D-CED
25	R	609	CLA	C3-C5-C6-C7
25	r	609	CLA	C3-C5-C6-C7
25	A	405	CLA	CBA-CGA-O2A-C1
25	C	510	CLA	CBA-CGA-O2A-C1
25	a	405	CLA	CBA-CGA-O2A-C1
25	c	510	CLA	CBA-CGA-O2A-C1
24	N	608	CHL	O1D-CGD-O2D-CED
25	9	603	CLA	O1D-CGD-O2D-CED
24	R	607	CHL	O1A-CGA-O2A-C1
25	5	614	CLA	O1A-CGA-O2A-C1
25	S	602	CLA	O1A-CGA-O2A-C1
25	Y	612	CLA	O1A-CGA-O2A-C1
25	c	512	CLA	O1A-CGA-O2A-C1
25	c	513	CLA	O1A-CGA-O2A-C1
25	y	612	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	S	608	CHL	O2A-C1-C2-C3
24	s	608	CHL	O2A-C1-C2-C3
25	C	504	CLA	C4-C3-C5-C6
25	C	513	CLA	C4-C3-C5-C6
25	p	604	CLA	C4-C3-C5-C6
25	c	504	CLA	C4-C3-C5-C6
25	C	504	CLA	C2-C3-C5-C6
25	C	513	CLA	C2-C3-C5-C6
25	p	604	CLA	C2-C3-C5-C6
25	c	504	CLA	C2-C3-C5-C6
25	c	501	CLA	CBD-CGD-O2D-CED
24	Y	607	CHL	C2A-CAA-CBA-CGA
24	0	607	CHL	C2A-CAA-CBA-CGA
24	y	607	CHL	C2A-CAA-CBA-CGA
25	C	501	CLA	C2A-CAA-CBA-CGA
25	G	614	CLA	C2A-CAA-CBA-CGA
25	c	501	CLA	C2A-CAA-CBA-CGA
25	g	614	CLA	C2A-CAA-CBA-CGA
24	7	607	CHL	O1A-CGA-O2A-C1
25	C	512	CLA	O1A-CGA-O2A-C1
25	p	614	CLA	O1A-CGA-O2A-C1
25	s	602	CLA	O1A-CGA-O2A-C1
35	A	412	SQD	O5-C1-O6-C44
35	B	621	SQD	O5-C1-O6-C44
35	a	412	SQD	O5-C1-O6-C44
35	b	621	SQD	O5-C1-O6-C44
24	R	608	CHL	C3-C5-C6-C7
24	r	608	CHL	C3-C5-C6-C7
24	7	607	CHL	CBA-CGA-O2A-C1
25	b	603	CLA	CBA-CGA-O2A-C1
25	n	613	CLA	CBA-CGA-O2A-C1
36	H	102	LMG	O6-C5-C6-O5
24	1	609	CHL	O1D-CGD-O2D-CED
24	0	608	CHL	O1D-CGD-O2D-CED
25	3	603	CLA	O1D-CGD-O2D-CED
25	B	615	CLA	O1D-CGD-O2D-CED
25	Y	604	CLA	O1D-CGD-O2D-CED
25	b	615	CLA	O1D-CGD-O2D-CED
25	y	604	CLA	O1D-CGD-O2D-CED
24	1	607	CHL	O1A-CGA-O2A-C1
24	1	605	CHL	O1D-CGD-O2D-CED
24	7	605	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	1	612	CLA	O1D-CGD-O2D-CED
25	G	603	CLA	O1D-CGD-O2D-CED
25	b	605	CLA	O1D-CGD-O2D-CED
25	c	507	CLA	O1D-CGD-O2D-CED
25	g	603	CLA	O1D-CGD-O2D-CED
25	B	605	CLA	O1D-CGD-O2D-CED
29	6	2630	LHG	C1-C2-C3-O3
29	l	101	LHG	C1-C2-C3-O3
24	3	607	CHL	O1A-CGA-O2A-C1
24	y	601	CHL	C3-C5-C6-C7
25	Y	614	CLA	C3-C5-C6-C7
25	y	613	CLA	C3-C5-C6-C7
25	y	614	CLA	C3-C5-C6-C7
24	4	606	CHL	O1D-CGD-O2D-CED
24	q	606	CHL	O1D-CGD-O2D-CED
25	Y	603	CLA	O1D-CGD-O2D-CED
25	0	602	CLA	O1D-CGD-O2D-CED
24	2	607	CHL	CBA-CGA-O2A-C1
24	3	607	CHL	CBA-CGA-O2A-C1
24	4	607	CHL	CBA-CGA-O2A-C1
24	6	606	CHL	CBA-CGA-O2A-C1
24	Y	607	CHL	CBA-CGA-O2A-C1
24	0	606	CHL	CBA-CGA-O2A-C1
24	8	607	CHL	CBA-CGA-O2A-C1
24	9	607	CHL	CBA-CGA-O2A-C1
24	y	607	CHL	CBA-CGA-O2A-C1
25	2	614	CLA	CBA-CGA-O2A-C1
25	4	614	CLA	CBA-CGA-O2A-C1
25	B	603	CLA	CBA-CGA-O2A-C1
25	B	613	CLA	CBA-CGA-O2A-C1
25	C	513	CLA	CBA-CGA-O2A-C1
25	D	402	CLA	CBA-CGA-O2A-C1
25	N	613	CLA	CBA-CGA-O2A-C1
25	R	603	CLA	CBA-CGA-O2A-C1
25	R	604	CLA	CBA-CGA-O2A-C1
25	R	613	CLA	CBA-CGA-O2A-C1
25	9	614	CLA	CBA-CGA-O2A-C1
25	q	614	CLA	CBA-CGA-O2A-C1
25	b	613	CLA	CBA-CGA-O2A-C1
25	d	402	CLA	CBA-CGA-O2A-C1
25	r	603	CLA	CBA-CGA-O2A-C1
25	r	613	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	3	613	CLA	CBD-CGD-O2D-CED
25	R	616	CLA	CBD-CGD-O2D-CED
25	r	616	CLA	CBD-CGD-O2D-CED
24	9	609	CHL	C2C-C3C-CAC-CBC
24	q	601	CHL	C13-C15-C16-C17
24	y	609	CHL	C8-C10-C11-C12
24	R	606	CHL	C15-C16-C17-C18
24	Y	609	CHL	C8-C10-C11-C12
24	Y	609	CHL	C15-C16-C17-C18
24	n	601	CHL	C15-C16-C17-C18
24	n	609	CHL	C8-C10-C11-C12
24	y	607	CHL	C15-C16-C17-C18
25	6	613	CLA	C13-C15-C16-C17
25	B	609	CLA	C15-C16-C17-C18
25	b	609	CLA	C15-C16-C17-C18
24	0	606	CHL	O1A-CGA-O2A-C1
25	C	513	CLA	O1A-CGA-O2A-C1
24	5	607	CHL	C2-C3-C5-C6
39	D	405	PL9	C12-C11-C9-C8
24	1	609	CHL	C14-C13-C15-C16
24	3	607	CHL	C11-C10-C8-C9
24	5	605	CHL	C11-C10-C8-C9
24	5	609	CHL	C11-C10-C8-C9
24	6	606	CHL	C14-C13-C15-C16
24	6	607	CHL	C14-C13-C15-C16
24	6	609	CHL	C14-C13-C15-C16
24	N	605	CHL	C11-C10-C8-C9
24	N	609	CHL	C11-C10-C8-C9
24	N	609	CHL	C14-C13-C15-C16
24	R	608	CHL	C6-C7-C8-C9
24	0	609	CHL	C14-C13-C15-C16
24	7	609	CHL	C14-C13-C15-C16
24	8	601	CHL	C6-C7-C8-C9
24	8	607	CHL	C11-C12-C13-C14
24	p	607	CHL	C11-C12-C13-C14
24	p	609	CHL	C11-C10-C8-C9
24	q	609	CHL	C11-C10-C8-C9
24	n	605	CHL	C11-C10-C8-C9
24	n	605	CHL	C11-C12-C13-C14
24	n	609	CHL	C11-C10-C8-C9
24	n	609	CHL	C14-C13-C15-C16
24	r	608	CHL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
25	B	602	CLA	C14-C13-C15-C16
25	B	605	CLA	C6-C7-C8-C9
25	C	506	CLA	C11-C10-C8-C9
25	N	610	CLA	C6-C7-C8-C9
25	R	616	CLA	C14-C13-C15-C16
25	b	602	CLA	C14-C13-C15-C16
25	b	605	CLA	C6-C7-C8-C9
25	c	506	CLA	C11-C10-C8-C9
25	n	610	CLA	C6-C7-C8-C9
25	r	616	CLA	C14-C13-C15-C16
24	p	607	CHL	O1D-CGD-O2D-CED
25	y	603	CLA	O1D-CGD-O2D-CED
25	S	609	CLA	CBD-CGD-O2D-CED
24	4	601	CHL	C13-C15-C16-C17
25	C	502	CLA	C10-C11-C12-C13
25	8	602	CLA	C10-C11-C12-C13
24	0	608	CHL	C2A-CAA-CBA-CGA
24	7	608	CHL	C2A-CAA-CBA-CGA
24	q	609	CHL	C2A-CAA-CBA-CGA
25	1	603	CLA	C2A-CAA-CBA-CGA
25	B	613	CLA	C2A-CAA-CBA-CGA
25	b	613	CLA	C2A-CAA-CBA-CGA
25	r	601	CLA	C2A-CAA-CBA-CGA
26	4	1620	LUT	C27-C28-C29-C39
26	Y	1621	LUT	C7-C8-C9-C19
26	8	1620	LUT	C27-C28-C29-C39
26	p	1620	LUT	C27-C28-C29-C39
26	p	1620	LUT	C31-C32-C33-C40
26	y	1621	LUT	C7-C8-C9-C19
27	0	1622	XAT	C31-C32-C33-C40
27	q	1622	XAT	C11-C12-C13-C20
28	2	1623	NEX	C31-C32-C33-C40
34	C	514	BCR	C37-C22-C23-C24
34	C	515	BCR	C7-C8-C9-C34
34	D	404	BCR	C7-C8-C9-C34
34	c	514	BCR	C37-C22-C23-C24
34	c	515	BCR	C7-C8-C9-C34
34	d	404	BCR	C7-C8-C9-C34
29	9	2630	LHG	C7-C8-C9-C10
24	6	606	CHL	O1A-CGA-O2A-C1
24	Y	607	CHL	O1A-CGA-O2A-C1
24	8	607	CHL	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	y	607	CHL	O1A-CGA-O2A-C1
25	4	614	CLA	O1A-CGA-O2A-C1
25	N	613	CLA	O1A-CGA-O2A-C1
25	R	613	CLA	O1A-CGA-O2A-C1
25	9	614	CLA	O1A-CGA-O2A-C1
25	q	614	CLA	O1A-CGA-O2A-C1
25	r	613	CLA	O1A-CGA-O2A-C1
24	2	609	CHL	C13-C15-C16-C17
24	3	605	CHL	C15-C16-C17-C18
24	3	609	CHL	C5-C6-C7-C8
24	4	609	CHL	C5-C6-C7-C8
24	6	607	CHL	C5-C6-C7-C8
24	N	601	CHL	C15-C16-C17-C18
24	7	607	CHL	C8-C10-C11-C12
24	r	606	CHL	C15-C16-C17-C18
25	1	610	CLA	C13-C15-C16-C17
25	6	604	CLA	C13-C15-C16-C17
25	B	606	CLA	C13-C15-C16-C17
25	B	617	CLA	C15-C16-C17-C18
25	C	510	CLA	C13-C15-C16-C17
25	Y	604	CLA	C10-C11-C12-C13
25	b	606	CLA	C13-C15-C16-C17
25	c	510	CLA	C13-C15-C16-C17
25	y	604	CLA	C10-C11-C12-C13
25	s	609	CLA	CBD-CGD-O2D-CED
37	C	524	DGD	O6E-C5E-C6E-O5E
37	c	524	DGD	O6E-C5E-C6E-O5E
25	C	513	CLA	C3-C5-C6-C7
24	9	608	CHL	C2A-CAA-CBA-CGA
24	q	608	CHL	C2A-CAA-CBA-CGA
25	r	604	CLA	CBA-CGA-O2A-C1
24	1	601	CHL	C15-C16-C17-C18
24	1	607	CHL	C13-C15-C16-C17
24	2	609	CHL	C5-C6-C7-C8
24	Y	607	CHL	C8-C10-C11-C12
24	q	609	CHL	C8-C10-C11-C12
24	y	609	CHL	C13-C15-C16-C17
25	2	603	CLA	C15-C16-C17-C18
25	4	613	CLA	C5-C6-C7-C8
25	A	405	CLA	C13-C15-C16-C17
25	C	506	CLA	C8-C10-C11-C12
25	C	512	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	D	403	CLA	C5-C6-C7-C8
25	G	602	CLA	C10-C11-C12-C13
25	Y	612	CLA	C13-C15-C16-C17
25	7	613	CLA	C10-C11-C12-C13
25	9	603	CLA	C8-C10-C11-C12
25	9	603	CLA	C15-C16-C17-C18
25	p	604	CLA	C13-C15-C16-C17
25	p	604	CLA	C15-C16-C17-C18
25	q	602	CLA	C8-C10-C11-C12
25	a	405	CLA	C13-C15-C16-C17
25	b	605	CLA	C8-C10-C11-C12
25	c	506	CLA	C8-C10-C11-C12
25	c	507	CLA	C15-C16-C17-C18
25	c	512	CLA	C5-C6-C7-C8
25	y	612	CLA	C13-C15-C16-C17
24	1	601	CHL	C10-C11-C12-C13
24	1	607	CHL	C8-C10-C11-C12
24	3	601	CHL	C8-C10-C11-C12
24	3	605	CHL	C5-C6-C7-C8
24	4	609	CHL	C15-C16-C17-C18
24	5	601	CHL	C13-C15-C16-C17
24	6	606	CHL	C10-C11-C12-C13
24	G	609	CHL	C8-C10-C11-C12
24	G	609	CHL	C15-C16-C17-C18
24	N	601	CHL	C8-C10-C11-C12
24	N	605	CHL	C13-C15-C16-C17
24	N	609	CHL	C8-C10-C11-C12
24	R	608	CHL	C5-C6-C7-C8
24	Y	606	CHL	C13-C15-C16-C17
24	Y	609	CHL	C13-C15-C16-C17
24	0	601	CHL	C13-C15-C16-C17
24	0	609	CHL	C8-C10-C11-C12
24	7	607	CHL	C13-C15-C16-C17
24	8	601	CHL	C8-C10-C11-C12
24	8	605	CHL	C5-C6-C7-C8
24	9	609	CHL	C5-C6-C7-C8
24	9	609	CHL	C13-C15-C16-C17
24	p	601	CHL	C13-C15-C16-C17
24	p	605	CHL	C13-C15-C16-C17
24	p	607	CHL	C8-C10-C11-C12
24	q	601	CHL	C10-C11-C12-C13
24	q	609	CHL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
24	g	609	CHL	C8-C10-C11-C12
24	g	609	CHL	C15-C16-C17-C18
24	n	605	CHL	C8-C10-C11-C12
24	y	606	CHL	C13-C15-C16-C17
24	y	607	CHL	C8-C10-C11-C12
24	y	609	CHL	C15-C16-C17-C18
24	r	608	CHL	C5-C6-C7-C8
25	1	613	CLA	C10-C11-C12-C13
25	2	603	CLA	C8-C10-C11-C12
25	4	602	CLA	C8-C10-C11-C12
25	6	610	CLA	C8-C10-C11-C12
25	B	602	CLA	C13-C15-C16-C17
25	B	603	CLA	C10-C11-C12-C13
25	B	605	CLA	C8-C10-C11-C12
25	C	503	CLA	C5-C6-C7-C8
25	C	507	CLA	C15-C16-C17-C18
25	C	508	CLA	C8-C10-C11-C12
25	R	616	CLA	C13-C15-C16-C17
25	0	604	CLA	C8-C10-C11-C12
25	0	604	CLA	C13-C15-C16-C17
25	0	610	CLA	C8-C10-C11-C12
25	7	610	CLA	C13-C15-C16-C17
25	q	610	CLA	C13-C15-C16-C17
25	b	602	CLA	C13-C15-C16-C17
25	b	603	CLA	C10-C11-C12-C13
25	b	617	CLA	C15-C16-C17-C18
25	c	508	CLA	C8-C10-C11-C12
25	c	513	CLA	C13-C15-C16-C17
25	d	403	CLA	C5-C6-C7-C8
25	r	616	CLA	C13-C15-C16-C17
24	0	607	CHL	O1D-CGD-O2D-CED
25	Y	612	CLA	O1D-CGD-O2D-CED
25	8	603	CLA	O1D-CGD-O2D-CED
25	y	612	CLA	O1D-CGD-O2D-CED
25	2	614	CLA	O1A-CGA-O2A-C1
25	B	613	CLA	O1A-CGA-O2A-C1
25	b	613	CLA	O1A-CGA-O2A-C1
29	1	2630	LHG	C7-C8-C9-C10
29	D	410	LHG	C23-C24-C25-C26
29	d	410	LHG	C23-C24-C25-C26
35	B	623	SQD	C23-C24-C25-C26
35	b	623	SQD	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
36	B	622	LMG	C28-C29-C30-C31
36	C	521	LMG	C28-C29-C30-C31
36	b	622	LMG	C28-C29-C30-C31
36	c	521	LMG	C28-C29-C30-C31
24	1	607	CHL	C5-C6-C7-C8
24	3	605	CHL	C8-C10-C11-C12
24	3	609	CHL	C13-C15-C16-C17
24	5	607	CHL	C8-C10-C11-C12
24	6	601	CHL	C13-C15-C16-C17
24	Y	601	CHL	C15-C16-C17-C18
24	7	607	CHL	C5-C6-C7-C8
24	p	609	CHL	C15-C16-C17-C18
24	q	601	CHL	C8-C10-C11-C12
24	g	601	CHL	C15-C16-C17-C18
24	n	601	CHL	C8-C10-C11-C12
24	n	607	CHL	C8-C10-C11-C12
25	3	603	CLA	C5-C6-C7-C8
25	3	613	CLA	C15-C16-C17-C18
25	4	602	CLA	C10-C11-C12-C13
25	A	410	CLA	C5-C6-C7-C8
25	B	610	CLA	C5-C6-C7-C8
25	C	505	CLA	C8-C10-C11-C12
25	C	513	CLA	C8-C10-C11-C12
25	G	602	CLA	C8-C10-C11-C12
25	7	602	CLA	C8-C10-C11-C12
25	8	613	CLA	C15-C16-C17-C18
25	9	602	CLA	C8-C10-C11-C12
25	a	410	CLA	C5-C6-C7-C8
25	b	610	CLA	C5-C6-C7-C8
25	c	505	CLA	C8-C10-C11-C12
25	g	602	CLA	C8-C10-C11-C12
25	g	602	CLA	C10-C11-C12-C13
25	n	610	CLA	C10-C11-C12-C13
24	n	607	CHL	CBA-CGA-O2A-C1
25	Y	613	CLA	CBA-CGA-O2A-C1
25	7	604	CLA	CBA-CGA-O2A-C1
25	y	613	CLA	CBA-CGA-O2A-C1
24	2	601	CHL	C15-C16-C17-C18
24	4	601	CHL	C8-C10-C11-C12
24	6	607	CHL	C8-C10-C11-C12
24	G	601	CHL	C15-C16-C17-C18
24	0	607	CHL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	7	601	CHL	C10-C11-C12-C13
24	8	605	CHL	C15-C16-C17-C18
24	8	609	CHL	C13-C15-C16-C17
24	9	601	CHL	C5-C6-C7-C8
25	1	602	CLA	C8-C10-C11-C12
25	B	608	CLA	C13-C15-C16-C17
25	B	614	CLA	C10-C11-C12-C13
25	C	508	CLA	C5-C6-C7-C8
25	C	513	CLA	C13-C15-C16-C17
25	N	610	CLA	C10-C11-C12-C13
25	0	613	CLA	C13-C15-C16-C17
25	7	604	CLA	C10-C11-C12-C13
25	8	603	CLA	C5-C6-C7-C8
25	q	602	CLA	C10-C11-C12-C13
25	b	608	CLA	C13-C15-C16-C17
25	b	614	CLA	C10-C11-C12-C13
25	c	508	CLA	C5-C6-C7-C8
29	2	2630	LHG	C7-C8-C9-C10
29	6	2630	LHG	C7-C8-C9-C10
29	G	2630	LHG	C7-C8-C9-C10
29	g	2630	LHG	C7-C8-C9-C10
24	8	606	CHL	CBD-CGD-O2D-CED
24	2	608	CHL	C2A-CAA-CBA-CGA
24	S	606	CHL	C2A-CAA-CBA-CGA
24	s	606	CHL	C2A-CAA-CBA-CGA
25	4	612	CLA	C2A-CAA-CBA-CGA
40	f	101	HEM	C3D-CAD-CBD-CGD
25	S	614	CLA	O2A-C1-C2-C3
25	s	614	CLA	O2A-C1-C2-C3
24	8	605	CHL	C8-C10-C11-C12
24	9	601	CHL	C15-C16-C17-C18
24	p	601	CHL	C15-C16-C17-C18
25	1	604	CLA	C10-C11-C12-C13
25	3	602	CLA	C10-C11-C12-C13
25	B	612	CLA	C13-C15-C16-C17
25	N	610	CLA	C5-C6-C7-C8
25	b	612	CLA	C13-C15-C16-C17
25	c	502	CLA	C10-C11-C12-C13
24	2	606	CHL	O1D-CGD-O2D-CED
33	A	408	PHO	O1D-CGD-O2D-CED
24	2	601	CHL	C6-C7-C8-C10
24	4	601	CHL	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
24	5	605	CHL	C6-C7-C8-C10
24	6	606	CHL	C12-C13-C15-C16
24	6	607	CHL	C11-C10-C8-C7
24	6	609	CHL	C12-C13-C15-C16
24	G	601	CHL	C6-C7-C8-C10
24	0	606	CHL	C12-C13-C15-C16
24	7	607	CHL	C11-C10-C8-C7
24	8	609	CHL	C11-C10-C8-C7
24	g	601	CHL	C6-C7-C8-C10
24	n	605	CHL	C12-C13-C15-C16
25	B	613	CLA	C12-C13-C15-C16
25	N	603	CLA	C11-C12-C13-C15
25	Y	610	CLA	C11-C12-C13-C15
25	b	613	CLA	C12-C13-C15-C16
25	c	511	CLA	C6-C7-C8-C10
25	n	603	CLA	C11-C12-C13-C15
25	y	610	CLA	C11-C12-C13-C15
26	q	1621	LUT	C29-C30-C31-C32
29	g	2630	LHG	C24-C23-O8-C6
24	6	607	CHL	C2A-CAA-CBA-CGA
24	6	608	CHL	C2A-CAA-CBA-CGA
25	1	614	CLA	C2A-CAA-CBA-CGA
25	G	602	CLA	C2A-CAA-CBA-CGA
25	R	604	CLA	C2A-CAA-CBA-CGA
25	7	603	CLA	C2A-CAA-CBA-CGA
25	7	614	CLA	C2A-CAA-CBA-CGA
25	g	602	CLA	C2A-CAA-CBA-CGA
24	5	609	CHL	O1D-CGD-O2D-CED
24	Y	606	CHL	O1D-CGD-O2D-CED
24	Y	608	CHL	O1D-CGD-O2D-CED
24	9	606	CHL	O1D-CGD-O2D-CED
24	p	609	CHL	O1D-CGD-O2D-CED
24	y	606	CHL	O1D-CGD-O2D-CED
24	y	608	CHL	O1D-CGD-O2D-CED
25	4	604	CLA	O1D-CGD-O2D-CED
25	5	614	CLA	O1D-CGD-O2D-CED
25	6	602	CLA	O1D-CGD-O2D-CED
25	R	611	CLA	O1D-CGD-O2D-CED
25	r	611	CLA	O1D-CGD-O2D-CED
33	a	408	PHO	O1D-CGD-O2D-CED
24	6	609	CHL	C8-C10-C11-C12
24	N	607	CHL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	Y	601	CHL	C13-C15-C16-C17
24	0	606	CHL	C10-C11-C12-C13
24	p	605	CHL	C5-C6-C7-C8
24	q	609	CHL	C5-C6-C7-C8
24	y	601	CHL	C15-C16-C17-C18
25	3	613	CLA	C5-C6-C7-C8
25	5	604	CLA	C13-C15-C16-C17
25	6	612	CLA	C10-C11-C12-C13
25	C	503	CLA	C8-C10-C11-C12
25	C	503	CLA	C15-C16-C17-C18
25	C	513	CLA	C15-C16-C17-C18
25	G	613	CLA	C15-C16-C17-C18
25	N	613	CLA	C10-C11-C12-C13
25	R	613	CLA	C8-C10-C11-C12
25	0	612	CLA	C10-C11-C12-C13
25	8	613	CLA	C5-C6-C7-C8
25	9	603	CLA	C5-C6-C7-C8
25	c	503	CLA	C15-C16-C17-C18
25	g	613	CLA	C15-C16-C17-C18
25	n	603	CLA	C5-C6-C7-C8
25	n	613	CLA	C10-C11-C12-C13
25	r	613	CLA	C8-C10-C11-C12
24	4	607	CHL	O1A-CGA-O2A-C1
25	B	603	CLA	O1A-CGA-O2A-C1
25	D	402	CLA	O1A-CGA-O2A-C1
25	R	603	CLA	O1A-CGA-O2A-C1
25	b	603	CLA	O1A-CGA-O2A-C1
25	r	603	CLA	O1A-CGA-O2A-C1
25	C	507	CLA	CBD-CGD-O2D-CED
25	9	602	CLA	CBD-CGD-O2D-CED
24	7	601	CHL	C13-C15-C16-C17
24	8	601	CHL	C5-C6-C7-C8
24	8	607	CHL	C8-C10-C11-C12
24	p	605	CHL	C15-C16-C17-C18
24	g	601	CHL	C13-C15-C16-C17
24	y	601	CHL	C5-C6-C7-C8
24	y	601	CHL	C13-C15-C16-C17
25	R	616	CLA	C15-C16-C17-C18
25	c	507	CLA	C13-C15-C16-C17
25	r	616	CLA	C15-C16-C17-C18
24	R	606	CHL	O1D-CGD-O2D-CED
24	q	609	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
24	r	606	CHL	O1D-CGD-O2D-CED
29	0	2630	LHG	C7-C8-C9-C10
29	y	2630	LHG	C7-C8-C9-C10
37	C	518	DGD	C1A-C2A-C3A-C4A
29	6	2630	LHG	O2-C2-C3-O3
29	G	2630	LHG	O2-C2-C3-O3
29	g	2630	LHG	O2-C2-C3-O3
29	l	101	LHG	O2-C2-C3-O3
25	Y	613	CLA	C3-C5-C6-C7
25	b	602	CLA	C3-C5-C6-C7
24	G	608	CHL	C2A-CAA-CBA-CGA
25	9	612	CLA	C2A-CAA-CBA-CGA
24	1	606	CHL	C13-C15-C16-C17
24	1	609	CHL	C8-C10-C11-C12
24	5	609	CHL	C5-C6-C7-C8
24	N	601	CHL	C13-C15-C16-C17
24	N	605	CHL	C8-C10-C11-C12
24	N	607	CHL	C13-C15-C16-C17
24	7	606	CHL	C13-C15-C16-C17
24	7	609	CHL	C8-C10-C11-C12
24	p	601	CHL	C8-C10-C11-C12
24	n	601	CHL	C13-C15-C16-C17
25	1	603	CLA	C10-C11-C12-C13
25	4	610	CLA	C13-C15-C16-C17
25	N	603	CLA	C5-C6-C7-C8
25	Y	604	CLA	C13-C15-C16-C17
25	c	502	CLA	C5-C6-C7-C8
25	c	503	CLA	C8-C10-C11-C12
25	c	511	CLA	C15-C16-C17-C18
25	n	610	CLA	C5-C6-C7-C8
25	y	604	CLA	C13-C15-C16-C17
25	y	610	CLA	C5-C6-C7-C8
24	N	607	CHL	CBA-CGA-O2A-C1
24	8	608	CHL	CBA-CGA-O2A-C1
24	p	607	CHL	CBA-CGA-O2A-C1
25	p	604	CLA	O1D-CGD-O2D-CED
24	9	607	CHL	O1A-CGA-O2A-C1
25	R	604	CLA	O1A-CGA-O2A-C1
25	d	402	CLA	O1A-CGA-O2A-C1
25	n	613	CLA	O1A-CGA-O2A-C1
25	2	614	CLA	O1D-CGD-O2D-CED
24	3	607	CHL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
24	8	605	CHL	C13-C15-C16-C17
24	p	607	CHL	C5-C6-C7-C8
24	p	609	CHL	C8-C10-C11-C12
24	n	609	CHL	C10-C11-C12-C13
25	6	602	CLA	C5-C6-C7-C8
25	6	612	CLA	C13-C15-C16-C17
25	A	405	CLA	C15-C16-C17-C18
25	C	504	CLA	C8-C10-C11-C12
25	C	507	CLA	C13-C15-C16-C17
25	C	511	CLA	C15-C16-C17-C18
25	G	613	CLA	C13-C15-C16-C17
25	Y	610	CLA	C5-C6-C7-C8
25	0	612	CLA	C13-C15-C16-C17
25	7	603	CLA	C10-C11-C12-C13
25	8	603	CLA	C10-C11-C12-C13
25	p	604	CLA	C10-C11-C12-C13
25	q	602	CLA	C15-C16-C17-C18
25	q	603	CLA	C8-C10-C11-C12
25	a	405	CLA	C15-C16-C17-C18
25	c	504	CLA	C8-C10-C11-C12
25	g	613	CLA	C13-C15-C16-C17
25	G	614	CLA	O1D-CGD-O2D-CED
25	9	614	CLA	O1D-CGD-O2D-CED
25	c	511	CLA	O1D-CGD-O2D-CED
24	2	607	CHL	O1A-CGA-O2A-C1
24	n	607	CHL	O1A-CGA-O2A-C1
37	C	524	DGD	C2B-C1B-O2G-C2G
37	c	524	DGD	C2B-C1B-O2G-C2G
24	1	601	CHL	C5-C6-C7-C8
24	2	609	CHL	C15-C16-C17-C18
24	3	607	CHL	C8-C10-C11-C12
24	5	601	CHL	C8-C10-C11-C12
24	5	605	CHL	C13-C15-C16-C17
24	5	605	CHL	C15-C16-C17-C18
24	G	601	CHL	C13-C15-C16-C17
24	N	609	CHL	C10-C11-C12-C13
24	R	606	CHL	C8-C10-C11-C12
24	8	607	CHL	C15-C16-C17-C18
24	q	609	CHL	C10-C11-C12-C13
24	n	607	CHL	C13-C15-C16-C17
24	r	606	CHL	C8-C10-C11-C12
25	2	602	CLA	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	2	603	CLA	C5-C6-C7-C8
25	3	610	CLA	C5-C6-C7-C8
25	5	604	CLA	C15-C16-C17-C18
25	B	606	CLA	C15-C16-C17-C18
25	R	610	CLA	C15-C16-C17-C18
25	8	610	CLA	C5-C6-C7-C8
25	b	606	CLA	C15-C16-C17-C18
29	2	2630	LHG	C3-O3-P-O6
29	2	2630	LHG	C4-O6-P-O3
29	5	2630	LHG	C4-O6-P-O3
29	C	2630	LHG	C4-O6-P-O3
29	D	408	LHG	C4-O6-P-O3
29	N	2630	LHG	C3-O3-P-O6
29	N	2630	LHG	C4-O6-P-O3
29	R	2630	LHG	C3-O3-P-O6
29	R	2630	LHG	C4-O6-P-O3
29	0	2630	LHG	C4-O6-P-O3
29	9	2630	LHG	C4-O6-P-O3
29	p	2630	LHG	C4-O6-P-O3
29	d	408	LHG	C4-O6-P-O3
29	l	101	LHG	C4-O6-P-O3
29	n	2630	LHG	C3-O3-P-O6
29	n	2630	LHG	C4-O6-P-O3
29	r	2630	LHG	C3-O3-P-O6
29	r	2630	LHG	C4-O6-P-O3
37	C	523	DGD	C1A-C2A-C3A-C4A
37	c	518	DGD	C1A-C2A-C3A-C4A
37	c	523	DGD	C1A-C2A-C3A-C4A
24	6	606	CHL	C3-C5-C6-C7
24	8	607	CHL	C3-C5-C6-C7
25	B	602	CLA	C3-C5-C6-C7
33	A	408	PHO	C3-C5-C6-C7
33	a	408	PHO	C3-C5-C6-C7
24	5	608	CHL	CBA-CGA-O2A-C1
24	n	608	CHL	CBA-CGA-O2A-C1
24	r	606	CHL	CBA-CGA-O2A-C1
25	R	601	CLA	CBA-CGA-O2A-C1
29	2	2630	LHG	C24-C23-O8-C6
29	G	2630	LHG	C24-C23-O8-C6
29	S	2630	LHG	C24-C23-O8-C6
25	5	613	CLA	O1D-CGD-O2D-CED
24	4	609	CHL	C8-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
24	8	607	CHL	C13-C15-C16-C17
24	9	609	CHL	C15-C16-C17-C18
24	n	605	CHL	C13-C15-C16-C17
25	B	615	CLA	C10-C11-C12-C13
25	B	616	CLA	C15-C16-C17-C18
25	Y	604	CLA	C8-C10-C11-C12
25	0	604	CLA	C15-C16-C17-C18
25	b	615	CLA	C10-C11-C12-C13
25	b	616	CLA	C15-C16-C17-C18
25	y	604	CLA	C8-C10-C11-C12
25	r	610	CLA	C15-C16-C17-C18
24	7	609	CHL	O1D-CGD-O2D-CED
24	2	609	CHL	C2C-C3C-CAC-CBC
25	2	612	CLA	C2A-CAA-CBA-CGA
29	7	2630	LHG	C7-C8-C9-C10
24	2	608	CHL	O1D-CGD-O2D-CED
24	3	609	CHL	C15-C16-C17-C18
25	C	502	CLA	C5-C6-C7-C8
25	C	502	CLA	C8-C10-C11-C12
25	p	602	CLA	C8-C10-C11-C12
25	c	501	CLA	C15-C16-C17-C18
25	a	407	CLA	CBD-CGD-O2D-CED
24	4	605	CHL	C2A-CAA-CBA-CGA
25	1	610	CLA	C2A-CAA-CBA-CGA
25	6	610	CLA	C2A-CAA-CBA-CGA
25	C	505	CLA	C2A-CAA-CBA-CGA
25	C	507	CLA	C2A-CAA-CBA-CGA
25	7	610	CLA	C2A-CAA-CBA-CGA
25	p	610	CLA	C2A-CAA-CBA-CGA
25	c	505	CLA	C2A-CAA-CBA-CGA
25	r	604	CLA	C2A-CAA-CBA-CGA
24	3	601	CHL	C16-C17-C18-C20
24	6	609	CHL	C16-C17-C18-C20
24	R	606	CHL	C16-C17-C18-C20
24	8	601	CHL	C16-C17-C18-C20
24	r	606	CHL	C16-C17-C18-C20
37	C	518	DGD	O6E-C5E-C6E-O5E
37	c	518	DGD	O6E-C5E-C6E-O5E
25	N	604	CLA	C3-C5-C6-C7
24	1	609	CHL	CBA-CGA-O2A-C1
24	3	608	CHL	CBA-CGA-O2A-C1
24	R	606	CHL	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
24	Y	606	CHL	CBA-CGA-O2A-C1
24	y	606	CHL	CBA-CGA-O2A-C1
25	6	614	CLA	CBA-CGA-O2A-C1
25	c	501	CLA	CBA-CGA-O2A-C1
29	s	2630	LHG	C24-C23-O8-C6
24	1	607	CHL	C15-C16-C17-C18
25	3	603	CLA	C10-C11-C12-C13
24	3	601	CHL	C5-C6-C7-C8
24	0	607	CHL	C15-C16-C17-C18
24	p	609	CHL	C5-C6-C7-C8
25	5	613	CLA	C13-C15-C16-C17
29	4	2630	LHG	C33-C34-C35-C36
29	6	2630	LHG	C27-C28-C29-C30
36	C	521	LMG	C30-C31-C32-C33
35	D	413	SQD	C8-C7-O47-C45
35	d	413	SQD	C8-C7-O47-C45
24	Y	601	CHL	C5-C6-C7-C8
25	G	612	CLA	C2A-CAA-CBA-CGA
25	g	612	CLA	C2A-CAA-CBA-CGA
29	6	2630	LHG	C14-C15-C16-C17
35	a	412	SQD	C9-C10-C11-C12
36	c	521	LMG	C30-C31-C32-C33
37	C	523	DGD	C6A-C7A-C8A-C9A
37	c	523	DGD	C6A-C7A-C8A-C9A
37	c	524	DGD	C4E-C5E-C6E-O5E
24	1	606	CHL	O1D-CGD-O2D-CED
25	7	604	CLA	O1D-CGD-O2D-CED
25	b	611	CLA	O1D-CGD-O2D-CED
25	g	614	CLA	O1D-CGD-O2D-CED
24	1	606	CHL	C16-C17-C18-C20
24	6	601	CHL	C16-C17-C18-C20
24	6	606	CHL	C16-C17-C18-C19
24	0	601	CHL	C16-C17-C18-C19
24	0	609	CHL	C16-C17-C18-C19
25	4	603	CLA	C16-C17-C18-C20
25	B	607	CLA	C16-C17-C18-C20
25	R	602	CLA	C11-C12-C13-C14
25	a	405	CLA	C16-C17-C18-C20
25	b	607	CLA	C16-C17-C18-C20
25	r	602	CLA	C11-C12-C13-C14
24	3	601	CHL	CBA-CGA-O2A-C1
29	Y	2630	LHG	C32-C33-C34-C35

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Mol	Chain	Res	Type	Atoms
29	0	2630	LHG	C14-C15-C16-C17
29	r	2630	LHG	C9-C10-C11-C12
35	A	412	SQD	C9-C10-C11-C12
36	s	2631	LMG	C39-C40-C41-C42
24	3	607	CHL	O1D-CGD-O2D-CED
24	3	609	CHL	O1D-CGD-O2D-CED
24	5	607	CHL	O1D-CGD-O2D-CED
25	C	511	CLA	O1D-CGD-O2D-CED
25	7	612	CLA	O1D-CGD-O2D-CED
35	D	413	SQD	O49-C7-O47-C45
35	d	413	SQD	O49-C7-O47-C45
37	C	524	DGD	O1B-C1B-O2G-C2G
37	c	524	DGD	O1B-C1B-O2G-C2G
24	6	607	CHL	C15-C16-C17-C18
37	C	524	DGD	C4E-C5E-C6E-O5E
24	4	605	CHL	CBD-CGD-O2D-CED
29	R	2630	LHG	C9-C10-C11-C12
24	Y	605	CHL	O1D-CGD-O2D-CED
24	y	605	CHL	O1D-CGD-O2D-CED
25	B	611	CLA	O1D-CGD-O2D-CED
25	N	604	CLA	O1D-CGD-O2D-CED
25	n	604	CLA	O1D-CGD-O2D-CED
24	N	607	CHL	O1A-CGA-O2A-C1
25	7	604	CLA	O1A-CGA-O2A-C1
29	y	2630	LHG	C32-C33-C34-C35
37	C	519	DGD	C5A-C6A-C7A-C8A
37	c	523	DGD	C7A-C8A-C9A-CAA
24	1	609	CHL	C15-C16-C17-C18
24	6	609	CHL	C15-C16-C17-C18
24	p	609	CHL	C13-C15-C16-C17
29	1	2630	LHG	O2-C2-C3-O3
29	2	2630	LHG	O2-C2-C3-O3
29	7	2630	LHG	O2-C2-C3-O3
29	q	2630	LHG	O2-C2-C3-O3
35	a	412	SQD	C24-C25-C26-C27
37	C	523	DGD	C7A-C8A-C9A-CAA
37	C	524	DGD	CCA-CDA-CEA-CFA
25	7	612	CLA	C3-C5-C6-C7
24	8	607	CHL	O1D-CGD-O2D-CED
36	A	413	LMG	C2-C1-O1-C7
36	a	413	LMG	C2-C1-O1-C7
25	C	501	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	1	2630	LHG	C14-C15-C16-C17
29	d	409	LHG	C24-C25-C26-C27
35	A	412	SQD	C24-C25-C26-C27
35	B	623	SQD	C15-C16-C17-C18
35	b	623	SQD	C15-C16-C17-C18
37	c	524	DGD	CCA-CDA-CEA-CFA
24	7	601	CHL	C15-C16-C17-C18
24	n	608	CHL	O1A-CGA-O2A-C1
25	Y	613	CLA	O1A-CGA-O2A-C1
25	c	501	CLA	O1A-CGA-O2A-C1
25	y	613	CLA	O1A-CGA-O2A-C1
29	g	2630	LHG	O10-C23-O8-C6
24	5	601	CHL	C16-C17-C18-C19
24	5	607	CHL	C16-C17-C18-C19
24	6	609	CHL	C16-C17-C18-C19
24	8	601	CHL	C16-C17-C18-C19
24	8	605	CHL	C16-C17-C18-C20
24	q	609	CHL	C16-C17-C18-C19
25	2	603	CLA	C16-C17-C18-C19
25	6	604	CLA	C16-C17-C18-C20
25	B	614	CLA	C16-C17-C18-C19
25	Y	611	CLA	C16-C17-C18-C20
25	9	603	CLA	C16-C17-C18-C19
25	b	614	CLA	C16-C17-C18-C19
25	y	611	CLA	C16-C17-C18-C20
25	r	610	CLA	C16-C17-C18-C20
24	R	607	CHL	O1D-CGD-O2D-CED
24	8	609	CHL	O1D-CGD-O2D-CED
25	0	613	CLA	O1D-CGD-O2D-CED
24	R	608	CHL	C4-C3-C5-C6
24	0	607	CHL	C4-C3-C5-C6
24	r	608	CHL	C4-C3-C5-C6
25	5	603	CLA	C4-C3-C5-C6
39	D	405	PL9	C15-C14-C16-C17
29	D	409	LHG	C24-C25-C26-C27
29	L	101	LHG	C9-C10-C11-C12
29	7	2630	LHG	C14-C15-C16-C17
29	9	2630	LHG	C18-C19-C20-C21
29	l	101	LHG	C9-C10-C11-C12
25	5	603	CLA	C2-C3-C5-C6
24	4	609	CHL	C6-C7-C8-C9
24	Y	607	CHL	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
24	Y	609	CHL	C11-C12-C13-C14
24	y	609	CHL	C11-C12-C13-C14
25	C	511	CLA	C6-C7-C8-C9
25	D	403	CLA	C11-C12-C13-C14
25	R	610	CLA	C11-C10-C8-C9
25	8	604	CLA	C14-C13-C15-C16
25	p	602	CLA	C6-C7-C8-C9
25	q	602	CLA	C14-C13-C15-C16
25	c	511	CLA	C6-C7-C8-C9
25	d	403	CLA	C11-C12-C13-C14
25	r	610	CLA	C11-C10-C8-C9
25	r	613	CLA	C6-C7-C8-C9
24	5	601	CHL	O1D-CGD-O2D-CED
24	r	607	CHL	O1D-CGD-O2D-CED
25	3	610	CLA	O1D-CGD-O2D-CED
25	G	613	CLA	O1D-CGD-O2D-CED
29	L	101	LHG	C18-C19-C20-C21
29	l	101	LHG	C18-C19-C20-C21
24	0	607	CHL	C13-C15-C16-C17
24	7	601	CHL	C5-C6-C7-C8
24	n	605	CHL	C10-C11-C12-C13
25	C	504	CLA	C10-C11-C12-C13
25	7	612	CLA	C8-C10-C11-C12
25	c	504	CLA	C10-C11-C12-C13
24	1	608	CHL	C2A-CAA-CBA-CGA
24	S	601	CHL	C2A-CAA-CBA-CGA
24	s	601	CHL	C2A-CAA-CBA-CGA
25	5	602	CLA	C2A-CAA-CBA-CGA
25	5	614	CLA	C2A-CAA-CBA-CGA
25	R	601	CLA	C2A-CAA-CBA-CGA
25	0	610	CLA	C2A-CAA-CBA-CGA
24	Y	606	CHL	O1A-CGA-O2A-C1
24	y	606	CHL	O1A-CGA-O2A-C1
25	r	604	CLA	O1A-CGA-O2A-C1
29	2	2630	LHG	C27-C28-C29-C30
36	A	413	LMG	C11-C12-C13-C14
36	a	413	LMG	C11-C12-C13-C14
29	N	2630	LHG	O1-C1-C2-C3
29	n	2630	LHG	O1-C1-C2-C3
26	p	1621	LUT	C27-C28-C29-C30
24	8	601	CHL	C3-C5-C6-C7
24	p	607	CHL	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	n	604	CLA	C3-C5-C6-C7
24	3	601	CHL	C15-C16-C17-C18
24	Y	607	CHL	C15-C16-C17-C18
24	7	606	CHL	C8-C10-C11-C12
25	0	602	CLA	C5-C6-C7-C8
25	c	502	CLA	C8-C10-C11-C12
24	3	609	CHL	C2C-C3C-CAC-CBC
29	5	2630	LHG	C13-C14-C15-C16
37	C	518	DGD	C4A-C5A-C6A-C7A
37	c	519	DGD	C5A-C6A-C7A-C8A
25	C	512	CLA	O1D-CGD-O2D-CED
29	C	2630	LHG	C29-C30-C31-C32
29	S	2630	LHG	C12-C13-C14-C15
29	Y	2630	LHG	C34-C35-C36-C37
29	c	2630	LHG	C29-C30-C31-C32
29	s	2630	LHG	C12-C13-C14-C15
29	y	2630	LHG	C34-C35-C36-C37
37	c	518	DGD	C4A-C5A-C6A-C7A
37	c	518	DGD	CAB-CBB-CCB-CDB
24	3	601	CHL	C16-C17-C18-C19
24	3	605	CHL	C16-C17-C18-C20
24	3	607	CHL	C16-C17-C18-C19
24	3	607	CHL	C16-C17-C18-C20
24	4	609	CHL	C16-C17-C18-C19
24	5	609	CHL	C16-C17-C18-C19
24	G	601	CHL	C16-C17-C18-C20
24	G	609	CHL	C16-C17-C18-C20
24	R	606	CHL	C16-C17-C18-C19
24	0	601	CHL	C16-C17-C18-C20
24	0	609	CHL	C16-C17-C18-C20
24	7	606	CHL	C16-C17-C18-C20
24	p	601	CHL	C16-C17-C18-C19
24	p	609	CHL	C16-C17-C18-C20
24	q	601	CHL	C16-C17-C18-C20
24	g	601	CHL	C16-C17-C18-C20
24	g	609	CHL	C16-C17-C18-C20
24	r	606	CHL	C16-C17-C18-C19
25	A	405	CLA	C16-C17-C18-C20
25	B	607	CLA	C16-C17-C18-C19
25	R	610	CLA	C16-C17-C18-C19
25	R	610	CLA	C16-C17-C18-C20
25	b	607	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
25	r	610	CLA	C16-C17-C18-C19
36	A	413	LMG	O6-C1-O1-C7
36	a	413	LMG	O6-C1-O1-C7
24	4	609	CHL	C10-C11-C12-C13
24	9	609	CHL	C8-C10-C11-C12
25	q	602	CLA	C13-C15-C16-C17
36	S	2631	LMG	C39-C40-C41-C42
37	C	518	DGD	CAB-CBB-CCB-CDB
24	p	601	CHL	CBD-CGD-O2D-CED
25	B	613	CLA	CBD-CGD-O2D-CED
25	b	613	CLA	CBD-CGD-O2D-CED
24	0	605	CHL	O1D-CGD-O2D-CED
25	c	512	CLA	O1D-CGD-O2D-CED
24	8	609	CHL	C2C-C3C-CAC-CBC
29	y	2630	LHG	C14-C15-C16-C17
35	b	621	SQD	C18-C19-C20-C21
37	C	519	DGD	C8B-C9B-CAB-CBB
36	D	411	LMG	C10-C11-C12-C13
36	d	411	LMG	C10-C11-C12-C13
24	5	601	CHL	C5-C6-C7-C8
24	5	605	CHL	C8-C10-C11-C12
24	5	609	CHL	C8-C10-C11-C12
25	5	604	CLA	C10-C11-C12-C13
25	B	607	CLA	C10-C11-C12-C13
25	C	501	CLA	C15-C16-C17-C18
25	C	508	CLA	C15-C16-C17-C18
25	R	613	CLA	C5-C6-C7-C8
25	b	607	CLA	C8-C10-C11-C12
25	b	607	CLA	C10-C11-C12-C13
25	c	508	CLA	C15-C16-C17-C18
25	r	613	CLA	C5-C6-C7-C8
24	3	608	CHL	O1A-CGA-O2A-C1
29	G	2630	LHG	O10-C23-O8-C6
35	B	621	SQD	C18-C19-C20-C21
24	S	606	CHL	O1D-CGD-O2D-CED
25	8	613	CLA	O1D-CGD-O2D-CED
29	D	409	LHG	C13-C14-C15-C16
29	d	409	LHG	C13-C14-C15-C16
24	G	609	CHL	O1D-CGD-O2D-CED
24	g	609	CHL	O1D-CGD-O2D-CED
24	2	606	CHL	C3A-C2A-CAA-CBA
24	2	607	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	3	606	CHL	C3A-C2A-CAA-CBA
24	3	607	CHL	C3A-C2A-CAA-CBA
24	4	601	CHL	C3A-C2A-CAA-CBA
24	4	605	CHL	C3A-C2A-CAA-CBA
24	5	607	CHL	C3A-C2A-CAA-CBA
24	G	607	CHL	C3A-C2A-CAA-CBA
24	N	605	CHL	C3A-C2A-CAA-CBA
24	N	606	CHL	C3A-C2A-CAA-CBA
24	N	607	CHL	C3A-C2A-CAA-CBA
24	R	606	CHL	C3A-C2A-CAA-CBA
24	Y	606	CHL	C3A-C2A-CAA-CBA
24	0	607	CHL	C3A-C2A-CAA-CBA
24	8	607	CHL	C3A-C2A-CAA-CBA
24	9	606	CHL	C3A-C2A-CAA-CBA
24	9	607	CHL	C3A-C2A-CAA-CBA
24	p	607	CHL	C3A-C2A-CAA-CBA
24	q	607	CHL	C3A-C2A-CAA-CBA
24	q	609	CHL	C3A-C2A-CAA-CBA
24	g	607	CHL	C3A-C2A-CAA-CBA
24	n	605	CHL	C3A-C2A-CAA-CBA
24	n	606	CHL	C3A-C2A-CAA-CBA
24	n	607	CHL	C3A-C2A-CAA-CBA
24	y	606	CHL	C3A-C2A-CAA-CBA
24	r	606	CHL	C3A-C2A-CAA-CBA
25	1	603	CLA	C3A-C2A-CAA-CBA
25	2	603	CLA	C3A-C2A-CAA-CBA
25	3	603	CLA	C3A-C2A-CAA-CBA
25	3	612	CLA	C3A-C2A-CAA-CBA
25	3	613	CLA	C3A-C2A-CAA-CBA
25	4	603	CLA	C3A-C2A-CAA-CBA
25	4	612	CLA	C3A-C2A-CAA-CBA
25	5	603	CLA	C3A-C2A-CAA-CBA
25	6	603	CLA	C3A-C2A-CAA-CBA
25	A	405	CLA	C3A-C2A-CAA-CBA
25	D	402	CLA	C3A-C2A-CAA-CBA
25	N	603	CLA	C3A-C2A-CAA-CBA
25	R	601	CLA	C3A-C2A-CAA-CBA
25	R	604	CLA	C3A-C2A-CAA-CBA
25	S	605	CLA	C3A-C2A-CAA-CBA
25	Y	603	CLA	C3A-C2A-CAA-CBA
25	0	603	CLA	C3A-C2A-CAA-CBA
25	7	603	CLA	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	8	603	CLA	C3A-C2A-CAA-CBA
25	8	612	CLA	C3A-C2A-CAA-CBA
25	8	613	CLA	C3A-C2A-CAA-CBA
25	9	603	CLA	C3A-C2A-CAA-CBA
25	p	603	CLA	C3A-C2A-CAA-CBA
25	q	603	CLA	C3A-C2A-CAA-CBA
25	q	612	CLA	C3A-C2A-CAA-CBA
25	a	405	CLA	C3A-C2A-CAA-CBA
25	d	402	CLA	C3A-C2A-CAA-CBA
25	n	603	CLA	C3A-C2A-CAA-CBA
25	s	605	CLA	C3A-C2A-CAA-CBA
25	y	603	CLA	C3A-C2A-CAA-CBA
25	r	604	CLA	C3A-C2A-CAA-CBA
33	A	409	PHO	C3A-C2A-CAA-CBA
33	a	409	PHO	C3A-C2A-CAA-CBA
24	3	605	CHL	C13-C15-C16-C17
24	5	609	CHL	C13-C15-C16-C17
25	B	607	CLA	C8-C10-C11-C12
29	p	2630	LHG	C17-C18-C19-C20
29	Y	2630	LHG	C7-C8-C9-C10
24	s	606	CHL	O1D-CGD-O2D-CED
36	h	102	LMG	C4-C5-C6-O5
24	5	608	CHL	O1A-CGA-O2A-C1
24	p	607	CHL	O1A-CGA-O2A-C1
24	3	605	CHL	C16-C17-C18-C19
24	5	609	CHL	C16-C17-C18-C20
24	6	601	CHL	C16-C17-C18-C19
24	G	601	CHL	C16-C17-C18-C19
24	g	601	CHL	C16-C17-C18-C19
24	g	609	CHL	C16-C17-C18-C19
25	4	603	CLA	C16-C17-C18-C19
25	B	614	CLA	C16-C17-C18-C20
25	R	602	CLA	C11-C12-C13-C15
25	Y	604	CLA	C16-C17-C18-C19
25	Y	604	CLA	C16-C17-C18-C20
25	b	614	CLA	C16-C17-C18-C20
25	y	604	CLA	C16-C17-C18-C19
25	y	604	CLA	C16-C17-C18-C20
25	r	602	CLA	C11-C12-C13-C15
29	Y	2630	LHG	C13-C14-C15-C16
36	A	413	LMG	C14-C15-C16-C17
36	a	413	LMG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
37	C	519	DGD	CAB-CBB-CCB-CDB
24	2	609	CHL	O1D-CGD-O2D-CED
24	Y	609	CHL	O1D-CGD-O2D-CED
25	q	612	CLA	O1D-CGD-O2D-CED
29	6	2630	LHG	C4-C5-C6-O8
36	H	102	LMG	C7-C8-C9-O8
37	C	523	DGD	C1G-C2G-C3G-O3G
37	c	523	DGD	C1G-C2G-C3G-O3G
24	y	609	CHL	CBD-CGD-O2D-CED
24	8	605	CHL	C3-C5-C6-C7
25	c	513	CLA	C3-C5-C6-C7
24	8	601	CHL	C15-C16-C17-C18
24	6	607	CHL	C4-C3-C5-C6
25	2	603	CLA	C4-C3-C5-C6
25	6	611	CLA	C4-C3-C5-C6
25	B	604	CLA	C4-C3-C5-C6
25	9	603	CLA	C4-C3-C5-C6
25	b	604	CLA	C4-C3-C5-C6
39	d	405	PL9	C15-C14-C16-C17
24	6	607	CHL	C2-C3-C5-C6
24	R	608	CHL	C2-C3-C5-C6
24	0	607	CHL	C2-C3-C5-C6
24	p	607	CHL	C2-C3-C5-C6
24	r	608	CHL	C2-C3-C5-C6
25	2	603	CLA	C2-C3-C5-C6
25	6	611	CLA	C2-C3-C5-C6
25	9	603	CLA	C2-C3-C5-C6
39	D	405	PL9	C13-C14-C16-C17
39	d	405	PL9	C13-C14-C16-C17
36	B	622	LMG	C11-C10-O7-C8
36	D	412	LMG	C11-C10-O7-C8
36	b	622	LMG	C11-C10-O7-C8
36	d	412	LMG	C11-C10-O7-C8
25	5	611	CLA	O1D-CGD-O2D-CED
24	9	609	CHL	C4C-C3C-CAC-CBC
24	p	606	CHL	C2A-CAA-CBA-CGA
24	q	607	CHL	C2A-CAA-CBA-CGA
25	c	503	CLA	C2A-CAA-CBA-CGA
29	5	2630	LHG	O1-C1-C2-O2
29	6	2630	LHG	O1-C1-C2-O2
29	C	2630	LHG	O1-C1-C2-O2
29	Y	2630	LHG	C9-C10-C11-C12

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Mol	Chain	Res	Type	Atoms
25	y	610	CLA	O1D-CGD-O2D-CED
24	8	608	CHL	O1A-CGA-O2A-C1
25	R	601	CLA	O1A-CGA-O2A-C1
29	s	2630	LHG	O10-C23-O8-C6
24	1	601	CHL	C16-C17-C18-C19
24	2	609	CHL	C16-C17-C18-C20
24	G	609	CHL	C16-C17-C18-C19
24	8	605	CHL	C16-C17-C18-C19
25	C	508	CLA	C16-C17-C18-C19
25	D	403	CLA	C16-C17-C18-C19
25	c	508	CLA	C16-C17-C18-C19
25	d	403	CLA	C16-C17-C18-C19
29	9	2630	LHG	O2-C2-C3-O3
24	3	609	CHL	C8-C10-C11-C12
24	g	609	CHL	C5-C6-C7-C8
25	B	606	CLA	C10-C11-C12-C13
25	Y	611	CLA	C13-C15-C16-C17
25	8	610	CLA	C10-C11-C12-C13
25	b	606	CLA	C10-C11-C12-C13
36	s	2631	LMG	C20-C21-C22-C23
25	c	502	CLA	C3-C5-C6-C7
35	a	412	SQD	C30-C31-C32-C33
24	1	609	CHL	O1A-CGA-O2A-C1
24	3	601	CHL	O1A-CGA-O2A-C1
24	R	606	CHL	O1A-CGA-O2A-C1
24	r	606	CHL	O1A-CGA-O2A-C1
25	6	614	CLA	O1A-CGA-O2A-C1
25	C	501	CLA	O1A-CGA-O2A-C1
29	2	2630	LHG	O10-C23-O8-C6
29	S	2630	LHG	O10-C23-O8-C6
24	2	609	CHL	C8-C10-C11-C12
25	y	611	CLA	C13-C15-C16-C17
37	C	523	DGD	CEA-CFA-CGA-CHA
37	c	523	DGD	CEA-CFA-CGA-CHA
36	B	622	LMG	O9-C10-O7-C8
36	D	412	LMG	O9-C10-O7-C8
36	b	622	LMG	O9-C10-O7-C8
36	d	412	LMG	O9-C10-O7-C8
24	Y	607	CHL	C2-C1-O2A-CGA
24	y	607	CHL	C2-C1-O2A-CGA
29	D	409	LHG	C12-C13-C14-C15
29	q	2630	LHG	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
29	d	409	LHG	C12-C13-C14-C15
36	D	411	LMG	C31-C32-C33-C34
37	c	519	DGD	C6A-C7A-C8A-C9A
25	5	610	CLA	C8-C10-C11-C12
25	Y	611	CLA	C15-C16-C17-C18
25	7	604	CLA	C5-C6-C7-C8
25	y	602	CLA	C15-C16-C17-C18
25	y	611	CLA	C15-C16-C17-C18
29	q	2630	LHG	C9-C10-C11-C12
29	y	2630	LHG	C9-C10-C11-C12
37	C	519	DGD	C6A-C7A-C8A-C9A
24	5	607	CHL	C16-C17-C18-C20
24	0	606	CHL	C16-C17-C18-C19
25	6	604	CLA	C16-C17-C18-C19
37	C	519	DGD	C1B-C2B-C3B-C4B
37	c	519	DGD	C1B-C2B-C3B-C4B
24	3	601	CHL	C3-C5-C6-C7
26	1	1620	LUT	C1-C6-C7-C8
26	3	1620	LUT	C1-C6-C7-C8
26	3	1620	LUT	C5-C6-C7-C8
26	4	1621	LUT	C1-C6-C7-C8
26	4	1621	LUT	C5-C6-C7-C8
26	5	1620	LUT	C1-C6-C7-C8
26	5	1620	LUT	C5-C6-C7-C8
26	6	1620	LUT	C5-C6-C7-C8
26	G	1620	LUT	C1-C6-C7-C8
26	G	1620	LUT	C5-C6-C7-C8
26	N	1620	LUT	C5-C6-C7-C8
26	N	1621	LUT	C5-C6-C7-C8
26	0	1620	LUT	C1-C6-C7-C8
26	0	1620	LUT	C5-C6-C7-C8
26	8	1620	LUT	C1-C6-C7-C8
26	8	1620	LUT	C5-C6-C7-C8
26	p	1620	LUT	C1-C6-C7-C8
26	p	1620	LUT	C5-C6-C7-C8
26	p	1621	LUT	C5-C6-C7-C8
26	q	1620	LUT	C5-C6-C7-C8
26	q	1621	LUT	C1-C6-C7-C8
26	q	1621	LUT	C5-C6-C7-C8
26	g	1620	LUT	C1-C6-C7-C8
26	g	1620	LUT	C5-C6-C7-C8
26	n	1620	LUT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	n	1621	LUT	C5-C6-C7-C8
34	A	411	BCR	C23-C24-C25-C26
34	A	411	BCR	C23-C24-C25-C30
34	B	618	BCR	C1-C6-C7-C8
34	B	618	BCR	C5-C6-C7-C8
34	C	514	BCR	C1-C6-C7-C8
34	C	514	BCR	C5-C6-C7-C8
34	C	515	BCR	C5-C6-C7-C8
34	C	516	BCR	C23-C24-C25-C26
34	C	516	BCR	C23-C24-C25-C30
34	H	101	BCR	C23-C24-C25-C26
34	a	411	BCR	C23-C24-C25-C26
34	a	411	BCR	C23-C24-C25-C30
34	b	618	BCR	C1-C6-C7-C8
34	b	618	BCR	C5-C6-C7-C8
34	c	514	BCR	C1-C6-C7-C8
34	c	514	BCR	C5-C6-C7-C8
34	c	516	BCR	C23-C24-C25-C26
34	c	516	BCR	C23-C24-C25-C30
34	h	101	BCR	C23-C24-C25-C26
29	2	2630	LHG	C18-C19-C20-C21
36	d	411	LMG	C31-C32-C33-C34
24	p	601	CHL	CBA-CGA-O2A-C1
24	q	607	CHL	CBA-CGA-O2A-C1
25	1	603	CLA	CBA-CGA-O2A-C1
25	B	602	CLA	CBA-CGA-O2A-C1
25	B	605	CLA	CBA-CGA-O2A-C1
25	C	511	CLA	CBA-CGA-O2A-C1
25	b	602	CLA	CBA-CGA-O2A-C1
25	b	605	CLA	CBA-CGA-O2A-C1
24	2	601	CHL	C8-C10-C11-C12
24	G	609	CHL	C5-C6-C7-C8
24	Y	607	CHL	C5-C6-C7-C8
24	7	609	CHL	C15-C16-C17-C18
24	p	605	CHL	C8-C10-C11-C12
25	4	613	CLA	C15-C16-C17-C18
25	B	602	CLA	C15-C16-C17-C18
25	C	507	CLA	C8-C10-C11-C12
25	D	402	CLA	C10-C11-C12-C13
25	Y	602	CLA	C15-C16-C17-C18
25	Y	612	CLA	C10-C11-C12-C13
25	7	610	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
25	b	602	CLA	C15-C16-C17-C18
25	y	612	CLA	C10-C11-C12-C13
29	1	2630	LHG	C24-C25-C26-C27
35	A	412	SQD	C26-C27-C28-C29
35	a	412	SQD	C26-C27-C28-C29
36	S	2631	LMG	C19-C20-C21-C22
36	S	2631	LMG	C20-C21-C22-C23
29	D	409	LHG	C7-C8-C9-C10
24	6	601	CHL	C10-C11-C12-C13
24	0	601	CHL	C10-C11-C12-C13
25	B	611	CLA	C15-C16-C17-C18
25	b	611	CLA	C15-C16-C17-C18
33	A	408	PHO	C15-C16-C17-C18
33	a	408	PHO	C15-C16-C17-C18
35	A	412	SQD	C30-C31-C32-C33
36	s	2631	LMG	C16-C17-C18-C19
25	4	613	CLA	C4-C3-C5-C6
25	5	604	CLA	C4-C3-C5-C6
25	7	612	CLA	C4-C3-C5-C6
24	S	601	CHL	O1D-CGD-O2D-CED
25	p	610	CLA	O1D-CGD-O2D-CED
24	1	607	CHL	C11-C10-C8-C7
24	1	609	CHL	C11-C12-C13-C15
24	1	609	CHL	C12-C13-C15-C16
24	N	605	CHL	C6-C7-C8-C10
24	N	605	CHL	C11-C10-C8-C7
24	R	608	CHL	C6-C7-C8-C10
24	Y	601	CHL	C11-C10-C8-C7
24	Y	607	CHL	C11-C10-C8-C7
24	0	609	CHL	C2-C3-C5-C6
24	7	609	CHL	C11-C12-C13-C15
24	p	607	CHL	C11-C10-C8-C7
24	q	609	CHL	C2-C3-C5-C6
24	q	609	CHL	C11-C10-C8-C7
24	n	605	CHL	C6-C7-C8-C10
24	y	607	CHL	C11-C10-C8-C7
24	r	608	CHL	C6-C7-C8-C10
25	1	604	CLA	C12-C13-C15-C16
25	1	610	CLA	C11-C12-C13-C15
25	1	611	CLA	C2-C3-C5-C6
25	3	603	CLA	C11-C10-C8-C7
25	4	610	CLA	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
25	6	604	CLA	C11-C12-C13-C15
25	B	607	CLA	C11-C12-C13-C15
25	B	613	CLA	C6-C7-C8-C10
25	C	505	CLA	C11-C10-C8-C7
25	C	506	CLA	C11-C10-C8-C7
25	C	511	CLA	C6-C7-C8-C10
25	D	402	CLA	C11-C10-C8-C7
25	G	613	CLA	C12-C13-C15-C16
25	R	610	CLA	C11-C10-C8-C7
25	R	616	CLA	C6-C7-C8-C10
25	R	616	CLA	C11-C12-C13-C15
25	Y	604	CLA	C12-C13-C15-C16
25	0	604	CLA	C2-C3-C5-C6
25	7	604	CLA	C12-C13-C15-C16
25	7	610	CLA	C11-C12-C13-C15
25	7	612	CLA	C12-C13-C15-C16
25	8	603	CLA	C11-C10-C8-C7
25	8	604	CLA	C12-C13-C15-C16
25	p	602	CLA	C6-C7-C8-C10
25	b	607	CLA	C11-C12-C13-C15
25	b	613	CLA	C6-C7-C8-C10
25	c	505	CLA	C11-C10-C8-C7
25	c	506	CLA	C11-C10-C8-C7
25	d	403	CLA	C11-C12-C13-C15
25	g	613	CLA	C12-C13-C15-C16
25	y	604	CLA	C12-C13-C15-C16
25	r	610	CLA	C11-C10-C8-C7
25	r	616	CLA	C6-C7-C8-C10
25	r	616	CLA	C11-C12-C13-C15
33	A	408	PHO	C2-C3-C5-C6
33	a	408	PHO	C2-C3-C5-C6
25	B	605	CLA	O1A-CGA-O2A-C1
36	b	622	LMG	C12-C13-C14-C15
24	1	606	CHL	C8-C10-C11-C12
24	p	601	CHL	C10-C11-C12-C13
24	y	609	CHL	C5-C6-C7-C8
24	r	607	CHL	C5-C6-C7-C8
25	4	613	CLA	C13-C15-C16-C17
25	B	614	CLA	C5-C6-C7-C8
25	b	614	CLA	C5-C6-C7-C8
26	7	1621	LUT	C29-C30-C31-C32
24	5	605	CHL	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
29	d	409	LHG	C7-C8-C9-C10
35	B	621	SQD	C7-C8-C9-C10
35	b	621	SQD	C7-C8-C9-C10
36	s	2631	LMG	C28-C29-C30-C31
24	7	609	CHL	CBA-CGA-O2A-C1
24	8	601	CHL	CBA-CGA-O2A-C1
24	p	608	CHL	CBA-CGA-O2A-C1
25	1	613	CLA	CBA-CGA-O2A-C1
25	S	610	CLA	CBA-CGA-O2A-C1
25	0	614	CLA	CBA-CGA-O2A-C1
25	7	613	CLA	CBA-CGA-O2A-C1
25	8	613	CLA	CBA-CGA-O2A-C1
25	s	610	CLA	CBA-CGA-O2A-C1
25	r	601	CLA	CBA-CGA-O2A-C1
24	1	606	CHL	C2A-CAA-CBA-CGA
24	6	606	CHL	C2A-CAA-CBA-CGA
24	8	605	CHL	C2A-CAA-CBA-CGA
25	2	611	CLA	C2A-CAA-CBA-CGA
25	3	614	CLA	C2A-CAA-CBA-CGA
25	G	613	CLA	C2A-CAA-CBA-CGA
25	S	602	CLA	C2A-CAA-CBA-CGA
25	Y	610	CLA	C2A-CAA-CBA-CGA
25	8	614	CLA	C2A-CAA-CBA-CGA
25	9	611	CLA	C2A-CAA-CBA-CGA
25	b	604	CLA	C2A-CAA-CBA-CGA
25	g	613	CLA	C2A-CAA-CBA-CGA
25	s	602	CLA	C2A-CAA-CBA-CGA
24	R	607	CHL	C5-C6-C7-C8
29	C	2630	LHG	C33-C34-C35-C36
29	n	2630	LHG	C26-C27-C28-C29
35	B	621	SQD	C9-C10-C11-C12
36	a	413	LMG	C30-C31-C32-C33
24	4	601	CHL	O1D-CGD-O2D-CED
29	0	2630	LHG	C27-C28-C29-C30
35	b	621	SQD	C9-C10-C11-C12
36	A	413	LMG	C30-C31-C32-C33
24	S	607	CHL	O1D-CGD-O2D-CED
24	7	606	CHL	O1D-CGD-O2D-CED
24	s	607	CHL	O1D-CGD-O2D-CED
25	8	610	CLA	O1D-CGD-O2D-CED
24	7	607	CHL	C15-C16-C17-C18
24	8	609	CHL	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
24	y	607	CHL	C5-C6-C7-C8
25	4	610	CLA	C5-C6-C7-C8
29	C	2630	LHG	C11-C10-C9-C8
29	N	2630	LHG	C11-C10-C9-C8
36	B	622	LMG	C12-C13-C14-C15
24	q	607	CHL	O1A-CGA-O2A-C1
25	1	603	CLA	O1A-CGA-O2A-C1
25	b	605	CLA	O1A-CGA-O2A-C1
24	N	605	CHL	CBD-CGD-O2D-CED
25	A	407	CLA	CBD-CGD-O2D-CED
25	7	611	CLA	CBD-CGD-O2D-CED
25	3	613	CLA	CBA-CGA-O2A-C1
24	Y	606	CHL	C16-C17-C18-C20
24	0	607	CHL	C16-C17-C18-C20
24	p	605	CHL	C16-C17-C18-C19
24	y	606	CHL	C16-C17-C18-C20
25	Y	611	CLA	C16-C17-C18-C19
25	q	603	CLA	C16-C17-C18-C20
25	y	611	CLA	C16-C17-C18-C19
24	3	607	CHL	C13-C15-C16-C17
25	3	610	CLA	C10-C11-C12-C13
25	C	501	CLA	O1D-CGD-O2D-CED
29	d	409	LHG	C14-C15-C16-C17
29	C	2630	LHG	C8-C7-O7-C5
29	c	2630	LHG	C8-C7-O7-C5
35	A	412	SQD	C8-C7-O47-C45
35	a	412	SQD	C8-C7-O47-C45
29	C	2630	LHG	C32-C33-C34-C35
29	y	2630	LHG	C26-C27-C28-C29
25	B	614	CLA	C15-C16-C17-C18
25	b	614	CLA	C15-C16-C17-C18
24	8	601	CHL	CBD-CGD-O2D-CED
24	9	609	CHL	CBD-CGD-O2D-CED
29	D	409	LHG	C14-C15-C16-C17
36	B	622	LMG	C10-C11-C12-C13
37	c	519	DGD	CAB-CBB-CCB-CDB
25	b	602	CLA	C5-C6-C7-C8
37	C	519	DGD	O1G-C1G-C2G-O2G
37	C	524	DGD	O1G-C1G-C2G-O2G
37	c	519	DGD	O1G-C1G-C2G-O2G
37	c	524	DGD	O1G-C1G-C2G-O2G
36	S	2631	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
36	s	2631	LMG	O6-C5-C6-O5
36	D	411	LMG	C17-C18-C19-C20
36	d	411	LMG	C17-C18-C19-C20
37	c	519	DGD	C8B-C9B-CAB-CBB
25	G	610	CLA	CBD-CGD-O2D-CED
25	g	610	CLA	CBD-CGD-O2D-CED
24	s	601	CHL	O1D-CGD-O2D-CED
24	q	609	CHL	C16-C17-C18-C20
25	l	610	CLA	C16-C17-C18-C19
25	a	405	CLA	C16-C17-C18-C19
29	0	2630	LHG	C32-C33-C34-C35
24	G	601	CHL	C10-C11-C12-C13
24	N	601	CHL	C10-C11-C12-C13
24	R	606	CHL	C13-C15-C16-C17
24	n	601	CHL	C10-C11-C12-C13
25	q	603	CLA	C15-C16-C17-C18
24	p	607	CHL	C4-C3-C5-C6
24	q	609	CHL	C4-C3-C5-C6
25	2	602	CLA	C4-C3-C5-C6
25	0	604	CLA	C4-C3-C5-C6
25	7	613	CLA	C4-C3-C5-C6
33	A	408	PHO	C4-C3-C5-C6
33	a	408	PHO	C4-C3-C5-C6
39	D	405	PL9	C30-C29-C31-C32
39	d	405	PL9	C30-C29-C31-C32
25	4	613	CLA	C2-C3-C5-C6
25	B	604	CLA	C2-C3-C5-C6
25	b	604	CLA	C2-C3-C5-C6
37	C	523	DGD	CBA-CCA-CDA-CEA
37	c	523	DGD	CBA-CCA-CDA-CEA
24	1	607	CHL	C11-C10-C8-C9
24	1	609	CHL	C11-C12-C13-C14
24	2	601	CHL	C6-C7-C8-C9
24	3	609	CHL	C11-C12-C13-C14
24	6	607	CHL	C11-C10-C8-C9
24	G	601	CHL	C6-C7-C8-C9
24	N	607	CHL	C14-C13-C15-C16
24	Y	601	CHL	C11-C10-C8-C9
24	7	607	CHL	C11-C10-C8-C9
24	7	609	CHL	C11-C12-C13-C14
24	8	609	CHL	C11-C12-C13-C14
24	g	601	CHL	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
24	n	607	CHL	C14-C13-C15-C16
24	y	601	CHL	C11-C10-C8-C9
24	y	607	CHL	C11-C10-C8-C9
25	1	604	CLA	C14-C13-C15-C16
25	1	610	CLA	C11-C12-C13-C14
25	1	612	CLA	C14-C13-C15-C16
25	3	603	CLA	C11-C10-C8-C9
25	4	610	CLA	C11-C12-C13-C14
25	6	604	CLA	C11-C10-C8-C9
25	6	604	CLA	C11-C12-C13-C14
25	C	510	CLA	C6-C7-C8-C9
25	D	402	CLA	C11-C10-C8-C9
25	G	613	CLA	C14-C13-C15-C16
25	R	616	CLA	C6-C7-C8-C9
25	R	616	CLA	C11-C12-C13-C14
25	Y	604	CLA	C14-C13-C15-C16
25	Y	610	CLA	C11-C12-C13-C14
25	0	604	CLA	C11-C10-C8-C9
25	7	604	CLA	C14-C13-C15-C16
25	7	610	CLA	C11-C12-C13-C14
25	8	603	CLA	C11-C10-C8-C9
25	q	613	CLA	C14-C13-C15-C16
25	c	510	CLA	C6-C7-C8-C9
25	d	402	CLA	C11-C10-C8-C9
25	g	613	CLA	C14-C13-C15-C16
25	y	604	CLA	C14-C13-C15-C16
25	r	616	CLA	C6-C7-C8-C9
25	r	616	CLA	C11-C12-C13-C14
25	Y	610	CLA	O1D-CGD-O2D-CED
25	g	611	CLA	O1D-CGD-O2D-CED
25	1	611	CLA	CBD-CGD-O2D-CED
29	6	2630	LHG	C26-C27-C28-C29
36	h	102	LMG	C32-C33-C34-C35
24	3	605	CHL	C2A-CAA-CBA-CGA
24	3	608	CHL	C2A-CAA-CBA-CGA
24	R	606	CHL	C2A-CAA-CBA-CGA
24	7	606	CHL	C2A-CAA-CBA-CGA
24	8	608	CHL	C2A-CAA-CBA-CGA
24	r	606	CHL	C2A-CAA-CBA-CGA
25	B	604	CLA	C2A-CAA-CBA-CGA
25	C	503	CLA	C2A-CAA-CBA-CGA
25	N	602	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	N	613	CLA	C2A-CAA-CBA-CGA
25	Y	602	CLA	C2A-CAA-CBA-CGA
25	Y	603	CLA	C2A-CAA-CBA-CGA
25	p	602	CLA	C2A-CAA-CBA-CGA
25	n	602	CLA	C2A-CAA-CBA-CGA
25	y	602	CLA	C2A-CAA-CBA-CGA
36	H	102	LMG	C32-C33-C34-C35
24	3	609	CHL	CBA-CGA-O2A-C1
24	N	605	CHL	C10-C11-C12-C13
24	p	601	CHL	C5-C6-C7-C8
25	2	610	CLA	C10-C11-C12-C13
25	3	604	CLA	C13-C15-C16-C17
25	B	602	CLA	C5-C6-C7-C8
26	3	1620	LUT	C27-C28-C29-C30
27	0	1622	XAT	C31-C32-C33-C34
27	7	1622	XAT	C31-C32-C33-C34
24	8	601	CHL	O1A-CGA-O2A-C1
24	p	601	CHL	O1A-CGA-O2A-C1
25	B	602	CLA	O1A-CGA-O2A-C1
25	C	511	CLA	O1A-CGA-O2A-C1
25	b	602	CLA	O1A-CGA-O2A-C1
24	1	609	CHL	C1A-C2A-CAA-CBA
24	2	601	CHL	C1A-C2A-CAA-CBA
24	2	606	CHL	C1A-C2A-CAA-CBA
24	2	607	CHL	C1A-C2A-CAA-CBA
24	2	608	CHL	C1A-C2A-CAA-CBA
24	3	607	CHL	C1A-C2A-CAA-CBA
24	G	605	CHL	C1A-C2A-CAA-CBA
24	G	608	CHL	C1A-C2A-CAA-CBA
24	G	609	CHL	C1A-C2A-CAA-CBA
24	N	605	CHL	C1A-C2A-CAA-CBA
24	N	606	CHL	C1A-C2A-CAA-CBA
24	N	607	CHL	C1A-C2A-CAA-CBA
24	R	606	CHL	C1A-C2A-CAA-CBA
24	Y	605	CHL	C1A-C2A-CAA-CBA
24	Y	609	CHL	C1A-C2A-CAA-CBA
24	7	608	CHL	C1A-C2A-CAA-CBA
24	8	607	CHL	C1A-C2A-CAA-CBA
24	9	601	CHL	C1A-C2A-CAA-CBA
24	9	606	CHL	C1A-C2A-CAA-CBA
24	9	607	CHL	C1A-C2A-CAA-CBA
24	9	608	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	q	607	CHL	C1A-C2A-CAA-CBA
24	q	609	CHL	C1A-C2A-CAA-CBA
24	g	605	CHL	C1A-C2A-CAA-CBA
24	g	608	CHL	C1A-C2A-CAA-CBA
24	g	609	CHL	C1A-C2A-CAA-CBA
24	n	605	CHL	C1A-C2A-CAA-CBA
24	n	606	CHL	C1A-C2A-CAA-CBA
24	n	607	CHL	C1A-C2A-CAA-CBA
24	y	605	CHL	C1A-C2A-CAA-CBA
24	y	609	CHL	C1A-C2A-CAA-CBA
24	r	606	CHL	C1A-C2A-CAA-CBA
25	1	603	CLA	C1A-C2A-CAA-CBA
25	1	604	CLA	C1A-C2A-CAA-CBA
25	1	610	CLA	C1A-C2A-CAA-CBA
25	1	614	CLA	C1A-C2A-CAA-CBA
25	2	603	CLA	C1A-C2A-CAA-CBA
25	2	614	CLA	C1A-C2A-CAA-CBA
25	3	603	CLA	C1A-C2A-CAA-CBA
25	3	604	CLA	C1A-C2A-CAA-CBA
25	3	611	CLA	C1A-C2A-CAA-CBA
25	3	614	CLA	C1A-C2A-CAA-CBA
25	4	603	CLA	C1A-C2A-CAA-CBA
25	4	610	CLA	C1A-C2A-CAA-CBA
25	5	603	CLA	C1A-C2A-CAA-CBA
25	5	604	CLA	C1A-C2A-CAA-CBA
25	5	611	CLA	C1A-C2A-CAA-CBA
25	5	614	CLA	C1A-C2A-CAA-CBA
25	6	603	CLA	C1A-C2A-CAA-CBA
25	6	610	CLA	C1A-C2A-CAA-CBA
25	A	405	CLA	C1A-C2A-CAA-CBA
25	A	406	CLA	C1A-C2A-CAA-CBA
25	A	407	CLA	C1A-C2A-CAA-CBA
25	B	602	CLA	C1A-C2A-CAA-CBA
25	B	606	CLA	C1A-C2A-CAA-CBA
25	B	612	CLA	C1A-C2A-CAA-CBA
25	C	503	CLA	C1A-C2A-CAA-CBA
25	C	508	CLA	C1A-C2A-CAA-CBA
25	C	511	CLA	C1A-C2A-CAA-CBA
25	D	402	CLA	C1A-C2A-CAA-CBA
25	G	611	CLA	C1A-C2A-CAA-CBA
25	G	614	CLA	C1A-C2A-CAA-CBA
25	N	614	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	R	601	CLA	C1A-C2A-CAA-CBA
25	S	604	CLA	C1A-C2A-CAA-CBA
25	S	610	CLA	C1A-C2A-CAA-CBA
25	S	611	CLA	C1A-C2A-CAA-CBA
25	Y	603	CLA	C1A-C2A-CAA-CBA
25	Y	604	CLA	C1A-C2A-CAA-CBA
25	Y	610	CLA	C1A-C2A-CAA-CBA
25	Y	614	CLA	C1A-C2A-CAA-CBA
25	0	603	CLA	C1A-C2A-CAA-CBA
25	0	604	CLA	C1A-C2A-CAA-CBA
25	0	610	CLA	C1A-C2A-CAA-CBA
25	7	603	CLA	C1A-C2A-CAA-CBA
25	7	610	CLA	C1A-C2A-CAA-CBA
25	7	614	CLA	C1A-C2A-CAA-CBA
25	8	603	CLA	C1A-C2A-CAA-CBA
25	8	604	CLA	C1A-C2A-CAA-CBA
25	8	611	CLA	C1A-C2A-CAA-CBA
25	8	614	CLA	C1A-C2A-CAA-CBA
25	9	603	CLA	C1A-C2A-CAA-CBA
25	9	610	CLA	C1A-C2A-CAA-CBA
25	9	614	CLA	C1A-C2A-CAA-CBA
25	p	603	CLA	C1A-C2A-CAA-CBA
25	p	604	CLA	C1A-C2A-CAA-CBA
25	p	610	CLA	C1A-C2A-CAA-CBA
25	p	611	CLA	C1A-C2A-CAA-CBA
25	p	614	CLA	C1A-C2A-CAA-CBA
25	q	603	CLA	C1A-C2A-CAA-CBA
25	q	604	CLA	C1A-C2A-CAA-CBA
25	q	610	CLA	C1A-C2A-CAA-CBA
25	q	614	CLA	C1A-C2A-CAA-CBA
25	a	405	CLA	C1A-C2A-CAA-CBA
25	a	406	CLA	C1A-C2A-CAA-CBA
25	a	407	CLA	C1A-C2A-CAA-CBA
25	b	602	CLA	C1A-C2A-CAA-CBA
25	b	606	CLA	C1A-C2A-CAA-CBA
25	b	612	CLA	C1A-C2A-CAA-CBA
25	c	508	CLA	C1A-C2A-CAA-CBA
25	c	511	CLA	C1A-C2A-CAA-CBA
25	d	402	CLA	C1A-C2A-CAA-CBA
25	g	611	CLA	C1A-C2A-CAA-CBA
25	g	614	CLA	C1A-C2A-CAA-CBA
25	n	611	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	n	614	CLA	C1A-C2A-CAA-CBA
25	s	604	CLA	C1A-C2A-CAA-CBA
25	s	610	CLA	C1A-C2A-CAA-CBA
25	s	611	CLA	C1A-C2A-CAA-CBA
25	y	603	CLA	C1A-C2A-CAA-CBA
25	y	604	CLA	C1A-C2A-CAA-CBA
25	y	610	CLA	C1A-C2A-CAA-CBA
25	y	614	CLA	C1A-C2A-CAA-CBA
25	r	601	CLA	C1A-C2A-CAA-CBA
24	2	609	CHL	C16-C17-C18-C19
24	4	609	CHL	C16-C17-C18-C20
24	5	601	CHL	C16-C17-C18-C20
24	6	607	CHL	C16-C17-C18-C19
24	Y	606	CHL	C16-C17-C18-C19
24	0	606	CHL	C16-C17-C18-C20
24	0	607	CHL	C16-C17-C18-C19
24	p	601	CHL	C16-C17-C18-C20
24	q	601	CHL	C16-C17-C18-C19
24	y	606	CHL	C16-C17-C18-C19
25	2	603	CLA	C16-C17-C18-C20
25	B	609	CLA	C16-C17-C18-C19
25	C	508	CLA	C16-C17-C18-C20
25	9	603	CLA	C16-C17-C18-C20
25	q	603	CLA	C16-C17-C18-C19
25	c	510	CLA	C16-C17-C18-C19
25	c	513	CLA	C16-C17-C18-C20
25	d	403	CLA	C16-C17-C18-C20
29	q	2630	LHG	C27-C28-C29-C30
26	1	1621	LUT	C29-C30-C31-C32
25	G	611	CLA	O1D-CGD-O2D-CED
24	1	601	CHL	C8-C10-C11-C12
24	g	601	CHL	C10-C11-C12-C13
24	r	606	CHL	C13-C15-C16-C17
25	6	602	CLA	C10-C11-C12-C13
29	6	2630	LHG	C4-O6-P-O3
29	D	408	LHG	C3-O3-P-O6
29	d	409	LHG	C3-O3-P-O6
29	l	101	LHG	C3-O3-P-O6
29	c	2630	LHG	C33-C34-C35-C36
35	D	413	SQD	C11-C10-C9-C8
24	0	606	CHL	C3-C5-C6-C7
29	Y	2630	LHG	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
35	d	413	SQD	C11-C10-C9-C8
24	Y	609	CHL	C5-C6-C7-C8
25	1	603	CLA	C8-C10-C11-C12
25	5	602	CLA	C8-C10-C11-C12
25	R	610	CLA	C13-C15-C16-C17
25	7	603	CLA	C8-C10-C11-C12
29	4	2630	LHG	O6-C4-C5-C6
24	n	609	CHL	O1D-CGD-O2D-CED
25	3	613	CLA	O1D-CGD-O2D-CED
36	b	622	LMG	C10-C11-C12-C13
24	9	601	CHL	C13-C15-C16-C17
25	1	612	CLA	C8-C10-C11-C12
25	r	610	CLA	C13-C15-C16-C17
24	7	606	CHL	C16-C17-C18-C19
24	p	609	CHL	C16-C17-C18-C19
25	A	405	CLA	C16-C17-C18-C19
25	B	611	CLA	C16-C17-C18-C19
25	b	611	CLA	C16-C17-C18-C19
25	c	508	CLA	C16-C17-C18-C20
29	3	2630	LHG	C18-C19-C20-C21
37	C	524	DGD	C6A-C7A-C8A-C9A
24	4	601	CHL	C5-C6-C7-C8
24	G	609	CHL	C13-C15-C16-C17
29	9	2630	LHG	C27-C28-C29-C30
24	5	607	CHL	CBA-CGA-O2A-C1
24	q	601	CHL	CBA-CGA-O2A-C1
29	c	2630	LHG	O9-C7-O7-C5
24	3	607	CHL	C4-C3-C5-C6
24	4	609	CHL	C4-C3-C5-C6
24	0	609	CHL	C4-C3-C5-C6
25	1	611	CLA	C4-C3-C5-C6
25	1	612	CLA	C4-C3-C5-C6
25	1	613	CLA	C4-C3-C5-C6
25	5	604	CLA	C2-C3-C5-C6
25	7	612	CLA	C2-C3-C5-C6
40	F	101	HEM	C2A-CAA-CBA-CGA
29	2	2630	LHG	C9-C10-C11-C12
29	9	2630	LHG	C13-C14-C15-C16
29	d	409	LHG	C34-C35-C36-C37
29	s	2630	LHG	C25-C26-C27-C28
35	B	623	SQD	C16-C17-C18-C19
37	C	519	DGD	CAA-CBA-CCA-CDA

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Mol	Chain	Res	Type	Atoms
37	c	524	DGD	C6A-C7A-C8A-C9A
25	c	501	CLA	O1D-CGD-O2D-CED
29	S	2630	LHG	C25-C26-C27-C28
24	p	608	CHL	O1A-CGA-O2A-C1
25	0	614	CLA	O1A-CGA-O2A-C1
29	4	2630	LHG	O2-C2-C3-O3
24	Y	607	CHL	C10-C11-C12-C13
25	6	611	CLA	C2A-CAA-CBA-CGA
24	6	606	CHL	C16-C17-C18-C20
24	9	609	CHL	C16-C17-C18-C20
25	B	609	CLA	C16-C17-C18-C20
25	D	403	CLA	C16-C17-C18-C20
25	7	610	CLA	C16-C17-C18-C19
24	Y	601	CHL	C3-C5-C6-C7
29	1	2630	LHG	C4-C5-C6-O8
29	2	2630	LHG	C11-C12-C13-C14
29	G	2630	LHG	C17-C18-C19-C20
29	N	2630	LHG	C4-C5-C6-O8
29	7	2630	LHG	C4-C5-C6-O8
29	n	2630	LHG	C4-C5-C6-O8
29	y	2630	LHG	C4-C5-C6-O8
29	y	2630	LHG	C11-C10-C9-C8
36	S	2631	LMG	C7-C8-C9-O8
36	h	102	LMG	C7-C8-C9-O8
36	s	2631	LMG	C7-C8-C9-O8
37	C	524	DGD	O1G-C1G-C2G-C3G
37	c	524	DGD	O1G-C1G-C2G-C3G
24	g	609	CHL	C13-C15-C16-C17
25	N	602	CLA	C5-C6-C7-C8
35	A	412	SQD	C11-C12-C13-C14
24	7	609	CHL	O1A-CGA-O2A-C1
25	S	610	CLA	O1A-CGA-O2A-C1
25	s	610	CLA	O1A-CGA-O2A-C1
25	r	601	CLA	O1A-CGA-O2A-C1
24	N	601	CHL	C5-C6-C7-C8
24	N	607	CHL	C15-C16-C17-C18
25	D	403	CLA	C8-C10-C11-C12
29	9	2630	LHG	C9-C10-C11-C12
35	a	412	SQD	C11-C12-C13-C14
37	C	520	DGD	C9B-CAB-CBB-CCB
37	c	520	DGD	C9B-CAB-CBB-CCB
36	D	412	LMG	O6-C5-C6-O5

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Mol	Chain	Res	Type	Atoms
36	d	412	LMG	O6-C5-C6-O5
24	q	601	CHL	O1A-CGA-O2A-C1
25	8	613	CLA	O1A-CGA-O2A-C1
25	b	609	CLA	C16-C17-C18-C20
24	N	609	CHL	O1D-CGD-O2D-CED
29	C	2630	LHG	C10-C11-C12-C13
29	0	2630	LHG	C24-C25-C26-C27
29	N	2630	LHG	O1-C1-C2-O2
29	p	2630	LHG	O1-C1-C2-O2
29	n	2630	LHG	O1-C1-C2-O2
29	s	2630	LHG	O1-C1-C2-O2
25	1	613	CLA	O1A-CGA-O2A-C1
29	8	2630	LHG	C18-C19-C20-C21
29	9	2630	LHG	C11-C12-C13-C14
24	N	605	CHL	O1D-CGD-O2D-CED
24	n	601	CHL	C5-C6-C7-C8
24	n	607	CHL	C15-C16-C17-C18
25	c	513	CLA	C15-C16-C17-C18
25	d	403	CLA	C8-C10-C11-C12
36	D	411	LMG	O6-C5-C6-O5
36	d	411	LMG	O6-C5-C6-O5
24	6	609	CHL	C4-C3-C5-C6
25	3	603	CLA	C4-C3-C5-C6
25	6	604	CLA	C4-C3-C5-C6
29	p	2630	LHG	C15-C16-C17-C18
37	C	523	DGD	CAA-CBA-CCA-CDA
37	c	523	DGD	CAA-CBA-CCA-CDA
25	6	604	CLA	C2-C3-C5-C6
25	7	613	CLA	C2-C3-C5-C6
24	1	606	CHL	C16-C17-C18-C19
25	C	510	CLA	C16-C17-C18-C19
25	C	510	CLA	C16-C17-C18-C20
25	0	604	CLA	C16-C17-C18-C20
25	b	609	CLA	C16-C17-C18-C19
25	c	510	CLA	C16-C17-C18-C20
24	5	601	CHL	CBA-CGA-O2A-C1
25	2	613	CLA	CBA-CGA-O2A-C1
25	7	603	CLA	CBA-CGA-O2A-C1
25	9	613	CLA	CBA-CGA-O2A-C1
29	D	410	LHG	C24-C23-O8-C6
29	d	410	LHG	C24-C23-O8-C6
29	q	2630	LHG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
25	g	604	CLA	CBD-CGD-O2D-CED
24	2	601	CHL	C13-C15-C16-C17
24	5	601	CHL	C15-C16-C17-C18
25	0	602	CLA	C10-C11-C12-C13
29	D	410	LHG	C34-C35-C36-C37
24	8	606	CHL	O1D-CGD-O2D-CED
25	6	602	CLA	C2A-CAA-CBA-CGA
25	c	502	CLA	C2A-CAA-CBA-CGA
24	6	607	CHL	C13-C15-C16-C17
25	b	613	CLA	C13-C15-C16-C17
25	C	513	CLA	C2-C1-O2A-CGA
25	6	614	CLA	C6-C7-C8-C9
29	R	2630	LHG	C24-C25-C26-C27
29	d	410	LHG	C34-C35-C36-C37
25	0	614	CLA	C6-C7-C8-C9
25	9	602	CLA	O1D-CGD-O2D-CED
25	B	613	CLA	C13-C15-C16-C17
25	b	612	CLA	C10-C11-C12-C13
25	n	602	CLA	C5-C6-C7-C8
29	y	2630	LHG	C13-C14-C15-C16
24	1	606	CHL	CBA-CGA-O2A-C1
24	8	609	CHL	CBA-CGA-O2A-C1
24	q	605	CHL	CBA-CGA-O2A-C1
25	1	612	CLA	CBA-CGA-O2A-C1
29	5	2630	LHG	C24-C23-O8-C6
29	5	2630	LHG	O6-C4-C5-O7
24	6	607	CHL	C16-C17-C18-C20
24	9	609	CHL	C16-C17-C18-C19
24	p	605	CHL	C16-C17-C18-C20
29	y	2630	LHG	C27-C28-C29-C30
25	B	612	CLA	C10-C11-C12-C13
29	3	2630	LHG	O2-C2-C3-O3
24	4	605	CHL	O1D-CGD-O2D-CED
25	R	616	CLA	O1D-CGD-O2D-CED
24	3	609	CHL	O1A-CGA-O2A-C1
24	5	607	CHL	O1A-CGA-O2A-C1
25	3	613	CLA	O1A-CGA-O2A-C1
25	7	613	CLA	O1A-CGA-O2A-C1
29	r	2630	LHG	C24-C25-C26-C27
25	B	607	CLA	C15-C16-C17-C18
25	B	609	CLA	C10-C11-C12-C13
25	r	616	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
35	B	621	SQD	C33-C34-C35-C36
35	b	621	SQD	C33-C34-C35-C36
24	q	607	CHL	CAA-CBA-CGA-O2A
29	6	2630	LHG	O7-C5-C6-O8
29	Y	2630	LHG	O7-C5-C6-O8
29	y	2630	LHG	O7-C5-C6-O8
36	H	102	LMG	O7-C8-C9-O8
36	h	102	LMG	O7-C8-C9-O8
25	C	507	CLA	O1D-CGD-O2D-CED
29	N	2630	LHG	C26-C27-C28-C29
29	C	2630	LHG	O9-C7-O7-C5
24	5	609	CHL	C15-C16-C17-C18
24	0	606	CHL	C13-C15-C16-C17
25	Y	602	CLA	C8-C10-C11-C12
25	b	607	CLA	C15-C16-C17-C18
25	y	602	CLA	C8-C10-C11-C12
33	A	409	PHO	CHA-CBD-CGD-O1D
33	A	409	PHO	CHA-CBD-CGD-O2D
33	a	409	PHO	CHA-CBD-CGD-O1D
33	a	409	PHO	CHA-CBD-CGD-O2D
29	D	409	LHG	C34-C35-C36-C37
25	7	603	CLA	C4-C3-C5-C6
25	p	603	CLA	C4-C3-C5-C6
39	d	405	PL9	C12-C13-C14-C15
24	2	609	CHL	C4C-C3C-CAC-CBC
36	c	521	LMG	C29-C30-C31-C32
37	C	523	DGD	C8A-C9A-CAA-CBA
37	c	523	DGD	C8A-C9A-CAA-CBA
25	b	609	CLA	C10-C11-C12-C13
24	1	601	CHL	C6-C7-C8-C10
24	1	607	CHL	C11-C12-C13-C15
24	3	601	CHL	C12-C13-C15-C16
24	3	609	CHL	C11-C12-C13-C15
24	4	609	CHL	C2-C3-C5-C6
24	5	605	CHL	C11-C12-C13-C15
24	5	605	CHL	C12-C13-C15-C16
24	6	609	CHL	C2-C3-C5-C6
24	N	601	CHL	C11-C10-C8-C7
24	N	609	CHL	C11-C10-C8-C7
24	0	607	CHL	C11-C10-C8-C7
24	0	607	CHL	C12-C13-C15-C16
24	0	609	CHL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	8	601	CHL	C6-C7-C8-C10
24	8	601	CHL	C11-C12-C13-C15
24	8	601	CHL	C12-C13-C15-C16
24	8	607	CHL	C6-C7-C8-C10
24	8	609	CHL	C11-C12-C13-C15
24	9	601	CHL	C6-C7-C8-C10
24	p	609	CHL	C11-C12-C13-C15
24	p	609	CHL	C12-C13-C15-C16
24	q	601	CHL	C12-C13-C15-C16
24	n	601	CHL	C11-C10-C8-C7
24	n	605	CHL	C11-C10-C8-C7
24	n	609	CHL	C11-C12-C13-C15
24	y	601	CHL	C11-C10-C8-C7
24	y	607	CHL	C11-C12-C13-C15
25	1	603	CLA	C12-C13-C15-C16
25	1	611	CLA	C11-C12-C13-C15
25	1	612	CLA	C11-C10-C8-C7
25	1	612	CLA	C12-C13-C15-C16
25	1	613	CLA	C6-C7-C8-C10
25	1	613	CLA	C12-C13-C15-C16
25	4	603	CLA	C12-C13-C15-C16
25	5	603	CLA	C11-C10-C8-C7
25	5	613	CLA	C6-C7-C8-C10
25	6	602	CLA	C6-C7-C8-C10
25	6	604	CLA	C11-C10-C8-C7
25	6	612	CLA	C12-C13-C15-C16
25	6	613	CLA	C6-C7-C8-C10
25	6	613	CLA	C11-C10-C8-C7
25	B	602	CLA	C11-C12-C13-C15
25	B	602	CLA	C12-C13-C15-C16
25	B	603	CLA	C6-C7-C8-C10
25	C	502	CLA	C11-C10-C8-C7
25	C	504	CLA	C11-C10-C8-C7
25	C	507	CLA	C12-C13-C15-C16
25	C	510	CLA	C6-C7-C8-C10
25	C	512	CLA	C12-C13-C15-C16
25	N	613	CLA	C12-C13-C15-C16
25	R	602	CLA	C6-C7-C8-C10
25	0	602	CLA	C6-C7-C8-C10
25	0	604	CLA	C11-C10-C8-C7
25	0	612	CLA	C12-C13-C15-C16
25	0	613	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	7	603	CLA	C12-C13-C15-C16
25	7	613	CLA	C12-C13-C15-C16
25	8	602	CLA	C11-C12-C13-C15
25	p	610	CLA	C11-C10-C8-C7
25	p	613	CLA	C12-C13-C15-C16
25	q	602	CLA	C6-C7-C8-C10
25	q	613	CLA	C6-C7-C8-C10
25	q	613	CLA	C12-C13-C15-C16
25	b	602	CLA	C11-C12-C13-C15
25	b	602	CLA	C12-C13-C15-C16
25	b	603	CLA	C6-C7-C8-C10
25	c	502	CLA	C11-C10-C8-C7
25	c	510	CLA	C6-C7-C8-C10
25	c	511	CLA	C11-C12-C13-C15
25	c	513	CLA	C11-C10-C8-C7
25	c	513	CLA	C11-C12-C13-C15
25	d	402	CLA	C11-C10-C8-C7
25	n	613	CLA	C12-C13-C15-C16
25	r	602	CLA	C6-C7-C8-C10
29	c	2630	LHG	C32-C33-C34-C35
24	1	607	CHL	C11-C12-C13-C14
24	5	605	CHL	C11-C12-C13-C14
24	Y	607	CHL	C11-C12-C13-C14
24	0	607	CHL	C11-C10-C8-C9
24	0	609	CHL	C11-C12-C13-C14
24	8	609	CHL	C11-C10-C8-C9
24	n	605	CHL	C14-C13-C15-C16
24	y	607	CHL	C11-C12-C13-C14
25	1	602	CLA	C11-C12-C13-C14
25	1	603	CLA	C11-C12-C13-C14
25	1	612	CLA	C11-C10-C8-C9
25	1	613	CLA	C14-C13-C15-C16
25	2	603	CLA	C14-C13-C15-C16
25	3	602	CLA	C6-C7-C8-C9
25	3	602	CLA	C11-C12-C13-C14
25	4	603	CLA	C14-C13-C15-C16
25	5	602	CLA	C6-C7-C8-C9
25	5	604	CLA	C6-C7-C8-C9
25	5	613	CLA	C6-C7-C8-C9
25	6	603	CLA	C14-C13-C15-C16
25	6	613	CLA	C6-C7-C8-C9
25	B	602	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	B	603	CLA	C6-C7-C8-C9
25	B	604	CLA	C11-C12-C13-C14
25	B	607	CLA	C11-C10-C8-C9
25	B	615	CLA	C6-C7-C8-C9
25	B	617	CLA	C6-C7-C8-C9
25	C	502	CLA	C11-C10-C8-C9
25	C	507	CLA	C14-C13-C15-C16
25	C	512	CLA	C11-C10-C8-C9
25	N	613	CLA	C11-C10-C8-C9
25	N	613	CLA	C14-C13-C15-C16
25	R	602	CLA	C6-C7-C8-C9
25	Y	602	CLA	C6-C7-C8-C9
25	Y	602	CLA	C11-C12-C13-C14
25	Y	603	CLA	C14-C13-C15-C16
25	Y	612	CLA	C11-C10-C8-C9
25	0	602	CLA	C6-C7-C8-C9
25	0	611	CLA	C14-C13-C15-C16
25	7	602	CLA	C11-C12-C13-C14
25	7	610	CLA	C6-C7-C8-C9
25	7	611	CLA	C11-C12-C13-C14
25	7	612	CLA	C14-C13-C15-C16
25	7	613	CLA	C14-C13-C15-C16
25	8	602	CLA	C6-C7-C8-C9
25	8	602	CLA	C11-C12-C13-C14
25	9	603	CLA	C14-C13-C15-C16
25	p	604	CLA	C6-C7-C8-C9
25	p	613	CLA	C6-C7-C8-C9
25	q	602	CLA	C6-C7-C8-C9
25	q	613	CLA	C6-C7-C8-C9
25	q	613	CLA	C11-C10-C8-C9
25	b	602	CLA	C11-C12-C13-C14
25	b	603	CLA	C6-C7-C8-C9
25	b	604	CLA	C11-C12-C13-C14
25	b	607	CLA	C11-C10-C8-C9
25	b	615	CLA	C6-C7-C8-C9
25	b	617	CLA	C6-C7-C8-C9
25	c	502	CLA	C11-C10-C8-C9
25	c	507	CLA	C14-C13-C15-C16
25	c	512	CLA	C11-C10-C8-C9
25	c	512	CLA	C14-C13-C15-C16
25	n	613	CLA	C11-C10-C8-C9
25	n	613	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	y	602	CLA	C6-C7-C8-C9
25	y	602	CLA	C11-C12-C13-C14
25	y	610	CLA	C11-C12-C13-C14
25	y	612	CLA	C11-C10-C8-C9
25	r	602	CLA	C6-C7-C8-C9
24	7	606	CHL	CBA-CGA-O2A-C1
24	g	601	CHL	CBA-CGA-O2A-C1
25	D	403	CLA	CBA-CGA-O2A-C1
25	7	611	CLA	C15-C16-C17-C18
25	7	613	CLA	C5-C6-C7-C8
25	q	610	CLA	C15-C16-C17-C18
25	b	608	CLA	C15-C16-C17-C18
25	7	602	CLA	C2A-CAA-CBA-CGA
25	y	610	CLA	C2A-CAA-CBA-CGA
29	S	2630	LHG	C11-C10-C9-C8
24	5	601	CHL	O1A-CGA-O2A-C1
26	3	1620	LUT	C31-C32-C33-C40
34	D	404	BCR	C37-C22-C23-C24
34	d	404	BCR	C37-C22-C23-C24
24	5	605	CHL	C16-C17-C18-C20
25	B	616	CLA	C16-C17-C18-C20
25	b	616	CLA	C16-C17-C18-C20
26	4	1621	LUT	C11-C12-C13-C14
27	1	1622	XAT	C31-C32-C33-C34
34	D	404	BCR	C21-C22-C23-C24
34	b	620	BCR	C7-C8-C9-C10
34	d	404	BCR	C21-C22-C23-C24
37	C	518	DGD	O6D-C5D-C6D-O5D
37	c	518	DGD	O6D-C5D-C6D-O5D
24	p	607	CHL	C13-C15-C16-C17
25	4	603	CLA	C13-C15-C16-C17
25	B	608	CLA	C15-C16-C17-C18
29	Y	2630	LHG	C27-C28-C29-C30
29	g	2630	LHG	C17-C18-C19-C20
29	s	2630	LHG	C11-C10-C9-C8
36	C	521	LMG	C29-C30-C31-C32
25	4	613	CLA	CBA-CGA-O2A-C1
24	6	606	CHL	C13-C15-C16-C17
25	6	604	CLA	C15-C16-C17-C18
25	b	610	CLA	C13-C15-C16-C17
29	7	2630	LHG	C24-C25-C26-C27
35	B	623	SQD	C24-C25-C26-C27

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Mol	Chain	Res	Type	Atoms
35	b	623	SQD	C16-C17-C18-C19
37	C	520	DGD	C7B-C8B-C9B-CAB
25	0	604	CLA	C16-C17-C18-C19
25	B	610	CLA	C13-C15-C16-C17
25	9	613	CLA	C5-C6-C7-C8
29	1	2630	LHG	O6-C4-C5-C6
29	7	2630	LHG	O6-C4-C5-C6
29	p	2630	LHG	O6-C4-C5-C6
29	y	2630	LHG	C12-C13-C14-C15
29	1	2630	LHG	C23-C24-C25-C26
29	7	2630	LHG	C23-C24-C25-C26
25	N	604	CLA	CBA-CGA-O2A-C1
24	r	608	CHL	CBD-CGD-O2D-CED
24	2	609	CHL	C10-C11-C12-C13
24	0	609	CHL	C13-C15-C16-C17
24	r	608	CHL	C10-C11-C12-C13
24	y	609	CHL	O1D-CGD-O2D-CED
24	q	601	CHL	C4-C3-C5-C6
25	B	612	CLA	C4-C3-C5-C6
25	C	512	CLA	C4-C3-C5-C6
25	b	612	CLA	C4-C3-C5-C6
25	c	505	CLA	C4-C3-C5-C6
25	1	613	CLA	C2-C3-C5-C6
25	7	603	CLA	C2-C3-C5-C6
25	p	603	CLA	C2-C3-C5-C6
29	Y	2630	LHG	C23-C24-C25-C26
25	B	612	CLA	C5-C6-C7-C8
25	b	612	CLA	C5-C6-C7-C8
29	8	2630	LHG	O2-C2-C3-O3
25	7	603	CLA	O1A-CGA-O2A-C1
37	c	520	DGD	C7B-C8B-C9B-CAB
25	C	502	CLA	C3-C5-C6-C7
25	D	402	CLA	C3-C5-C6-C7
25	B	602	CLA	C16-C17-C18-C20
25	B	617	CLA	C16-C17-C18-C19
25	b	602	CLA	C16-C17-C18-C20
25	b	617	CLA	C16-C17-C18-C19
25	S	609	CLA	O1D-CGD-O2D-CED
25	D	402	CLA	C2A-CAA-CBA-CGA
24	G	601	CHL	CBA-CGA-O2A-C1
25	c	511	CLA	CBA-CGA-O2A-C1
24	5	607	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
24	R	608	CHL	CBD-CGD-O2D-CED
25	s	609	CLA	O1D-CGD-O2D-CED
24	1	608	CHL	C3A-C2A-CAA-CBA
24	0	606	CHL	C3A-C2A-CAA-CBA
24	7	608	CHL	C3A-C2A-CAA-CBA
25	6	613	CLA	C3A-C2A-CAA-CBA
25	B	608	CLA	C3A-C2A-CAA-CBA
25	b	608	CLA	C3A-C2A-CAA-CBA
36	A	413	LMG	C35-C36-C37-C38
36	a	413	LMG	C35-C36-C37-C38
26	6	1621	LUT	C29-C30-C31-C32
26	0	1621	LUT	C29-C30-C31-C32
37	C	518	DGD	CDB-CEB-CFB-CGB
29	S	2630	LHG	C23-C24-C25-C26
24	3	605	CHL	C3-C5-C6-C7
25	d	402	CLA	C3-C5-C6-C7
25	1	604	CLA	C5-C6-C7-C8
25	0	613	CLA	CBA-CGA-O2A-C1
25	d	403	CLA	CBA-CGA-O2A-C1
25	n	604	CLA	CBA-CGA-O2A-C1
24	3	609	CHL	C4C-C3C-CAC-CBC
25	r	604	CLA	O2A-C1-C2-C3
24	9	609	CHL	C10-C11-C12-C13
25	4	610	CLA	C10-C11-C12-C13
25	B	614	CLA	C8-C10-C11-C12
25	8	610	CLA	C15-C16-C17-C18
25	b	614	CLA	C8-C10-C11-C12
25	c	505	CLA	C10-C11-C12-C13
25	c	506	CLA	C5-C6-C7-C8
25	c	507	CLA	C8-C10-C11-C12
29	Y	2630	LHG	C4-C5-C6-O8
35	B	621	SQD	O6-C44-C45-C46
35	b	621	SQD	O6-C44-C45-C46
36	A	413	LMG	C7-C8-C9-O8
36	a	413	LMG	C7-C8-C9-O8
37	C	520	DGD	O1G-C1G-C2G-C3G
37	c	520	DGD	O1G-C1G-C2G-C3G
35	a	412	SQD	O49-C7-O47-C45
29	s	2630	LHG	C23-C24-C25-C26
29	r	2630	LHG	C23-C24-C25-C26
36	S	2631	LMG	C28-C29-C30-C31
37	c	519	DGD	CAA-CBA-CCA-CDA

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Mol	Chain	Res	Type	Atoms
24	y	606	CHL	C15-C16-C17-C18
35	b	621	SQD	C11-C12-C13-C14
25	1	612	CLA	C3-C5-C6-C7
35	B	621	SQD	C11-C12-C13-C14
37	c	518	DGD	CDB-CEB-CFB-CGB
25	C	505	CLA	C10-C11-C12-C13
25	b	605	CLA	C5-C6-C7-C8
25	C	505	CLA	C4-C3-C5-C6
24	1	601	CHL	C16-C17-C18-C20
25	1	612	CLA	C2-C3-C5-C6
29	9	2630	LHG	C10-C11-C12-C13
25	1	603	CLA	CBD-CGD-O2D-CED
29	Y	2630	LHG	C11-C10-C9-C8
29	r	2630	LHG	C11-C10-C9-C8
24	Y	606	CHL	C15-C16-C17-C18
24	0	609	CHL	C15-C16-C17-C18
24	3	601	CHL	C3C-C2C-CMC-OMC
24	3	606	CHL	C3C-C2C-CMC-OMC
24	4	601	CHL	C3C-C2C-CMC-OMC
24	4	605	CHL	C3C-C2C-CMC-OMC
24	5	606	CHL	C3C-C2C-CMC-OMC
24	N	606	CHL	C3C-C2C-CMC-OMC
24	N	607	CHL	C3C-C2C-CMC-OMC
24	R	608	CHL	C3C-C2C-CMC-OMC
24	Y	606	CHL	C3C-C2C-CMC-OMC
24	0	609	CHL	C3C-C2C-CMC-OMC
24	7	606	CHL	C3C-C2C-CMC-OMC
24	7	609	CHL	C3C-C2C-CMC-OMC
24	8	607	CHL	C3C-C2C-CMC-OMC
24	q	601	CHL	C3C-C2C-CMC-OMC
24	n	606	CHL	C3C-C2C-CMC-OMC
24	n	607	CHL	C3C-C2C-CMC-OMC
24	y	606	CHL	C3C-C2C-CMC-OMC
24	r	608	CHL	C3C-C2C-CMC-OMC
29	D	409	LHG	C3-O3-P-O6
29	R	2630	LHG	C23-C24-C25-C26
24	1	606	CHL	O1A-CGA-O2A-C1
24	q	605	CHL	O1A-CGA-O2A-C1
24	g	601	CHL	O1A-CGA-O2A-C1
25	2	613	CLA	O1A-CGA-O2A-C1
24	p	601	CHL	O1D-CGD-O2D-CED
25	B	613	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	a	407	CLA	O1D-CGD-O2D-CED
25	b	613	CLA	O1D-CGD-O2D-CED
25	4	603	CLA	C3-C5-C6-C7
24	0	605	CHL	C2A-CAA-CBA-CGA
25	2	602	CLA	C2A-CAA-CBA-CGA
25	p	614	CLA	C2A-CAA-CBA-CGA
25	r	612	CLA	C2A-CAA-CBA-CGA
24	n	609	CHL	C13-C15-C16-C17
25	B	605	CLA	C5-C6-C7-C8
29	1	2630	LHG	O6-C4-C5-O7
37	C	518	DGD	C4D-C5D-C6D-O5D
37	c	518	DGD	C4D-C5D-C6D-O5D
35	A	412	SQD	O49-C7-O47-C45
25	S	604	CLA	CBA-CGA-O2A-C1
39	D	405	PL9	C12-C13-C14-C15
24	8	609	CHL	O1A-CGA-O2A-C1
29	d	410	LHG	O10-C23-O8-C6
37	C	520	DGD	O6D-C5D-C6D-O5D
37	c	520	DGD	O6D-C5D-C6D-O5D
24	8	607	CHL	C16-C17-C18-C19
25	B	611	CLA	C16-C17-C18-C20
25	b	611	CLA	C16-C17-C18-C20
24	R	608	CHL	C10-C11-C12-C13
25	b	603	CLA	C13-C15-C16-C17
29	R	2630	LHG	C11-C10-C9-C8
24	8	609	CHL	C4C-C3C-CAC-CBC
35	b	623	SQD	C32-C33-C34-C35
25	1	612	CLA	O1A-CGA-O2A-C1
25	9	613	CLA	O1A-CGA-O2A-C1
29	5	2630	LHG	O10-C23-O8-C6
29	D	410	LHG	O10-C23-O8-C6
29	Y	2630	LHG	C14-C15-C16-C17
29	1	2630	LHG	O7-C5-C6-O8
29	7	2630	LHG	O7-C5-C6-O8
36	D	411	LMG	O1-C7-C8-O7
37	C	519	DGD	O2G-C2G-C3G-O3G
37	C	520	DGD	O1G-C1G-C2G-O2G
37	c	519	DGD	O2G-C2G-C3G-O3G
37	c	520	DGD	O1G-C1G-C2G-O2G
25	s	604	CLA	CBA-CGA-O2A-C1
25	7	611	CLA	O1D-CGD-O2D-CED
24	p	609	CHL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
29	r	2630	LHG	C12-C13-C14-C15
29	4	2630	LHG	C23-C24-C25-C26
25	1	610	CLA	C16-C17-C18-C20
25	N	613	CLA	C16-C17-C18-C20
25	b	602	CLA	C16-C17-C18-C19
25	c	513	CLA	C16-C17-C18-C19
25	n	613	CLA	C16-C17-C18-C20
29	R	2630	LHG	C12-C13-C14-C15
29	p	2630	LHG	C16-C17-C18-C19
35	b	623	SQD	C24-C25-C26-C27
25	2	613	CLA	C5-C6-C7-C8
25	B	606	CLA	C5-C6-C7-C8
25	b	606	CLA	C5-C6-C7-C8
25	d	402	CLA	C10-C11-C12-C13
24	3	607	CHL	C2-C1-O2A-CGA
24	4	607	CHL	C2-C1-O2A-CGA
24	8	607	CHL	C2-C1-O2A-CGA
25	C	511	CLA	C2-C1-O2A-CGA
25	R	612	CLA	C2-C1-O2A-CGA
25	B	612	CLA	C2-C3-C5-C6
25	b	612	CLA	C2-C3-C5-C6
25	c	505	CLA	C2-C3-C5-C6
29	s	2630	LHG	C28-C29-C30-C31
25	C	506	CLA	C5-C6-C7-C8
25	8	604	CLA	C13-C15-C16-C17
24	2	609	CHL	C11-C12-C13-C14
24	5	605	CHL	C14-C13-C15-C16
24	6	606	CHL	C11-C10-C8-C9
24	6	609	CHL	C11-C12-C13-C14
24	N	605	CHL	C14-C13-C15-C16
24	N	607	CHL	C11-C12-C13-C14
24	R	606	CHL	C11-C12-C13-C14
24	7	607	CHL	C11-C12-C13-C14
24	9	609	CHL	C11-C12-C13-C14
24	9	609	CHL	C14-C13-C15-C16
24	p	605	CHL	C6-C7-C8-C9
24	p	607	CHL	C11-C10-C8-C9
24	r	606	CHL	C11-C12-C13-C14
25	1	611	CLA	C11-C12-C13-C14
25	5	613	CLA	C14-C13-C15-C16
25	6	602	CLA	C6-C7-C8-C9
25	6	602	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	6	613	CLA	C11-C10-C8-C9
25	6	613	CLA	C14-C13-C15-C16
25	B	613	CLA	C14-C13-C15-C16
25	C	508	CLA	C11-C10-C8-C9
25	C	512	CLA	C14-C13-C15-C16
25	D	402	CLA	C11-C12-C13-C14
25	G	613	CLA	C11-C10-C8-C9
25	N	602	CLA	C11-C12-C13-C14
25	R	610	CLA	C11-C12-C13-C14
25	R	613	CLA	C6-C7-C8-C9
25	0	602	CLA	C11-C12-C13-C14
25	7	603	CLA	C11-C12-C13-C14
25	p	613	CLA	C14-C13-C15-C16
25	q	603	CLA	C11-C12-C13-C14
25	b	613	CLA	C14-C13-C15-C16
25	c	508	CLA	C11-C10-C8-C9
25	c	513	CLA	C11-C12-C13-C14
25	g	613	CLA	C11-C10-C8-C9
25	y	603	CLA	C14-C13-C15-C16
25	r	610	CLA	C11-C12-C13-C14
25	1	613	CLA	C5-C6-C7-C8
25	6	612	CLA	C8-C10-C11-C12
25	7	610	CLA	C15-C16-C17-C18
25	y	603	CLA	C5-C6-C7-C8
33	A	409	PHO	C1A-C2A-CAA-CBA
25	D	403	CLA	O1A-CGA-O2A-C1
29	s	2630	LHG	C11-C12-C13-C14
36	h	102	LMG	C16-C17-C18-C19
24	p	608	CHL	C2A-CAA-CBA-CGA
25	R	612	CLA	C2A-CAA-CBA-CGA
25	Y	613	CLA	C2A-CAA-CBA-CGA
25	0	602	CLA	C2A-CAA-CBA-CGA
25	8	613	CLA	C2A-CAA-CBA-CGA
25	9	602	CLA	C2A-CAA-CBA-CGA
25	q	602	CLA	C2A-CAA-CBA-CGA
25	n	613	CLA	C2A-CAA-CBA-CGA
25	y	603	CLA	C2A-CAA-CBA-CGA
25	y	613	CLA	C2A-CAA-CBA-CGA
25	B	602	CLA	C16-C17-C18-C19
25	B	617	CLA	C16-C17-C18-C20
35	a	412	SQD	C23-C24-C25-C26
25	4	604	CLA	O2A-C1-C2-C3

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Mol	Chain	Res	Type	Atoms
25	B	608	CLA	C3-C5-C6-C7
26	1	1620	LUT	C5-C6-C7-C8
26	2	1620	LUT	C1-C6-C7-C8
26	2	1620	LUT	C5-C6-C7-C8
26	4	1620	LUT	C5-C6-C7-C8
26	5	1621	LUT	C5-C6-C7-C8
26	S	1620	LUT	C5-C6-C7-C8
26	Y	1621	LUT	C5-C6-C7-C8
26	0	1621	LUT	C5-C6-C7-C8
26	7	1620	LUT	C1-C6-C7-C8
26	7	1620	LUT	C5-C6-C7-C8
26	7	1621	LUT	C1-C6-C7-C8
26	7	1621	LUT	C5-C6-C7-C8
26	9	1620	LUT	C5-C6-C7-C8
26	s	1620	LUT	C5-C6-C7-C8
26	y	1621	LUT	C5-C6-C7-C8
34	B	620	BCR	C23-C24-C25-C26
34	B	620	BCR	C23-C24-C25-C30
34	C	515	BCR	C1-C6-C7-C8
34	b	620	BCR	C23-C24-C25-C26
34	b	620	BCR	C23-C24-C25-C30
34	c	515	BCR	C1-C6-C7-C8
34	c	515	BCR	C5-C6-C7-C8
27	n	1622	XAT	C31-C32-C33-C40
35	B	623	SQD	C32-C33-C34-C35
25	1	611	CLA	O1D-CGD-O2D-CED
26	4	1620	LUT	C27-C28-C29-C30
26	Y	1621	LUT	C7-C8-C9-C10
26	8	1620	LUT	C27-C28-C29-C30
26	p	1620	LUT	C27-C28-C29-C30
26	y	1621	LUT	C7-C8-C9-C10
27	n	1622	XAT	C31-C32-C33-C34
28	2	1623	NEX	C31-C32-C33-C34
34	B	620	BCR	C7-C8-C9-C10
34	C	515	BCR	C7-C8-C9-C10
34	D	404	BCR	C7-C8-C9-C10
34	d	404	BCR	C7-C8-C9-C10
24	1	606	CHL	C15-C16-C17-C18
24	3	601	CHL	C10-C11-C12-C13
24	7	609	CHL	C13-C15-C16-C17
29	9	2630	LHG	C23-C24-C25-C26
37	C	523	DGD	C3B-C4B-C5B-C6B

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Mol	Chain	Res	Type	Atoms
37	c	523	DGD	C3B-C4B-C5B-C6B
29	S	2630	LHG	C11-C12-C13-C14
35	A	412	SQD	C31-C32-C33-C34
36	s	2631	LMG	C42-C43-C44-C45
25	B	616	CLA	C16-C17-C18-C19
25	7	610	CLA	C16-C17-C18-C20
25	b	616	CLA	C16-C17-C18-C19
35	A	412	SQD	C23-C24-C25-C26
35	b	623	SQD	C25-C26-C27-C28
25	1	611	CLA	C15-C16-C17-C18
25	B	616	CLA	C5-C6-C7-C8
25	0	612	CLA	C8-C10-C11-C12
24	p	607	CHL	CAA-CBA-CGA-O2A
35	B	623	SQD	C25-C26-C27-C28
24	1	606	CHL	C11-C12-C13-C15
24	2	601	CHL	C11-C12-C13-C15
24	2	609	CHL	C11-C12-C13-C15
24	3	601	CHL	C6-C7-C8-C10
24	3	601	CHL	C11-C10-C8-C7
24	3	605	CHL	C12-C13-C15-C16
24	4	601	CHL	C11-C10-C8-C7
24	4	609	CHL	C11-C10-C8-C7
24	5	601	CHL	C11-C10-C8-C7
24	5	607	CHL	C11-C12-C13-C15
24	5	609	CHL	C12-C13-C15-C16
24	6	606	CHL	C11-C12-C13-C15
24	6	607	CHL	C6-C7-C8-C10
24	6	609	CHL	C11-C12-C13-C15
24	G	609	CHL	C11-C12-C13-C15
24	N	605	CHL	C11-C12-C13-C15
24	N	609	CHL	C11-C12-C13-C15
24	R	606	CHL	C11-C12-C13-C15
24	Y	601	CHL	C11-C12-C13-C15
24	Y	606	CHL	C11-C12-C13-C15
24	Y	607	CHL	C11-C12-C13-C15
24	0	609	CHL	C11-C12-C13-C15
24	7	606	CHL	C11-C12-C13-C15
24	7	607	CHL	C11-C12-C13-C15
24	7	609	CHL	C12-C13-C15-C16
24	8	605	CHL	C11-C12-C13-C15
24	9	601	CHL	C11-C10-C8-C7
24	9	609	CHL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
24	9	609	CHL	C12-C13-C15-C16
24	p	605	CHL	C12-C13-C15-C16
24	q	601	CHL	C11-C10-C8-C7
24	q	609	CHL	C11-C12-C13-C15
24	g	609	CHL	C11-C12-C13-C15
24	n	605	CHL	C11-C12-C13-C15
24	n	609	CHL	C11-C10-C8-C7
24	y	601	CHL	C11-C12-C13-C15
24	y	606	CHL	C11-C12-C13-C15
24	r	606	CHL	C11-C12-C13-C15
25	1	602	CLA	C6-C7-C8-C10
25	1	602	CLA	C11-C12-C13-C15
25	1	610	CLA	C6-C7-C8-C10
25	2	603	CLA	C12-C13-C15-C16
25	3	602	CLA	C6-C7-C8-C10
25	3	602	CLA	C11-C12-C13-C15
25	4	602	CLA	C6-C7-C8-C10
25	4	610	CLA	C12-C13-C15-C16
25	4	613	CLA	C11-C10-C8-C7
25	4	613	CLA	C12-C13-C15-C16
25	5	602	CLA	C6-C7-C8-C10
25	5	604	CLA	C6-C7-C8-C10
25	5	613	CLA	C12-C13-C15-C16
25	6	602	CLA	C11-C12-C13-C15
25	6	603	CLA	C12-C13-C15-C16
25	6	611	CLA	C12-C13-C15-C16
25	B	604	CLA	C11-C12-C13-C15
25	B	606	CLA	C12-C13-C15-C16
25	B	607	CLA	C11-C10-C8-C7
25	B	607	CLA	C12-C13-C15-C16
25	B	615	CLA	C6-C7-C8-C10
25	B	617	CLA	C6-C7-C8-C10
25	C	505	CLA	C2-C3-C5-C6
25	C	512	CLA	C11-C10-C8-C7
25	D	402	CLA	C11-C12-C13-C15
25	D	403	CLA	C11-C12-C13-C15
25	G	603	CLA	C11-C10-C8-C7
25	G	610	CLA	C12-C13-C15-C16
25	G	613	CLA	C11-C10-C8-C7
25	N	602	CLA	C11-C12-C13-C15
25	N	613	CLA	C11-C10-C8-C7
25	Y	602	CLA	C6-C7-C8-C10

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Mol	Chain	Res	Type	Atoms
25	Y	602	CLA	C11-C12-C13-C15
25	Y	603	CLA	C12-C13-C15-C16
25	Y	604	CLA	C6-C7-C8-C10
25	Y	612	CLA	C11-C10-C8-C7
25	0	602	CLA	C11-C12-C13-C15
25	0	611	CLA	C12-C13-C15-C16
25	7	602	CLA	C6-C7-C8-C10
25	7	602	CLA	C11-C12-C13-C15
25	7	610	CLA	C6-C7-C8-C10
25	7	611	CLA	C11-C12-C13-C15
25	8	602	CLA	C6-C7-C8-C10
25	9	603	CLA	C12-C13-C15-C16
25	p	603	CLA	C12-C13-C15-C16
25	p	604	CLA	C6-C7-C8-C10
25	p	613	CLA	C6-C7-C8-C10
25	p	613	CLA	C11-C10-C8-C7
25	q	613	CLA	C11-C10-C8-C7
25	b	604	CLA	C11-C12-C13-C15
25	b	606	CLA	C12-C13-C15-C16
25	b	607	CLA	C11-C10-C8-C7
25	b	607	CLA	C12-C13-C15-C16
25	b	615	CLA	C6-C7-C8-C10
25	b	617	CLA	C6-C7-C8-C10
25	c	504	CLA	C11-C10-C8-C7
25	c	507	CLA	C12-C13-C15-C16
25	c	512	CLA	C11-C10-C8-C7
25	c	512	CLA	C12-C13-C15-C16
25	d	402	CLA	C11-C12-C13-C15
25	g	603	CLA	C11-C10-C8-C7
25	g	610	CLA	C12-C13-C15-C16
25	g	613	CLA	C11-C10-C8-C7
25	n	613	CLA	C11-C10-C8-C7
25	y	602	CLA	C6-C7-C8-C10
25	y	602	CLA	C11-C12-C13-C15
25	y	603	CLA	C12-C13-C15-C16
25	y	604	CLA	C6-C7-C8-C10
25	y	612	CLA	C11-C10-C8-C7
24	7	606	CHL	O1A-CGA-O2A-C1
35	a	412	SQD	C31-C32-C33-C34
36	S	2631	LMG	C42-C43-C44-C45
24	N	609	CHL	C13-C15-C16-C17
26	G	1621	LUT	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
26	g	1621	LUT	C29-C30-C31-C32
34	H	101	BCR	C9-C10-C11-C12
34	h	101	BCR	C9-C10-C11-C12
25	b	617	CLA	C16-C17-C18-C20
36	H	102	LMG	C16-C17-C18-C19
29	S	2630	LHG	C28-C29-C30-C31
25	l	610	CLA	C8-C10-C11-C12
25	b	616	CLA	C5-C6-C7-C8
25	4	613	CLA	O1A-CGA-O2A-C1
24	6	605	CHL	C2A-CAA-CBA-CGA
25	3	613	CLA	C2A-CAA-CBA-CGA
25	d	402	CLA	C2A-CAA-CBA-CGA
25	n	604	CLA	C2A-CAA-CBA-CGA
24	p	606	CHL	CBD-CGD-O2D-CED
25	6	613	CLA	C15-C16-C17-C18
25	g	603	CLA	C15-C16-C17-C18
24	2	609	CHL	C3-C5-C6-C7
24	y	609	CHL	C3-C5-C6-C7
25	R	616	CLA	C3-C5-C6-C7
25	r	616	CLA	C3-C5-C6-C7
37	C	523	DGD	CDB-CEB-CFB-CGB
37	c	523	DGD	CDB-CEB-CFB-CGB
24	Y	601	CHL	C16-C17-C18-C19
24	9	601	CHL	C8-C10-C11-C12
25	C	504	CLA	CBA-CGA-O2A-C1
25	q	604	CLA	CBA-CGA-O2A-C1
29	9	2630	LHG	C24-C23-O8-C6
29	D	408	LHG	C29-C30-C31-C32
29	d	408	LHG	C29-C30-C31-C32
29	4	2630	LHG	C10-C11-C12-C13
36	D	412	LMG	C15-C16-C17-C18
36	H	102	LMG	C17-C18-C19-C20
24	8	601	CHL	O1D-CGD-O2D-CED
24	3	607	CHL	C5-C6-C7-C8
25	B	603	CLA	C13-C15-C16-C17
25	G	603	CLA	C15-C16-C17-C18
25	Y	603	CLA	C5-C6-C7-C8
25	7	610	CLA	C8-C10-C11-C12
24	3	606	CHL	CBD-CGD-O2D-CED
29	4	2630	LHG	C11-C12-C13-C14
29	p	2630	LHG	C14-C15-C16-C17
29	c	2630	LHG	C14-C15-C16-C17

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Mol	Chain	Res	Type	Atoms
36	d	412	LMG	C15-C16-C17-C18
24	1	605	CHL	CAD-CBD-CGD-O2D
24	2	601	CHL	CAD-CBD-CGD-O2D
24	G	605	CHL	CAD-CBD-CGD-O2D
24	N	606	CHL	CAD-CBD-CGD-O2D
24	R	607	CHL	CAD-CBD-CGD-O2D
24	0	601	CHL	CAD-CBD-CGD-O2D
24	7	605	CHL	CAD-CBD-CGD-O2D
24	7	608	CHL	CAD-CBD-CGD-O2D
24	9	607	CHL	CAD-CBD-CGD-O2D
24	q	608	CHL	CAD-CBD-CGD-O2D
24	g	605	CHL	CAD-CBD-CGD-O2D
24	n	606	CHL	CAD-CBD-CGD-O2D
24	r	607	CHL	CAD-CBD-CGD-O2D
25	1	603	CLA	CAD-CBD-CGD-O2D
25	1	604	CLA	CAD-CBD-CGD-O2D
25	2	602	CLA	CAD-CBD-CGD-O2D
25	3	602	CLA	CAD-CBD-CGD-O2D
25	3	612	CLA	CAD-CBD-CGD-O2D
25	3	614	CLA	CAD-CBD-CGD-O2D
25	4	604	CLA	CAD-CBD-CGD-O2D
25	4	613	CLA	CAD-CBD-CGD-O2D
25	5	610	CLA	CAD-CBD-CGD-O2D
25	5	614	CLA	CAD-CBD-CGD-O2D
25	A	410	CLA	CAD-CBD-CGD-O2D
25	B	607	CLA	CAD-CBD-CGD-O2D
25	B	610	CLA	CAD-CBD-CGD-O2D
25	C	501	CLA	CAD-CBD-CGD-O2D
25	C	506	CLA	CAD-CBD-CGD-O2D
25	G	610	CLA	CAD-CBD-CGD-O2D
25	G	614	CLA	CAD-CBD-CGD-O2D
25	N	610	CLA	CAD-CBD-CGD-O2D
25	N	614	CLA	CAD-CBD-CGD-O2D
25	R	603	CLA	CAD-CBD-CGD-O2D
25	R	609	CLA	CAD-CBD-CGD-O2D
25	R	610	CLA	CAD-CBD-CGD-O2D
25	R	611	CLA	CAD-CBD-CGD-O2D
25	S	614	CLA	CAD-CBD-CGD-O2D
25	Y	602	CLA	CAD-CBD-CGD-O2D
25	0	603	CLA	CAD-CBD-CGD-O2D
25	0	614	CLA	CAD-CBD-CGD-O2D
25	8	602	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	8	612	CLA	CAD-CBD-CGD-O2D
25	8	614	CLA	CAD-CBD-CGD-O2D
25	p	602	CLA	CAD-CBD-CGD-O2D
25	p	610	CLA	CAD-CBD-CGD-O2D
25	q	610	CLA	CAD-CBD-CGD-O2D
25	q	614	CLA	CAD-CBD-CGD-O2D
25	a	410	CLA	CAD-CBD-CGD-O2D
25	b	607	CLA	CAD-CBD-CGD-O2D
25	b	608	CLA	CAD-CBD-CGD-O2D
25	b	610	CLA	CAD-CBD-CGD-O2D
25	c	501	CLA	CAD-CBD-CGD-O2D
25	g	610	CLA	CAD-CBD-CGD-O2D
25	g	614	CLA	CAD-CBD-CGD-O2D
25	n	610	CLA	CAD-CBD-CGD-O2D
25	n	613	CLA	CAD-CBD-CGD-O2D
25	n	614	CLA	CAD-CBD-CGD-O2D
25	s	614	CLA	CAD-CBD-CGD-O2D
25	y	602	CLA	CAD-CBD-CGD-O2D
25	r	603	CLA	CAD-CBD-CGD-O2D
25	r	609	CLA	CAD-CBD-CGD-O2D
25	r	610	CLA	CAD-CBD-CGD-O2D
25	r	611	CLA	CAD-CBD-CGD-O2D
33	A	408	PHO	CAD-CBD-CGD-O2D
33	a	408	PHO	CAD-CBD-CGD-O2D
24	5	607	CHL	C5-C6-C7-C8
25	G	610	CLA	C13-C15-C16-C17
25	c	504	CLA	CBA-CGA-O2A-C1
24	N	605	CHL	C4-C3-C5-C6
24	n	605	CHL	C4-C3-C5-C6
25	Y	603	CLA	C4-C3-C5-C6
25	b	608	CLA	C4-C3-C5-C6
25	C	512	CLA	C16-C17-C18-C20
25	c	506	CLA	C2-C3-C5-C6
36	S	2631	LMG	C18-C19-C20-C21
29	R	2630	LHG	C4-C5-C6-O8
29	q	2630	LHG	C4-C5-C6-O8
29	r	2630	LHG	C4-C5-C6-O8
36	D	411	LMG	O1-C7-C8-C9
36	d	411	LMG	O1-C7-C8-C9
37	C	519	DGD	O1G-C1G-C2G-C3G
37	c	519	DGD	O1G-C1G-C2G-C3G
37	c	519	DGD	C1G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
25	G	602	CLA	CBD-CGD-O2D-CED
25	S	604	CLA	O1A-CGA-O2A-C1
25	c	511	CLA	O1A-CGA-O2A-C1
29	4	2630	LHG	C9-C10-C11-C12
29	C	2630	LHG	O6-C4-C5-O7
29	L	101	LHG	O6-C4-C5-O7
29	7	2630	LHG	O6-C4-C5-O7
29	p	2630	LHG	O6-C4-C5-O7
24	1	606	CHL	C5-C6-C7-C8
25	C	506	CLA	C13-C15-C16-C17
25	g	610	CLA	C13-C15-C16-C17
25	g	610	CLA	C15-C16-C17-C18
25	G	614	CLA	O2A-C1-C2-C3
25	N	611	CLA	O2A-C1-C2-C3
25	S	602	CLA	O2A-C1-C2-C3
25	n	611	CLA	O2A-C1-C2-C3
25	s	602	CLA	O2A-C1-C2-C3
25	G	610	CLA	O1D-CGD-O2D-CED
36	h	102	LMG	C17-C18-C19-C20
24	0	606	CHL	C2A-CAA-CBA-CGA
25	1	602	CLA	C2A-CAA-CBA-CGA
25	C	502	CLA	C2A-CAA-CBA-CGA
25	N	604	CLA	C2A-CAA-CBA-CGA
25	9	602	CLA	C15-C16-C17-C18
25	c	506	CLA	C13-C15-C16-C17
36	d	411	LMG	C14-C15-C16-C17
24	Y	601	CHL	C16-C17-C18-C20
24	7	601	CHL	C16-C17-C18-C20
24	8	607	CHL	C16-C17-C18-C20
25	c	512	CLA	C16-C17-C18-C20
25	g	610	CLA	O1D-CGD-O2D-CED
24	R	608	CHL	CHA-CBD-CGD-O1D
24	R	608	CHL	CHA-CBD-CGD-O2D
24	S	606	CHL	CHA-CBD-CGD-O1D
24	S	606	CHL	CHA-CBD-CGD-O2D
24	Y	607	CHL	CHA-CBD-CGD-O2D
24	s	606	CHL	CHA-CBD-CGD-O1D
24	s	606	CHL	CHA-CBD-CGD-O2D
24	y	607	CHL	CHA-CBD-CGD-O2D
24	r	608	CHL	CHA-CBD-CGD-O1D
24	r	608	CHL	CHA-CBD-CGD-O2D
25	1	602	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	1	602	CLA	CHA-CBD-CGD-O2D
25	1	613	CLA	CHA-CBD-CGD-O1D
25	1	613	CLA	CHA-CBD-CGD-O2D
25	2	611	CLA	CHA-CBD-CGD-O2D
25	3	611	CLA	CHA-CBD-CGD-O2D
25	4	611	CLA	CHA-CBD-CGD-O1D
25	4	611	CLA	CHA-CBD-CGD-O2D
25	4	612	CLA	CHA-CBD-CGD-O1D
25	4	612	CLA	CHA-CBD-CGD-O2D
25	5	603	CLA	CHA-CBD-CGD-O1D
25	B	603	CLA	CHA-CBD-CGD-O1D
25	B	603	CLA	CHA-CBD-CGD-O2D
25	B	605	CLA	CHA-CBD-CGD-O1D
25	B	605	CLA	CHA-CBD-CGD-O2D
25	B	606	CLA	CHA-CBD-CGD-O1D
25	B	606	CLA	CHA-CBD-CGD-O2D
25	C	511	CLA	CHA-CBD-CGD-O1D
25	C	511	CLA	CHA-CBD-CGD-O2D
25	N	611	CLA	CHA-CBD-CGD-O1D
25	R	616	CLA	CHA-CBD-CGD-O1D
25	7	602	CLA	CHA-CBD-CGD-O1D
25	7	602	CLA	CHA-CBD-CGD-O2D
25	7	604	CLA	CHA-CBD-CGD-O2D
25	9	602	CLA	CHA-CBD-CGD-O1D
25	q	611	CLA	CHA-CBD-CGD-O1D
25	b	603	CLA	CHA-CBD-CGD-O1D
25	b	603	CLA	CHA-CBD-CGD-O2D
25	b	605	CLA	CHA-CBD-CGD-O2D
25	b	606	CLA	CHA-CBD-CGD-O1D
25	b	606	CLA	CHA-CBD-CGD-O2D
25	c	505	CLA	CHA-CBD-CGD-O1D
25	r	616	CLA	CHA-CBD-CGD-O1D
25	p	602	CLA	C3-C5-C6-C7
24	G	601	CHL	O1A-CGA-O2A-C1
25	d	403	CLA	O1A-CGA-O2A-C1
25	n	604	CLA	O1A-CGA-O2A-C1
29	l	101	LHG	C17-C18-C19-C20
36	D	411	LMG	C14-C15-C16-C17
29	q	2630	LHG	O7-C5-C6-O8
29	r	2630	LHG	O7-C5-C6-O8
36	d	411	LMG	O1-C7-C8-O7
37	C	523	DGD	O2G-C2G-C3G-O3G

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Mol	Chain	Res	Type	Atoms
37	c	523	DGD	O2G-C2G-C3G-O3G
25	A	407	CLA	O1D-CGD-O2D-CED
24	7	601	CHL	C8-C10-C11-C12
24	7	606	CHL	C5-C6-C7-C8
25	G	610	CLA	C15-C16-C17-C18
29	L	101	LHG	C17-C18-C19-C20
24	N	609	CHL	C16-C17-C18-C20
24	9	609	CHL	O1D-CGD-O2D-CED
25	G	602	CLA	O1D-CGD-O2D-CED
29	d	408	LHG	C31-C32-C33-C34
25	b	610	CLA	C15-C16-C17-C18
25	C	506	CLA	C4-C3-C5-C6
25	c	506	CLA	C4-C3-C5-C6
25	y	603	CLA	C4-C3-C5-C6
29	D	408	LHG	C31-C32-C33-C34
29	y	2630	LHG	C18-C19-C20-C21
25	N	604	CLA	O1A-CGA-O2A-C1
25	s	604	CLA	O1A-CGA-O2A-C1
25	3	603	CLA	C2-C3-C5-C6
25	C	506	CLA	C2-C3-C5-C6
29	s	2630	LHG	O9-C7-O7-C5
25	B	610	CLA	C15-C16-C17-C18
25	Y	610	CLA	C15-C16-C17-C18
24	1	606	CHL	C11-C12-C13-C14
24	2	609	CHL	C14-C13-C15-C16
24	4	601	CHL	C14-C13-C15-C16
24	4	609	CHL	C11-C12-C13-C14
24	Y	606	CHL	C11-C12-C13-C14
24	7	606	CHL	C11-C12-C13-C14
24	9	601	CHL	C11-C10-C8-C9
24	q	601	CHL	C11-C10-C8-C9
24	y	606	CHL	C11-C12-C13-C14
25	4	602	CLA	C6-C7-C8-C9
25	4	603	CLA	C11-C10-C8-C9
25	4	610	CLA	C14-C13-C15-C16
25	4	613	CLA	C14-C13-C15-C16
25	5	613	CLA	C11-C10-C8-C9
25	6	611	CLA	C14-C13-C15-C16
25	B	610	CLA	C11-C12-C13-C14
25	C	505	CLA	C11-C12-C13-C14
25	G	610	CLA	C14-C13-C15-C16
25	0	613	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	b	610	CLA	C11-C12-C13-C14
25	c	505	CLA	C11-C12-C13-C14
25	d	402	CLA	C11-C12-C13-C14
25	g	610	CLA	C14-C13-C15-C16
24	p	606	CHL	O1D-CGD-O2D-CED
29	2	2630	LHG	C10-C11-C12-C13
29	s	2630	LHG	C29-C30-C31-C32
25	C	504	CLA	O1A-CGA-O2A-C1
25	q	604	CLA	O1A-CGA-O2A-C1
25	g	604	CLA	O1D-CGD-O2D-CED
25	Y	612	CLA	C8-C10-C11-C12
25	y	612	CLA	C8-C10-C11-C12
35	A	412	SQD	C4-C5-C6-S
35	a	412	SQD	C4-C5-C6-S
24	5	601	CHL	C3-C5-C6-C7
24	9	609	CHL	C3-C5-C6-C7
29	L	101	LHG	C34-C35-C36-C37
29	Y	2630	LHG	C26-C27-C28-C29
29	7	2630	LHG	C35-C36-C37-C38
25	5	613	CLA	C2A-CAA-CBA-CGA
26	1	1621	LUT	C11-C12-C13-C20
27	4	1622	XAT	C11-C12-C13-C20
28	3	1623	NEX	C31-C32-C33-C40
28	0	1623	NEX	C11-C12-C13-C20
29	1	2630	LHG	C35-C36-C37-C38
35	b	621	SQD	C10-C11-C12-C13
34	c	515	BCR	C7-C8-C9-C10
29	G	2630	LHG	C25-C26-C27-C28
24	7	609	CHL	C1A-C2A-CAA-CBA
24	9	609	CHL	C1A-C2A-CAA-CBA
24	q	601	CHL	C1A-C2A-CAA-CBA
24	n	608	CHL	C1A-C2A-CAA-CBA
25	2	610	CLA	C1A-C2A-CAA-CBA
25	4	612	CLA	C1A-C2A-CAA-CBA
25	5	602	CLA	C1A-C2A-CAA-CBA
25	5	610	CLA	C1A-C2A-CAA-CBA
25	B	607	CLA	C1A-C2A-CAA-CBA
25	B	610	CLA	C1A-C2A-CAA-CBA
25	C	505	CLA	C1A-C2A-CAA-CBA
25	G	602	CLA	C1A-C2A-CAA-CBA
25	N	602	CLA	C1A-C2A-CAA-CBA
25	N	610	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	R	610	CLA	C1A-C2A-CAA-CBA
25	q	612	CLA	C1A-C2A-CAA-CBA
25	b	607	CLA	C1A-C2A-CAA-CBA
25	g	602	CLA	C1A-C2A-CAA-CBA
25	n	602	CLA	C1A-C2A-CAA-CBA
25	n	610	CLA	C1A-C2A-CAA-CBA
25	r	610	CLA	C1A-C2A-CAA-CBA
29	y	2630	LHG	C23-C24-C25-C26
24	y	601	CHL	C16-C17-C18-C20
29	R	2630	LHG	O9-C7-O7-C5
25	C	512	CLA	C15-C16-C17-C18
25	C	513	CLA	C5-C6-C7-C8
29	s	2630	LHG	C8-C7-O7-C5
29	S	2630	LHG	C29-C30-C31-C32
24	N	609	CHL	CBA-CGA-O2A-C1
35	B	621	SQD	C10-C11-C12-C13
24	3	606	CHL	O1D-CGD-O2D-CED
29	3	2630	LHG	C3-O3-P-O6
29	8	2630	LHG	C3-O3-P-O6
29	q	2630	LHG	C3-O3-P-O6
29	d	408	LHG	C3-O3-P-O6
29	l	101	LHG	C34-C35-C36-C37
36	B	622	LMG	C36-C37-C38-C39
36	b	622	LMG	C36-C37-C38-C39
29	g	2630	LHG	C25-C26-C27-C28
24	7	609	CHL	C4-C3-C5-C6
25	B	608	CLA	C4-C3-C5-C6
24	3	607	CHL	C2-C3-C5-C6
25	2	602	CLA	C2-C3-C5-C6
25	y	603	CLA	C2-C3-C5-C6
25	0	613	CLA	O1A-CGA-O2A-C1
29	1	2630	LHG	C4-O6-P-O4
29	2	2630	LHG	C3-O3-P-O4
29	2	2630	LHG	C4-O6-P-O4
29	6	2630	LHG	C4-O6-P-O4
29	C	2630	LHG	C4-O6-P-O5
29	D	408	LHG	C3-O3-P-O4
29	D	409	LHG	C4-O6-P-O4
29	R	2630	LHG	C4-O6-P-O4
29	7	2630	LHG	C4-O6-P-O4
29	9	2630	LHG	C3-O3-P-O4
29	9	2630	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
29	c	2630	LHG	C4-O6-P-O5
29	d	408	LHG	C3-O3-P-O4
29	d	409	LHG	C4-O6-P-O4
29	l	101	LHG	C3-O3-P-O4
29	l	101	LHG	C4-O6-P-O4
29	r	2630	LHG	C4-O6-P-O4
25	3	611	CLA	O2A-C1-C2-C3
25	5	611	CLA	O2A-C1-C2-C3
25	A	407	CLA	O2A-C1-C2-C3
25	R	612	CLA	O2A-C1-C2-C3
25	S	613	CLA	O2A-C1-C2-C3
25	8	611	CLA	O2A-C1-C2-C3
25	a	407	CLA	O2A-C1-C2-C3
25	g	614	CLA	O2A-C1-C2-C3
25	s	613	CLA	O2A-C1-C2-C3
25	r	612	CLA	O2A-C1-C2-C3
24	7	606	CHL	C15-C16-C17-C18
24	g	609	CHL	C10-C11-C12-C13
25	c	512	CLA	C15-C16-C17-C18
25	y	610	CLA	C15-C16-C17-C18
29	Y	2630	LHG	C24-C23-O8-C6
33	a	409	PHO	CBA-CGA-O2A-C1
29	5	2630	LHG	O6-C4-C5-C6
29	L	101	LHG	O6-C4-C5-C6
29	l	101	LHG	O6-C4-C5-C6
36	H	102	LMG	C13-C14-C15-C16
25	c	504	CLA	O1A-CGA-O2A-C1
25	S	614	CLA	C2A-CAA-CBA-CGA
25	p	613	CLA	C2A-CAA-CBA-CGA
25	s	614	CLA	C2A-CAA-CBA-CGA
25	b	608	CLA	C3-C5-C6-C7
25	c	505	CLA	C5-C6-C7-C8
29	d	409	LHG	C25-C26-C27-C28
35	a	412	SQD	C12-C13-C14-C15
37	c	519	DGD	C2B-C1B-O2G-C2G
25	q	602	CLA	C16-C17-C18-C19
24	S	606	CHL	CAD-CBD-CGD-O1D
24	s	606	CHL	CAD-CBD-CGD-O1D
25	2	611	CLA	CAD-CBD-CGD-O1D
25	4	611	CLA	CAD-CBD-CGD-O1D
25	5	611	CLA	CAD-CBD-CGD-O1D
25	6	604	CLA	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	B	602	CLA	CAD-CBD-CGD-O1D
25	B	605	CLA	CAD-CBD-CGD-O1D
25	B	606	CLA	CAD-CBD-CGD-O1D
25	G	611	CLA	CAD-CBD-CGD-O1D
25	S	603	CLA	CAD-CBD-CGD-O1D
25	Y	614	CLA	CAD-CBD-CGD-O1D
25	0	604	CLA	CAD-CBD-CGD-O1D
25	7	604	CLA	CAD-CBD-CGD-O1D
25	9	602	CLA	CAD-CBD-CGD-O1D
25	9	611	CLA	CAD-CBD-CGD-O1D
25	p	611	CLA	CAD-CBD-CGD-O1D
25	q	611	CLA	CAD-CBD-CGD-O1D
25	b	602	CLA	CAD-CBD-CGD-O1D
25	b	605	CLA	CAD-CBD-CGD-O1D
25	b	606	CLA	CAD-CBD-CGD-O1D
25	g	611	CLA	CAD-CBD-CGD-O1D
25	s	603	CLA	CAD-CBD-CGD-O1D
25	s	604	CLA	CAD-CBD-CGD-O1D
25	y	614	CLA	CAD-CBD-CGD-O1D
29	q	2630	LHG	O8-C23-C24-C25
25	R	610	CLA	C10-C11-C12-C13
25	r	610	CLA	C10-C11-C12-C13
25	5	602	CLA	C15-C16-C17-C18
37	C	523	DGD	C1B-C2B-C3B-C4B
37	c	523	DGD	C1B-C2B-C3B-C4B
29	C	2630	LHG	C15-C16-C17-C18
24	n	609	CHL	CBA-CGA-O2A-C1
25	c	503	CLA	CBA-CGA-O2A-C1
33	A	409	PHO	CBA-CGA-O2A-C1
29	G	2630	LHG	C1-C2-C3-O3
29	g	2630	LHG	C1-C2-C3-O3
29	C	2630	LHG	C34-C35-C36-C37
35	A	412	SQD	C12-C13-C14-C15
24	R	607	CHL	C6-C7-C8-C10
24	y	609	CHL	C16-C17-C18-C19
24	r	607	CHL	C6-C7-C8-C10
24	2	609	CHL	C12-C13-C15-C16
24	3	601	CHL	C11-C12-C13-C15
24	3	605	CHL	C11-C12-C13-C15
24	4	601	CHL	C11-C12-C13-C15
24	4	601	CHL	C12-C13-C15-C16
24	4	609	CHL	C11-C12-C13-C15

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Mol	Chain	Res	Type	Atoms
24	5	609	CHL	C11-C12-C13-C15
24	6	601	CHL	C12-C13-C15-C16
24	6	607	CHL	C12-C13-C15-C16
24	R	606	CHL	C11-C10-C8-C7
24	R	606	CHL	C12-C13-C15-C16
24	0	601	CHL	C12-C13-C15-C16
24	0	606	CHL	C11-C12-C13-C15
24	8	601	CHL	C11-C10-C8-C7
24	8	605	CHL	C12-C13-C15-C16
24	8	606	CHL	C3A-C2A-CAA-CBA
24	p	609	CHL	C11-C10-C8-C7
24	q	601	CHL	C2-C3-C5-C6
24	r	606	CHL	C11-C10-C8-C7
24	r	606	CHL	C12-C13-C15-C16
25	1	604	CLA	C6-C7-C8-C10
25	2	602	CLA	C11-C12-C13-C15
25	3	603	CLA	C12-C13-C15-C16
25	3	613	CLA	C11-C10-C8-C7
25	4	603	CLA	C11-C10-C8-C7
25	5	603	CLA	C12-C13-C15-C16
25	5	613	CLA	C11-C10-C8-C7
25	6	612	CLA	C6-C7-C8-C10
25	B	605	CLA	C6-C7-C8-C10
25	B	608	CLA	C12-C13-C15-C16
25	B	616	CLA	C12-C13-C15-C16
25	C	502	CLA	C12-C13-C15-C16
25	C	505	CLA	C11-C12-C13-C15
25	C	505	CLA	C12-C13-C15-C16
25	C	506	CLA	C11-C12-C13-C15
25	C	511	CLA	C11-C12-C13-C15
25	Y	612	CLA	C6-C7-C8-C10
25	Y	613	CLA	C11-C10-C8-C7
25	0	612	CLA	C6-C7-C8-C10
25	7	604	CLA	C6-C7-C8-C10
25	7	613	CLA	C6-C7-C8-C10
25	8	603	CLA	C12-C13-C15-C16
25	8	613	CLA	C11-C10-C8-C7
25	p	603	CLA	C11-C10-C8-C7
25	q	603	CLA	C11-C10-C8-C7
25	q	603	CLA	C12-C13-C15-C16
25	q	610	CLA	C6-C7-C8-C10
25	q	610	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	b	605	CLA	C6-C7-C8-C10
25	b	608	CLA	C6-C7-C8-C10
25	b	608	CLA	C12-C13-C15-C16
25	b	616	CLA	C12-C13-C15-C16
25	c	505	CLA	C11-C12-C13-C15
25	c	505	CLA	C12-C13-C15-C16
25	c	506	CLA	C11-C12-C13-C15
25	y	612	CLA	C6-C7-C8-C10
25	y	613	CLA	C11-C10-C8-C7
29	c	2630	LHG	O6-C4-C5-O7
29	l	101	LHG	O6-C4-C5-O7
39	D	405	PL9	C28-C29-C31-C32
39	d	405	PL9	C28-C29-C31-C32
29	2	2630	LHG	C13-C14-C15-C16
24	2	605	CHL	CAA-CBA-CGA-O2A
24	G	607	CHL	CAA-CBA-CGA-O2A
25	y	602	CLA	C10-C11-C12-C13
29	R	2630	LHG	C8-C7-O7-C5
37	C	519	DGD	C2B-C1B-O2G-C2G
29	G	2630	LHG	C24-C25-C26-C27
29	g	2630	LHG	C24-C25-C26-C27
24	5	609	CHL	C2C-C3C-CAC-CBC
25	p	610	CLA	C8-C10-C11-C12
24	p	605	CHL	CBD-CGD-O2D-CED
24	r	608	CHL	C2A-CAA-CBA-CGA
25	4	602	CLA	C2A-CAA-CBA-CGA
25	5	603	CLA	C2A-CAA-CBA-CGA
25	R	602	CLA	C2A-CAA-CBA-CGA
25	R	616	CLA	C2A-CAA-CBA-CGA
25	p	603	CLA	C2A-CAA-CBA-CGA
25	r	602	CLA	C2A-CAA-CBA-CGA
25	r	616	CLA	C2A-CAA-CBA-CGA
24	1	607	CHL	C16-C17-C18-C19
24	0	609	CHL	C2C-C3C-CAC-CBC
24	3	601	CHL	C1C-C2C-CMC-OMC
24	3	606	CHL	C1C-C2C-CMC-OMC
24	4	601	CHL	C1C-C2C-CMC-OMC
24	4	605	CHL	C1C-C2C-CMC-OMC
24	4	609	CHL	C1C-C2C-CMC-OMC
24	5	601	CHL	C1C-C2C-CMC-OMC
24	5	605	CHL	C1C-C2C-CMC-OMC
24	5	606	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
24	5	607	CHL	C1C-C2C-CMC-OMC
24	5	608	CHL	C1C-C2C-CMC-OMC
24	6	601	CHL	C1C-C2C-CMC-OMC
24	6	608	CHL	C1C-C2C-CMC-OMC
24	G	608	CHL	C1C-C2C-CMC-OMC
24	N	606	CHL	C1C-C2C-CMC-OMC
24	N	607	CHL	C1C-C2C-CMC-OMC
24	R	608	CHL	C1C-C2C-CMC-OMC
24	S	608	CHL	C1C-C2C-CMC-OMC
24	Y	607	CHL	C1C-C2C-CMC-OMC
24	0	601	CHL	C1C-C2C-CMC-OMC
24	0	609	CHL	C1C-C2C-CMC-OMC
24	7	609	CHL	C1C-C2C-CMC-OMC
24	8	607	CHL	C1C-C2C-CMC-OMC
24	p	607	CHL	C1C-C2C-CMC-OMC
24	n	606	CHL	C1C-C2C-CMC-OMC
24	n	607	CHL	C1C-C2C-CMC-OMC
24	s	608	CHL	C1C-C2C-CMC-OMC
24	y	607	CHL	C1C-C2C-CMC-OMC
24	r	608	CHL	C1C-C2C-CMC-OMC
37	C	519	DGD	C1G-C2G-C3G-O3G
29	R	2630	LHG	O7-C5-C6-O8
35	B	621	SQD	O6-C44-C45-O47
35	b	621	SQD	O6-C44-C45-O47
36	A	413	LMG	O7-C8-C9-O8
36	a	413	LMG	O7-C8-C9-O8
25	l	610	CLA	C15-C16-C17-C18
24	p	609	CHL	C4C-C3C-CAC-CBC
29	D	409	LHG	C25-C26-C27-C28
29	n	2630	LHG	C11-C10-C9-C8
36	A	413	LMG	C15-C16-C17-C18
36	a	413	LMG	C15-C16-C17-C18
37	C	519	DGD	C5D-C6D-O5D-C1E
37	c	519	DGD	C5D-C6D-O5D-C1E
25	Y	602	CLA	C10-C11-C12-C13
24	Y	609	CHL	C3-C5-C6-C7
29	9	2630	LHG	O10-C23-O8-C6
33	A	409	PHO	O1A-CGA-O2A-C1
33	a	409	PHO	O1A-CGA-O2A-C1
25	Y	604	CLA	C4-C3-C5-C6
25	y	604	CLA	C4-C3-C5-C6
29	4	2630	LHG	C24-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
24	9	605	CHL	CAA-CBA-CGA-O2A
24	g	607	CHL	CAA-CBA-CGA-O2A
24	G	609	CHL	C10-C11-C12-C13
25	p	604	CLA	C5-C6-C7-C8
24	2	601	CHL	C11-C12-C13-C14
24	3	601	CHL	C11-C10-C8-C9
24	3	601	CHL	C11-C12-C13-C14
24	3	605	CHL	C14-C13-C15-C16
24	4	601	CHL	C6-C7-C8-C9
24	5	605	CHL	C6-C7-C8-C9
24	G	609	CHL	C11-C12-C13-C14
24	N	605	CHL	C6-C7-C8-C9
24	R	606	CHL	C14-C13-C15-C16
24	Y	601	CHL	C11-C12-C13-C14
24	Y	601	CHL	C14-C13-C15-C16
24	0	606	CHL	C11-C10-C8-C9
24	8	601	CHL	C11-C10-C8-C9
24	8	601	CHL	C11-C12-C13-C14
24	8	605	CHL	C11-C12-C13-C14
24	p	609	CHL	C11-C12-C13-C14
24	p	609	CHL	C14-C13-C15-C16
24	q	609	CHL	C11-C12-C13-C14
24	g	609	CHL	C11-C12-C13-C14
24	y	601	CHL	C11-C12-C13-C14
24	r	606	CHL	C6-C7-C8-C9
24	r	606	CHL	C14-C13-C15-C16
25	1	602	CLA	C6-C7-C8-C9
25	1	610	CLA	C6-C7-C8-C9
25	4	613	CLA	C11-C10-C8-C9
25	5	603	CLA	C11-C10-C8-C9
25	B	607	CLA	C14-C13-C15-C16
25	C	504	CLA	C11-C10-C8-C9
25	C	513	CLA	C11-C12-C13-C14
25	G	603	CLA	C11-C10-C8-C9
25	Y	604	CLA	C6-C7-C8-C9
25	7	602	CLA	C6-C7-C8-C9
25	7	612	CLA	C11-C10-C8-C9
25	7	613	CLA	C6-C7-C8-C9
25	p	613	CLA	C11-C10-C8-C9
25	q	603	CLA	C14-C13-C15-C16
25	b	607	CLA	C14-C13-C15-C16
25	c	504	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	g	603	CLA	C11-C10-C8-C9
25	n	603	CLA	C11-C12-C13-C14
25	y	604	CLA	C6-C7-C8-C9
25	y	613	CLA	C11-C10-C8-C9
25	c	503	CLA	O1A-CGA-O2A-C1
25	R	609	CLA	C2C-C3C-CAC-CBC
29	2	2630	LHG	C16-C17-C18-C19
35	b	623	SQD	C11-C12-C13-C14
24	7	607	CHL	C16-C17-C18-C19
24	y	601	CHL	C16-C17-C18-C19
25	n	613	CLA	C16-C17-C18-C19
24	8	609	CHL	C8-C10-C11-C12
25	r	609	CLA	C2C-C3C-CAC-CBC
24	R	608	CHL	C2A-CAA-CBA-CGA
25	5	604	CLA	C3-C5-C6-C7
35	B	623	SQD	C11-C12-C13-C14
24	N	605	CHL	C16-C17-C18-C19
24	N	609	CHL	C16-C17-C18-C19
25	N	613	CLA	C16-C17-C18-C19
25	q	602	CLA	C16-C17-C18-C20
27	q	1622	XAT	C11-C12-C13-C14
29	r	2630	LHG	O9-C7-O7-C5
25	C	505	CLA	C5-C6-C7-C8
36	h	102	LMG	C13-C14-C15-C16
25	1	603	CLA	O1D-CGD-O2D-CED
24	7	609	CHL	C2-C3-C5-C6
24	n	605	CHL	C2-C3-C5-C6
25	b	608	CLA	C2-C3-C5-C6
24	y	607	CHL	C10-C11-C12-C13
25	G	610	CLA	C16-C17-C18-C20
25	g	610	CLA	C16-C17-C18-C20
36	b	622	LMG	C18-C19-C20-C21
36	H	102	LMG	C35-C36-C37-C38
24	1	608	CHL	C1-C2-C3-C4
24	2	606	CHL	C1-C2-C3-C4
24	2	607	CHL	C1-C2-C3-C4
24	3	608	CHL	C1-C2-C3-C4
24	4	606	CHL	C1-C2-C3-C4
24	4	607	CHL	C1-C2-C3-C4
24	5	608	CHL	C1-C2-C3-C4
24	6	608	CHL	C1-C2-C3-C4
24	G	606	CHL	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
24	G	607	CHL	C1-C2-C3-C4
24	N	608	CHL	C1-C2-C3-C4
24	Y	608	CHL	C1-C2-C3-C4
24	0	608	CHL	C1-C2-C3-C4
24	7	608	CHL	C1-C2-C3-C4
24	8	608	CHL	C1-C2-C3-C4
24	9	606	CHL	C1-C2-C3-C4
24	9	607	CHL	C1-C2-C3-C4
24	p	608	CHL	C1-C2-C3-C4
24	q	606	CHL	C1-C2-C3-C4
24	q	607	CHL	C1-C2-C3-C4
24	g	606	CHL	C1-C2-C3-C4
24	g	607	CHL	C1-C2-C3-C4
24	n	608	CHL	C1-C2-C3-C4
24	y	608	CHL	C1-C2-C3-C4
25	2	604	CLA	C1-C2-C3-C4
25	2	614	CLA	C1-C2-C3-C4
25	3	611	CLA	C1-C2-C3-C4
25	3	614	CLA	C1-C2-C3-C4
25	4	604	CLA	C1-C2-C3-C4
25	4	614	CLA	C1-C2-C3-C4
25	5	611	CLA	C1-C2-C3-C4
25	5	614	CLA	C1-C2-C3-C4
25	G	604	CLA	C1-C2-C3-C4
25	G	614	CLA	C1-C2-C3-C4
25	N	611	CLA	C1-C2-C3-C4
25	N	614	CLA	C1-C2-C3-C4
25	R	601	CLA	C1-C2-C3-C4
25	R	611	CLA	C1-C2-C3-C4
25	R	612	CLA	C1-C2-C3-C4
25	S	602	CLA	C1-C2-C3-C4
25	S	604	CLA	C1-C2-C3-C4
25	S	610	CLA	C1-C2-C3-C4
25	S	611	CLA	C1-C2-C3-C4
25	S	613	CLA	C1-C2-C3-C4
25	8	611	CLA	C1-C2-C3-C4
25	8	614	CLA	C1-C2-C3-C4
25	9	604	CLA	C1-C2-C3-C4
25	9	614	CLA	C1-C2-C3-C4
25	p	611	CLA	C1-C2-C3-C4
25	p	614	CLA	C1-C2-C3-C4
25	q	604	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
25	q	614	CLA	C1-C2-C3-C4
25	g	604	CLA	C1-C2-C3-C4
25	g	614	CLA	C1-C2-C3-C4
25	n	611	CLA	C1-C2-C3-C4
25	n	614	CLA	C1-C2-C3-C4
25	s	602	CLA	C1-C2-C3-C4
25	s	604	CLA	C1-C2-C3-C4
25	s	610	CLA	C1-C2-C3-C4
25	s	611	CLA	C1-C2-C3-C4
25	s	613	CLA	C1-C2-C3-C4
25	r	601	CLA	C1-C2-C3-C4
25	r	611	CLA	C1-C2-C3-C4
25	r	612	CLA	C1-C2-C3-C4
36	B	622	LMG	C18-C19-C20-C21
25	2	602	CLA	C15-C16-C17-C18
35	D	413	SQD	C44-C45-O47-C7
35	d	413	SQD	C44-C45-O47-C7
29	C	2630	LHG	O6-C4-C5-C6
29	c	2630	LHG	O6-C4-C5-C6
25	3	612	CLA	C2A-CAA-CBA-CGA
25	0	613	CLA	C2A-CAA-CBA-CGA
25	8	612	CLA	C2A-CAA-CBA-CGA
29	S	2630	LHG	O9-C7-O7-C5
29	3	2630	LHG	C24-C23-O8-C6
24	1	607	CHL	C2-C1-O2A-CGA
24	3	605	CHL	C2-C1-O2A-CGA
24	4	609	CHL	C2-C1-O2A-CGA
24	7	607	CHL	C2-C1-O2A-CGA
24	8	605	CHL	C2-C1-O2A-CGA
24	p	601	CHL	C2-C1-O2A-CGA
24	p	607	CHL	C2-C1-O2A-CGA
25	C	505	CLA	C2-C1-O2A-CGA
25	R	611	CLA	C2-C1-O2A-CGA
25	p	604	CLA	C2-C1-O2A-CGA
25	c	503	CLA	C2-C1-O2A-CGA
25	r	611	CLA	C2-C1-O2A-CGA
25	r	612	CLA	C2-C1-O2A-CGA
35	A	412	SQD	C14-C15-C16-C17
36	h	102	LMG	C35-C36-C37-C38
29	D	409	LHG	C28-C29-C30-C31
24	N	609	CHL	O1A-CGA-O2A-C1
25	A	410	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
29	N	2630	LHG	C27-C28-C29-C30
35	a	412	SQD	C14-C15-C16-C17
24	3	607	CHL	C2C-C3C-CAC-CBC
29	4	2630	LHG	O6-C4-C5-O7
24	n	605	CHL	O1D-CGD-O2D-CED
25	g	602	CLA	O1D-CGD-O2D-CED
26	4	1620	LUT	C1-C6-C7-C8
26	5	1621	LUT	C1-C6-C7-C8
26	6	1621	LUT	C1-C6-C7-C8
26	6	1621	LUT	C5-C6-C7-C8
26	S	1620	LUT	C1-C6-C7-C8
26	Y	1621	LUT	C1-C6-C7-C8
26	9	1620	LUT	C1-C6-C7-C8
26	s	1620	LUT	C1-C6-C7-C8
26	y	1621	LUT	C1-C6-C7-C8
24	N	605	CHL	C2-C3-C5-C6
25	Y	603	CLA	C2-C3-C5-C6
29	Y	2630	LHG	O10-C23-O8-C6
33	A	409	PHO	C8-C10-C11-C12
24	4	607	CHL	CAA-CBA-CGA-O2A
29	r	2630	LHG	C25-C26-C27-C28
24	R	607	CHL	C6-C7-C8-C9
29	S	2630	LHG	C8-C7-O7-C5
29	r	2630	LHG	C8-C7-O7-C5
33	a	409	PHO	C8-C10-C11-C12
24	4	606	CHL	C2A-CAA-CBA-CGA
29	4	2630	LHG	C3-O3-P-O6
29	5	2630	LHG	C3-O3-P-O6
29	G	2630	LHG	C3-O3-P-O6
29	G	2630	LHG	C4-O6-P-O3
29	L	101	LHG	C3-O3-P-O6
29	S	2630	LHG	C3-O3-P-O6
29	0	2630	LHG	C3-O3-P-O6
29	p	2630	LHG	C3-O3-P-O6
29	g	2630	LHG	C3-O3-P-O6
29	g	2630	LHG	C4-O6-P-O3
29	s	2630	LHG	C3-O3-P-O6
29	R	2630	LHG	C25-C26-C27-C28
24	Y	609	CHL	C16-C17-C18-C19
35	b	623	SQD	C12-C13-C14-C15
29	0	2630	LHG	C4-C5-C6-O8
24	5	609	CHL	C4C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
24	n	607	CHL	C5-C6-C7-C8
24	3	607	CHL	C6-C7-C8-C10
24	y	609	CHL	C11-C12-C13-C15
25	1	603	CLA	C11-C12-C13-C15
25	B	608	CLA	C6-C7-C8-C10
25	B	610	CLA	C11-C12-C13-C15
25	C	513	CLA	C11-C12-C13-C15
25	7	612	CLA	C11-C10-C8-C7
25	b	610	CLA	C11-C12-C13-C15
25	c	502	CLA	C12-C13-C15-C16
25	y	603	CLA	C11-C10-C8-C7
29	D	410	LHG	C29-C30-C31-C32
29	d	410	LHG	C29-C30-C31-C32
24	q	601	CHL	C3-C5-C6-C7
24	3	605	CHL	C11-C12-C13-C14
24	4	601	CHL	C11-C10-C8-C9
24	6	606	CHL	C11-C12-C13-C14
24	N	601	CHL	C11-C10-C8-C9
24	N	609	CHL	C11-C12-C13-C14
24	0	606	CHL	C11-C12-C13-C14
24	8	605	CHL	C14-C13-C15-C16
24	n	601	CHL	C11-C10-C8-C9
24	n	605	CHL	C6-C7-C8-C9
24	n	609	CHL	C11-C12-C13-C14
24	y	601	CHL	C14-C13-C15-C16
25	1	603	CLA	C14-C13-C15-C16
25	1	604	CLA	C6-C7-C8-C9
25	1	613	CLA	C6-C7-C8-C9
25	3	613	CLA	C11-C10-C8-C9
25	6	612	CLA	C6-C7-C8-C9
25	6	612	CLA	C14-C13-C15-C16
25	B	607	CLA	C11-C12-C13-C14
25	B	608	CLA	C14-C13-C15-C16
25	C	505	CLA	C14-C13-C15-C16
25	N	603	CLA	C11-C12-C13-C14
25	Y	612	CLA	C6-C7-C8-C9
25	Y	613	CLA	C11-C10-C8-C9
25	0	612	CLA	C14-C13-C15-C16
25	0	613	CLA	C11-C10-C8-C9
25	7	604	CLA	C6-C7-C8-C9
25	8	613	CLA	C11-C10-C8-C9
25	p	603	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
25	p	603	CLA	C14-C13-C15-C16
25	p	610	CLA	C11-C10-C8-C9
25	q	603	CLA	C11-C10-C8-C9
25	q	610	CLA	C6-C7-C8-C9
25	b	607	CLA	C11-C12-C13-C14
25	b	608	CLA	C14-C13-C15-C16
25	c	505	CLA	C14-C13-C15-C16
25	c	513	CLA	C11-C10-C8-C9
25	y	612	CLA	C6-C7-C8-C9
25	R	602	CLA	C8-C10-C11-C12
34	C	516	BCR	C15-C16-C17-C18
34	c	516	BCR	C15-C16-C17-C18
24	r	607	CHL	C6-C7-C8-C9
29	1	2630	LHG	C32-C33-C34-C35
33	A	408	PHO	CBA-CGA-O2A-C1
33	a	408	PHO	CBA-CGA-O2A-C1
25	6	602	CLA	C8-C10-C11-C12
25	b	615	CLA	C13-C15-C16-C17
25	r	602	CLA	C8-C10-C11-C12
36	C	521	LMG	C32-C33-C34-C35
36	h	102	LMG	C31-C32-C33-C34
28	9	1623	NEX	C31-C32-C33-C40
25	C	511	CLA	C16-C17-C18-C20
29	0	2630	LHG	O2-C2-C3-O3
25	B	615	CLA	C13-C15-C16-C17
25	0	613	CLA	C15-C16-C17-C18
25	q	613	CLA	C13-C15-C16-C17
29	7	2630	LHG	C15-C16-C17-C18
29	4	2630	LHG	C1-C2-C3-O3
29	q	2630	LHG	C1-C2-C3-O3
36	C	521	LMG	C33-C34-C35-C36
25	7	610	CLA	C4-C3-C5-C6
25	C	512	CLA	C2-C3-C5-C6
25	7	614	CLA	C6-C7-C8-C9
24	7	608	CHL	CBA-CGA-O2A-C1
36	c	521	LMG	C32-C33-C34-C35
24	n	609	CHL	O1A-CGA-O2A-C1
29	3	2630	LHG	O10-C23-O8-C6
33	a	408	PHO	O1A-CGA-O2A-C1
35	D	413	SQD	O10-C23-O48-C46
35	d	413	SQD	O10-C23-O48-C46
25	a	410	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
24	3	607	CHL	C4C-C3C-CAC-CBC
25	1	614	CLA	C5-C6-C7-C8
24	2	601	CHL	C5-C6-C7-C8
25	p	603	CLA	C5-C6-C7-C8
25	R	604	CLA	O2A-C1-C2-C3
33	A	408	PHO	O1A-CGA-O2A-C1
35	D	413	SQD	C24-C23-O48-C46
35	d	413	SQD	C24-C23-O48-C46
24	p	607	CHL	C2A-CAA-CBA-CGA
25	B	615	CLA	C2A-CAA-CBA-CGA
25	b	615	CLA	C2A-CAA-CBA-CGA
35	b	623	SQD	O5-C1-O6-C44
36	S	2631	LMG	O6-C1-O1-C7
36	s	2631	LMG	O6-C1-O1-C7
34	B	618	BCR	C19-C20-C21-C22
34	b	618	BCR	C19-C20-C21-C22
37	C	519	DGD	O1B-C1B-O2G-C2G
24	7	608	CHL	O1A-CGA-O2A-C1
29	d	410	LHG	O6-C4-C5-O7
25	6	611	CLA	C16-C17-C18-C19
25	C	511	CLA	C16-C17-C18-C19
33	A	409	PHO	C16-C17-C18-C19
33	a	409	PHO	C16-C17-C18-C19
36	c	521	LMG	C33-C34-C35-C36
25	R	610	CLA	C4-C3-C5-C6
25	7	613	CLA	C13-C15-C16-C17
29	3	2630	LHG	C29-C30-C31-C32
29	D	408	LHG	C25-C26-C27-C28
29	4	2630	LHG	O10-C23-O8-C6
25	1	613	CLA	C13-C15-C16-C17
37	c	519	DGD	O1B-C1B-O2G-C2G
29	7	2630	LHG	C32-C33-C34-C35
25	4	612	CLA	CBD-CGD-O2D-CED
24	6	609	CHL	C2-C1-O2A-CGA
24	Y	609	CHL	C2-C1-O2A-CGA
24	0	608	CHL	C2-C1-O2A-CGA
24	0	609	CHL	C2-C1-O2A-CGA
25	1	611	CLA	C2-C1-O2A-CGA
25	C	506	CLA	C2-C1-O2A-CGA
25	R	603	CLA	C2-C1-O2A-CGA
25	c	513	CLA	C2-C1-O2A-CGA
25	r	603	CLA	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
33	A	409	PHO	C16-C17-C18-C20
33	a	409	PHO	C16-C17-C18-C20
29	d	408	LHG	C25-C26-C27-C28
24	S	601	CHL	CAA-CBA-CGA-O1A
40	F	101	HEM	CAD-CBD-CGD-O1D
25	1	613	CLA	C2A-CAA-CBA-CGA
25	4	613	CLA	C2A-CAA-CBA-CGA
25	6	613	CLA	C2A-CAA-CBA-CGA
25	7	613	CLA	C2A-CAA-CBA-CGA
25	c	507	CLA	C2A-CAA-CBA-CGA
29	2	2630	LHG	O7-C5-C6-O8
29	c	2630	LHG	C34-C35-C36-C37
24	6	606	CHL	C3A-C2A-CAA-CBA
24	8	601	CHL	C3A-C2A-CAA-CBA
24	9	609	CHL	C3A-C2A-CAA-CBA
24	q	601	CHL	C3A-C2A-CAA-CBA
24	n	608	CHL	C3A-C2A-CAA-CBA
25	4	613	CLA	C3A-C2A-CAA-CBA
25	B	605	CLA	C3A-C2A-CAA-CBA
25	B	610	CLA	C3A-C2A-CAA-CBA
25	q	613	CLA	C3A-C2A-CAA-CBA
25	b	605	CLA	C3A-C2A-CAA-CBA
25	b	610	CLA	C3A-C2A-CAA-CBA
25	c	511	CLA	C16-C17-C18-C19
24	0	609	CHL	C4C-C3C-CAC-CBC
24	q	607	CHL	O2A-C1-C2-C3
26	q	1621	LUT	C9-C10-C11-C12
25	1	603	CLA	C4-C3-C5-C6
25	6	613	CLA	C4-C3-C5-C6
25	N	613	CLA	C4-C3-C5-C6
25	c	512	CLA	C4-C3-C5-C6
25	n	613	CLA	C4-C3-C5-C6
25	r	610	CLA	C4-C3-C5-C6
25	n	613	CLA	C2-C3-C5-C6
24	1	609	CHL	C6-C7-C8-C9
24	3	605	CHL	C6-C7-C8-C9
24	N	609	CHL	C6-C7-C8-C9
24	R	606	CHL	C6-C7-C8-C9
24	Y	606	CHL	C14-C13-C15-C16
24	Y	609	CHL	C14-C13-C15-C16
24	0	607	CHL	C6-C7-C8-C9
24	7	606	CHL	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
24	n	607	CHL	C11-C12-C13-C14
24	n	609	CHL	C6-C7-C8-C9
24	y	606	CHL	C14-C13-C15-C16
24	y	609	CHL	C14-C13-C15-C16
25	1	604	CLA	C11-C12-C13-C14
25	3	603	CLA	C14-C13-C15-C16
25	3	613	CLA	C6-C7-C8-C9
25	4	603	CLA	C11-C12-C13-C14
25	B	611	CLA	C11-C12-C13-C14
25	C	502	CLA	C6-C7-C8-C9
25	C	508	CLA	C11-C12-C13-C14
25	7	603	CLA	C14-C13-C15-C16
25	7	604	CLA	C11-C12-C13-C14
25	8	613	CLA	C6-C7-C8-C9
25	q	610	CLA	C14-C13-C15-C16
25	b	611	CLA	C11-C12-C13-C14
25	c	502	CLA	C6-C7-C8-C9
25	c	508	CLA	C11-C12-C13-C14
24	8	609	CHL	C16-C17-C18-C19
24	8	609	CHL	C16-C17-C18-C20
25	c	511	CLA	C16-C17-C18-C20
29	d	409	LHG	C28-C29-C30-C31
24	g	605	CHL	CBA-CGA-O2A-C1
35	B	621	SQD	C13-C14-C15-C16
36	b	622	LMG	C16-C17-C18-C19
35	B	623	SQD	C12-C13-C14-C15
25	B	605	CLA	C15-C16-C17-C18
28	1	1623	NEX	C39-C29-C30-C31
28	2	1623	NEX	C39-C29-C30-C31
28	3	1623	NEX	C39-C29-C30-C31
28	4	1623	NEX	C39-C29-C30-C31
28	5	1623	NEX	C39-C29-C30-C31
28	6	1623	NEX	C39-C29-C30-C31
28	G	1623	NEX	C39-C29-C30-C31
28	N	1623	NEX	C39-C29-C30-C31
28	R	623	NEX	C39-C29-C30-C31
28	S	1623	NEX	C39-C29-C30-C31
28	Y	1623	NEX	C39-C29-C30-C31
28	0	1623	NEX	C39-C29-C30-C31
28	7	1623	NEX	C39-C29-C30-C31
28	8	1623	NEX	C39-C29-C30-C31
28	9	1623	NEX	C39-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
28	p	1623	NEX	C39-C29-C30-C31
28	q	1623	NEX	C39-C29-C30-C31
28	g	1623	NEX	C39-C29-C30-C31
28	n	1623	NEX	C39-C29-C30-C31
28	s	1623	NEX	C39-C29-C30-C31
28	y	1623	NEX	C39-C29-C30-C31
28	r	623	NEX	C39-C29-C30-C31
29	3	2630	LHG	C1-C2-C3-O3
29	8	2630	LHG	C1-C2-C3-O3
35	b	621	SQD	C13-C14-C15-C16
24	G	607	CHL	C2A-CAA-CBA-CGA
25	y	613	CLA	C8-C10-C11-C12
25	1	614	CLA	C6-C7-C8-C9
25	7	614	CLA	C5-C6-C7-C8
36	H	102	LMG	C31-C32-C33-C34
37	C	519	DGD	O1A-C1A-O1G-C1G
36	H	102	LMG	C4-C5-C6-O5
24	q	607	CHL	CAA-CBA-CGA-O1A
24	N	605	CHL	C16-C17-C18-C20
29	l	101	LHG	C15-C16-C17-C18
24	3	606	CHL	CAA-CBA-CGA-O1A
24	s	601	CHL	CAA-CBA-CGA-O1A
25	n	612	CLA	CAA-CBA-CGA-O1A
26	4	1621	LUT	C7-C8-C9-C19
26	N	1621	LUT	C7-C8-C9-C19
26	n	1621	LUT	C7-C8-C9-C19
34	B	618	BCR	C36-C18-C19-C20
34	b	618	BCR	C36-C18-C19-C20
29	n	2630	LHG	C24-C25-C26-C27
29	5	2630	LHG	C11-C10-C9-C8
37	C	520	DGD	C4B-C5B-C6B-C7B
24	4	605	CHL	O1A-CGA-O2A-C1
24	6	606	CHL	C8-C10-C11-C12
24	8	607	CHL	C4-C3-C5-C6
25	a	410	CLA	C4-C3-C5-C6
25	g	610	CLA	C4-C3-C5-C6
24	3	608	CHL	C1A-C2A-CAA-CBA
24	R	608	CHL	C1A-C2A-CAA-CBA
24	S	606	CHL	C1A-C2A-CAA-CBA
24	7	606	CHL	C1A-C2A-CAA-CBA
24	8	601	CHL	C1A-C2A-CAA-CBA
24	8	608	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	s	606	CHL	C1A-C2A-CAA-CBA
24	r	608	CHL	C1A-C2A-CAA-CBA
25	B	608	CLA	C1A-C2A-CAA-CBA
25	C	502	CLA	C1A-C2A-CAA-CBA
25	C	504	CLA	C1A-C2A-CAA-CBA
25	8	610	CLA	C1A-C2A-CAA-CBA
25	p	602	CLA	C1A-C2A-CAA-CBA
25	q	613	CLA	C1A-C2A-CAA-CBA
25	b	608	CLA	C1A-C2A-CAA-CBA
25	b	610	CLA	C1A-C2A-CAA-CBA
25	c	502	CLA	C1A-C2A-CAA-CBA
25	c	504	CLA	C1A-C2A-CAA-CBA
25	c	505	CLA	C1A-C2A-CAA-CBA
29	4	2630	LHG	C34-C35-C36-C37
36	B	622	LMG	C16-C17-C18-C19
37	c	520	DGD	C4B-C5B-C6B-C7B
24	2	601	CHL	C11-C10-C8-C7
24	3	607	CHL	C11-C12-C13-C15
24	5	601	CHL	C12-C13-C15-C16
24	5	609	CHL	C11-C10-C8-C7
24	6	609	CHL	C11-C10-C8-C7
24	N	607	CHL	C11-C12-C13-C15
24	Y	609	CHL	C11-C12-C13-C15
24	8	607	CHL	C11-C12-C13-C15
24	p	607	CHL	C11-C12-C13-C15
24	y	601	CHL	C6-C7-C8-C10
25	5	604	CLA	C12-C13-C15-C16
25	6	613	CLA	C12-C13-C15-C16
25	Y	613	CLA	C6-C7-C8-C10
25	0	604	CLA	C12-C13-C15-C16
25	7	603	CLA	C11-C12-C13-C15
25	9	603	CLA	C11-C10-C8-C7
24	y	609	CHL	C2C-C3C-CAC-CBC
24	0	606	CHL	C8-C10-C11-C12
37	c	519	DGD	O1A-C1A-O1G-C1G
24	S	601	CHL	CAA-CBA-CGA-O2A
25	4	610	CLA	O1D-CGD-O2D-CED
24	6	606	CHL	C3C-C2C-CMC-OMC
24	8	606	CHL	C3C-C2C-CMC-OMC
24	g	607	CHL	C2A-CAA-CBA-CGA
25	B	617	CLA	C2A-CAA-CBA-CGA
25	9	610	CLA	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	b	617	CLA	C2A-CAA-CBA-CGA
33	A	408	PHO	C2A-CAA-CBA-CGA
33	a	408	PHO	C2A-CAA-CBA-CGA
24	1	607	CHL	C10-C11-C12-C13
24	7	607	CHL	C10-C11-C12-C13
25	G	610	CLA	C5-C6-C7-C8
25	0	602	CLA	C8-C10-C11-C12
25	g	610	CLA	C5-C6-C7-C8
24	8	606	CHL	CAA-CBA-CGA-O1A
24	4	607	CHL	O2A-C1-C2-C3
25	S	611	CLA	O2A-C1-C2-C3
25	q	604	CLA	O2A-C1-C2-C3
24	G	605	CHL	CBA-CGA-O2A-C1
29	y	2630	LHG	C24-C23-O8-C6
35	B	621	SQD	C27-C28-C29-C30
35	b	621	SQD	C27-C28-C29-C30
25	5	610	CLA	CBD-CGD-O2D-CED
24	1	609	CHL	C13-C15-C16-C17
24	8	606	CHL	CAA-CBA-CGA-O2A
25	p	612	CLA	CAA-CBA-CGA-O2A
40	F	101	HEM	CAD-CBD-CGD-O2D
29	1	2630	LHG	C15-C16-C17-C18
25	A	410	CLA	C4-C3-C5-C6
25	G	610	CLA	C4-C3-C5-C6
35	B	621	SQD	C34-C35-C36-C37
36	s	2631	LMG	C29-C30-C31-C32
25	Y	613	CLA	C8-C10-C11-C12
25	6	613	CLA	C2-C3-C5-C6
25	B	608	CLA	C2-C3-C5-C6
25	N	613	CLA	C2-C3-C5-C6
25	R	610	CLA	C2-C3-C5-C6
29	D	408	LHG	C24-C25-C26-C27
29	c	2630	LHG	C11-C10-C9-C8
29	L	101	LHG	C15-C16-C17-C18
29	8	2630	LHG	C29-C30-C31-C32
25	5	604	CLA	C5-C6-C7-C8
25	b	605	CLA	C15-C16-C17-C18
29	r	2630	LHG	C7-C8-C9-C10
36	H	102	LMG	O9-C10-O7-C8
25	B	604	CLA	C16-C17-C18-C20
28	1	1623	NEX	C28-C29-C30-C31
28	2	1623	NEX	C28-C29-C30-C31

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Mol	Chain	Res	Type	Atoms
28	3	1623	NEX	C28-C29-C30-C31
28	4	1623	NEX	C28-C29-C30-C31
28	5	1623	NEX	C28-C29-C30-C31
28	6	1623	NEX	C28-C29-C30-C31
28	G	1623	NEX	C28-C29-C30-C31
28	N	1623	NEX	C28-C29-C30-C31
28	R	623	NEX	C28-C29-C30-C31
28	S	1623	NEX	C28-C29-C30-C31
28	Y	1623	NEX	C28-C29-C30-C31
28	0	1623	NEX	C28-C29-C30-C31
28	7	1623	NEX	C28-C29-C30-C31
28	8	1623	NEX	C28-C29-C30-C31
28	9	1623	NEX	C28-C29-C30-C31
28	p	1623	NEX	C28-C29-C30-C31
28	q	1623	NEX	C28-C29-C30-C31
28	g	1623	NEX	C28-C29-C30-C31
28	n	1623	NEX	C28-C29-C30-C31
28	s	1623	NEX	C28-C29-C30-C31
28	y	1623	NEX	C28-C29-C30-C31
28	r	623	NEX	C28-C29-C30-C31
25	N	612	CLA	CAA-CBA-CGA-O1A
29	0	2630	LHG	O7-C5-C6-O8
25	2	604	CLA	CBA-CGA-O2A-C1
25	y	614	CLA	CBA-CGA-O2A-C1
35	b	621	SQD	C34-C35-C36-C37
24	p	605	CHL	O1D-CGD-O2D-CED
25	5	610	CLA	O1D-CGD-O2D-CED
29	d	410	LHG	C9-C10-C11-C12
28	y	1623	NEX	C33-C34-C35-C15
25	p	612	CLA	CAA-CBA-CGA-O1A
29	S	2630	LHG	C24-C25-C26-C27
29	R	2630	LHG	C7-C8-C9-C10
24	8	601	CHL	C10-C11-C12-C13
25	4	610	CLA	CBD-CGD-O2D-CED
25	2	604	CLA	O1A-CGA-O2A-C1
29	0	2630	LHG	C1-C2-C3-O3
29	n	2630	LHG	C1-C2-C3-O3
29	d	408	LHG	C24-C25-C26-C27
25	4	612	CLA	O1D-CGD-O2D-CED
24	Y	606	CHL	C4-C3-C5-C6
24	7	601	CHL	C4-C3-C5-C6
24	y	606	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	C	509	CLA	C4-C3-C5-C6
24	8	609	CHL	C2-C1-O2A-CGA
24	q	609	CHL	C2-C1-O2A-CGA
24	n	608	CHL	C2-C1-O2A-CGA
24	y	609	CHL	C2-C1-O2A-CGA
25	6	611	CLA	C2-C1-O2A-CGA
25	B	605	CLA	C2-C1-O2A-CGA
25	B	611	CLA	C2-C1-O2A-CGA
25	b	605	CLA	C2-C1-O2A-CGA
25	b	611	CLA	C2-C1-O2A-CGA
25	c	505	CLA	C2-C1-O2A-CGA
25	c	506	CLA	C2-C1-O2A-CGA
25	1	603	CLA	C2-C3-C5-C6
25	Y	604	CLA	C2-C3-C5-C6
25	7	610	CLA	C2-C3-C5-C6
25	8	603	CLA	C2-C3-C5-C6
25	y	604	CLA	C2-C3-C5-C6
25	r	610	CLA	C2-C3-C5-C6
24	G	605	CHL	C2-C1-O2A-CGA
24	g	605	CHL	O1A-CGA-O2A-C1
25	C	506	CLA	C10-C11-C12-C13
25	9	602	CLA	C13-C15-C16-C17
24	3	606	CHL	CAA-CBA-CGA-O2A
29	N	2630	LHG	C24-C25-C26-C27
24	2	609	CHL	C11-C10-C8-C9
24	p	609	CHL	C6-C7-C8-C9
25	A	405	CLA	C11-C12-C13-C14
25	C	502	CLA	C11-C12-C13-C14
25	0	603	CLA	C11-C10-C8-C9
25	n	602	CLA	C11-C12-C13-C14
25	y	603	CLA	C11-C10-C8-C9
37	c	519	DGD	C2A-C1A-O1G-C1G
24	Y	609	CHL	C2C-C3C-CAC-CBC
24	G	605	CHL	O1A-CGA-O2A-C1
24	g	605	CHL	C2-C1-O2A-CGA
29	0	2630	LHG	C13-C14-C15-C16
25	7	613	CLA	C3-C5-C6-C7
24	s	601	CHL	CAA-CBA-CGA-O2A
25	c	506	CLA	C10-C11-C12-C13
33	a	409	PHO	C1A-C2A-CAA-CBA
35	a	412	SQD	C29-C30-C31-C32
25	4	611	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	4	611	CLA	CAA-CBA-CGA-O2A
25	n	612	CLA	CAA-CBA-CGA-O2A
24	6	608	CHL	O2A-C1-C2-C3
24	G	606	CHL	O2A-C1-C2-C3
24	g	606	CHL	O2A-C1-C2-C3
25	s	611	CLA	O2A-C1-C2-C3
24	q	609	CHL	O1A-CGA-O2A-C1
25	y	614	CLA	O1A-CGA-O2A-C1
26	2	1621	LUT	C1-C6-C7-C8
26	2	1621	LUT	C5-C6-C7-C8
26	G	1621	LUT	C1-C6-C7-C8
26	R	620	LUT	C1-C6-C7-C8
26	Y	1620	LUT	C1-C6-C7-C8
26	Y	1620	LUT	C5-C6-C7-C8
26	0	1621	LUT	C1-C6-C7-C8
26	9	1621	LUT	C1-C6-C7-C8
26	y	1620	LUT	C1-C6-C7-C8
26	r	620	LUT	C1-C6-C7-C8
34	C	516	BCR	C1-C6-C7-C8
29	9	2630	LHG	C24-C25-C26-C27
35	B	621	SQD	C44-C45-C46-O48
35	b	621	SQD	C44-C45-C46-O48
25	N	612	CLA	CAA-CBA-CGA-O2A
24	4	605	CHL	C2-C1-O2A-CGA
24	6	609	CHL	O1A-CGA-O2A-C1
26	q	1621	LUT	C33-C34-C35-C15
26	n	1621	LUT	C29-C30-C31-C32
28	Y	1623	NEX	C33-C34-C35-C15
37	C	519	DGD	C2A-C1A-O1G-C1G
29	s	2630	LHG	C24-C25-C26-C27
24	1	601	CHL	C4-C3-C5-C6
24	1	609	CHL	C4-C3-C5-C6
24	N	609	CHL	C4-C3-C5-C6
24	0	606	CHL	C4-C3-C5-C6
25	Y	602	CLA	C4-C3-C5-C6
25	Y	611	CLA	C4-C3-C5-C6
39	D	405	PL9	C45-C44-C46-C47
39	d	405	PL9	C45-C44-C46-C47
27	8	1622	XAT	C31-C32-C33-C34
34	C	514	BCR	C21-C22-C23-C24
34	c	514	BCR	C21-C22-C23-C24
35	A	412	SQD	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
25	Y	611	CLA	C2-C3-C5-C6
29	7	2630	LHG	C26-C27-C28-C29
36	D	411	LMG	C8-C7-O1-C1
36	d	411	LMG	C8-C7-O1-C1
24	6	605	CHL	CAA-CBA-CGA-O2A
24	0	605	CHL	CAA-CBA-CGA-O2A
24	5	605	CHL	O1A-CGA-O2A-C1
25	p	611	CLA	CAA-CBA-CGA-O2A
36	a	413	LMG	C39-C40-C41-C42
24	3	609	CHL	C16-C17-C18-C19
25	b	604	CLA	C16-C17-C18-C20
36	A	413	LMG	C39-C40-C41-C42
25	6	603	CLA	C13-C15-C16-C17
29	D	410	LHG	O6-C4-C5-O7
24	6	605	CHL	CAA-CBA-CGA-O1A
25	S	612	CLA	CAA-CBA-CGA-O2A
25	s	612	CLA	CAA-CBA-CGA-O2A
25	s	611	CLA	C2A-CAA-CBA-CGA
25	g	602	CLA	C13-C15-C16-C17
24	8	607	CHL	CAA-CBA-CGA-O2A
36	H	102	LMG	C38-C39-C40-C41
24	p	601	CHL	C3-C5-C6-C7
24	0	605	CHL	CAA-CBA-CGA-O1A
25	c	506	CLA	C16-C17-C18-C20
25	G	602	CLA	C13-C15-C16-C17
24	6	606	CHL	C4-C3-C5-C6
25	1	610	CLA	C4-C3-C5-C6
25	5	602	CLA	C4-C3-C5-C6
25	8	603	CLA	C4-C3-C5-C6
25	y	602	CLA	C4-C3-C5-C6
39	D	405	PL9	C39-C41-C42-C43
24	N	601	CHL	C12-C13-C15-C16
24	Y	606	CHL	C2-C3-C5-C6
24	0	609	CHL	C11-C10-C8-C7
24	q	601	CHL	C11-C12-C13-C15
24	n	607	CHL	C11-C12-C13-C15
24	y	606	CHL	C2-C3-C5-C6
25	3	613	CLA	C6-C7-C8-C10
25	C	508	CLA	C11-C10-C8-C7
25	Y	603	CLA	C11-C10-C8-C7
25	0	603	CLA	C11-C10-C8-C7
25	0	613	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	8	613	CLA	C6-C7-C8-C10
25	c	508	CLA	C11-C10-C8-C7
25	y	611	CLA	C2-C3-C5-C6
24	N	607	CHL	C5-C6-C7-C8
26	4	1621	LUT	C29-C30-C31-C32
25	y	610	CLA	C16-C17-C18-C20
29	6	2630	LHG	C5-C4-O6-P
25	7	603	CLA	C15-C16-C17-C18
35	A	412	SQD	O6-C44-C45-O47
35	b	623	SQD	O47-C45-C46-O48
36	h	102	LMG	O9-C10-O7-C8
24	2	601	CHL	C2C-C3C-CAC-CBC
36	D	412	LMG	C12-C13-C14-C15
25	q	602	CLA	C3-C5-C6-C7
24	p	606	CHL	CAA-CBA-CGA-O2A
24	1	608	CHL	O2A-C1-C2-C3
24	2	606	CHL	O2A-C1-C2-C3
24	3	608	CHL	O2A-C1-C2-C3
24	N	608	CHL	O2A-C1-C2-C3
24	0	608	CHL	O2A-C1-C2-C3
24	7	608	CHL	O2A-C1-C2-C3
24	8	608	CHL	O2A-C1-C2-C3
24	9	606	CHL	O2A-C1-C2-C3
25	S	604	CLA	O2A-C1-C2-C3
25	s	604	CLA	O2A-C1-C2-C3
29	6	2630	LHG	O8-C23-C24-C25
29	2	2630	LHG	C28-C29-C30-C31
25	b	607	CLA	C5-C6-C7-C8
25	C	506	CLA	C16-C17-C18-C20
25	S	612	CLA	CAA-CBA-CGA-O1A
25	q	611	CLA	CAA-CBA-CGA-O2A
25	s	612	CLA	CAA-CBA-CGA-O1A
24	3	605	CHL	O1D-CGD-O2D-CED
24	4	605	CHL	CBA-CGA-O2A-C1
29	c	2630	LHG	C12-C13-C14-C15
36	d	412	LMG	C12-C13-C14-C15
24	1	606	CHL	CAA-CBA-CGA-O2A
24	9	607	CHL	CAA-CBA-CGA-O2A
25	4	603	CLA	CAA-CBA-CGA-O2A
24	3	609	CHL	C4-C3-C5-C6
24	Y	609	CHL	C4-C3-C5-C6
24	9	609	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
24	p	601	CHL	C4-C3-C5-C6
25	1	604	CLA	C4-C3-C5-C6
25	4	603	CLA	C4-C3-C5-C6
25	c	509	CLA	C4-C3-C5-C6
25	y	611	CLA	C4-C3-C5-C6
25	B	607	CLA	C5-C6-C7-C8
25	p	610	CLA	C10-C11-C12-C13
29	D	408	LHG	C14-C15-C16-C17
29	y	2630	LHG	C31-C32-C33-C34
36	S	2631	LMG	C29-C30-C31-C32
25	5	612	CLA	CAA-CBA-CGA-O2A
25	6	611	CLA	C16-C17-C18-C20
25	Y	614	CLA	CBA-CGA-O2A-C1
35	D	413	SQD	O48-C23-C24-C25
35	d	413	SQD	O48-C23-C24-C25
24	1	606	CHL	C14-C13-C15-C16
24	3	607	CHL	C6-C7-C8-C9
24	4	601	CHL	C11-C12-C13-C14
24	5	609	CHL	C6-C7-C8-C9
24	5	609	CHL	C11-C12-C13-C14
24	R	606	CHL	C11-C10-C8-C9
24	Y	607	CHL	C14-C13-C15-C16
24	8	607	CHL	C6-C7-C8-C9
24	q	601	CHL	C11-C12-C13-C14
24	r	606	CHL	C11-C10-C8-C9
25	B	616	CLA	C14-C13-C15-C16
25	C	501	CLA	C11-C10-C8-C9
25	C	502	CLA	C14-C13-C15-C16
25	C	505	CLA	C11-C10-C8-C9
25	C	506	CLA	C11-C12-C13-C14
25	Y	613	CLA	C6-C7-C8-C9
25	0	612	CLA	C6-C7-C8-C9
25	8	603	CLA	C14-C13-C15-C16
25	9	603	CLA	C11-C10-C8-C9
25	a	405	CLA	C11-C12-C13-C14
25	b	616	CLA	C14-C13-C15-C16
25	c	506	CLA	C11-C12-C13-C14
25	y	613	CLA	C6-C7-C8-C9
25	b	609	CLA	C13-C15-C16-C17
36	C	521	LMG	C20-C21-C22-C23
24	3	601	CHL	C3A-C2A-CAA-CBA
24	3	608	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
24	S	606	CHL	C3A-C2A-CAA-CBA
24	8	608	CHL	C3A-C2A-CAA-CBA
25	4	614	CLA	C3A-C2A-CAA-CBA
25	B	609	CLA	C3A-C2A-CAA-CBA
25	b	609	CLA	C3A-C2A-CAA-CBA
25	c	503	CLA	C3A-C2A-CAA-CBA
36	S	2631	LMG	C40-C41-C42-C43
24	2	607	CHL	CAA-CBA-CGA-O2A
25	q	603	CLA	CAA-CBA-CGA-O2A
29	2	2630	LHG	O7-C7-C8-C9
25	g	602	CLA	CBD-CGD-O2D-CED
29	d	408	LHG	C14-C15-C16-C17
24	2	608	CHL	CAD-CBD-CGD-O2D
24	4	605	CHL	CAD-CBD-CGD-O2D
24	6	601	CHL	CAD-CBD-CGD-O2D
24	G	606	CHL	CAD-CBD-CGD-O2D
24	R	606	CHL	CAD-CBD-CGD-O2D
24	0	607	CHL	CAD-CBD-CGD-O2D
24	9	601	CHL	CAD-CBD-CGD-O2D
24	p	608	CHL	CAD-CBD-CGD-O2D
24	q	605	CHL	CAD-CBD-CGD-O2D
24	g	606	CHL	CAD-CBD-CGD-O2D
24	g	607	CHL	CAD-CBD-CGD-O2D
24	r	606	CHL	CAD-CBD-CGD-O2D
25	1	610	CLA	CAD-CBD-CGD-O2D
25	2	604	CLA	CAD-CBD-CGD-O2D
25	2	610	CLA	CAD-CBD-CGD-O2D
25	3	610	CLA	CAD-CBD-CGD-O2D
25	3	613	CLA	CAD-CBD-CGD-O2D
25	4	603	CLA	CAD-CBD-CGD-O2D
25	4	610	CLA	CAD-CBD-CGD-O2D
25	4	614	CLA	CAD-CBD-CGD-O2D
25	5	602	CLA	CAD-CBD-CGD-O2D
25	6	602	CLA	CAD-CBD-CGD-O2D
25	6	610	CLA	CAD-CBD-CGD-O2D
25	6	614	CLA	CAD-CBD-CGD-O2D
25	B	604	CLA	CAD-CBD-CGD-O2D
25	B	608	CLA	CAD-CBD-CGD-O2D
25	B	613	CLA	CAD-CBD-CGD-O2D
25	B	614	CLA	CAD-CBD-CGD-O2D
25	C	508	CLA	CAD-CBD-CGD-O2D
25	C	509	CLA	CAD-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	C	510	CLA	CAD-CBD-CGD-O2D
25	C	513	CLA	CAD-CBD-CGD-O2D
25	G	604	CLA	CAD-CBD-CGD-O2D
25	N	613	CLA	CAD-CBD-CGD-O2D
25	Y	610	CLA	CAD-CBD-CGD-O2D
25	0	610	CLA	CAD-CBD-CGD-O2D
25	7	610	CLA	CAD-CBD-CGD-O2D
25	8	610	CLA	CAD-CBD-CGD-O2D
25	8	613	CLA	CAD-CBD-CGD-O2D
25	9	610	CLA	CAD-CBD-CGD-O2D
25	9	612	CLA	CAD-CBD-CGD-O2D
25	9	614	CLA	CAD-CBD-CGD-O2D
25	p	604	CLA	CAD-CBD-CGD-O2D
25	b	604	CLA	CAD-CBD-CGD-O2D
25	b	613	CLA	CAD-CBD-CGD-O2D
25	b	614	CLA	CAD-CBD-CGD-O2D
25	c	508	CLA	CAD-CBD-CGD-O2D
25	c	509	CLA	CAD-CBD-CGD-O2D
25	c	510	CLA	CAD-CBD-CGD-O2D
25	c	513	CLA	CAD-CBD-CGD-O2D
25	y	610	CLA	CAD-CBD-CGD-O2D
24	q	609	CHL	CBA-CGA-O2A-C1
24	3	609	CHL	C16-C17-C18-C20
25	y	610	CLA	C16-C17-C18-C19
24	5	608	CHL	C2A-CAA-CBA-CGA
25	3	602	CLA	C2A-CAA-CBA-CGA
29	q	2630	LHG	O9-C7-O7-C5
29	L	101	LHG	C13-C14-C15-C16
24	6	608	CHL	C2-C1-O2A-CGA
25	y	604	CLA	C2-C1-O2A-CGA
24	1	605	CHL	CAA-CBA-CGA-O2A
24	3	607	CHL	CAA-CBA-CGA-O2A
24	6	607	CHL	CAA-CBA-CGA-O2A
25	q	604	CLA	CAA-CBA-CGA-O2A
25	r	616	CLA	CAA-CBA-CGA-O2A
25	0	612	CLA	CBD-CGD-O2D-CED
24	6	609	CHL	CBA-CGA-O2A-C1
24	n	609	CHL	C4-C3-C5-C6
24	y	609	CHL	C4-C3-C5-C6
25	7	604	CLA	C4-C3-C5-C6
24	n	609	CHL	C16-C17-C18-C20
25	5	612	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
37	C	524	DGD	C2B-C3B-C4B-C5B
35	D	413	SQD	O5-C1-O6-C44
35	d	413	SQD	O5-C1-O6-C44
25	1	603	CLA	C15-C16-C17-C18
24	1	609	CHL	C2-C3-C5-C6
25	A	410	CLA	C2-C3-C5-C6
25	a	410	CLA	C2-C3-C5-C6
25	c	509	CLA	C2-C3-C5-C6
25	6	603	CLA	CAA-CBA-CGA-O2A
25	R	616	CLA	CAA-CBA-CGA-O2A
25	p	613	CLA	CAA-CBA-CGA-O2A
29	q	2630	LHG	O7-C7-C8-C9
26	4	1621	LUT	C7-C8-C9-C10
26	p	1620	LUT	C31-C32-C33-C34
27	3	1622	XAT	C31-C32-C33-C34
27	4	1622	XAT	C11-C12-C13-C14
28	3	1623	NEX	C31-C32-C33-C34
28	0	1623	NEX	C11-C12-C13-C14
39	d	405	PL9	C39-C41-C42-C43
27	q	1622	XAT	O24-C26-C27-C28
28	3	1623	NEX	O24-C26-C27-C28
28	4	1623	NEX	O24-C26-C27-C28
28	5	1623	NEX	O24-C26-C27-C28
28	6	1623	NEX	O24-C26-C27-C28
28	G	1623	NEX	O24-C26-C27-C28
28	0	1623	NEX	O24-C26-C27-C28
28	8	1623	NEX	O24-C26-C27-C28
28	p	1623	NEX	O24-C26-C27-C28
28	q	1623	NEX	O24-C26-C27-C28
28	g	1623	NEX	O24-C26-C27-C28
29	l	101	LHG	C14-C15-C16-C17
37	c	524	DGD	C2B-C3B-C4B-C5B
25	Y	614	CLA	O1A-CGA-O2A-C1
24	0	607	CHL	CAA-CBA-CGA-O2A
25	0	603	CLA	CAA-CBA-CGA-O2A
25	7	612	CLA	CAA-CBA-CGA-O2A
35	b	623	SQD	O47-C7-C8-C9
24	q	605	CHL	C2-C1-O2A-CGA
29	N	2630	LHG	C23-C24-C25-C26
24	5	608	CHL	O2A-C1-C2-C3
24	Y	608	CHL	O2A-C1-C2-C3
24	5	607	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
24	1	605	CHL	CAA-CBA-CGA-O1A
25	q	611	CLA	CAA-CBA-CGA-O1A
29	6	2630	LHG	C33-C34-C35-C36
24	1	601	CHL	O2A-C1-C2-C3
24	2	601	CHL	O2A-C1-C2-C3
24	3	601	CHL	O2A-C1-C2-C3
24	6	607	CHL	O2A-C1-C2-C3
24	Y	601	CHL	O2A-C1-C2-C3
24	Y	606	CHL	O2A-C1-C2-C3
24	0	601	CHL	O2A-C1-C2-C3
24	0	607	CHL	O2A-C1-C2-C3
24	7	601	CHL	O2A-C1-C2-C3
24	8	601	CHL	O2A-C1-C2-C3
24	y	606	CHL	O2A-C1-C2-C3
25	B	603	CLA	O2A-C1-C2-C3
25	D	402	CLA	O2A-C1-C2-C3
25	R	603	CLA	O2A-C1-C2-C3
25	b	603	CLA	O2A-C1-C2-C3
25	d	402	CLA	O2A-C1-C2-C3
25	r	603	CLA	O2A-C1-C2-C3
24	9	601	CHL	C2C-C3C-CAC-CBC
29	3	2630	LHG	C11-C12-C13-C14
24	9	606	CHL	CBA-CGA-O2A-C1
25	6	604	CLA	C2A-CAA-CBA-CGA
25	8	602	CLA	C2A-CAA-CBA-CGA
25	5	602	CLA	C13-C15-C16-C17
25	B	609	CLA	C13-C15-C16-C17
25	y	614	CLA	C5-C6-C7-C8
24	S	608	CHL	CAA-CBA-CGA-O2A
24	s	608	CHL	CAA-CBA-CGA-O2A
25	5	613	CLA	CAA-CBA-CGA-O2A
25	S	602	CLA	CAA-CBA-CGA-O2A
24	7	605	CHL	CAA-CBA-CGA-O2A
25	R	616	CLA	C16-C17-C18-C19
25	r	616	CLA	C16-C17-C18-C19
25	2	603	CLA	O1A-CGA-O2A-C1
24	1	601	CHL	CHA-CBD-CGD-O1D
24	1	601	CHL	CHA-CBD-CGD-O2D
24	G	601	CHL	CHA-CBD-CGD-O1D
24	G	601	CHL	CHA-CBD-CGD-O2D
24	0	606	CHL	CHA-CBD-CGD-O2D
24	7	601	CHL	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
24	g	601	CHL	CHA-CBD-CGD-O1D
24	g	601	CHL	CHA-CBD-CGD-O2D
25	1	604	CLA	CHA-CBD-CGD-O2D
25	1	612	CLA	CHA-CBD-CGD-O1D
25	2	603	CLA	CHA-CBD-CGD-O2D
25	2	612	CLA	CHA-CBD-CGD-O1D
25	4	602	CLA	CHA-CBD-CGD-O2D
25	6	612	CLA	CHA-CBD-CGD-O2D
25	B	602	CLA	CHA-CBD-CGD-O1D
25	B	613	CLA	CHA-CBD-CGD-O1D
25	B	617	CLA	CHA-CBD-CGD-O1D
25	C	503	CLA	CHA-CBD-CGD-O1D
25	C	503	CLA	CHA-CBD-CGD-O2D
25	C	505	CLA	CHA-CBD-CGD-O1D
25	G	602	CLA	CHA-CBD-CGD-O1D
25	G	602	CLA	CHA-CBD-CGD-O2D
25	G	612	CLA	CHA-CBD-CGD-O1D
25	N	604	CLA	CHA-CBD-CGD-O2D
25	N	611	CLA	CHA-CBD-CGD-O2D
25	N	612	CLA	CHA-CBD-CGD-O1D
25	N	612	CLA	CHA-CBD-CGD-O2D
25	R	604	CLA	CHA-CBD-CGD-O1D
25	R	604	CLA	CHA-CBD-CGD-O2D
25	R	616	CLA	CHA-CBD-CGD-O2D
25	S	602	CLA	CHA-CBD-CGD-O1D
25	S	602	CLA	CHA-CBD-CGD-O2D
25	S	604	CLA	CHA-CBD-CGD-O1D
25	S	609	CLA	CHA-CBD-CGD-O1D
25	S	609	CLA	CHA-CBD-CGD-O2D
25	Y	604	CLA	CHA-CBD-CGD-O1D
25	Y	604	CLA	CHA-CBD-CGD-O2D
25	Y	612	CLA	CHA-CBD-CGD-O1D
25	Y	612	CLA	CHA-CBD-CGD-O2D
25	7	603	CLA	CHA-CBD-CGD-O2D
25	7	612	CLA	CHA-CBD-CGD-O1D
25	8	612	CLA	CHA-CBD-CGD-O2D
25	9	602	CLA	CHA-CBD-CGD-O2D
25	9	603	CLA	CHA-CBD-CGD-O2D
25	9	604	CLA	CHA-CBD-CGD-O1D
25	q	611	CLA	CHA-CBD-CGD-O2D
25	q	612	CLA	CHA-CBD-CGD-O1D
25	q	612	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
25	q	613	CLA	CHA-CBD-CGD-O1D
25	q	613	CLA	CHA-CBD-CGD-O2D
25	b	602	CLA	CHA-CBD-CGD-O1D
25	b	608	CLA	CHA-CBD-CGD-O2D
25	b	613	CLA	CHA-CBD-CGD-O1D
25	b	617	CLA	CHA-CBD-CGD-O1D
25	b	617	CLA	CHA-CBD-CGD-O2D
25	c	503	CLA	CHA-CBD-CGD-O1D
25	c	503	CLA	CHA-CBD-CGD-O2D
25	g	602	CLA	CHA-CBD-CGD-O1D
25	g	602	CLA	CHA-CBD-CGD-O2D
25	g	612	CLA	CHA-CBD-CGD-O1D
25	g	613	CLA	CHA-CBD-CGD-O1D
25	g	613	CLA	CHA-CBD-CGD-O2D
25	n	604	CLA	CHA-CBD-CGD-O2D
25	n	611	CLA	CHA-CBD-CGD-O1D
25	n	611	CLA	CHA-CBD-CGD-O2D
25	n	612	CLA	CHA-CBD-CGD-O1D
25	n	612	CLA	CHA-CBD-CGD-O2D
25	s	604	CLA	CHA-CBD-CGD-O1D
25	s	609	CLA	CHA-CBD-CGD-O1D
25	s	609	CLA	CHA-CBD-CGD-O2D
25	y	604	CLA	CHA-CBD-CGD-O1D
25	y	604	CLA	CHA-CBD-CGD-O2D
25	y	612	CLA	CHA-CBD-CGD-O1D
25	y	612	CLA	CHA-CBD-CGD-O2D
25	r	604	CLA	CHA-CBD-CGD-O1D
25	r	604	CLA	CHA-CBD-CGD-O2D
25	r	616	CLA	CHA-CBD-CGD-O2D
26	N	1621	LUT	C29-C30-C31-C32
24	7	605	CHL	CAA-CBA-CGA-O1A
24	2	609	CHL	C4-C3-C5-C6
24	p	608	CHL	CAA-CBA-CGA-O2A
25	C	501	CLA	CAA-CBA-CGA-O2A
25	G	602	CLA	CAA-CBA-CGA-O2A
36	c	521	LMG	C20-C21-C22-C23
24	1	601	CHL	C2-C3-C5-C6
24	Y	609	CHL	C2-C3-C5-C6
24	0	606	CHL	C2-C3-C5-C6
25	1	604	CLA	C2-C3-C5-C6
25	Y	614	CLA	C5-C6-C7-C8
29	l	101	LHG	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
24	Y	607	CHL	C3-C5-C6-C7
24	5	601	CHL	C10-C11-C12-C13
29	d	410	LHG	O6-C4-C5-C6
24	p	606	CHL	CAA-CBA-CGA-O1A
25	R	616	CLA	C16-C17-C18-C20
25	r	616	CLA	C16-C17-C18-C20
25	5	611	CLA	CAA-CBA-CGA-O2A
25	g	602	CLA	CAA-CBA-CGA-O2A
25	s	602	CLA	CAA-CBA-CGA-O2A
29	2	2630	LHG	O8-C23-C24-C25
35	B	623	SQD	O47-C7-C8-C9
36	C	521	LMG	O8-C28-C29-C30
36	c	521	LMG	O8-C28-C29-C30
29	3	2630	LHG	C10-C11-C12-C13
29	L	101	LHG	C14-C15-C16-C17
35	a	412	SQD	O6-C44-C45-O47
25	2	602	CLA	C13-C15-C16-C17
25	3	612	CLA	CAA-CBA-CGA-O1A
29	y	2630	LHG	O10-C23-O8-C6
25	1	612	CLA	CAA-CBA-CGA-O2A
25	3	602	CLA	CAA-CBA-CGA-O2A
25	6	612	CLA	CAA-CBA-CGA-O2A
25	R	603	CLA	CAA-CBA-CGA-O2A
25	8	602	CLA	CAA-CBA-CGA-O2A
25	r	603	CLA	CAA-CBA-CGA-O2A
37	C	520	DGD	O1G-C1A-C2A-C3A
37	c	520	DGD	O1G-C1A-C2A-C3A
36	h	102	LMG	C14-C15-C16-C17
25	4	610	CLA	C2A-CAA-CBA-CGA
25	6	603	CLA	C2A-CAA-CBA-CGA
25	0	603	CLA	C2A-CAA-CBA-CGA
25	0	611	CLA	C2A-CAA-CBA-CGA
25	y	604	CLA	C2A-CAA-CBA-CGA
25	B	615	CLA	C16-C17-C18-C20
25	Y	610	CLA	C16-C17-C18-C20
40	f	101	HEM	CAA-CBA-CGA-O1A
25	c	504	CLA	C13-C15-C16-C17
25	6	613	CLA	CBA-CGA-O2A-C1
29	p	2630	LHG	C24-C23-O8-C6
29	5	2630	LHG	C7-C8-C9-C10
36	h	102	LMG	C38-C39-C40-C41
36	H	102	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
36	h	102	LMG	C11-C10-O7-C8
25	6	613	CLA	CAA-CBA-CGA-O2A
37	C	519	DGD	O1G-C1A-C2A-C3A
37	c	519	DGD	C7A-C8A-C9A-CAA
24	N	609	CHL	C12-C13-C15-C16
24	Y	607	CHL	C12-C13-C15-C16
24	7	601	CHL	C12-C13-C15-C16
24	n	609	CHL	C12-C13-C15-C16
25	4	603	CLA	C11-C12-C13-C15
25	5	602	CLA	C11-C12-C13-C15
25	B	615	CLA	C11-C12-C13-C15
25	C	501	CLA	C11-C10-C8-C7
25	C	502	CLA	C11-C12-C13-C15
25	C	506	CLA	C12-C13-C15-C16
25	0	603	CLA	C12-C13-C15-C16
25	b	615	CLA	C11-C12-C13-C15
25	c	506	CLA	C12-C13-C15-C16
25	c	507	CLA	C6-C7-C8-C10
25	n	602	CLA	C11-C12-C13-C15
25	y	613	CLA	C6-C7-C8-C10
25	C	512	CLA	C16-C17-C18-C19
25	Y	610	CLA	C16-C17-C18-C19
25	8	610	CLA	C16-C17-C18-C20
25	2	602	CLA	CAA-CBA-CGA-O2A
25	9	602	CLA	CAA-CBA-CGA-O2A
25	c	501	CLA	CAA-CBA-CGA-O2A
37	c	519	DGD	O1G-C1A-C2A-C3A
37	c	520	DGD	O2G-C1B-C2B-C3B
29	8	2630	LHG	C10-C11-C12-C13
24	2	601	CHL	C11-C10-C8-C9
24	5	609	CHL	C14-C13-C15-C16
24	6	601	CHL	C14-C13-C15-C16
24	0	601	CHL	C14-C13-C15-C16
24	7	601	CHL	C14-C13-C15-C16
24	9	601	CHL	C6-C7-C8-C9
24	9	601	CHL	C11-C12-C13-C14
25	2	602	CLA	C11-C12-C13-C14
25	5	603	CLA	C14-C13-C15-C16
25	C	506	CLA	C14-C13-C15-C16
25	R	609	CLA	C6-C7-C8-C9
25	Y	603	CLA	C11-C10-C8-C9
25	0	604	CLA	C14-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	9	602	CLA	C6-C7-C8-C9
25	b	608	CLA	C6-C7-C8-C9
25	b	615	CLA	C11-C12-C13-C14
25	c	502	CLA	C14-C13-C15-C16
25	c	505	CLA	C11-C10-C8-C9
25	c	506	CLA	C14-C13-C15-C16
25	c	511	CLA	C11-C12-C13-C14
25	r	609	CLA	C6-C7-C8-C9
28	5	1623	NEX	C13-C14-C15-C35
29	Y	2630	LHG	C33-C34-C35-C36
24	p	608	CHL	O2A-C1-C2-C3
24	y	608	CHL	O2A-C1-C2-C3
25	S	610	CLA	O2A-C1-C2-C3
25	n	614	CLA	O2A-C1-C2-C3
25	s	610	CLA	O2A-C1-C2-C3
25	9	603	CLA	O1A-CGA-O2A-C1
24	N	607	CHL	CAA-CBA-CGA-O2A
24	7	606	CHL	CAA-CBA-CGA-O2A
25	C	510	CLA	CAA-CBA-CGA-O2A
29	4	2630	LHG	O7-C7-C8-C9
29	9	2630	LHG	O7-C7-C8-C9
24	2	607	CHL	CAA-CBA-CGA-O1A
35	B	623	SQD	C4-C5-C6-S
35	b	623	SQD	C4-C5-C6-S
25	B	604	CLA	C16-C17-C18-C19
25	b	615	CLA	C16-C17-C18-C20
25	q	603	CLA	O1A-CGA-O2A-C1
24	4	607	CHL	C2A-CAA-CBA-CGA
24	8	606	CHL	C2A-CAA-CBA-CGA
25	5	610	CLA	C2A-CAA-CBA-CGA
25	B	608	CLA	C2A-CAA-CBA-CGA
25	S	611	CLA	C2A-CAA-CBA-CGA
25	Y	604	CLA	C2A-CAA-CBA-CGA
24	9	607	CHL	CAA-CBA-CGA-O1A
25	4	603	CLA	CAA-CBA-CGA-O1A
25	p	613	CLA	CAA-CBA-CGA-O1A
36	c	521	LMG	C17-C18-C19-C20
24	5	605	CHL	CAA-CBA-CGA-O2A
24	q	605	CHL	CAA-CBA-CGA-O2A
25	c	510	CLA	CAA-CBA-CGA-O2A
29	0	2630	LHG	O8-C23-C24-C25
37	C	520	DGD	O2G-C1B-C2B-C3B

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Mol	Chain	Res	Type	Atoms
25	2	603	CLA	CBA-CGA-O2A-C1
36	A	413	LMG	C29-C28-O8-C9
36	a	413	LMG	C29-C28-O8-C9
24	N	606	CHL	CAA-CBA-CGA-O1A
24	n	606	CHL	CAA-CBA-CGA-O1A
26	2	1621	LUT	C11-C12-C13-C20
29	q	2630	LHG	C23-C24-C25-C26
24	1	606	CHL	CAA-CBA-CGA-O1A
25	0	603	CLA	CAA-CBA-CGA-O1A
35	D	413	SQD	O10-C23-C24-C25
25	C	512	CLA	C10-C11-C12-C13
37	C	519	DGD	C7A-C8A-C9A-CAA
24	6	606	CHL	C2-C3-C5-C6
25	1	610	CLA	C2-C3-C5-C6
24	4	605	CHL	CAA-CBA-CGA-O2A
25	0	612	CLA	CAA-CBA-CGA-O2A
25	C	504	CLA	C13-C15-C16-C17
35	d	413	SQD	O10-C23-C24-C25
26	5	1620	LUT	C7-C8-C9-C10
26	N	1621	LUT	C7-C8-C9-C10
26	n	1621	LUT	C7-C8-C9-C10
28	9	1623	NEX	C31-C32-C33-C34
28	p	1623	NEX	C11-C12-C13-C14
24	5	605	CHL	CBA-CGA-O2A-C1
25	C	508	CLA	CBA-CGA-O2A-C1
29	8	2630	LHG	C24-C23-O8-C6
29	n	2630	LHG	C14-C15-C16-C17
35	B	621	SQD	C24-C25-C26-C27
35	b	621	SQD	C24-C25-C26-C27
24	3	601	CHL	C1A-C2A-CAA-CBA
24	4	606	CHL	C1A-C2A-CAA-CBA
24	5	608	CHL	C1A-C2A-CAA-CBA
24	Y	601	CHL	C1A-C2A-CAA-CBA
24	p	608	CHL	C1A-C2A-CAA-CBA
24	y	601	CHL	C1A-C2A-CAA-CBA
25	2	602	CLA	C1A-C2A-CAA-CBA
25	3	610	CLA	C1A-C2A-CAA-CBA
25	4	613	CLA	C1A-C2A-CAA-CBA
25	5	612	CLA	C1A-C2A-CAA-CBA
25	6	604	CLA	C1A-C2A-CAA-CBA
25	B	609	CLA	C1A-C2A-CAA-CBA
25	0	613	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	b	609	CLA	C1A-C2A-CAA-CBA
29	C	2630	LHG	C1-C2-C3-O3
29	N	2630	LHG	C1-C2-C3-O3
29	7	2630	LHG	C1-C2-C3-O3
29	S	2630	LHG	C32-C33-C34-C35
29	q	2630	LHG	C10-C11-C12-C13
24	0	607	CHL	CAA-CBA-CGA-O1A
24	7	606	CHL	CAA-CBA-CGA-O1A
25	R	616	CLA	CAA-CBA-CGA-O1A
25	q	604	CLA	CAA-CBA-CGA-O1A
36	a	413	LMG	C29-C30-C31-C32
25	Y	604	CLA	C2-C1-O2A-CGA
36	H	102	LMG	C29-C30-C31-C32
25	3	613	CLA	C8-C10-C11-C12
25	6	603	CLA	CBA-CGA-O2A-C1
25	C	507	CLA	CBA-CGA-O2A-C1
25	9	603	CLA	CBA-CGA-O2A-C1
25	q	603	CLA	CBA-CGA-O2A-C1
24	q	605	CHL	CAA-CBA-CGA-O1A
25	5	613	CLA	CAA-CBA-CGA-O1A
25	6	603	CLA	CAA-CBA-CGA-O1A
25	7	612	CLA	CAA-CBA-CGA-O1A
25	q	603	CLA	CAA-CBA-CGA-O1A
25	r	616	CLA	CAA-CBA-CGA-O1A
36	C	521	LMG	C17-C18-C19-C20
24	5	601	CHL	CAA-CBA-CGA-O2A
24	R	607	CHL	CAA-CBA-CGA-O2A
24	r	607	CHL	CAA-CBA-CGA-O2A
25	5	602	CLA	CAA-CBA-CGA-O2A
25	7	602	CLA	CAA-CBA-CGA-O2A
25	p	602	CLA	CAA-CBA-CGA-O2A
36	C	521	LMG	C35-C36-C37-C38
25	b	608	CLA	C2A-CAA-CBA-CGA
24	p	608	CHL	CAA-CBA-CGA-O1A
25	c	510	CLA	CAA-CBA-CGA-O1A
25	n	603	CLA	C13-C15-C16-C17
36	A	413	LMG	C29-C30-C31-C32
36	c	521	LMG	C35-C36-C37-C38
25	9	603	CLA	CAA-CBA-CGA-O2A
25	B	608	CLA	C10-C11-C12-C13
25	8	613	CLA	C8-C10-C11-C12
29	6	2630	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
25	9	602	CLA	C3-C5-C6-C7
25	2	602	CLA	CAA-CBA-CGA-O1A
25	C	510	CLA	CAA-CBA-CGA-O1A
37	c	520	DGD	O1B-C1B-C2B-C3B
25	6	603	CLA	O1A-CGA-O2A-C1
35	D	413	SQD	C2-C1-O6-C44
24	8	607	CHL	C5-C6-C7-C8
25	n	603	CLA	C10-C11-C12-C13
36	H	102	LMG	C14-C15-C16-C17
29	1	2630	LHG	C3-O3-P-O5
29	4	2630	LHG	C3-O3-P-O5
29	5	2630	LHG	C3-O3-P-O5
29	L	101	LHG	C3-O3-P-O4
29	Y	2630	LHG	C3-O3-P-O5
29	0	2630	LHG	C3-O3-P-O5
29	7	2630	LHG	C3-O3-P-O5
24	2	601	CHL	C4C-C3C-CAC-CBC
24	6	607	CHL	CAA-CBA-CGA-O1A
24	S	608	CHL	CAA-CBA-CGA-O1A
24	p	607	CHL	CAA-CBA-CGA-O1A
24	s	608	CHL	CAA-CBA-CGA-O1A
25	3	602	CLA	CAA-CBA-CGA-O1A
25	C	501	CLA	CAA-CBA-CGA-O1A
25	G	602	CLA	CAA-CBA-CGA-O1A
25	R	603	CLA	CAA-CBA-CGA-O1A
25	S	602	CLA	CAA-CBA-CGA-O1A
25	s	602	CLA	CAA-CBA-CGA-O1A
29	2	2630	LHG	O9-C7-C8-C9
29	6	2630	LHG	O10-C23-C24-C25
29	0	2630	LHG	O10-C23-C24-C25
29	q	2630	LHG	O9-C7-C8-C9
36	c	521	LMG	O10-C28-C29-C30
37	C	519	DGD	O1A-C1A-C2A-C3A
37	C	520	DGD	O1B-C1B-C2B-C3B
37	c	519	DGD	O1A-C1A-C2A-C3A
25	2	604	CLA	O2A-C1-C2-C3
25	N	614	CLA	O2A-C1-C2-C3
25	9	604	CLA	O2A-C1-C2-C3
25	7	611	CLA	CAA-CBA-CGA-O2A
25	8	604	CLA	CAA-CBA-CGA-O2A
26	R	620	LUT	C5-C6-C7-C8
26	g	1621	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	y	1620	LUT	C5-C6-C7-C8
26	r	620	LUT	C5-C6-C7-C8
34	C	516	BCR	C5-C6-C7-C8
34	c	516	BCR	C5-C6-C7-C8
25	6	613	CLA	CAA-CBA-CGA-O1A
25	9	602	CLA	CAA-CBA-CGA-O1A
25	r	603	CLA	CAA-CBA-CGA-O1A
29	9	2630	LHG	O9-C7-C8-C9
35	B	623	SQD	O49-C7-C8-C9
35	b	623	SQD	O49-C7-C8-C9
36	C	521	LMG	O10-C28-C29-C30
24	3	601	CHL	CAA-CBA-CGA-O2A
25	B	608	CLA	CAA-CBA-CGA-O2A
25	S	605	CLA	CAA-CBA-CGA-O2A
24	1	607	CHL	C16-C17-C18-C20
29	q	2630	LHG	C24-C25-C26-C27
25	2	614	CLA	C2A-CAA-CBA-CGA
25	9	613	CLA	C2A-CAA-CBA-CGA
25	9	614	CLA	C2A-CAA-CBA-CGA
25	q	610	CLA	C2A-CAA-CBA-CGA
25	c	501	CLA	CAA-CBA-CGA-O1A
24	y	609	CHL	C4C-C3C-CAC-CBC
25	q	602	CLA	CAA-CBA-CGA-O2A
25	g	602	CLA	CAA-CBA-CGA-O1A
24	8	607	CHL	C2-C3-C5-C6
24	7	601	CHL	C16-C17-C18-C19
29	g	2630	LHG	C29-C30-C31-C32
24	g	609	CHL	CAD-CBD-CGD-O1D
25	B	613	CLA	CAD-CBD-CGD-O1D
25	C	505	CLA	CAD-CBD-CGD-O1D
25	S	602	CLA	CAD-CBD-CGD-O1D
25	S	604	CLA	CAD-CBD-CGD-O1D
25	9	604	CLA	CAD-CBD-CGD-O1D
25	q	602	CLA	CAD-CBD-CGD-O1D
25	b	613	CLA	CAD-CBD-CGD-O1D
25	c	505	CLA	CAD-CBD-CGD-O1D
25	g	613	CLA	CAD-CBD-CGD-O1D
35	b	623	SQD	C5-C6-S-O7
37	C	520	DGD	O1A-C1A-C2A-C3A
37	c	520	DGD	O1A-C1A-C2A-C3A
25	b	604	CLA	C13-C15-C16-C17
29	C	2630	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
24	6	609	CHL	C11-C10-C8-C9
24	Y	606	CHL	C11-C10-C8-C9
24	y	601	CHL	C6-C7-C8-C9
24	y	606	CHL	C11-C10-C8-C9
25	2	603	CLA	C11-C10-C8-C9
25	5	602	CLA	C11-C12-C13-C14
25	5	604	CLA	C14-C13-C15-C16
25	5	610	CLA	C11-C10-C8-C9
25	A	410	CLA	C6-C7-C8-C9
25	B	604	CLA	C6-C7-C8-C9
25	B	615	CLA	C11-C12-C13-C14
25	0	603	CLA	C14-C13-C15-C16
25	a	410	CLA	C6-C7-C8-C9
25	b	604	CLA	C6-C7-C8-C9
25	c	501	CLA	C11-C10-C8-C9
25	c	502	CLA	C11-C12-C13-C14
25	c	507	CLA	C6-C7-C8-C9
25	6	604	CLA	C8-C10-C11-C12
25	0	603	CLA	O1A-CGA-O2A-C1
25	5	611	CLA	CAA-CBA-CGA-O1A
25	4	602	CLA	C3-C5-C6-C7
24	1	601	CHL	CAA-CBA-CGA-O2A
24	9	601	CHL	CAA-CBA-CGA-O2A
24	p	601	CHL	CAA-CBA-CGA-O2A
25	4	602	CLA	CAA-CBA-CGA-O2A
25	4	604	CLA	CAA-CBA-CGA-O2A
25	B	609	CLA	CAA-CBA-CGA-O2A
25	0	610	CLA	CAA-CBA-CGA-O2A
25	0	613	CLA	CAA-CBA-CGA-O2A
25	p	604	CLA	CAA-CBA-CGA-O2A
25	n	602	CLA	CAA-CBA-CGA-O2A
29	L	101	LHG	O7-C7-C8-C9
25	N	603	CLA	C13-C15-C16-C17
25	b	608	CLA	C10-C11-C12-C13
25	3	612	CLA	CAA-CBA-CGA-O2A
40	f	101	HEM	CAA-CBA-CGA-O2A
29	G	2630	LHG	C29-C30-C31-C32
24	p	601	CHL	C2A-CAA-CBA-CGA
25	2	610	CLA	C2A-CAA-CBA-CGA
24	Y	609	CHL	C4C-C3C-CAC-CBC
29	6	2630	LHG	C13-C14-C15-C16
29	L	101	LHG	C25-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
24	4	606	CHL	CAA-CBA-CGA-O2A
24	7	601	CHL	CAA-CBA-CGA-O2A
24	8	601	CHL	CAA-CBA-CGA-O2A
25	2	603	CLA	CAA-CBA-CGA-O2A
25	N	602	CLA	CAA-CBA-CGA-O2A
25	S	613	CLA	CAA-CBA-CGA-O2A
25	Y	602	CLA	CAA-CBA-CGA-O2A
25	b	609	CLA	CAA-CBA-CGA-O2A
25	s	613	CLA	CAA-CBA-CGA-O2A
25	y	602	CLA	CAA-CBA-CGA-O2A
29	S	2630	LHG	O7-C7-C8-C9
29	l	101	LHG	O7-C7-C8-C9
24	9	606	CHL	O1A-CGA-O2A-C1
25	4	604	CLA	O1A-CGA-O2A-C1
29	1	2630	LHG	C1-C2-C3-O3
24	8	609	CHL	C5-C6-C7-C8
25	R	609	CLA	C4C-C3C-CAC-CBC
25	y	603	CLA	C3-C5-C6-C7
25	8	602	CLA	CAA-CBA-CGA-O1A
25	p	602	CLA	CAA-CBA-CGA-O1A
29	s	2630	LHG	C32-C33-C34-C35
25	b	604	CLA	C16-C17-C18-C19
29	0	2630	LHG	C5-C4-O6-P
29	7	2630	LHG	C5-C4-O6-P
29	n	2630	LHG	C5-C4-O6-P
25	B	604	CLA	C13-C15-C16-C17
29	y	2630	LHG	C11-C12-C13-C14
25	C	508	CLA	O1A-CGA-O2A-C1
24	4	606	CHL	C3A-C2A-CAA-CBA
24	R	608	CHL	C3A-C2A-CAA-CBA
24	Y	606	CHL	C12-C13-C15-C16
24	7	601	CHL	C6-C7-C8-C10
24	7	606	CHL	C12-C13-C15-C16
24	9	601	CHL	C11-C12-C13-C15
24	p	605	CHL	C11-C12-C13-C15
24	q	601	CHL	C6-C7-C8-C10
24	n	601	CHL	C12-C13-C15-C16
24	s	606	CHL	C3A-C2A-CAA-CBA
24	y	606	CHL	C12-C13-C15-C16
24	y	609	CHL	C12-C13-C15-C16
24	r	608	CHL	C3A-C2A-CAA-CBA
25	2	603	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
25	5	610	CLA	C11-C10-C8-C7
25	5	612	CLA	C3A-C2A-CAA-CBA
25	B	603	CLA	C3A-C2A-CAA-CBA
25	B	604	CLA	C6-C7-C8-C10
25	B	612	CLA	C12-C13-C15-C16
25	C	503	CLA	C3A-C2A-CAA-CBA
25	C	513	CLA	C3A-C2A-CAA-CBA
25	N	610	CLA	C6-C7-C8-C10
25	R	609	CLA	C6-C7-C8-C10
25	R	616	CLA	C12-C13-C15-C16
25	9	602	CLA	C6-C7-C8-C10
25	q	614	CLA	C3A-C2A-CAA-CBA
25	b	603	CLA	C3A-C2A-CAA-CBA
25	b	604	CLA	C6-C7-C8-C10
25	b	612	CLA	C12-C13-C15-C16
25	c	501	CLA	C11-C10-C8-C7
25	c	512	CLA	C2-C3-C5-C6
25	n	610	CLA	C6-C7-C8-C10
25	r	609	CLA	C6-C7-C8-C10
25	r	616	CLA	C12-C13-C15-C16
24	R	607	CHL	CAA-CBA-CGA-O1A
24	r	607	CHL	CAA-CBA-CGA-O1A
25	5	602	CLA	CAA-CBA-CGA-O1A
25	6	612	CLA	CAA-CBA-CGA-O1A
24	5	608	CHL	CAA-CBA-CGA-O2A
24	6	606	CHL	CAA-CBA-CGA-O2A
24	n	607	CHL	CAA-CBA-CGA-O2A
24	n	608	CHL	CAA-CBA-CGA-O2A
25	6	610	CLA	CAA-CBA-CGA-O2A
25	B	614	CLA	CAA-CBA-CGA-O2A
25	b	608	CLA	CAA-CBA-CGA-O2A
25	b	614	CLA	CAA-CBA-CGA-O2A
29	D	409	LHG	O7-C7-C8-C9
29	d	409	LHG	O7-C7-C8-C9
29	g	2630	LHG	O8-C23-C24-C25
29	s	2630	LHG	O7-C7-C8-C9
24	g	601	CHL	C8-C10-C11-C12
25	r	609	CLA	C4C-C3C-CAC-CBC
26	1	1621	LUT	C11-C12-C13-C14
26	2	1621	LUT	C11-C12-C13-C14
26	3	1620	LUT	C31-C32-C33-C34
26	5	1620	LUT	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	G	1620	LUT	C27-C28-C29-C30
26	g	1620	LUT	C27-C28-C29-C30
34	B	618	BCR	C17-C18-C19-C20
34	b	618	BCR	C17-C18-C19-C20
24	5	601	CHL	CAA-CBA-CGA-O1A
25	4	604	CLA	CAA-CBA-CGA-O1A
25	B	609	CLA	CAA-CBA-CGA-O1A
25	0	612	CLA	CAA-CBA-CGA-O1A
25	7	602	CLA	CAA-CBA-CGA-O1A
25	9	603	CLA	CAA-CBA-CGA-O1A
29	S	2630	LHG	O9-C7-C8-C9
24	9	605	CHL	C2-C1-O2A-CGA
24	7	607	CHL	C16-C17-C18-C20
25	B	615	CLA	C16-C17-C18-C19
25	8	610	CLA	C16-C17-C18-C19
25	3	604	CLA	CAA-CBA-CGA-O2A
25	8	603	CLA	CAA-CBA-CGA-O2A
29	Y	2630	LHG	C17-C18-C19-C20
24	n	609	CHL	C15-C16-C17-C18
25	Y	612	CLA	C5-C6-C7-C8
25	c	509	CLA	C13-C15-C16-C17
29	d	410	LHG	C33-C34-C35-C36
24	7	601	CHL	CAA-CBA-CGA-O1A
25	1	612	CLA	CAA-CBA-CGA-O1A
25	6	610	CLA	CAA-CBA-CGA-O1A
25	Y	602	CLA	CAA-CBA-CGA-O1A
25	b	609	CLA	CAA-CBA-CGA-O1A
29	s	2630	LHG	O9-C7-C8-C9
40	F	101	HEM	CAA-CBA-CGA-O2A
25	C	509	CLA	C13-C15-C16-C17
25	9	610	CLA	C10-C11-C12-C13
24	2	605	CHL	C2-C1-O2A-CGA
29	D	410	LHG	C33-C34-C35-C36
29	y	2630	LHG	C33-C34-C35-C36
24	2	606	CHL	CAA-CBA-CGA-O2A
24	G	605	CHL	CAA-CBA-CGA-O2A
29	G	2630	LHG	O8-C23-C24-C25
24	8	607	CHL	C4C-C3C-CAC-CBC
36	B	622	LMG	C38-C39-C40-C41
24	7	609	CHL	C10-C11-C12-C13
25	y	612	CLA	C5-C6-C7-C8
25	s	613	CLA	CAA-CBA-CGA-O1A

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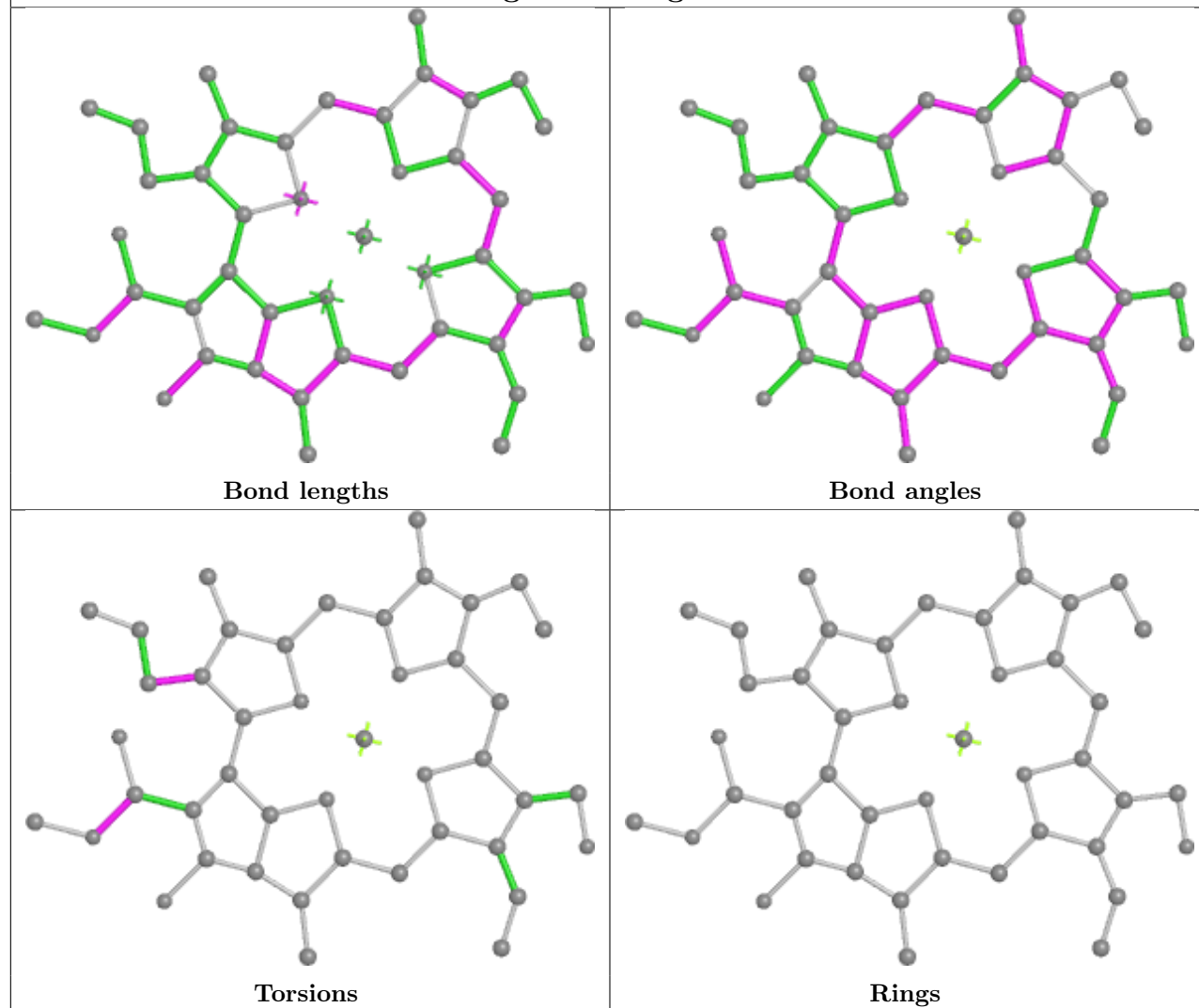
Mol	Chain	Res	Type	Atoms
25	y	602	CLA	CAA-CBA-CGA-O1A
29	4	2630	LHG	O9-C7-C8-C9
25	2	613	CLA	C2A-CAA-CBA-CGA
25	S	604	CLA	C2A-CAA-CBA-CGA
25	s	604	CLA	C2A-CAA-CBA-CGA
25	r	611	CLA	C2A-CAA-CBA-CGA
24	n	609	CHL	C16-C17-C18-C19
24	n	606	CHL	CAA-CBA-CGA-O2A
25	p	602	CLA	C15-C16-C17-C18
24	4	606	CHL	CAA-CBA-CGA-O1A
25	S	613	CLA	CAA-CBA-CGA-O1A
25	0	610	CLA	CAA-CBA-CGA-O1A
25	5	604	CLA	CAA-CBA-CGA-O2A
24	N	606	CHL	CAA-CBA-CGA-O2A

There are no ring outliers.

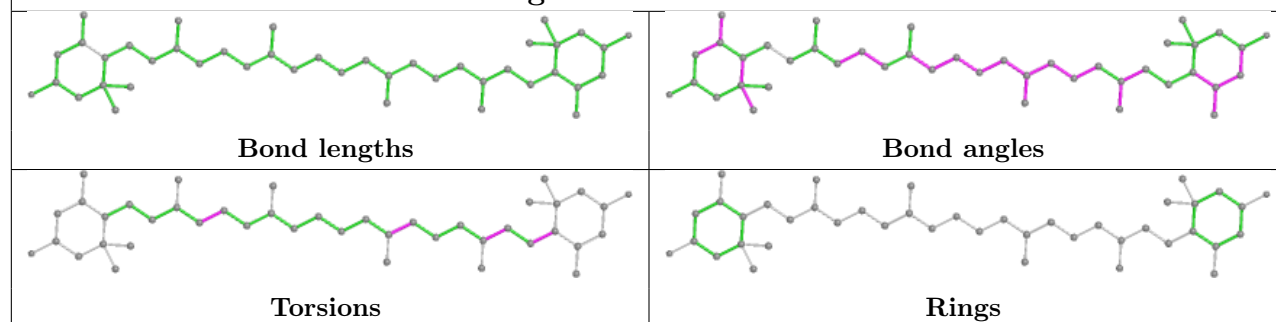
No monomer is involved in short contacts.

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.

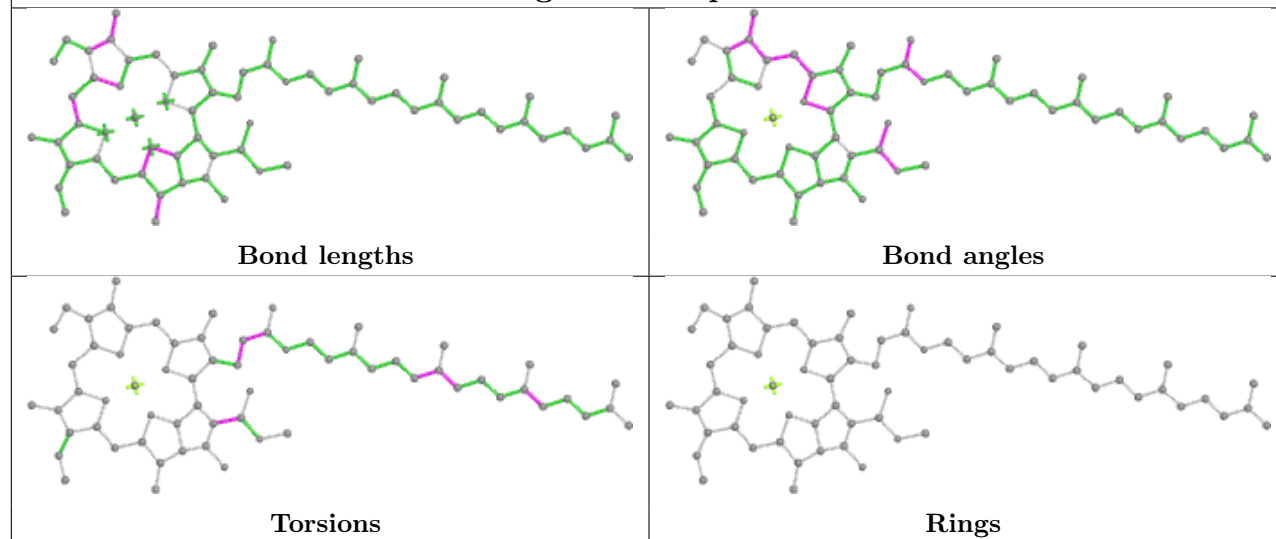
Ligand CHL g 608



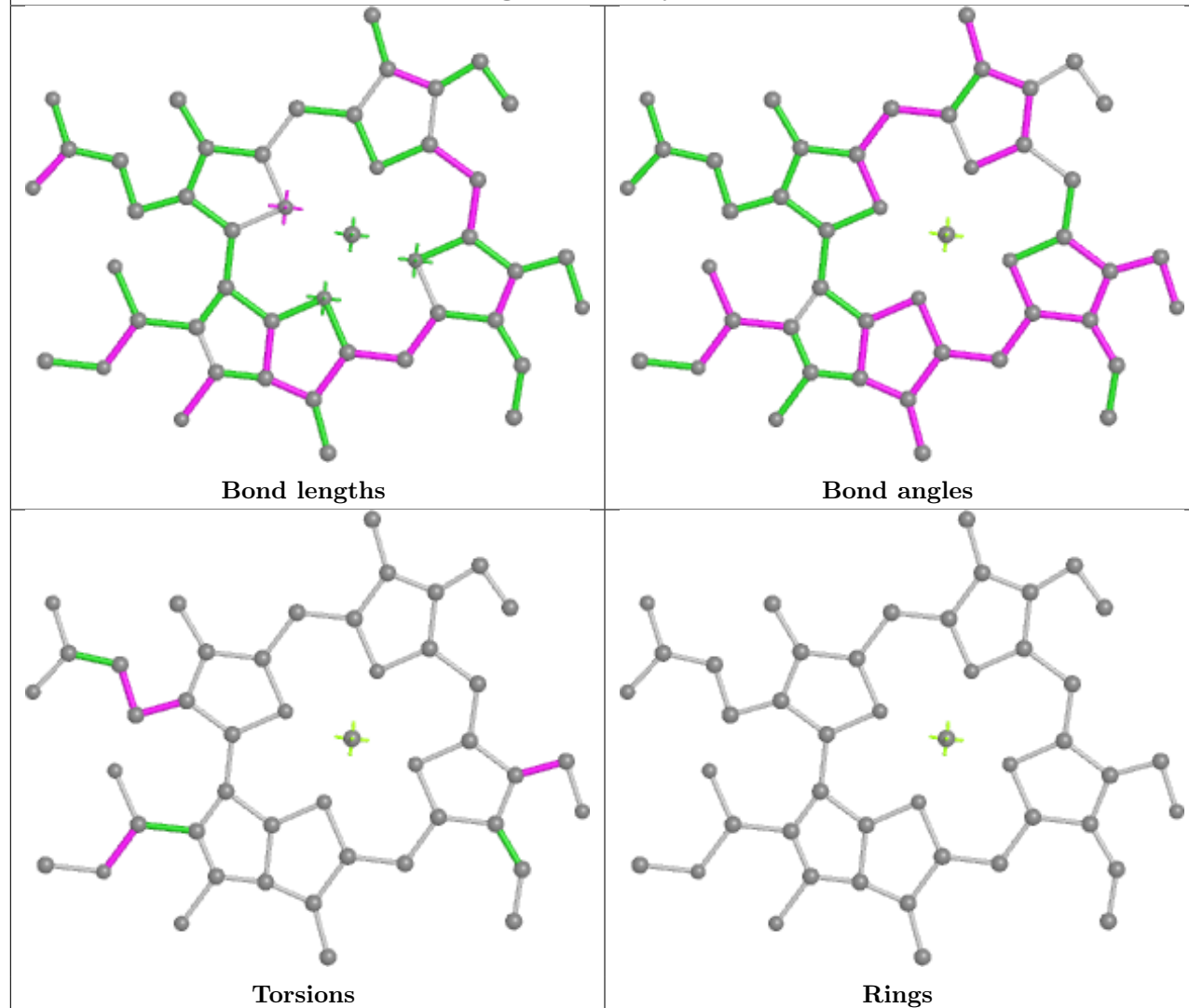
Ligand LUT 4 1621

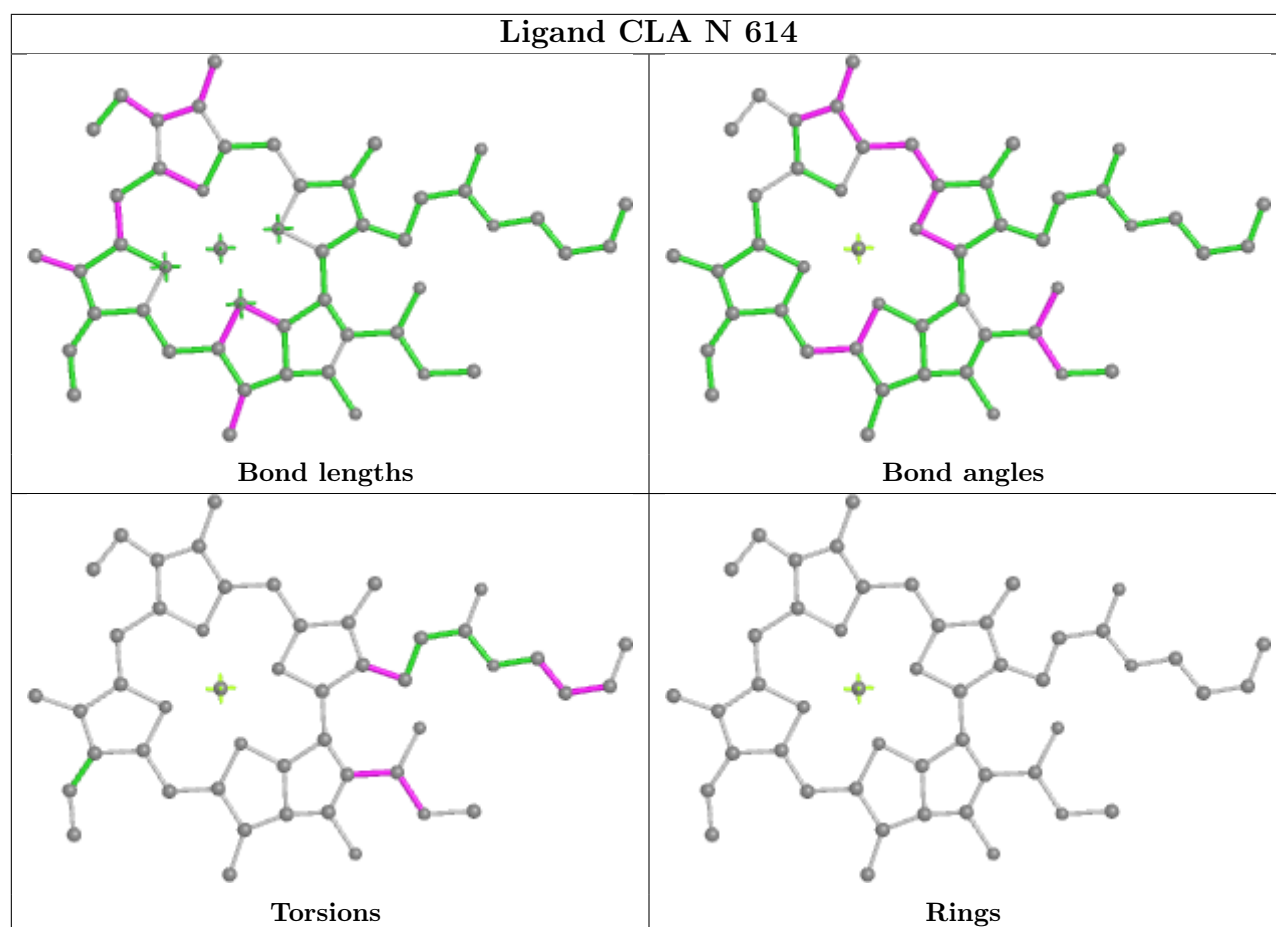


Ligand CLA p 613

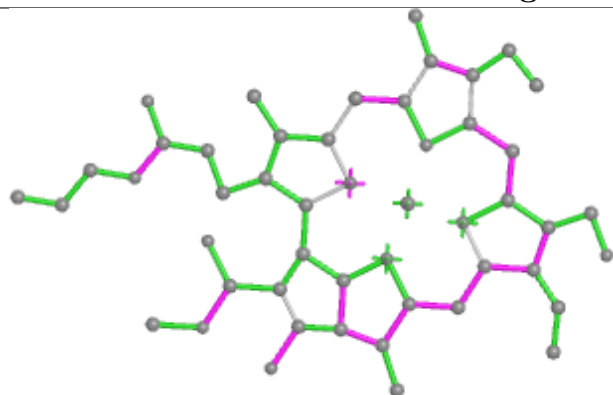


Ligand CHL y 605

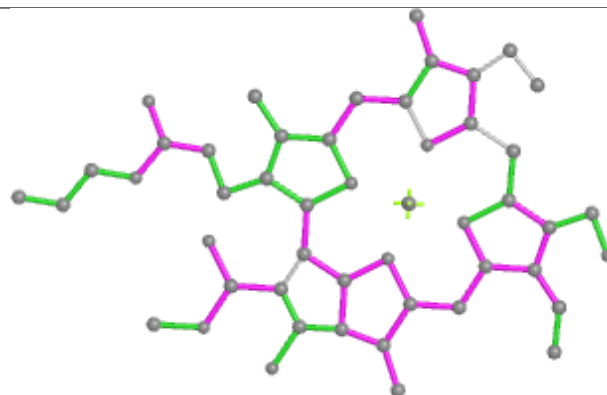




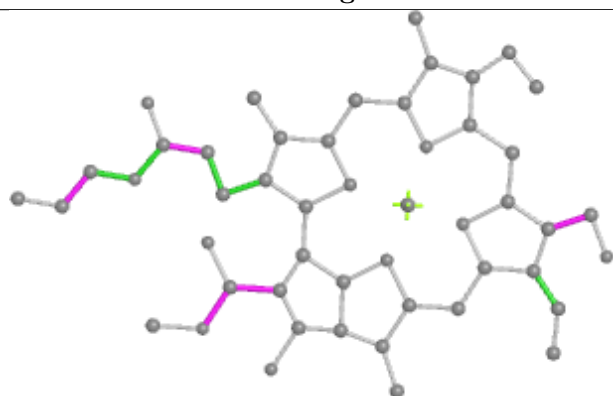
Ligand CHL s 608



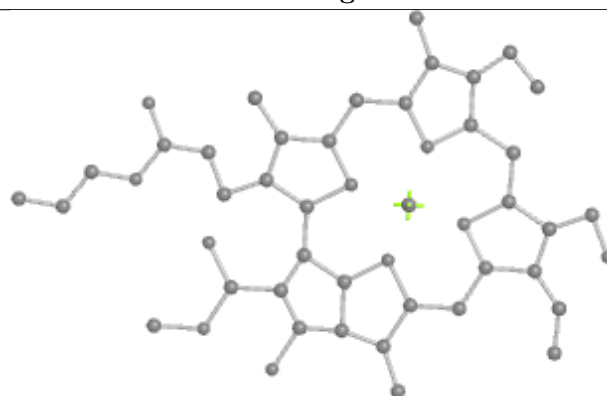
Bond lengths



Bond angles

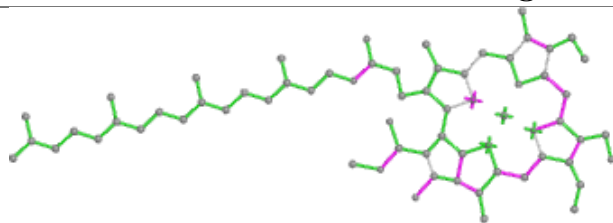


Torsions

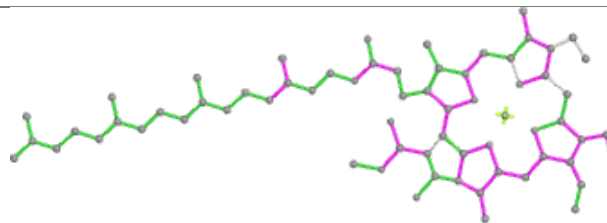


Rings

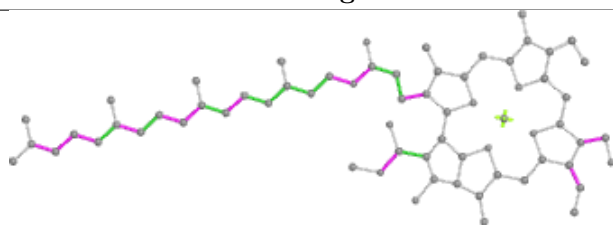
Ligand CHL 8 609



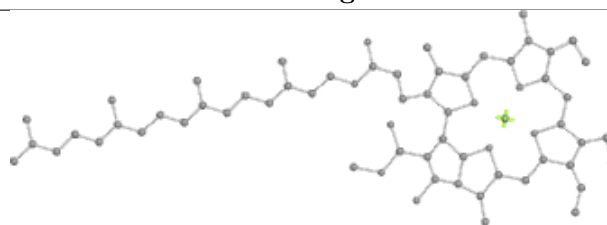
Bond lengths



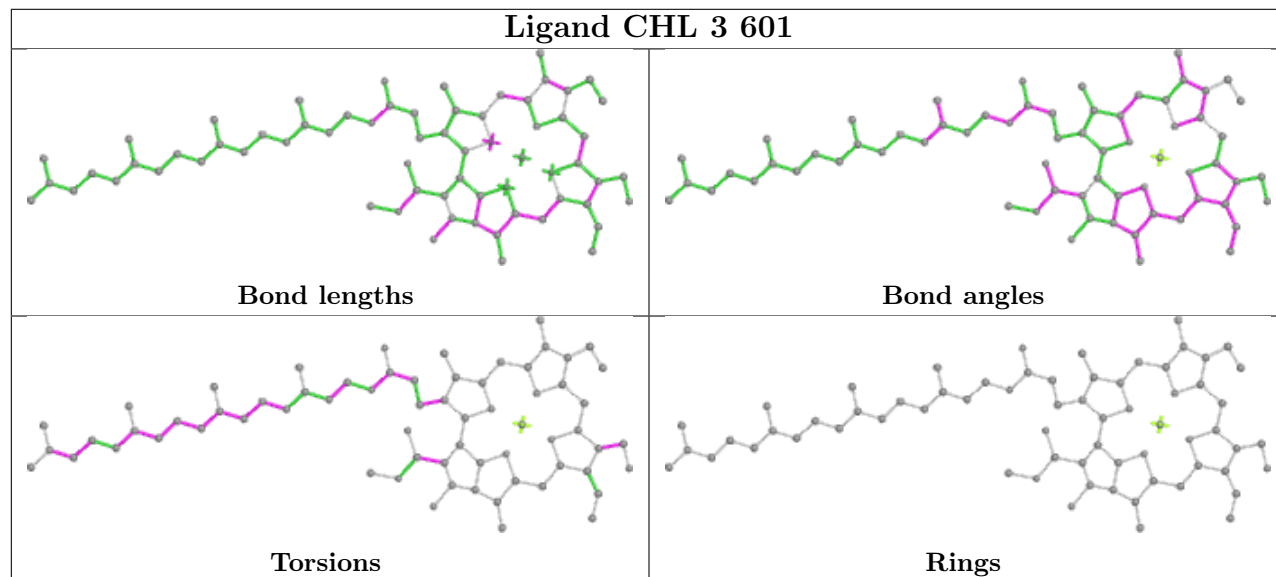
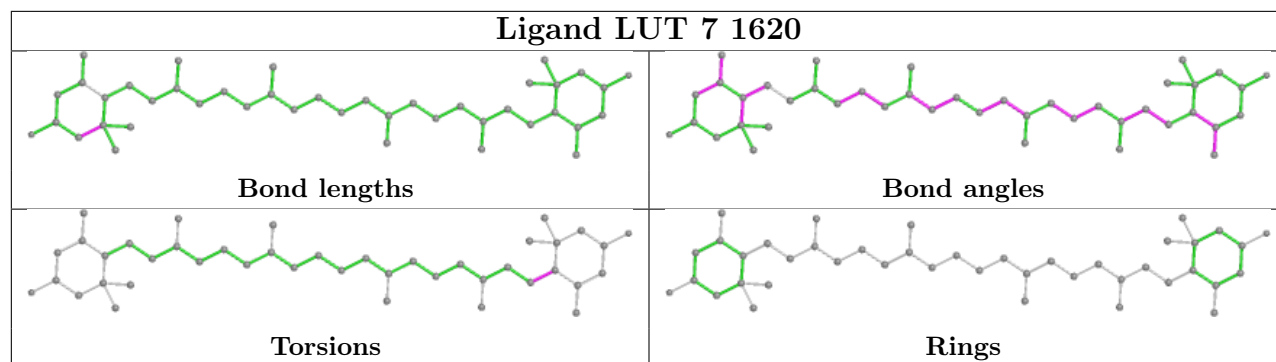
Bond angles



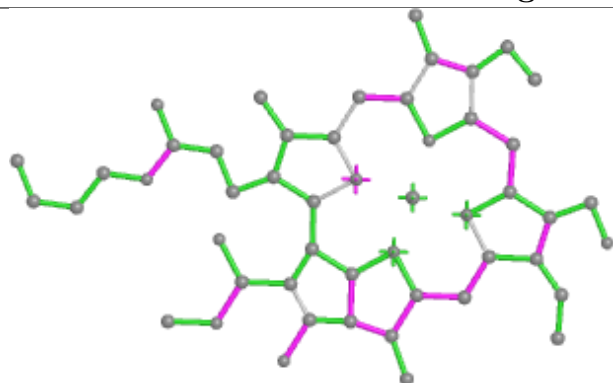
Torsions



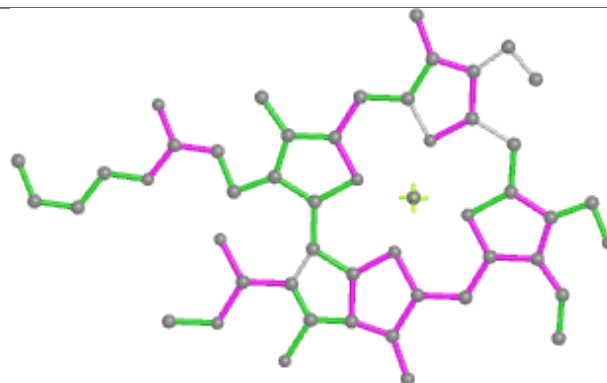
Rings



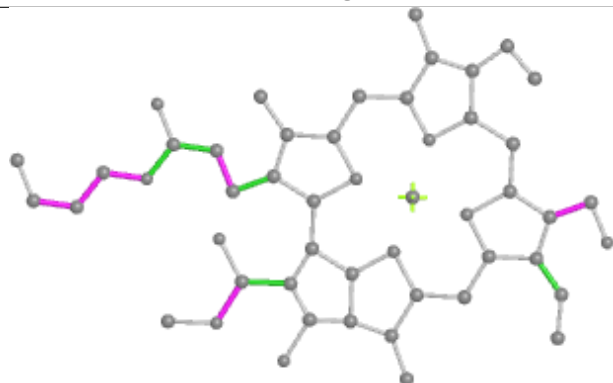
Ligand CHL 6 608



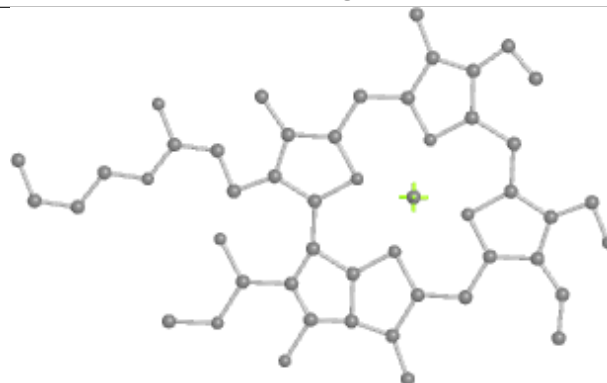
Bond lengths



Bond angles

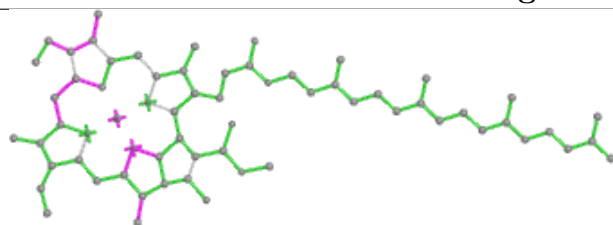


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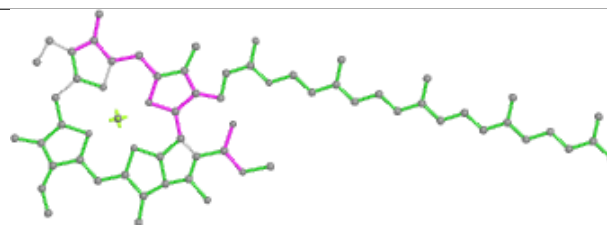


Rings

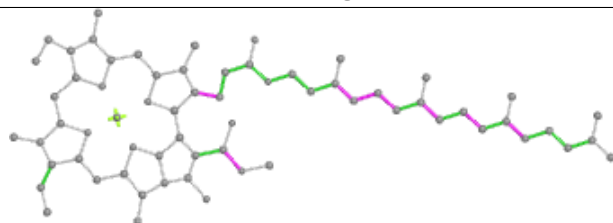
Ligand CLA 3 603



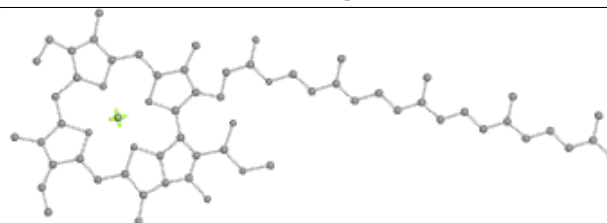
Bond lengths



Bond angles

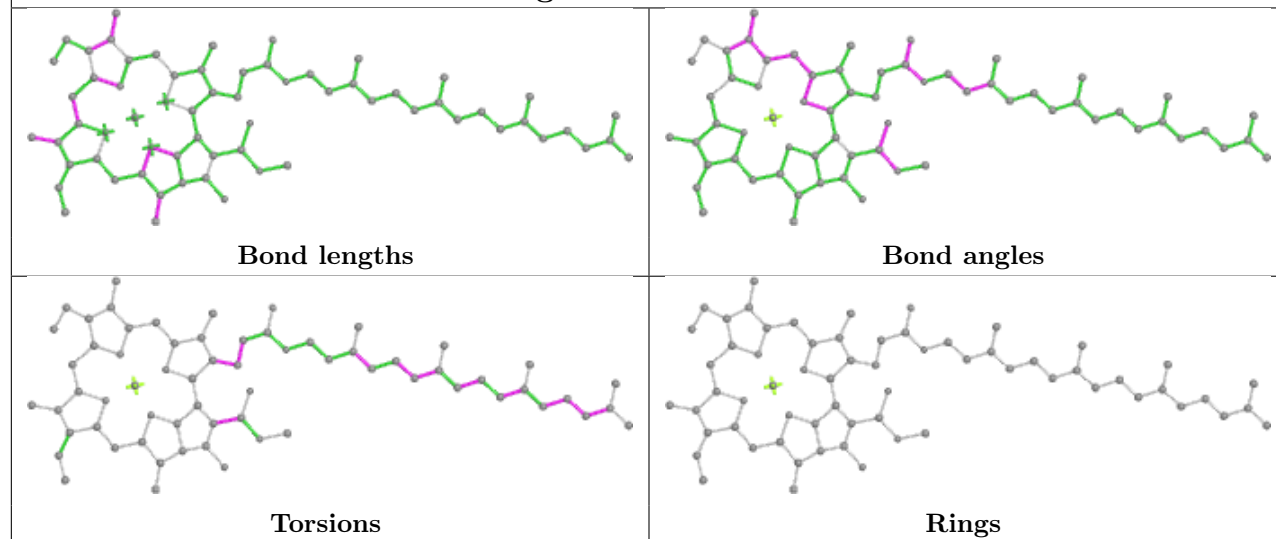


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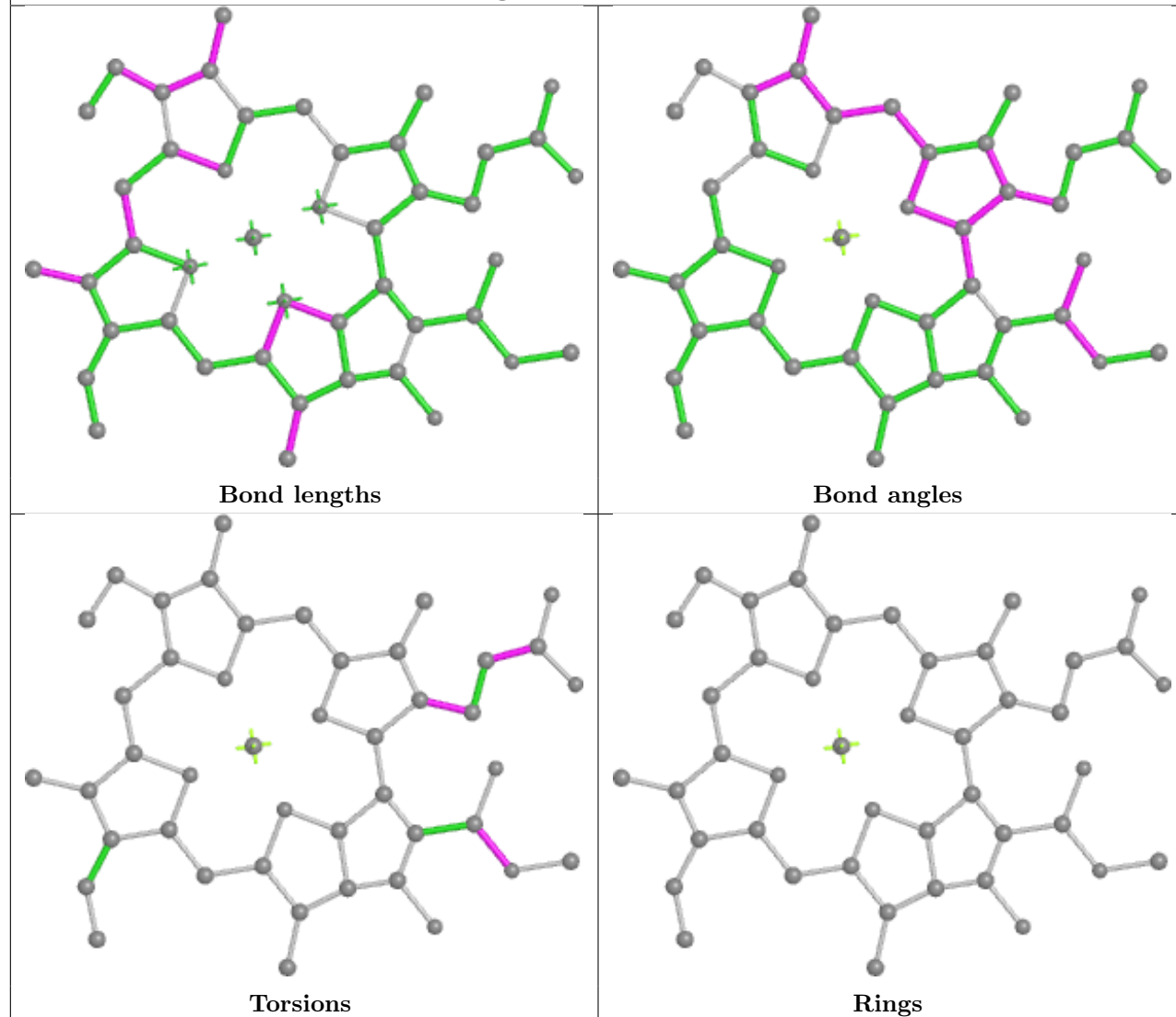


Rings

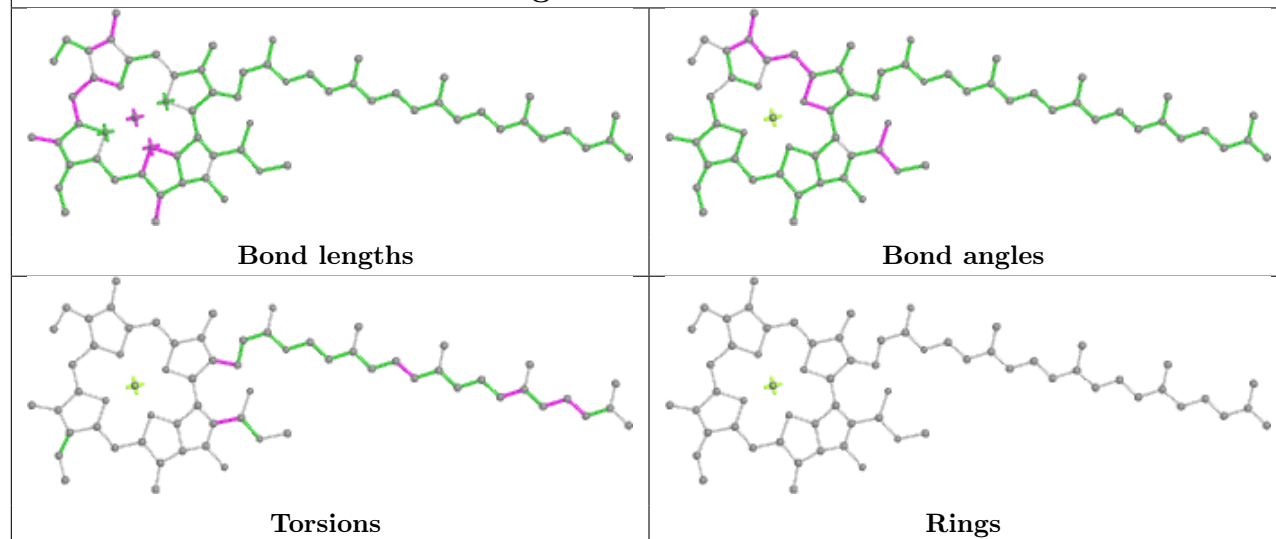
Ligand CLA 7 610



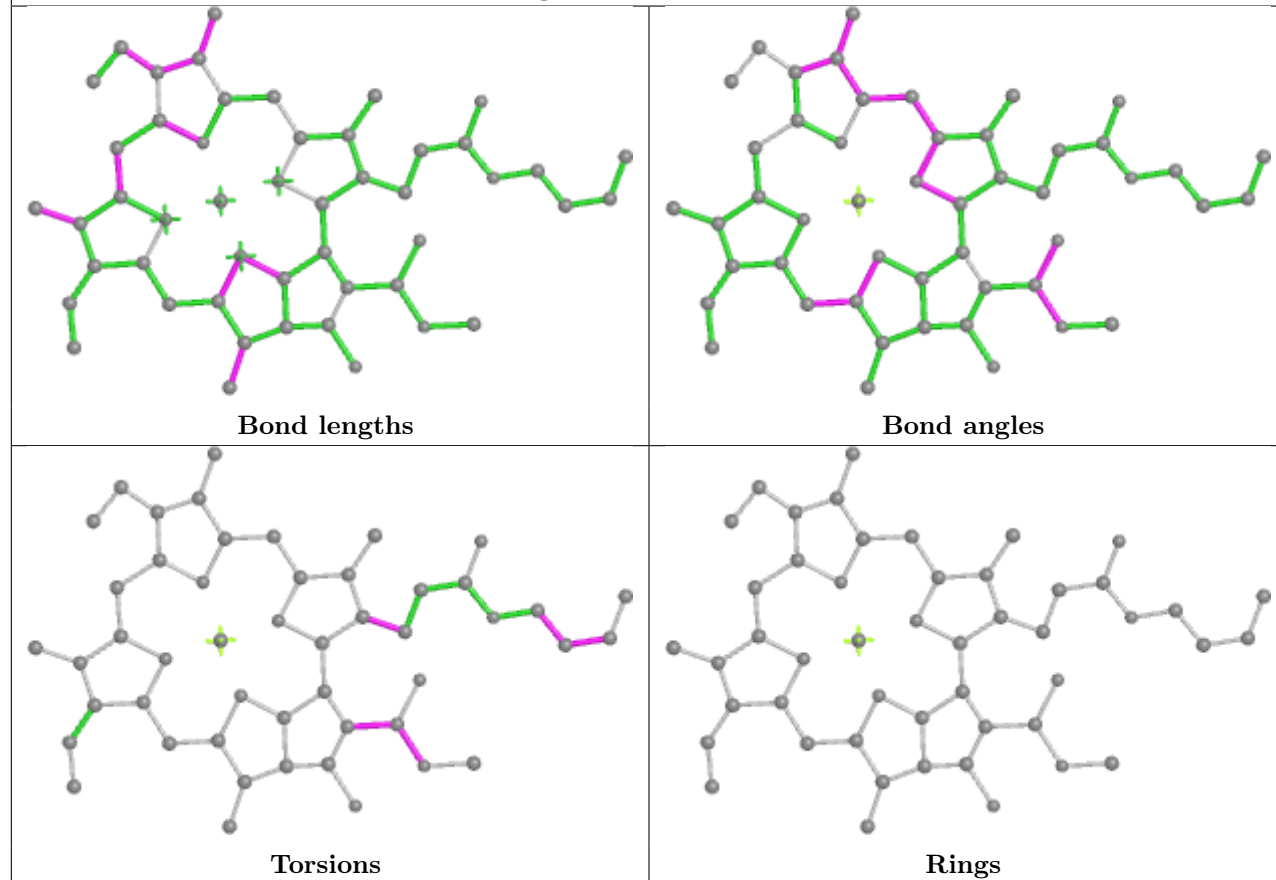
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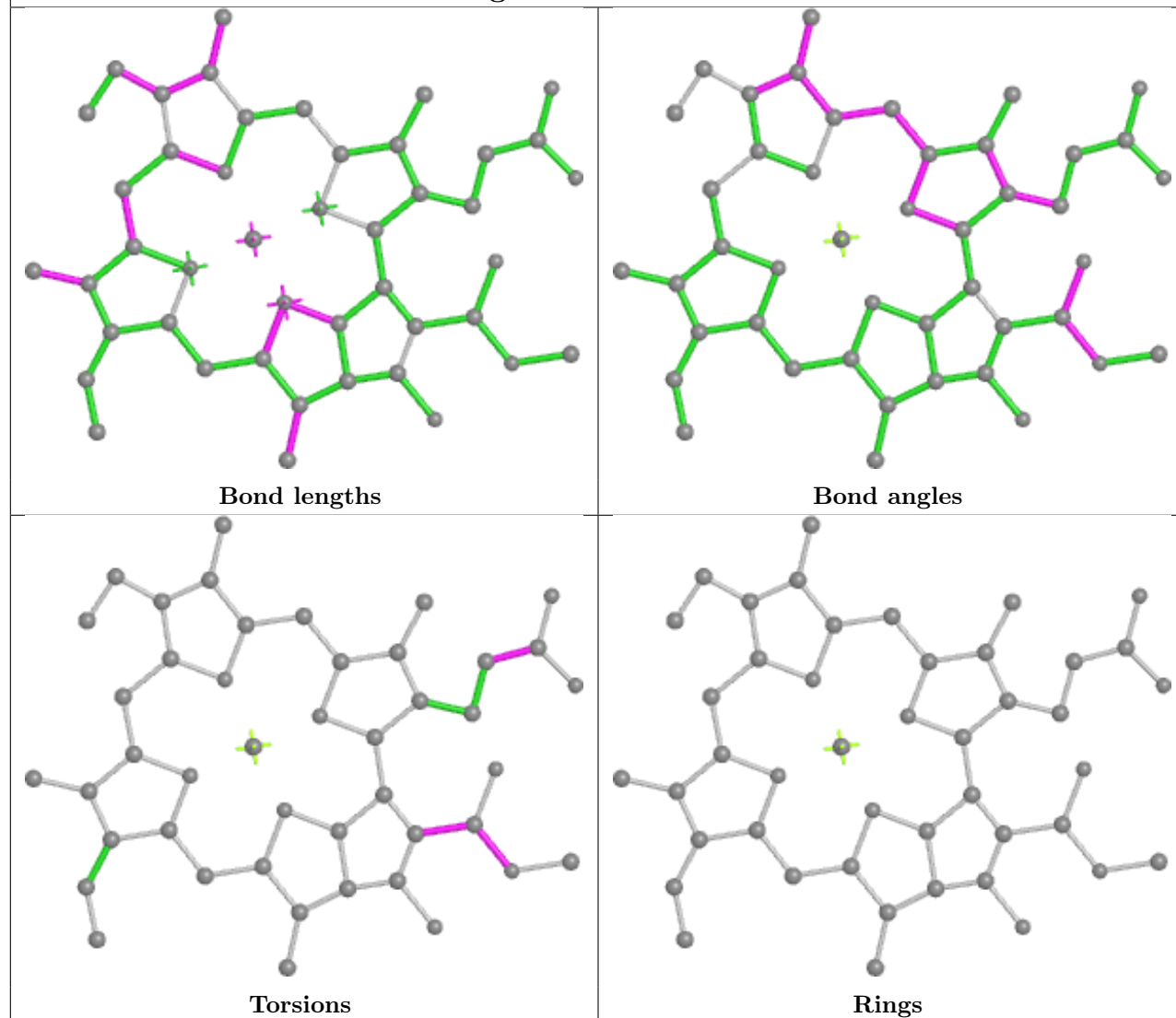
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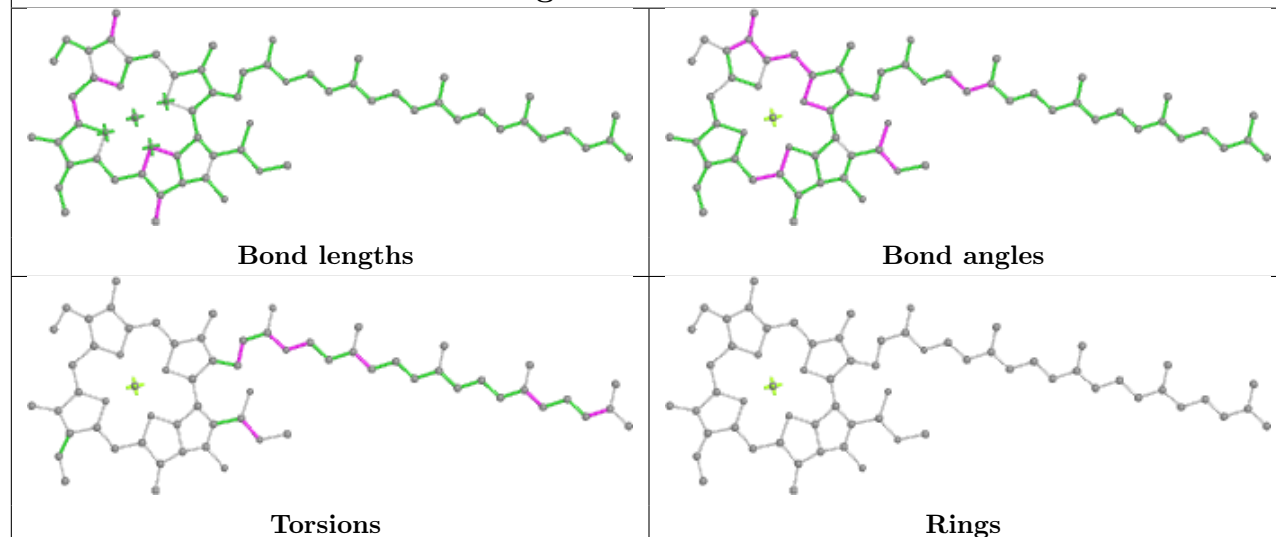
Ligand CLA n 614



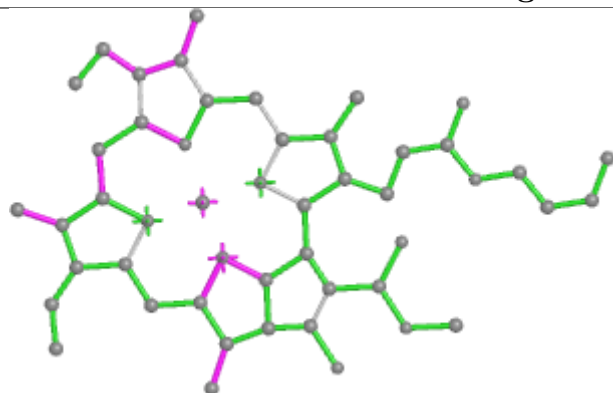
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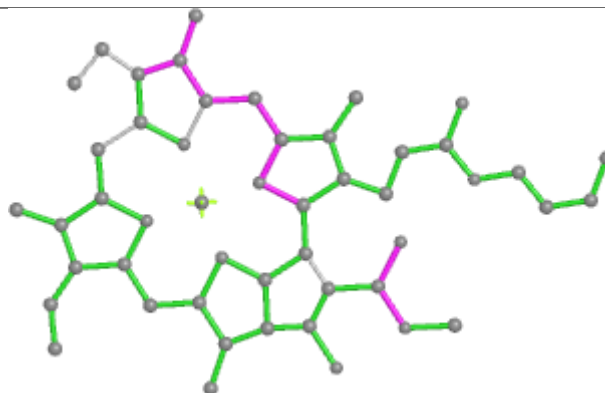
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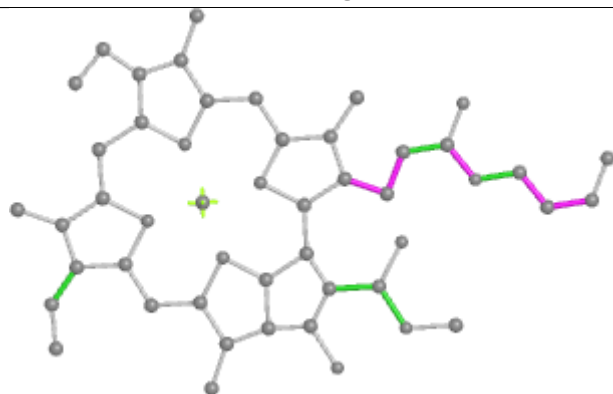
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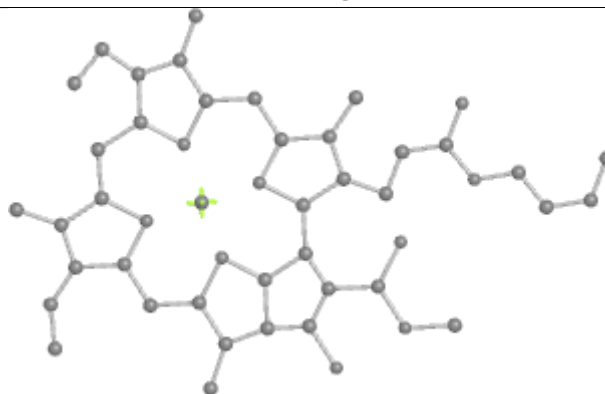
Bond lengths



Bond angles

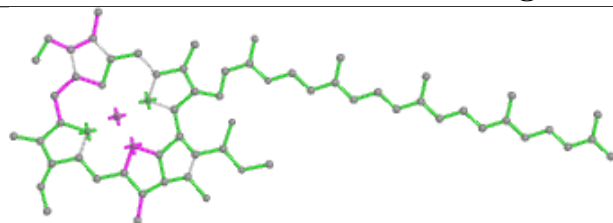


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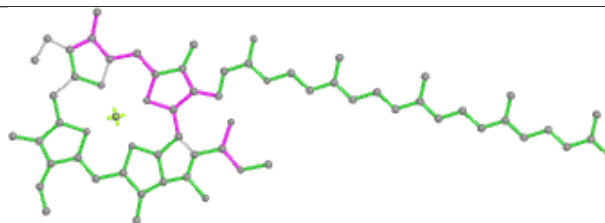


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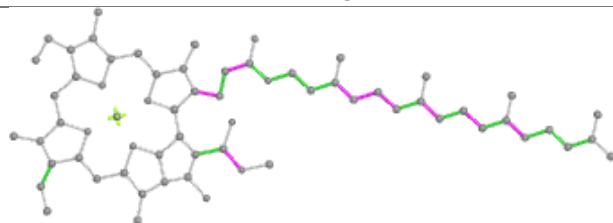
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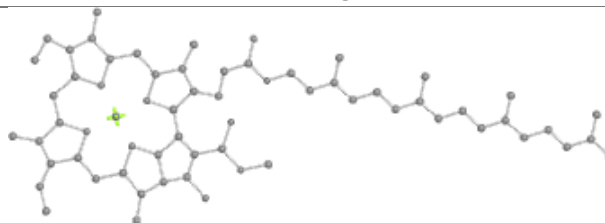
Bond lengths



Bond angles

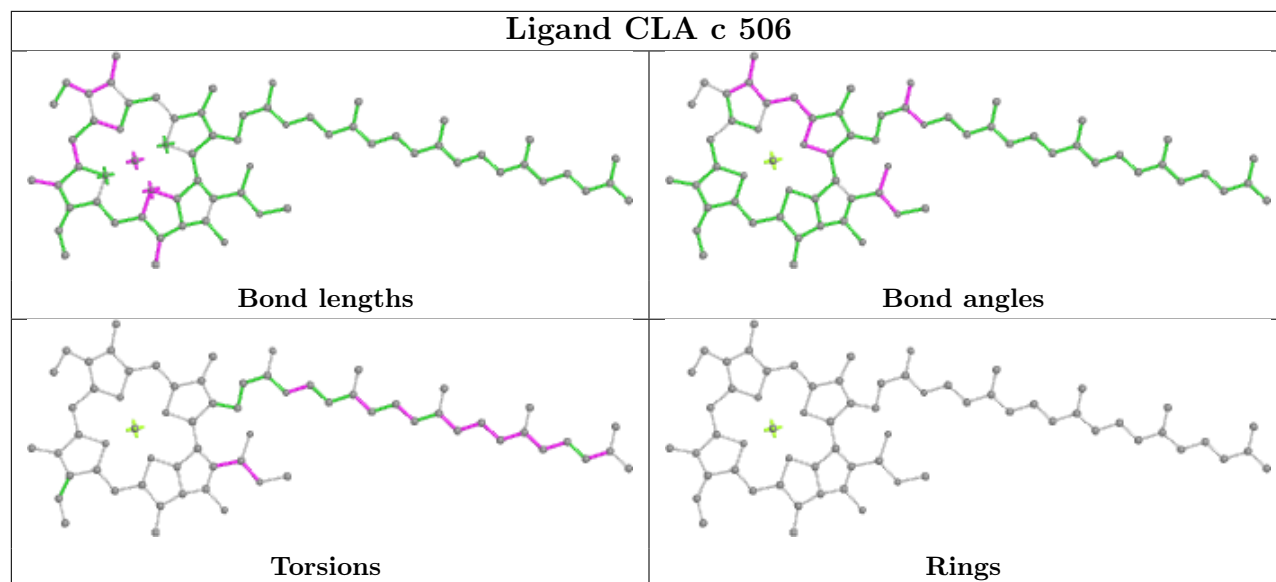


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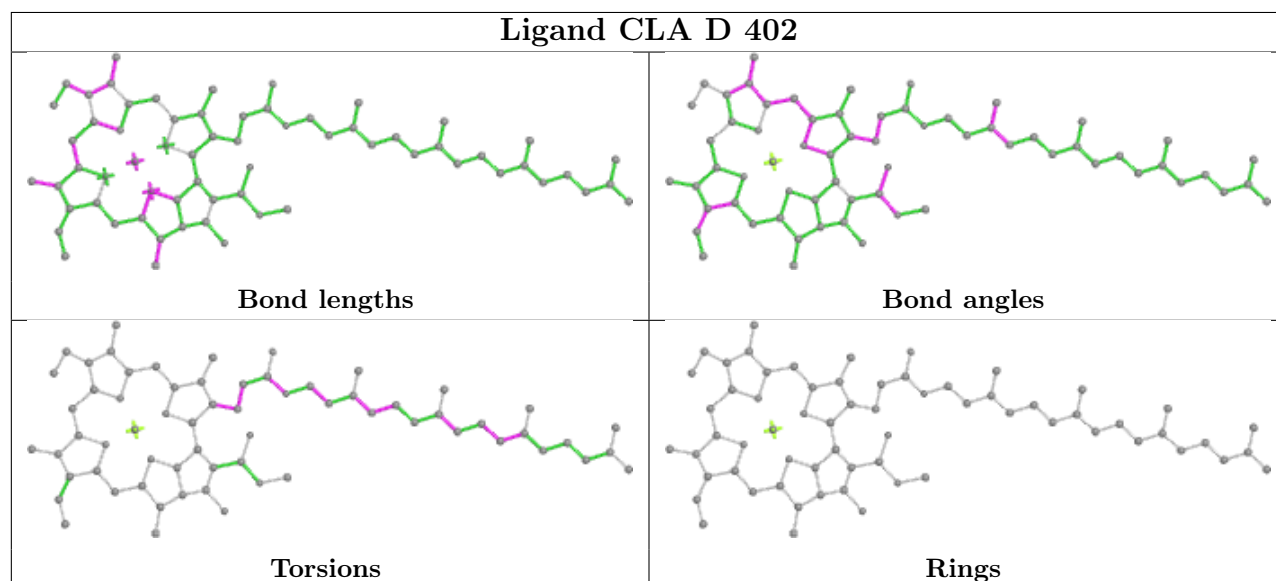


Rings

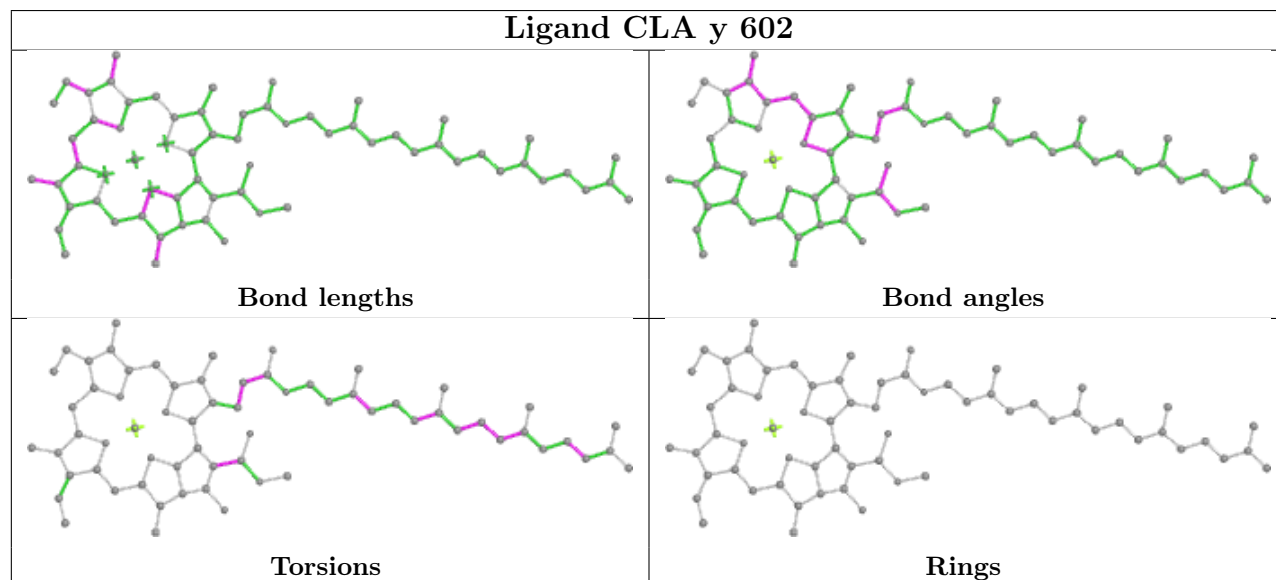
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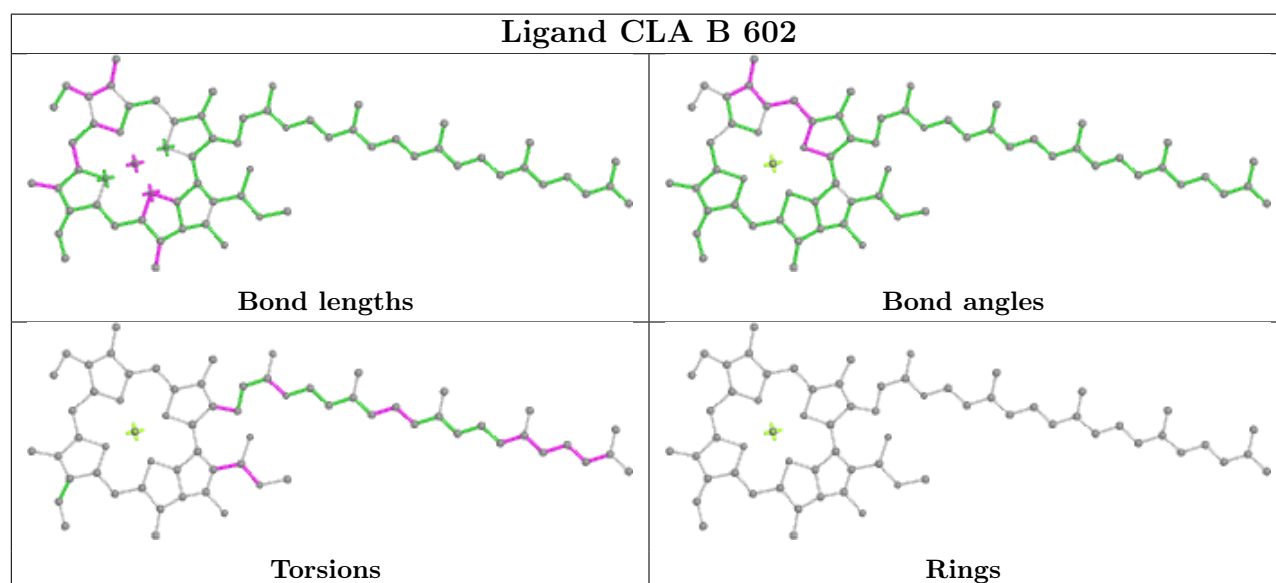
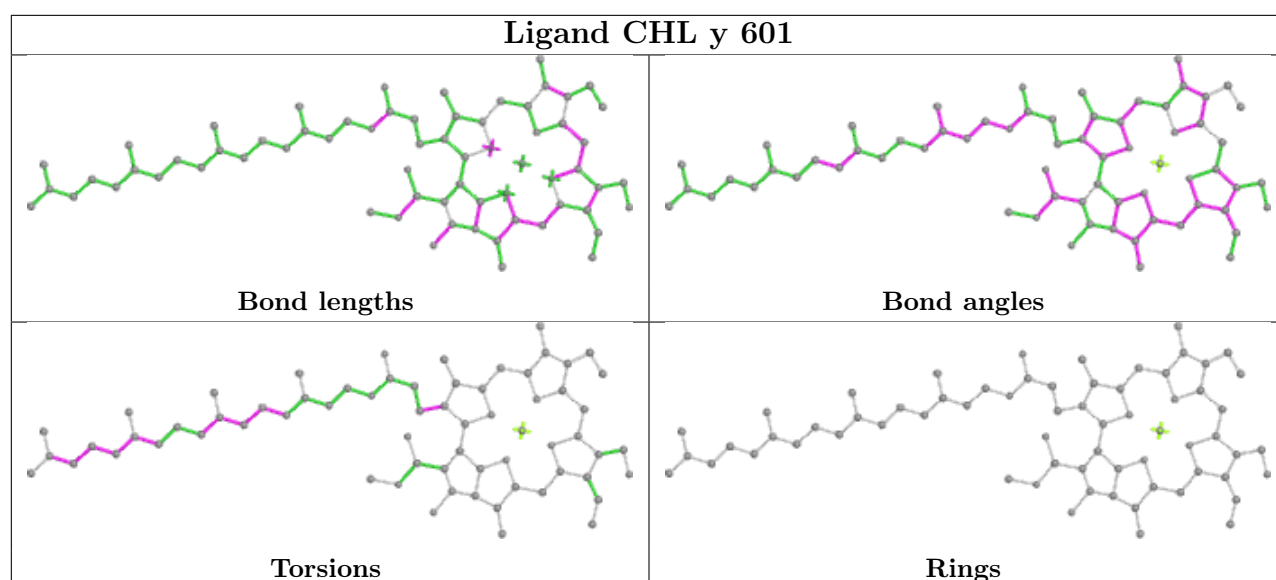
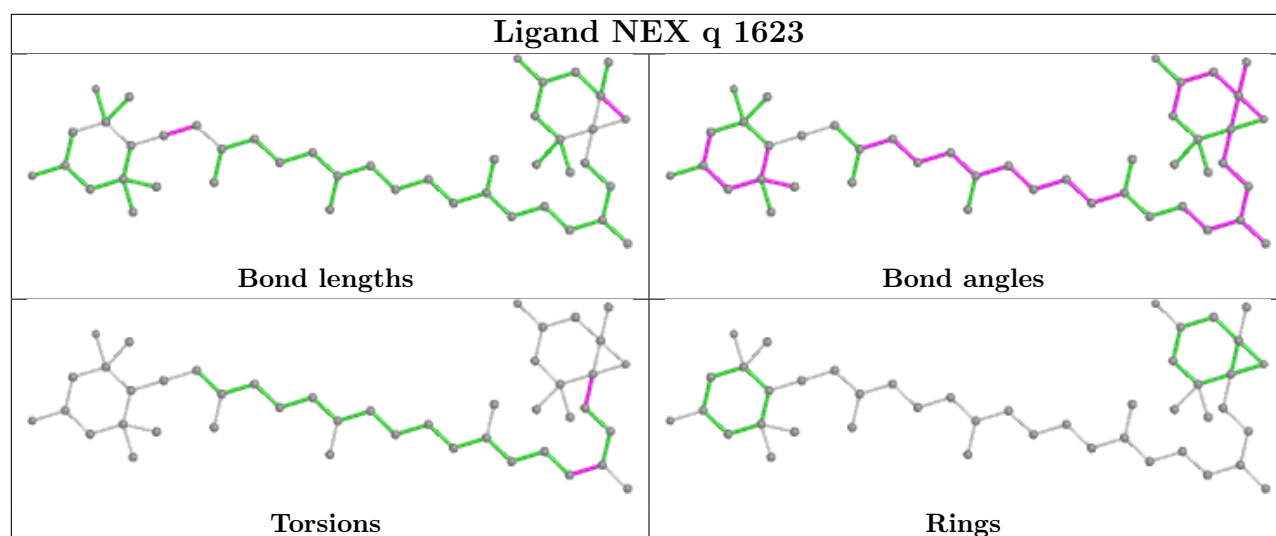


Ligand CLA D 402

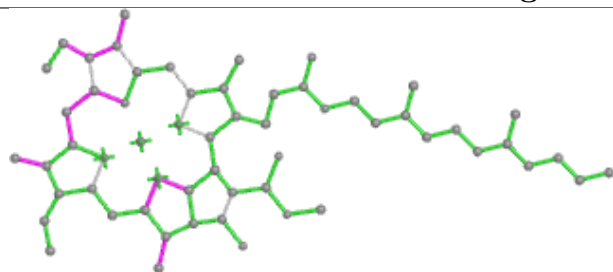


Ligand CLA y 602

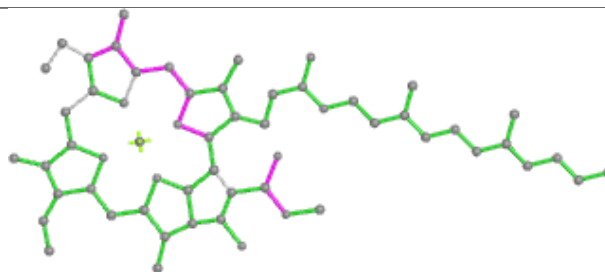




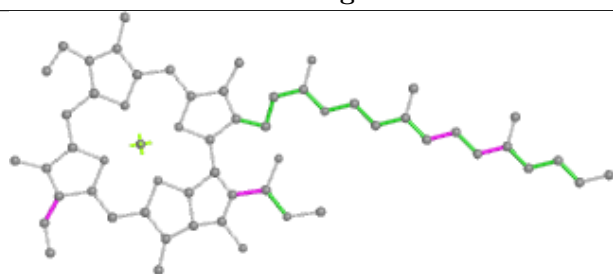
Ligand CLA r 609



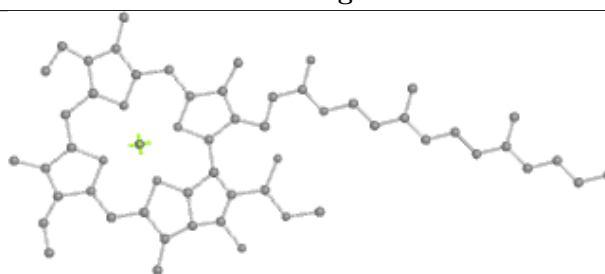
Bond lengths



Bond angles

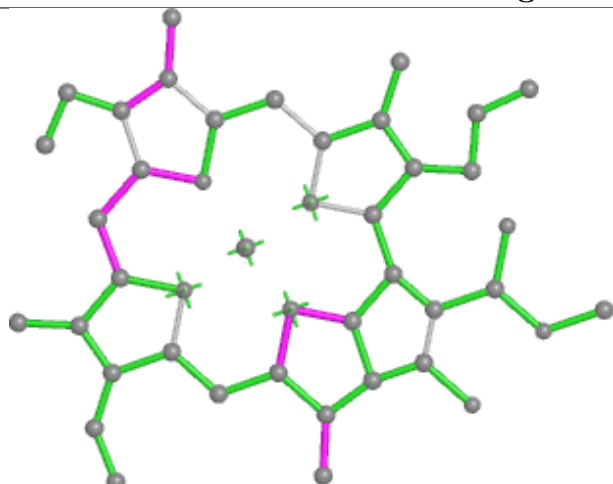


Torsions

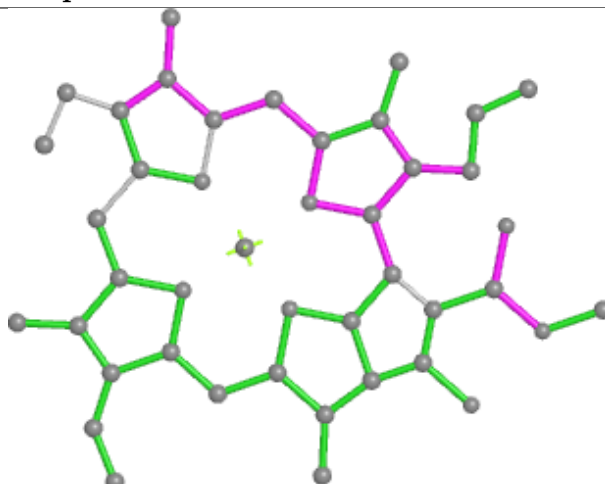


Rings

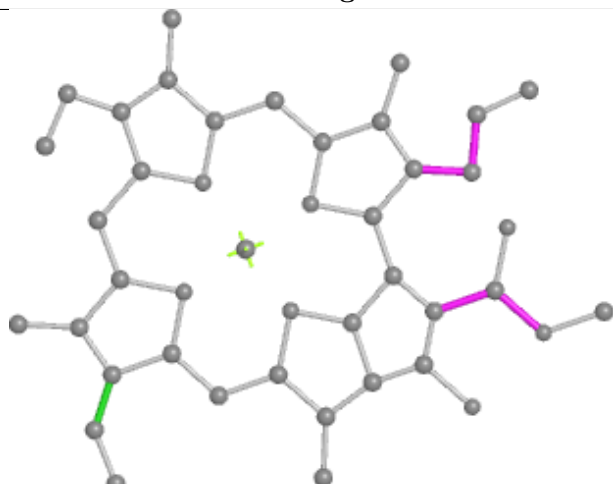
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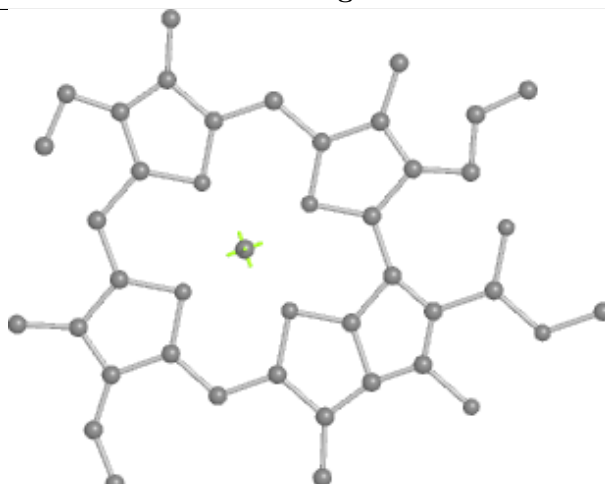
Bond lengths



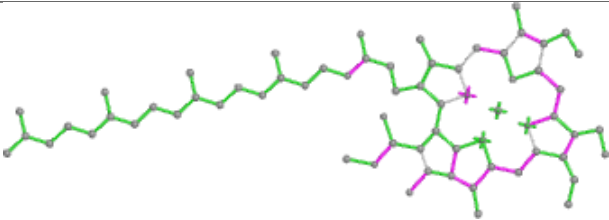
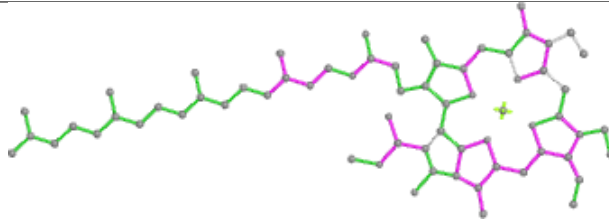
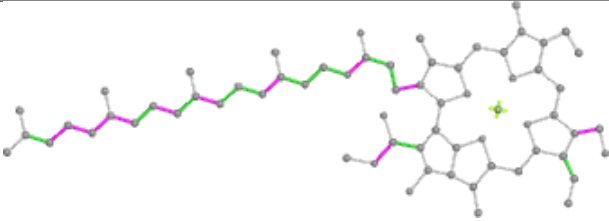
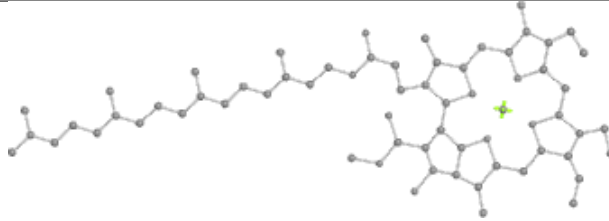
Bond angles

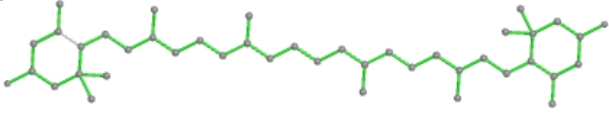
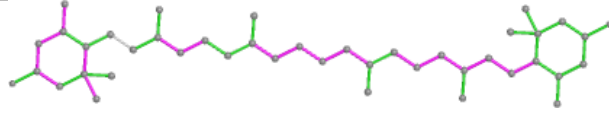
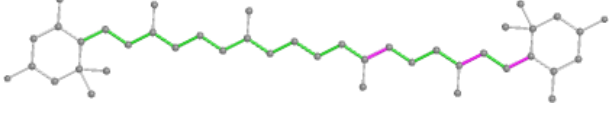
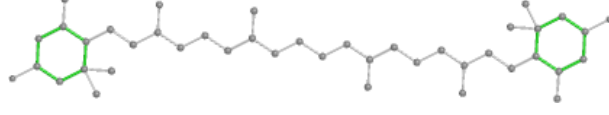


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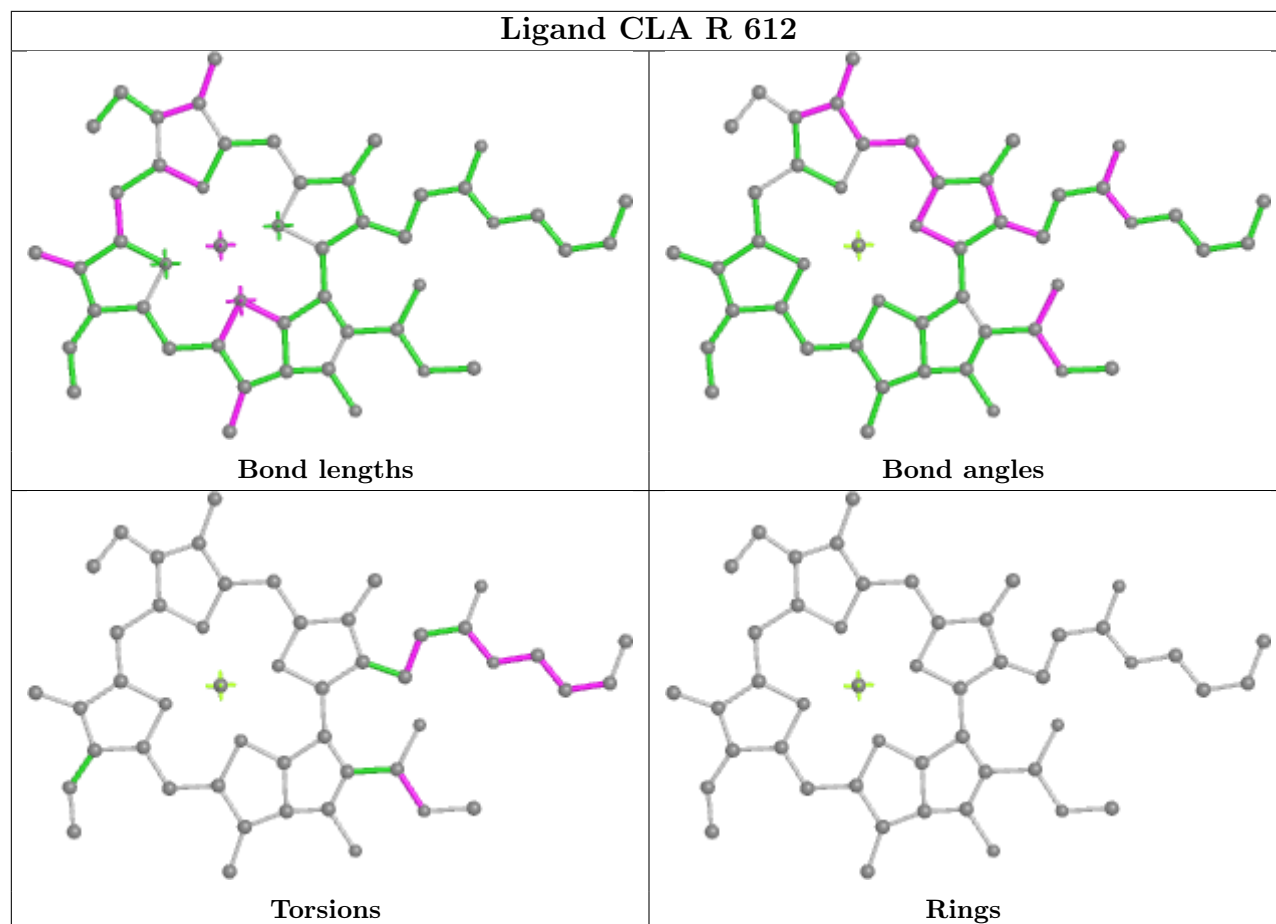


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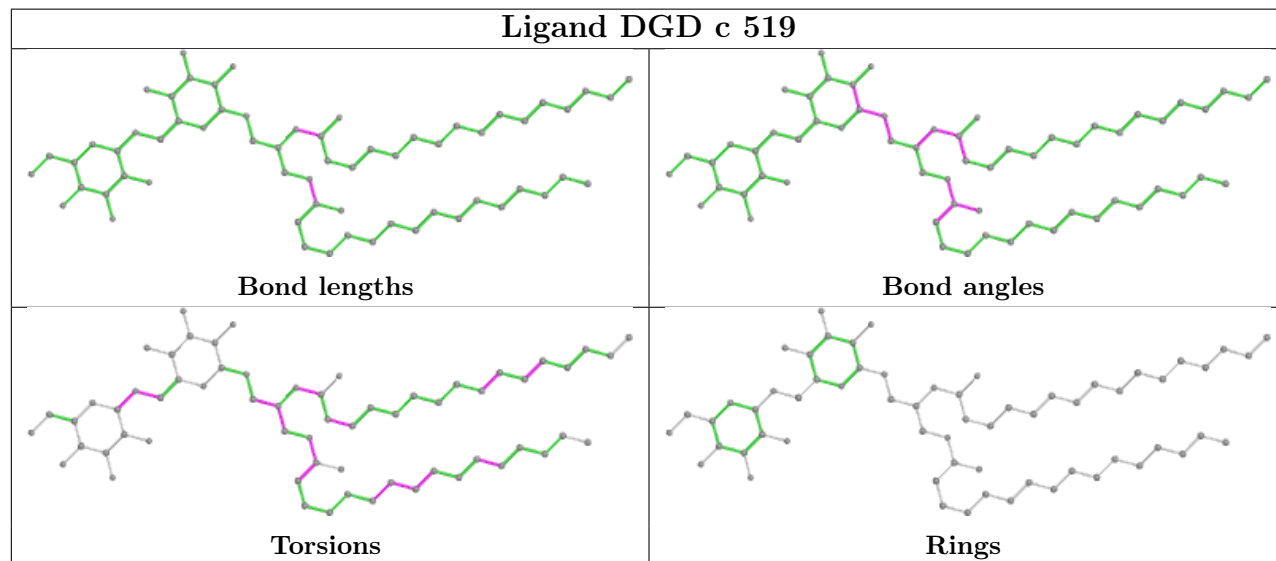
Ligand CHL 1 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

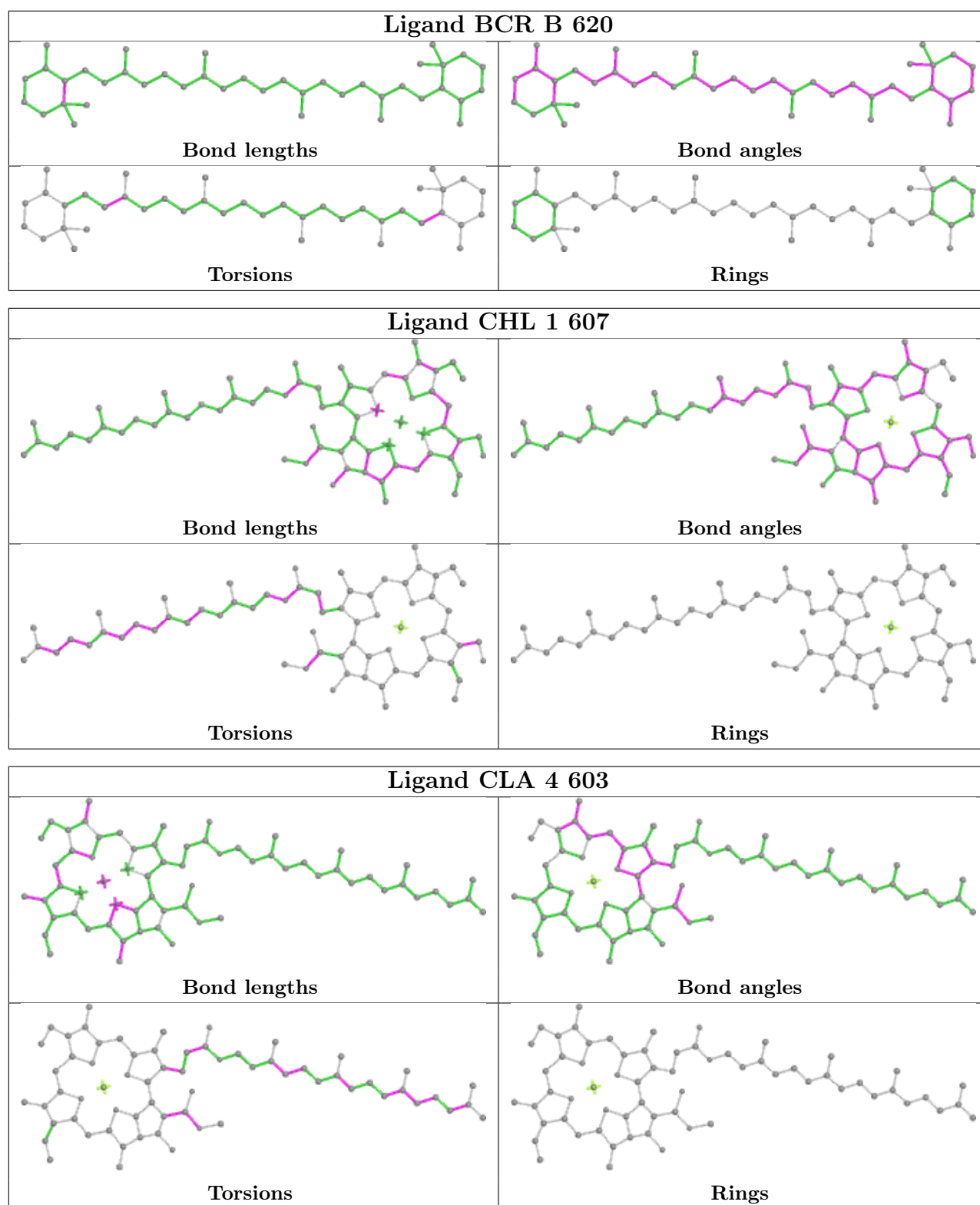
Ligand LUT 5 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA R 612

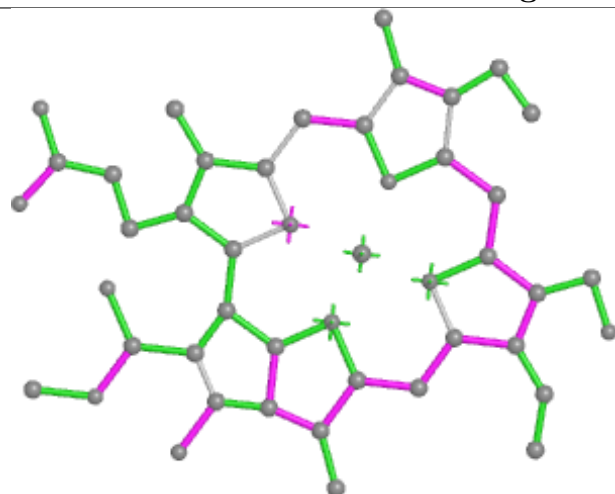


Ligand DGD c 519

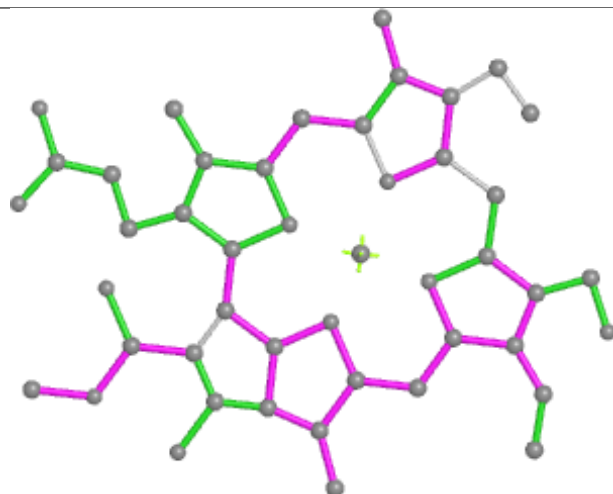




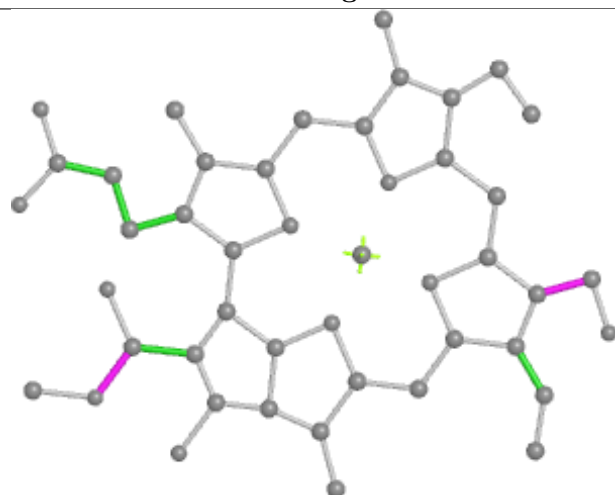
Ligand CHL 5 606



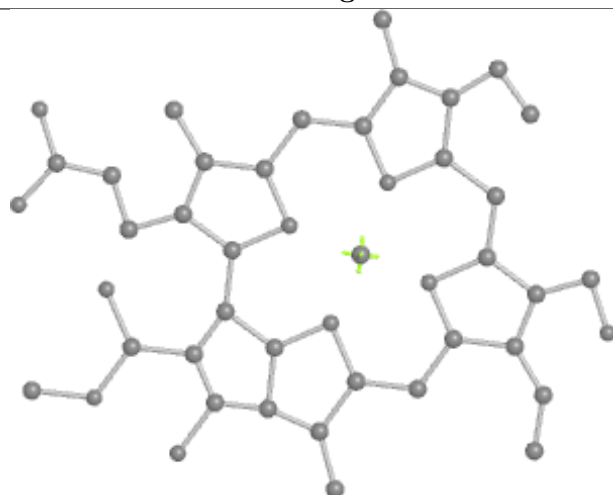
Bond lengths



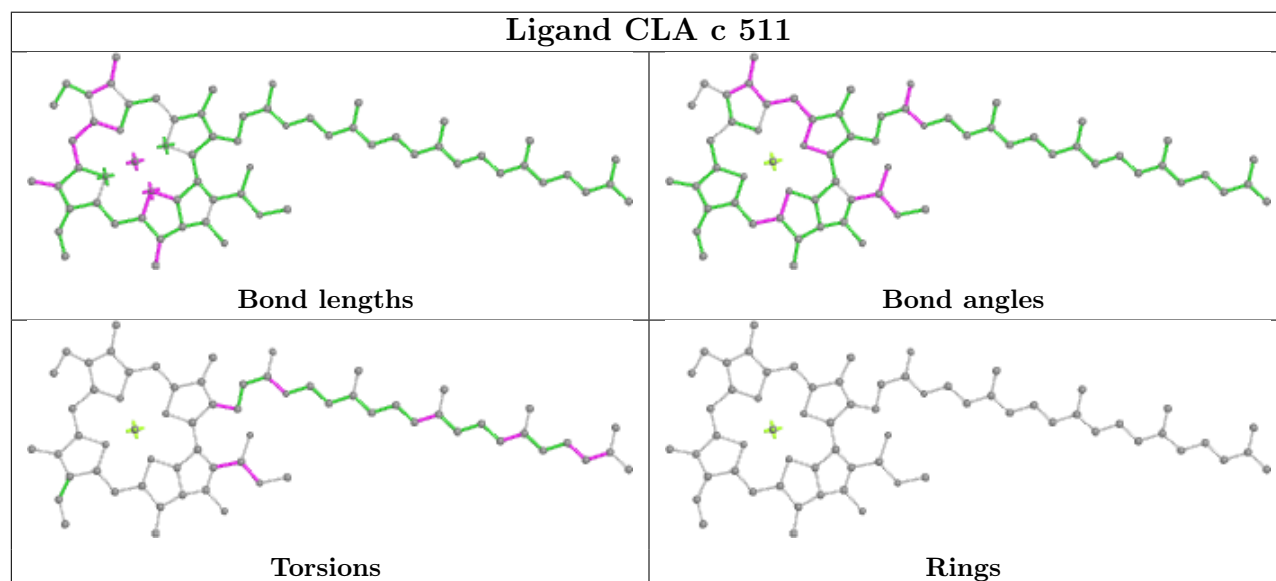
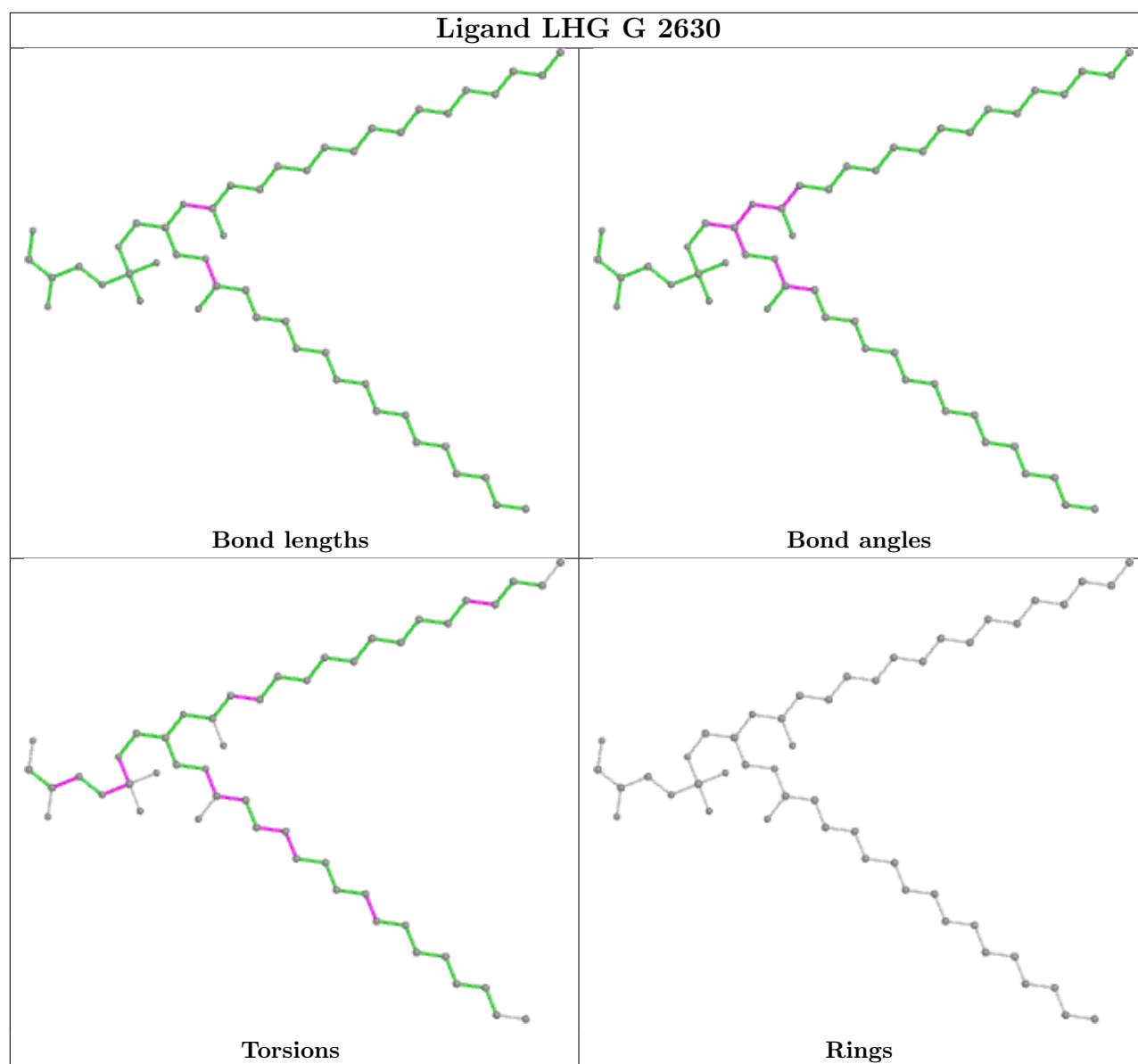
Bond angles

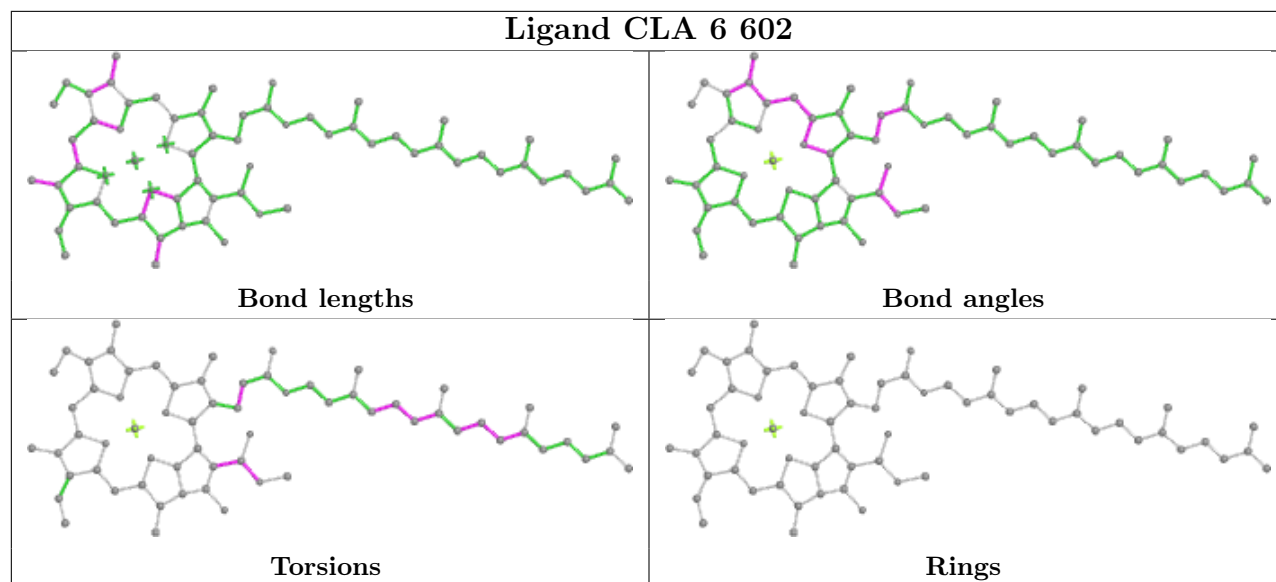
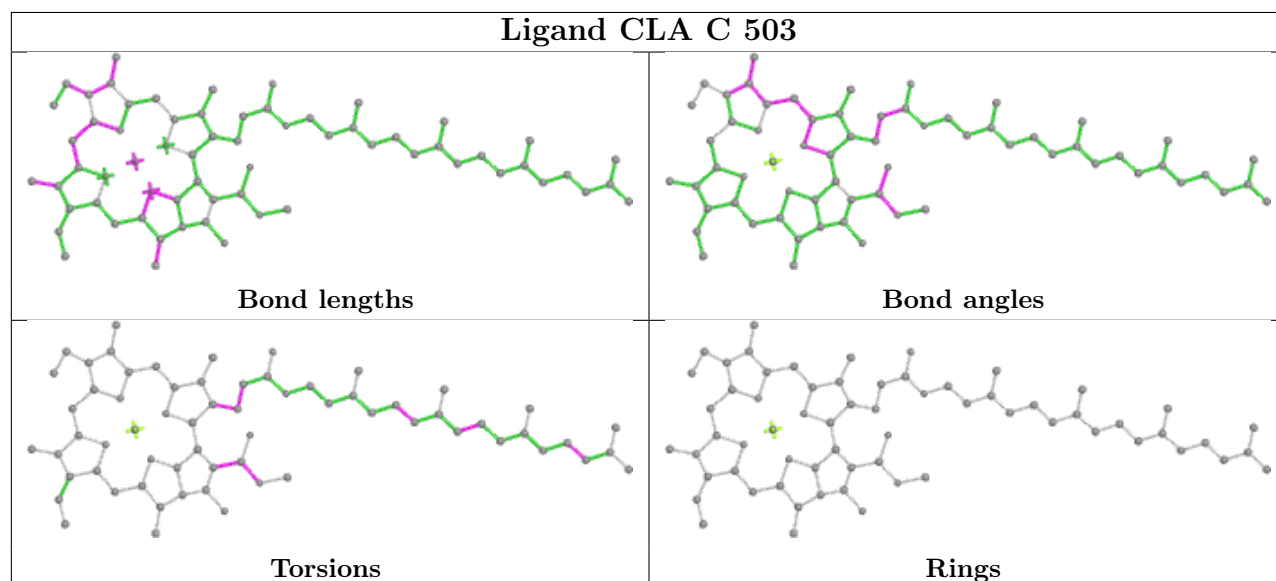
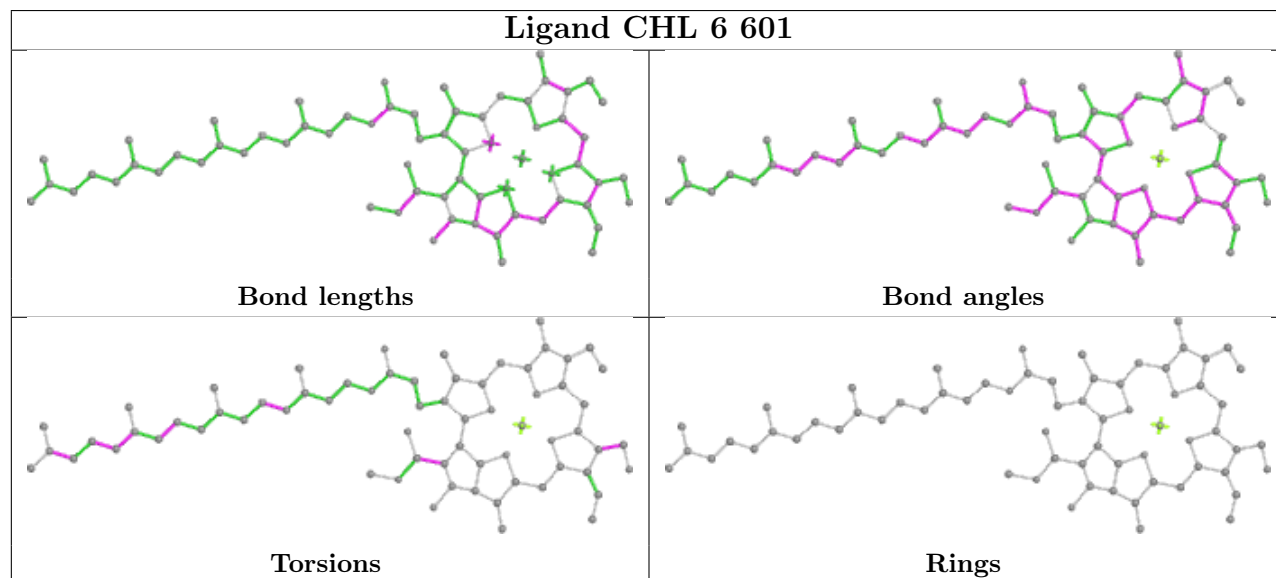


Torsions

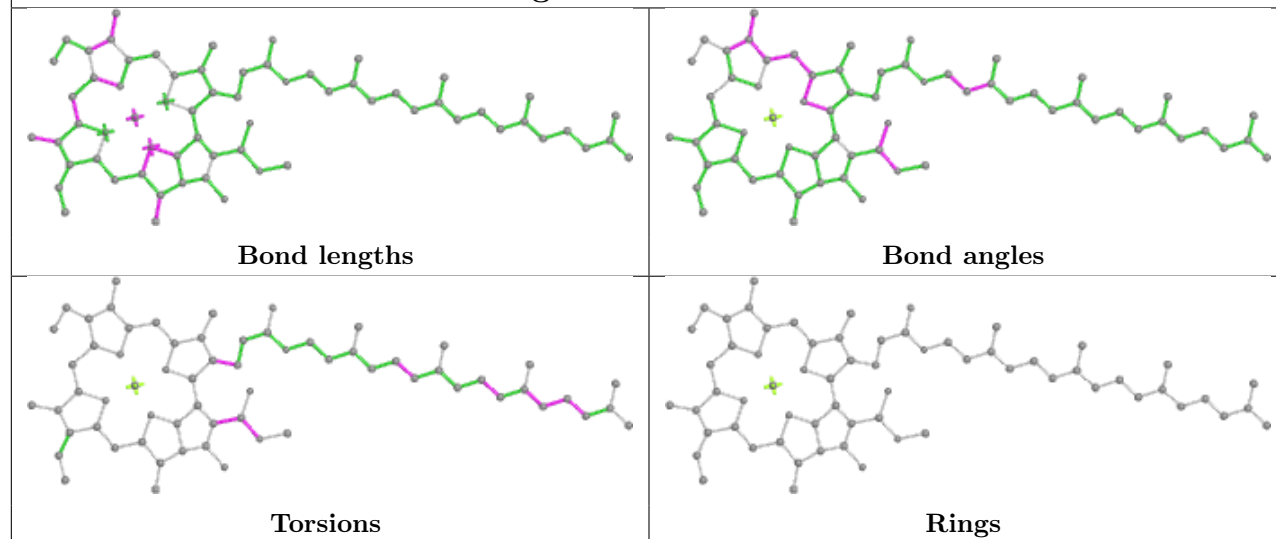


Rings

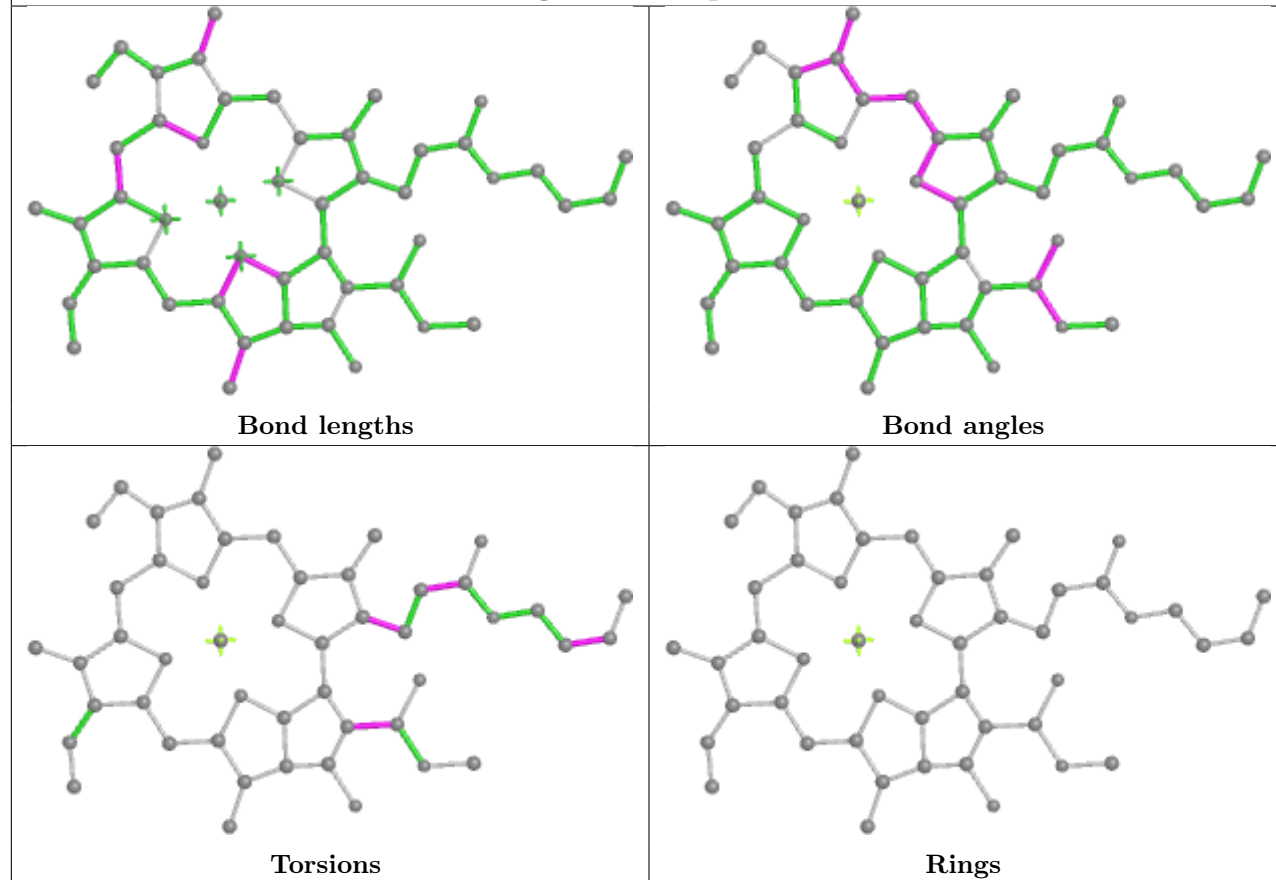


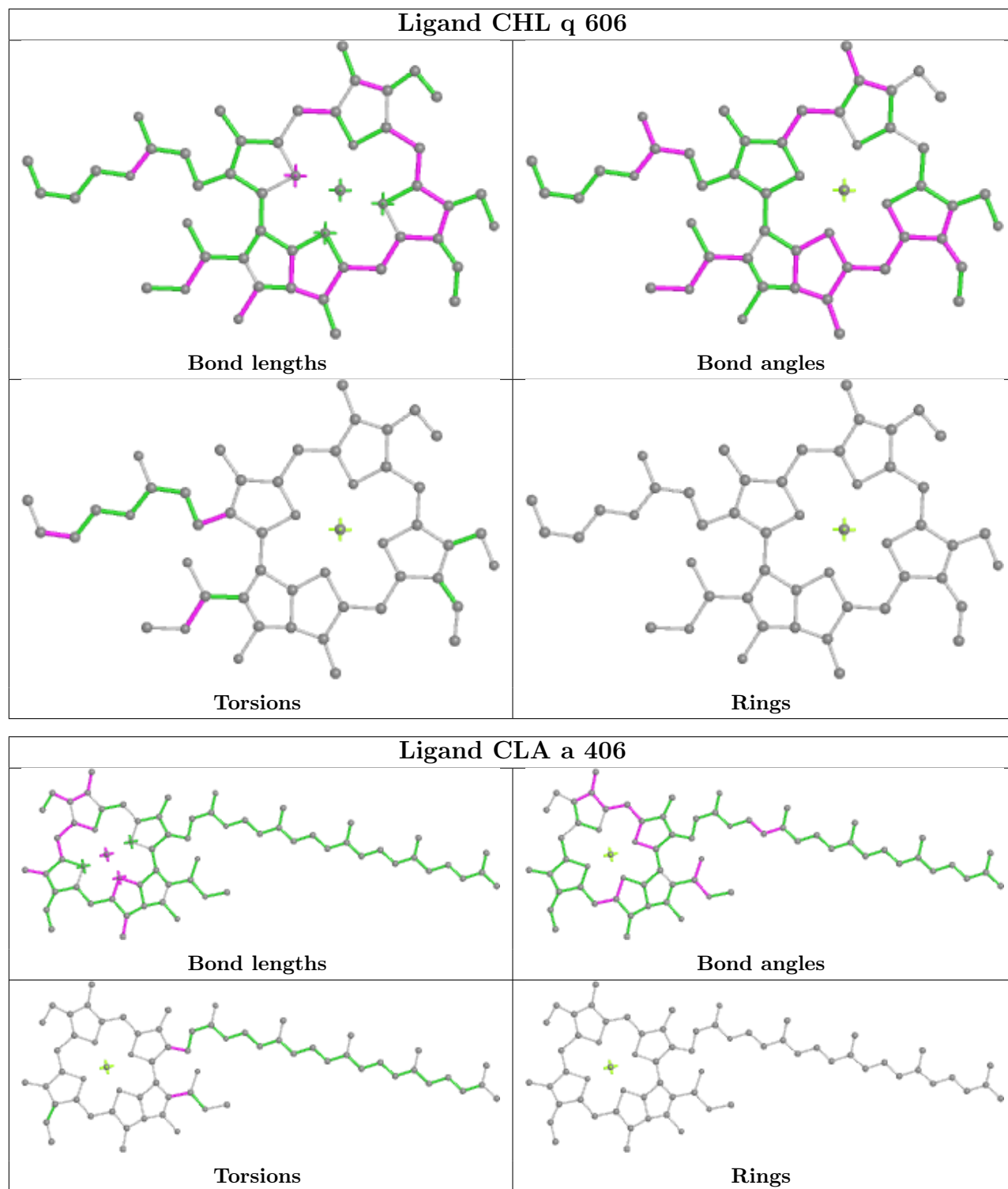
Ligand CLA 6 602**Ligand CLA C 503****Ligand CHL 6 601**

Ligand CLA B 606

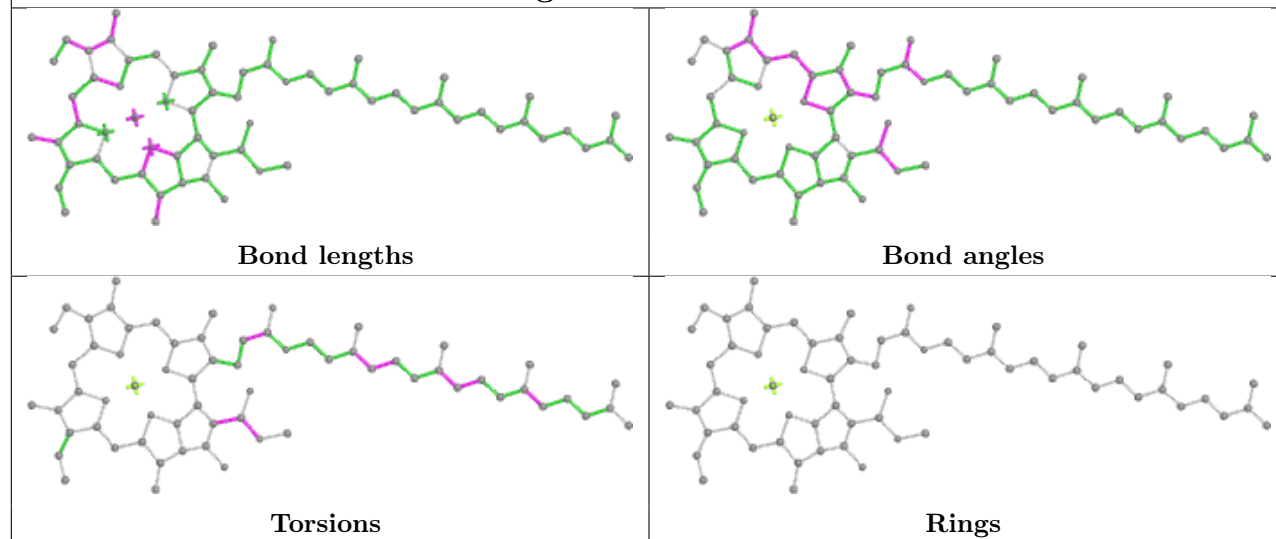


Ligand CLA p 611

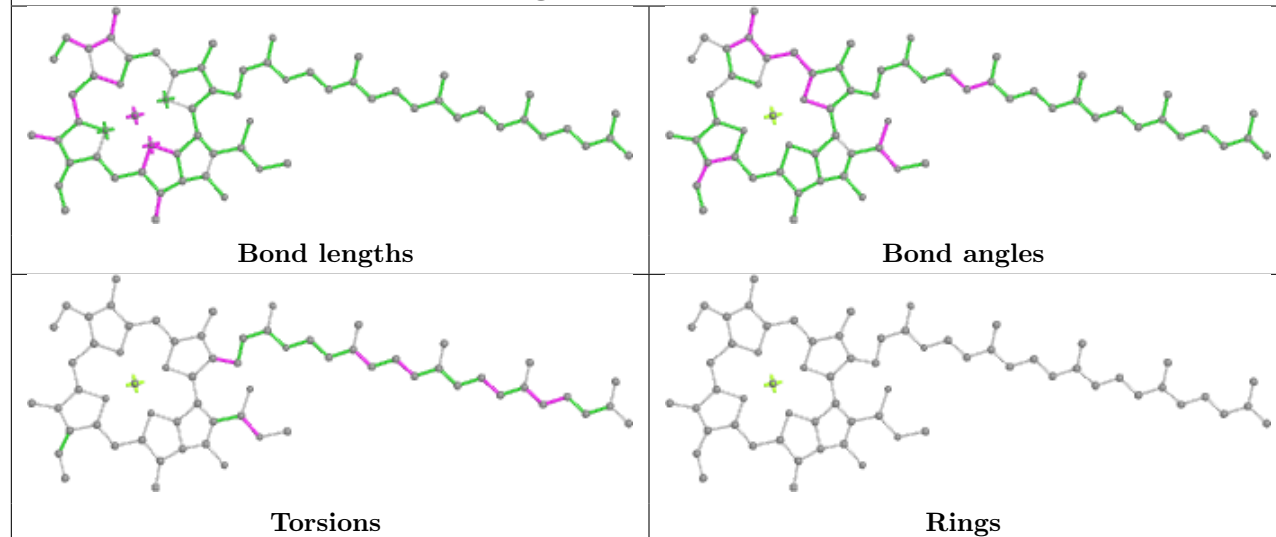


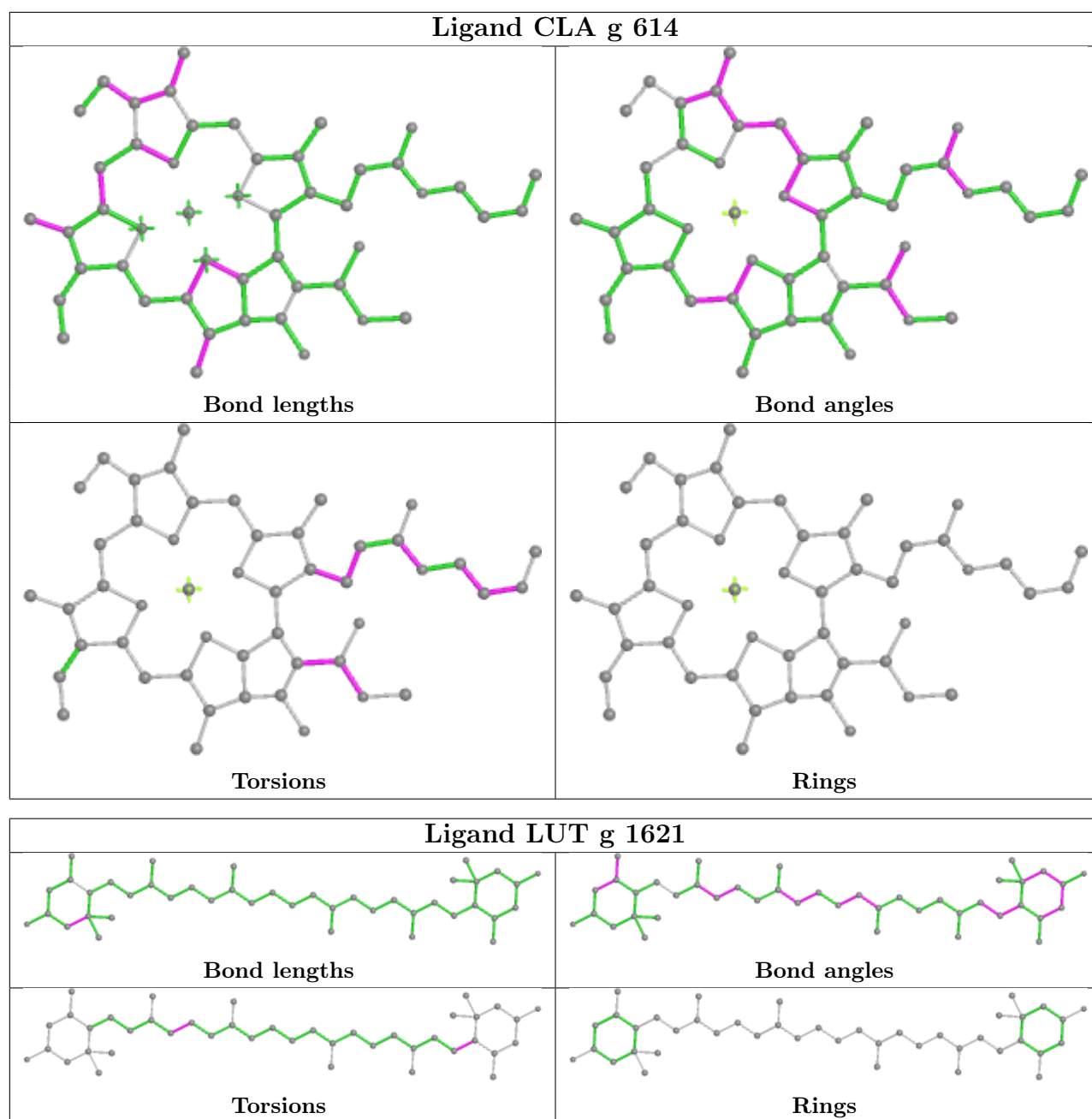


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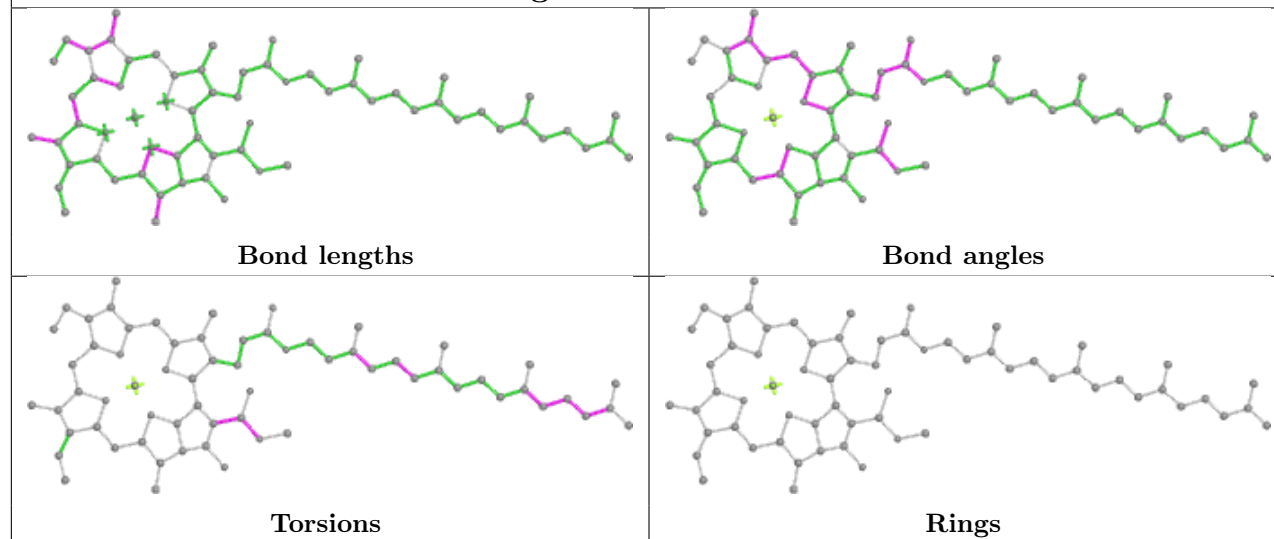


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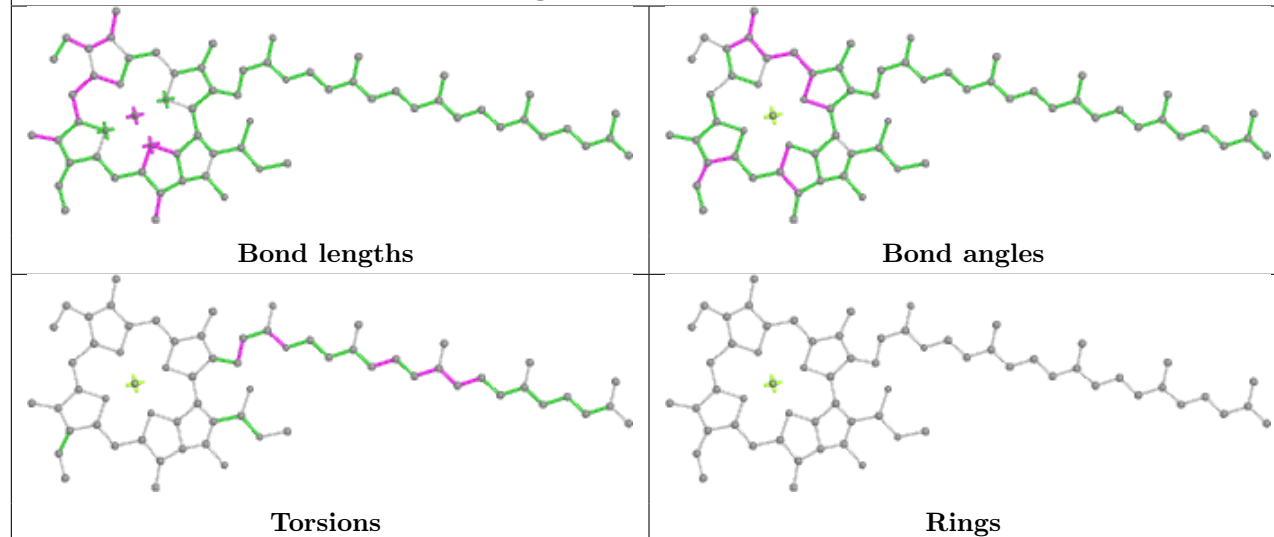




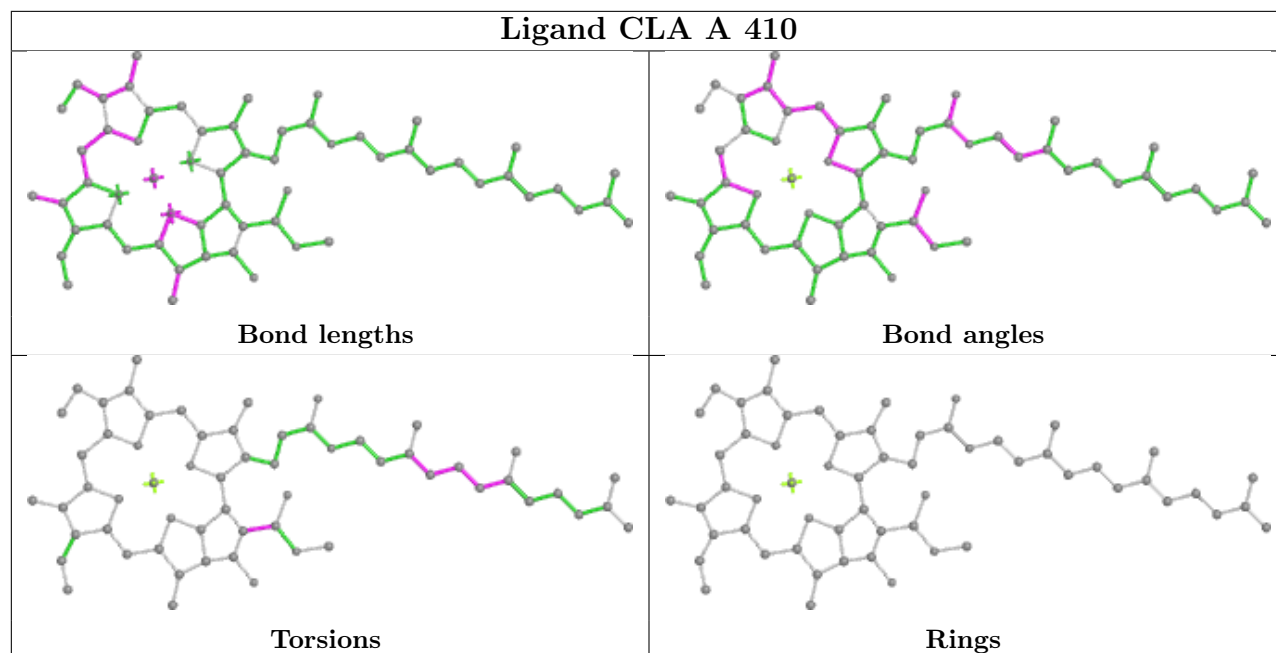
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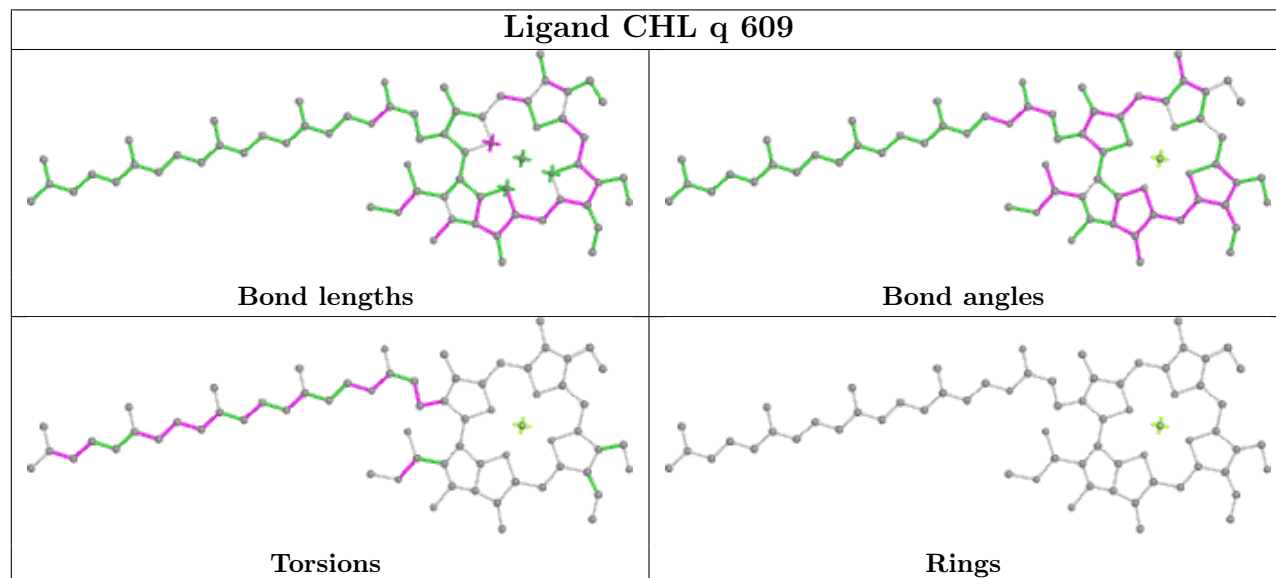
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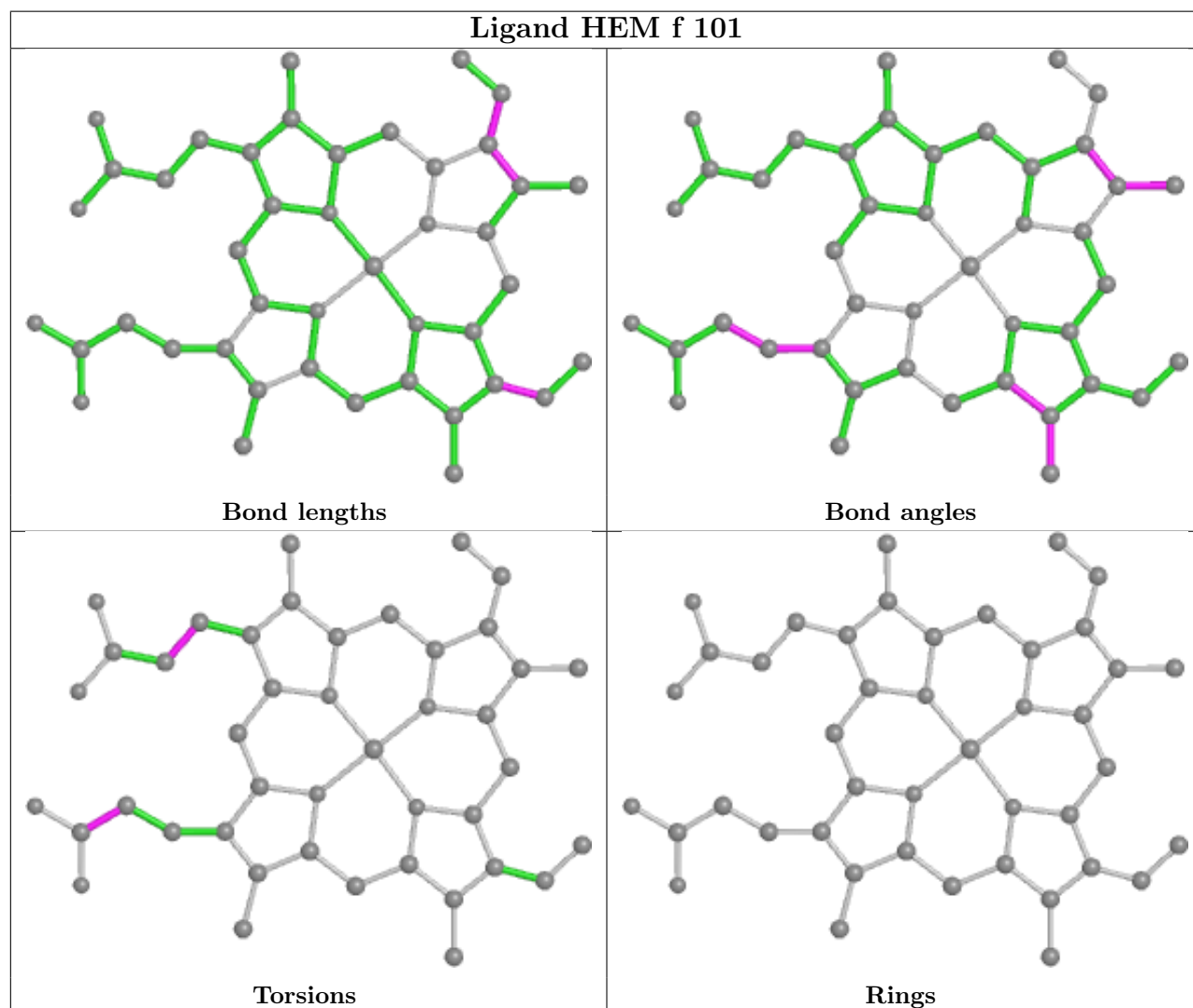
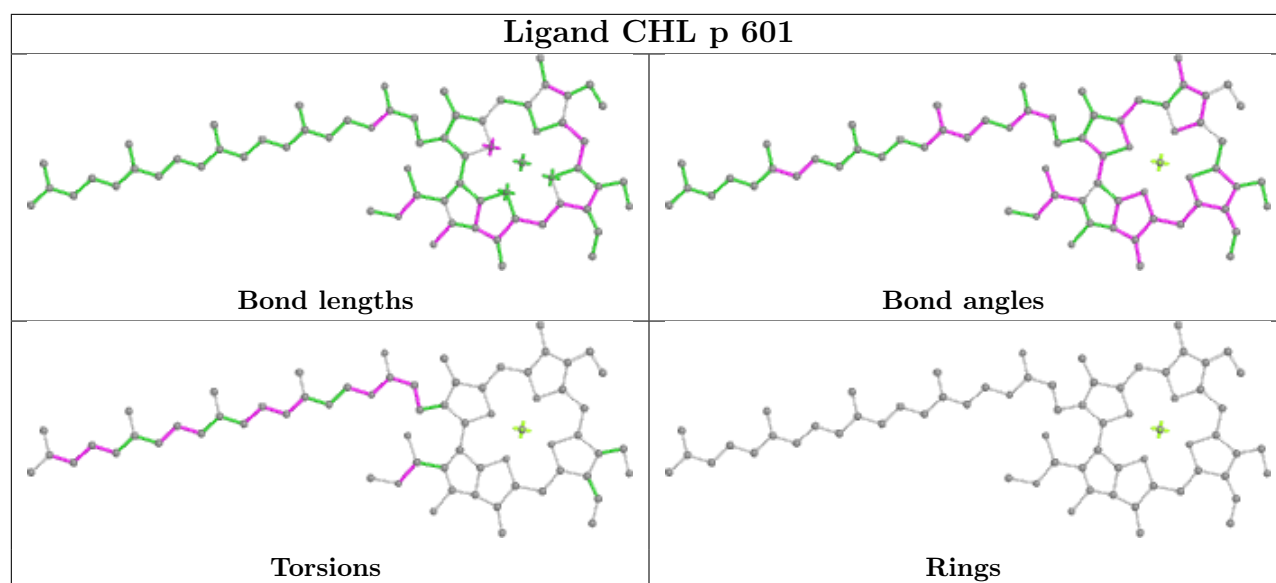


Ligand CLA A 410

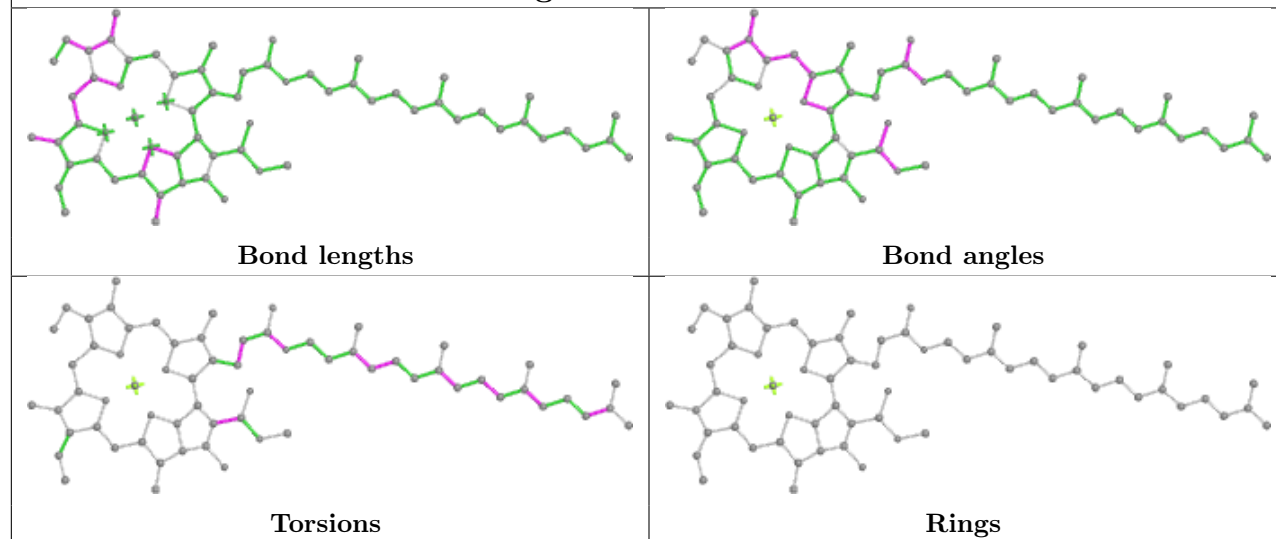


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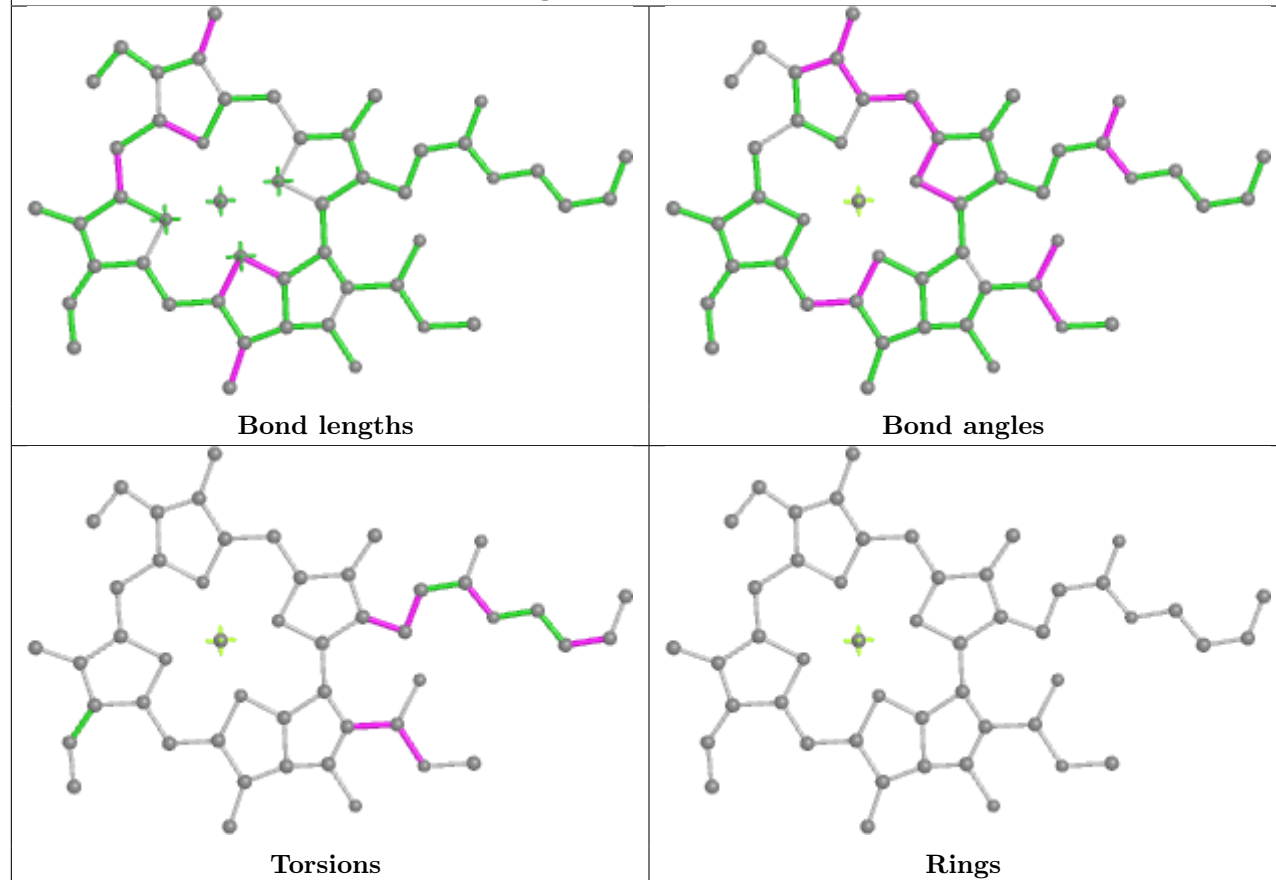




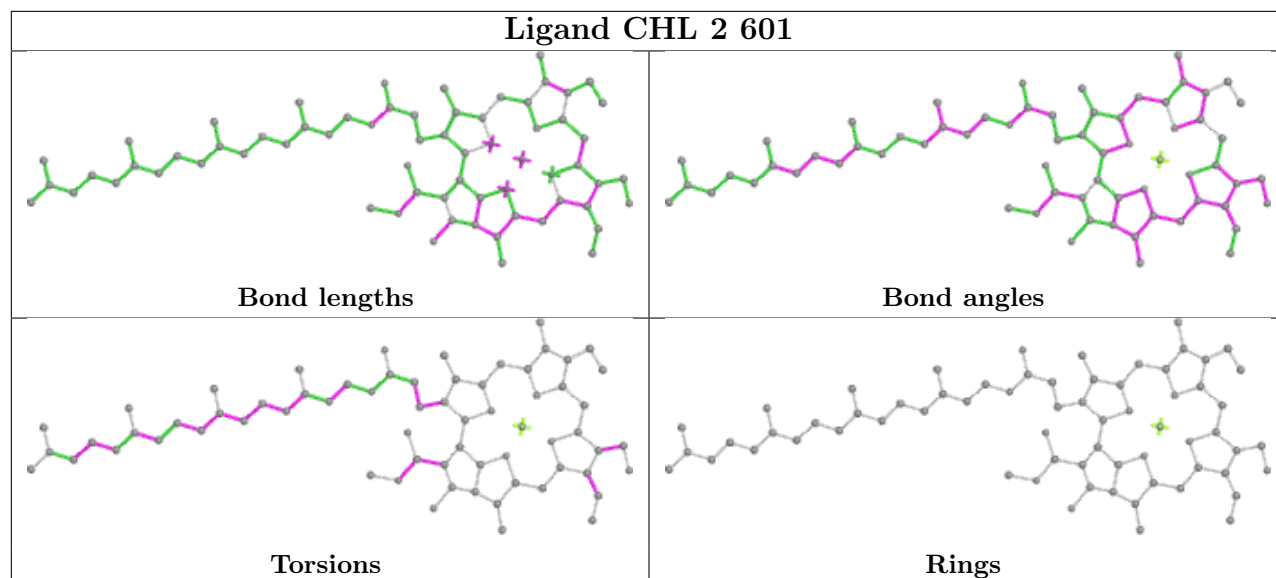
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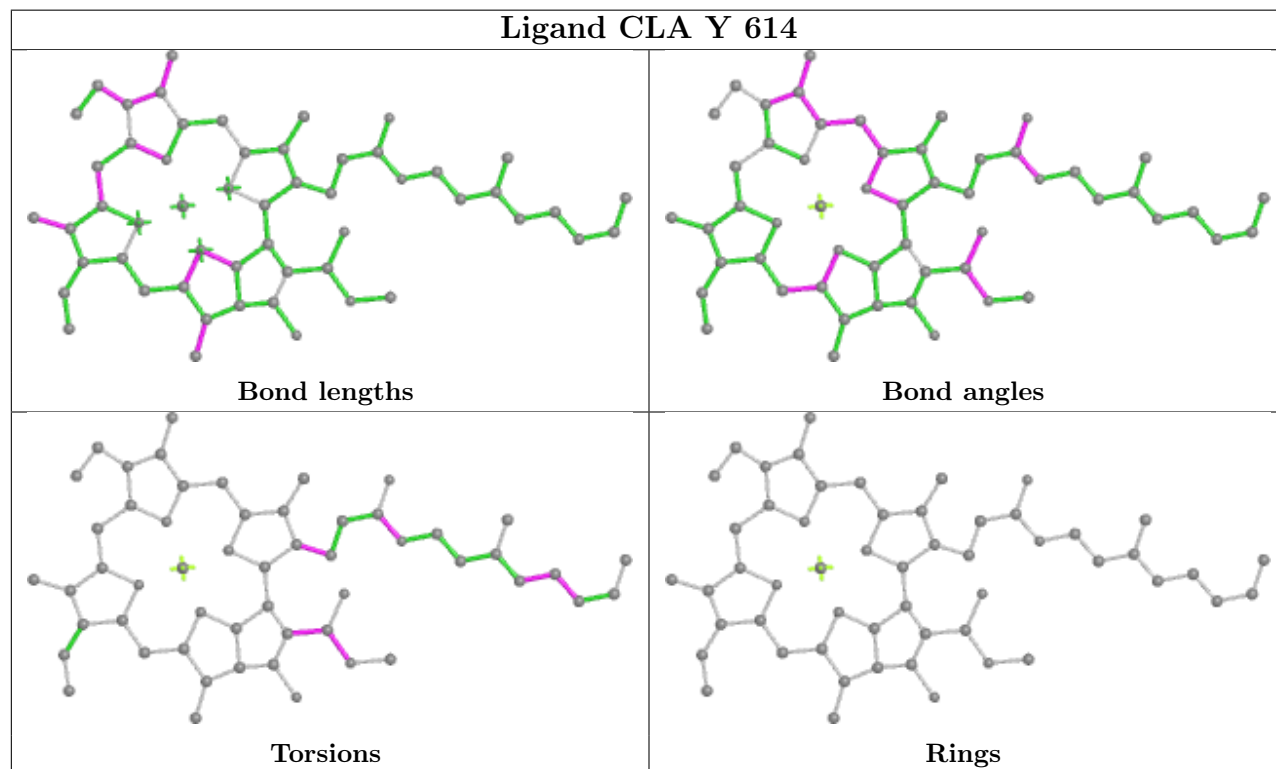
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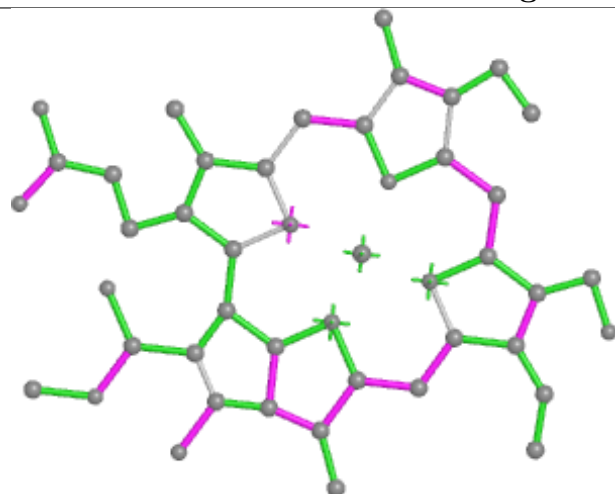
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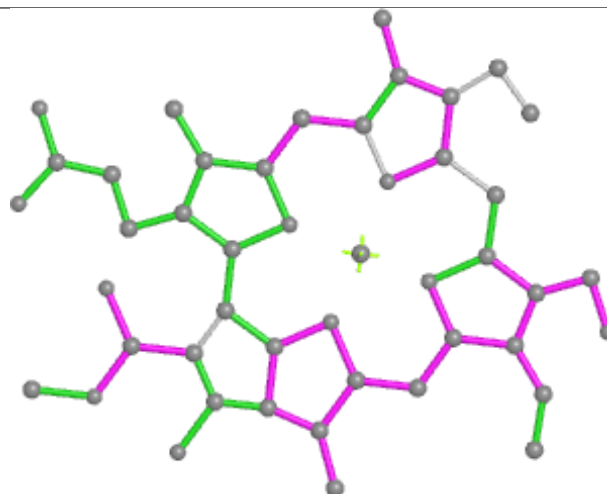
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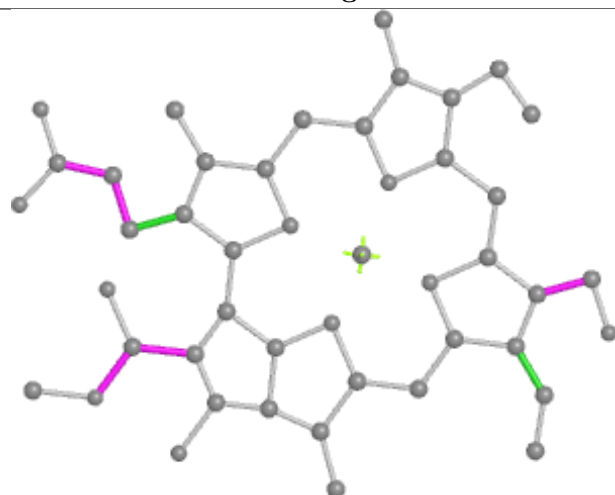
Ligand CHL 7 605



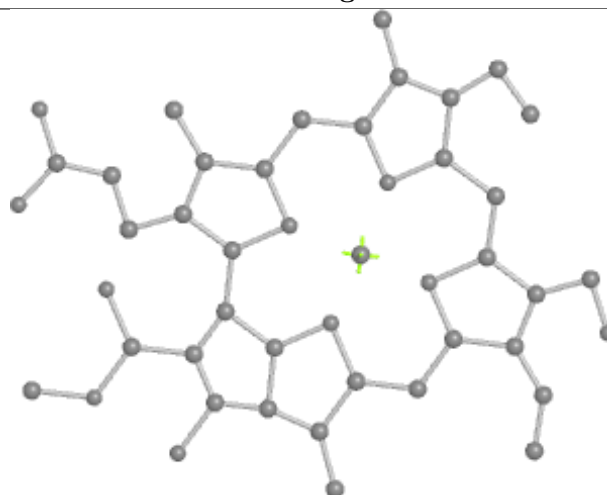
Bond lengths



Bond angles

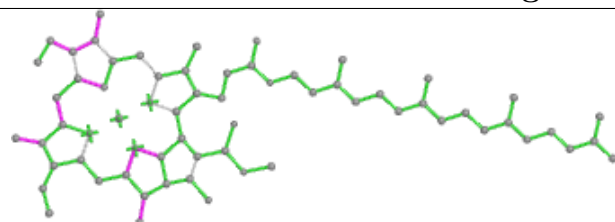


Torsions

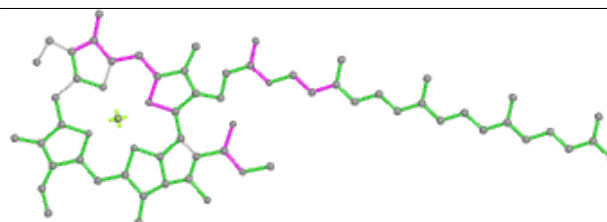


Rings

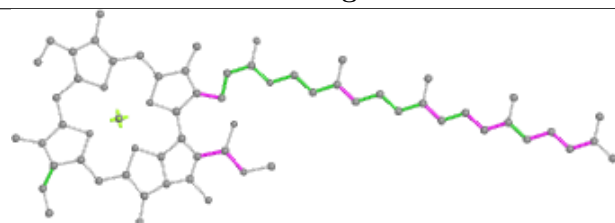
Ligand CLA r 610



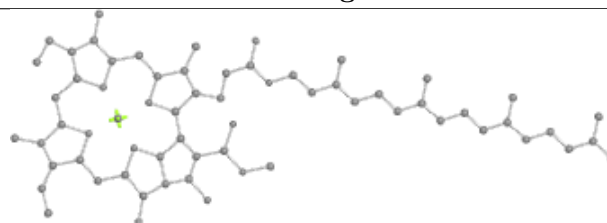
Bond lengths



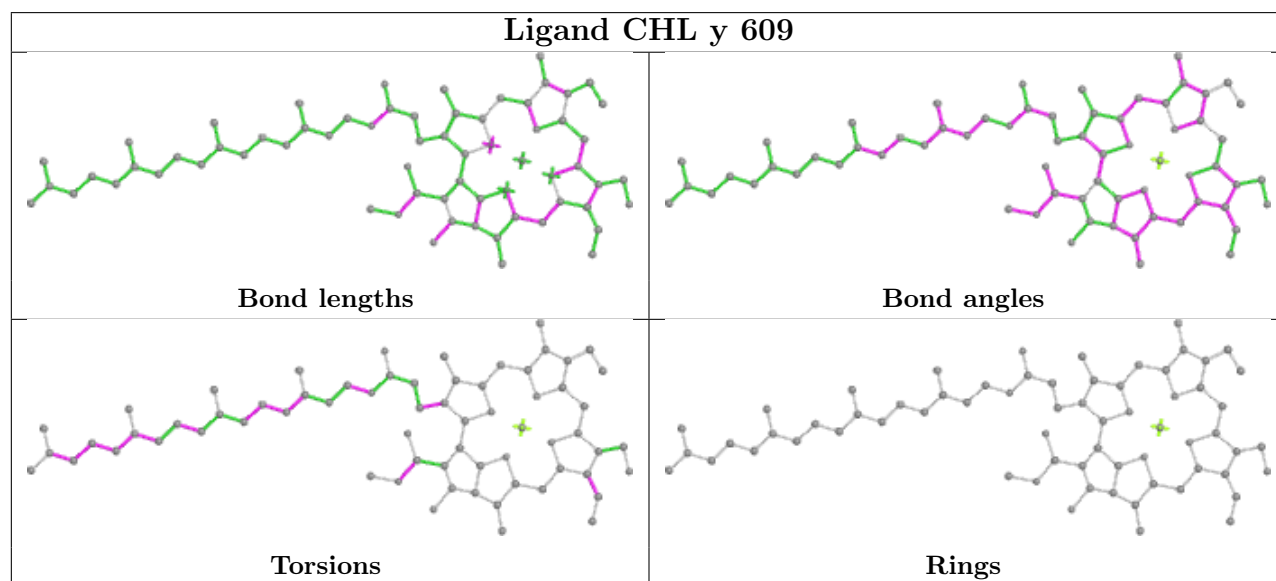
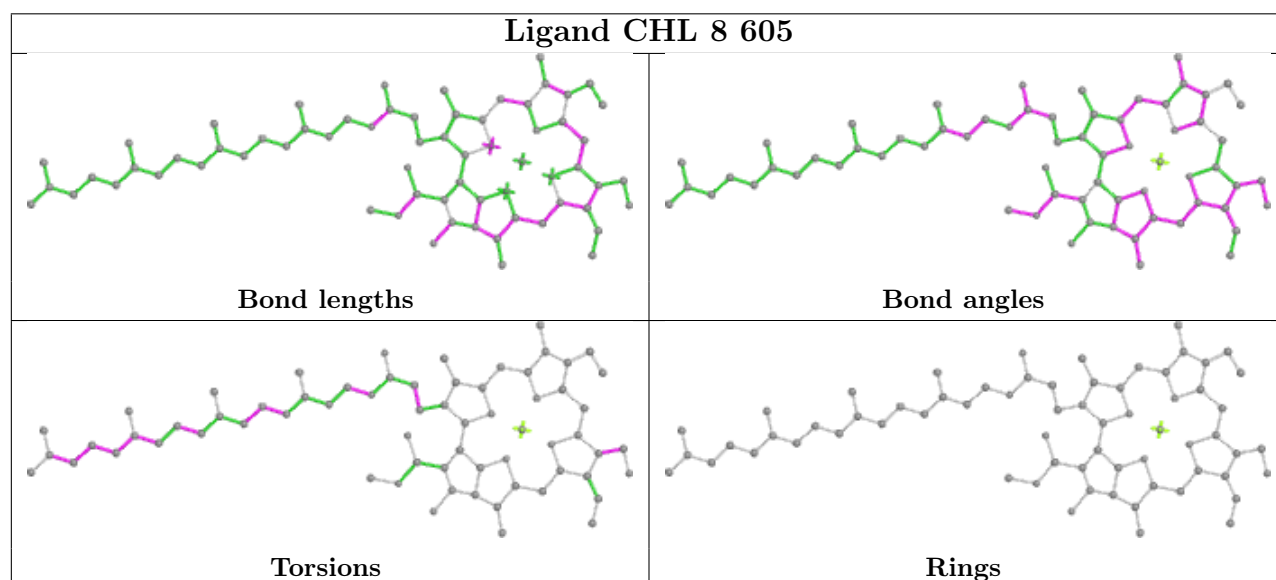
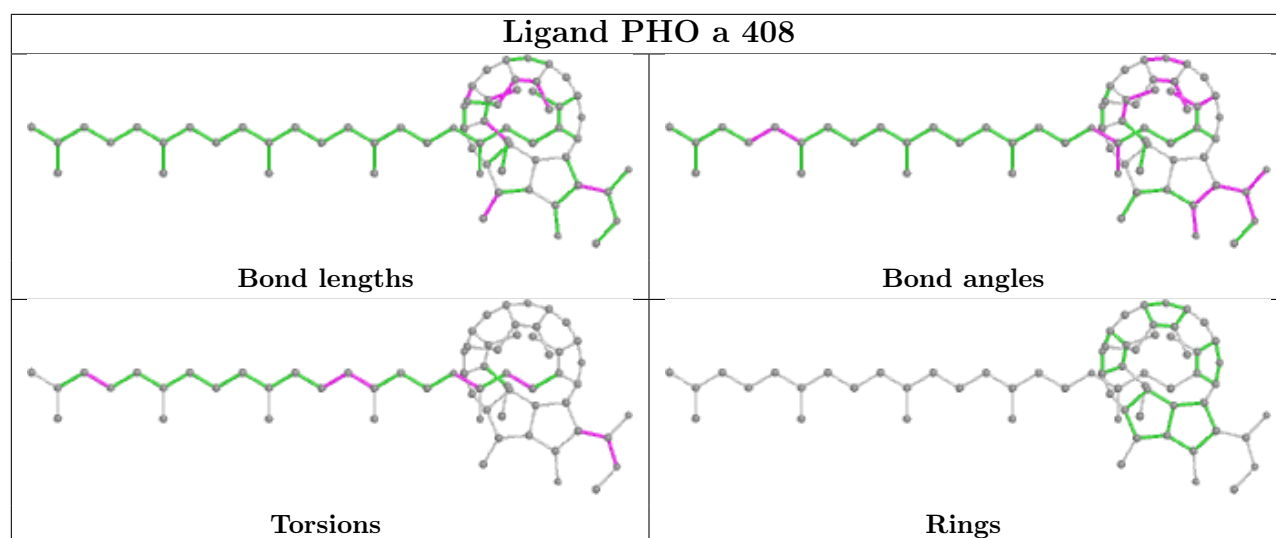
Bond angles



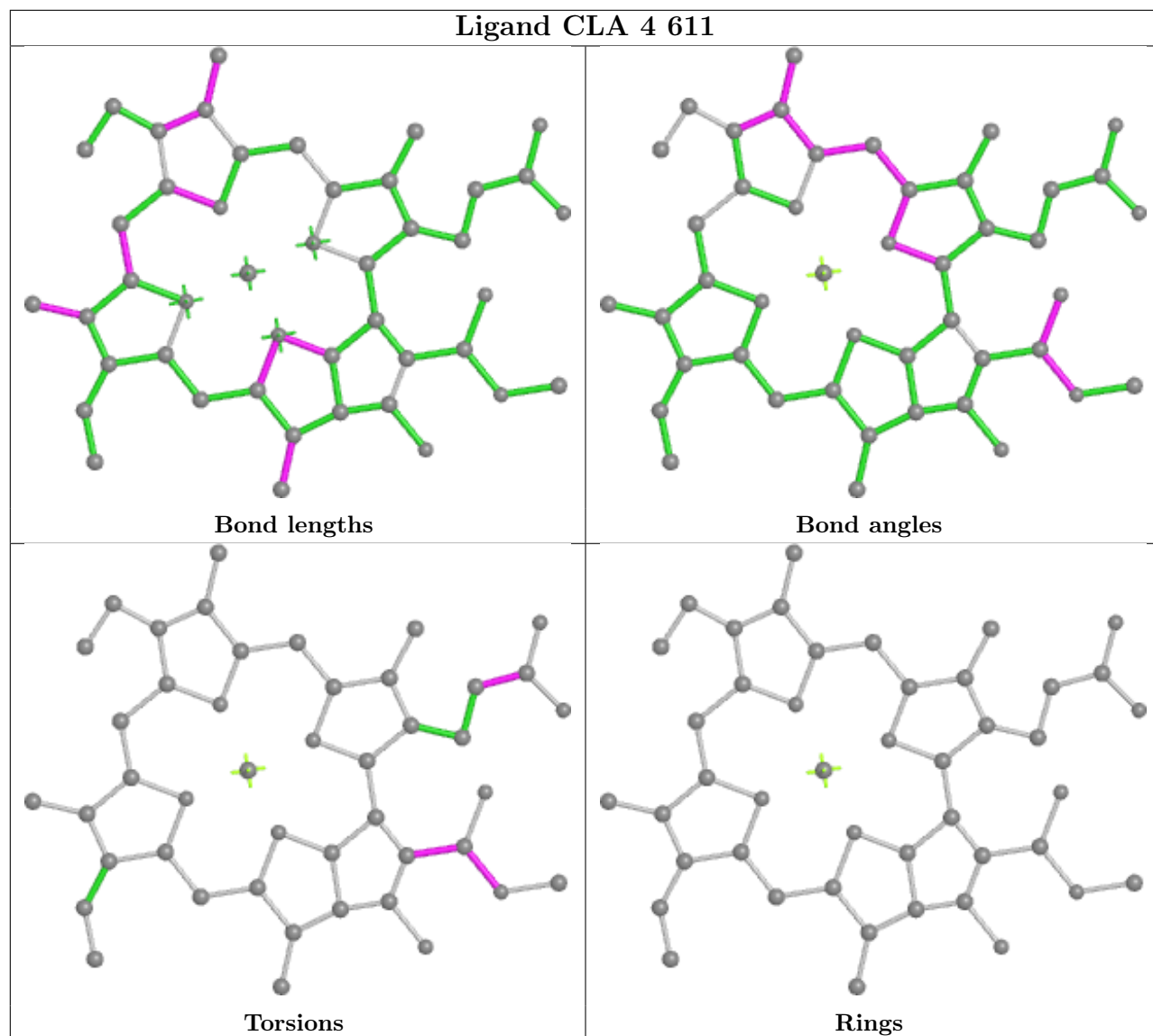
Torsions



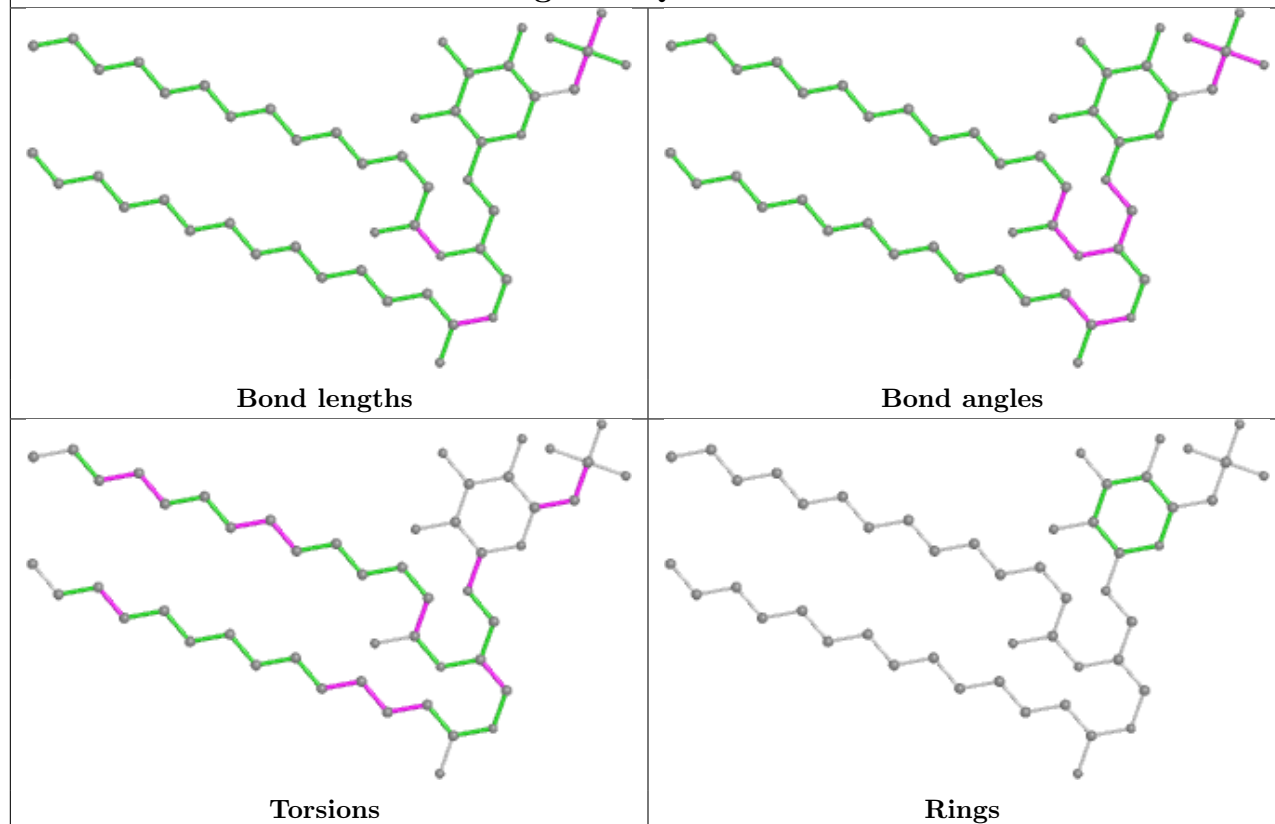
Rings



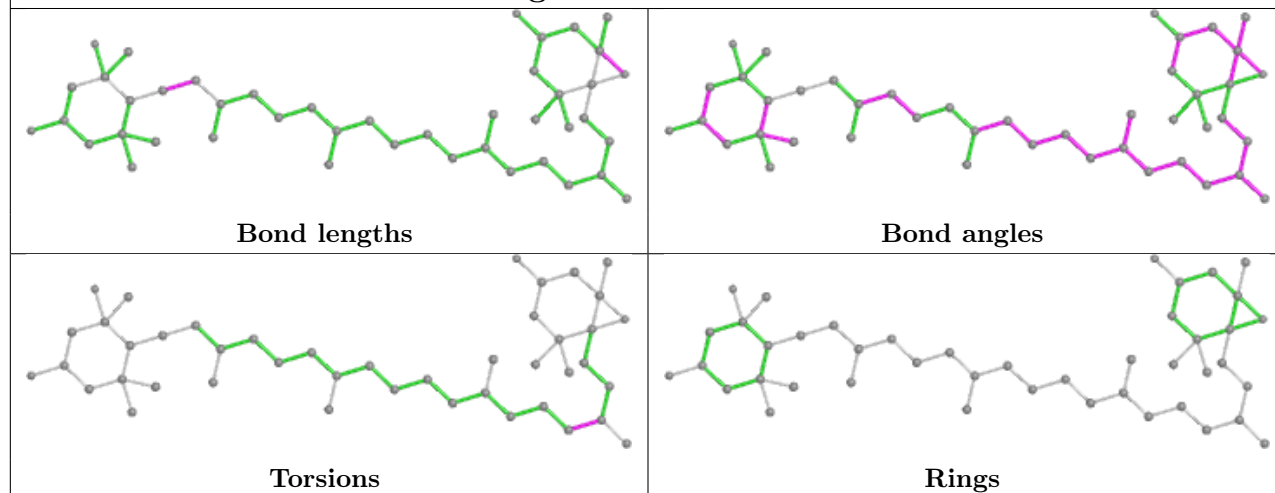
Ligand CLA 4 611

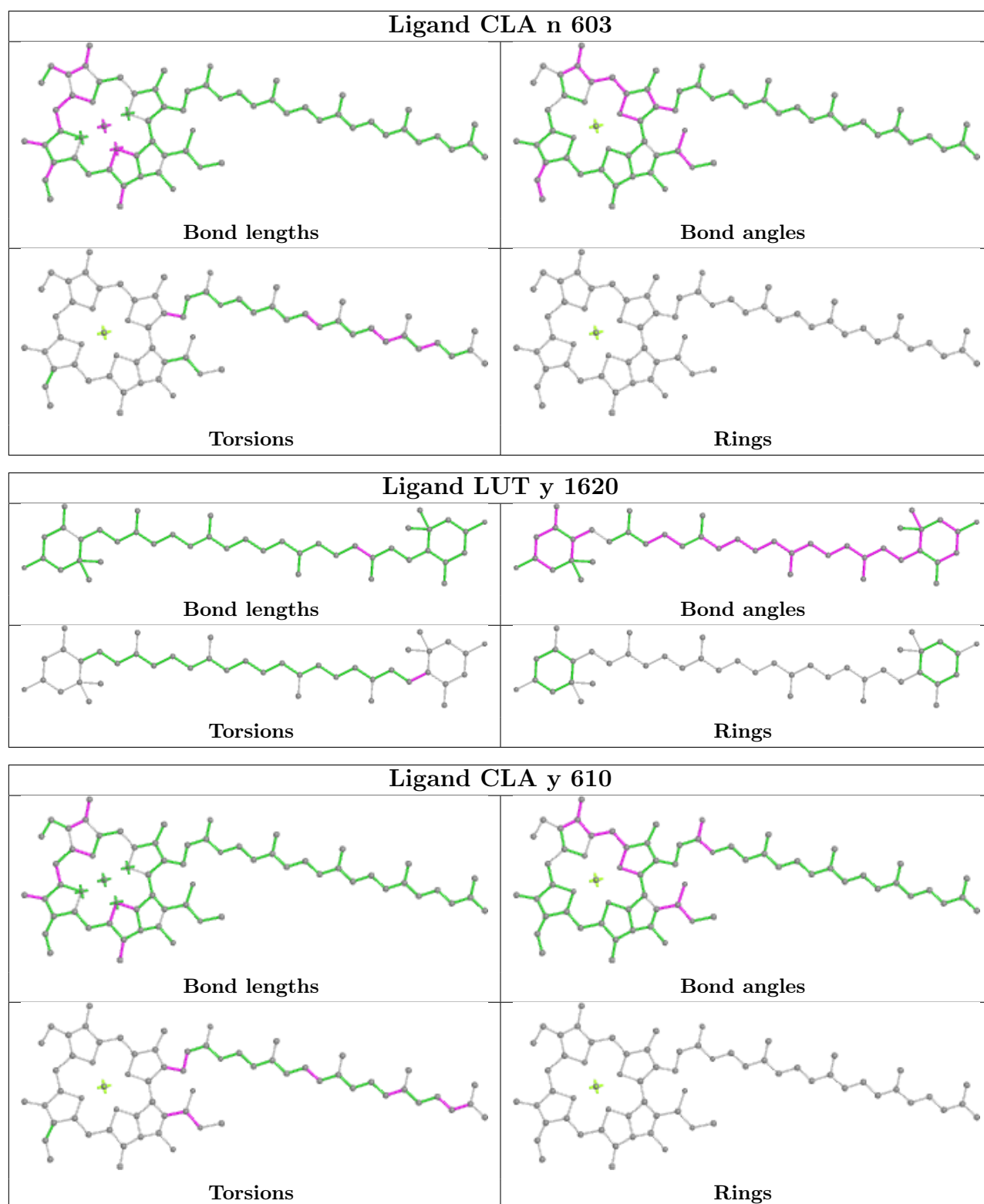


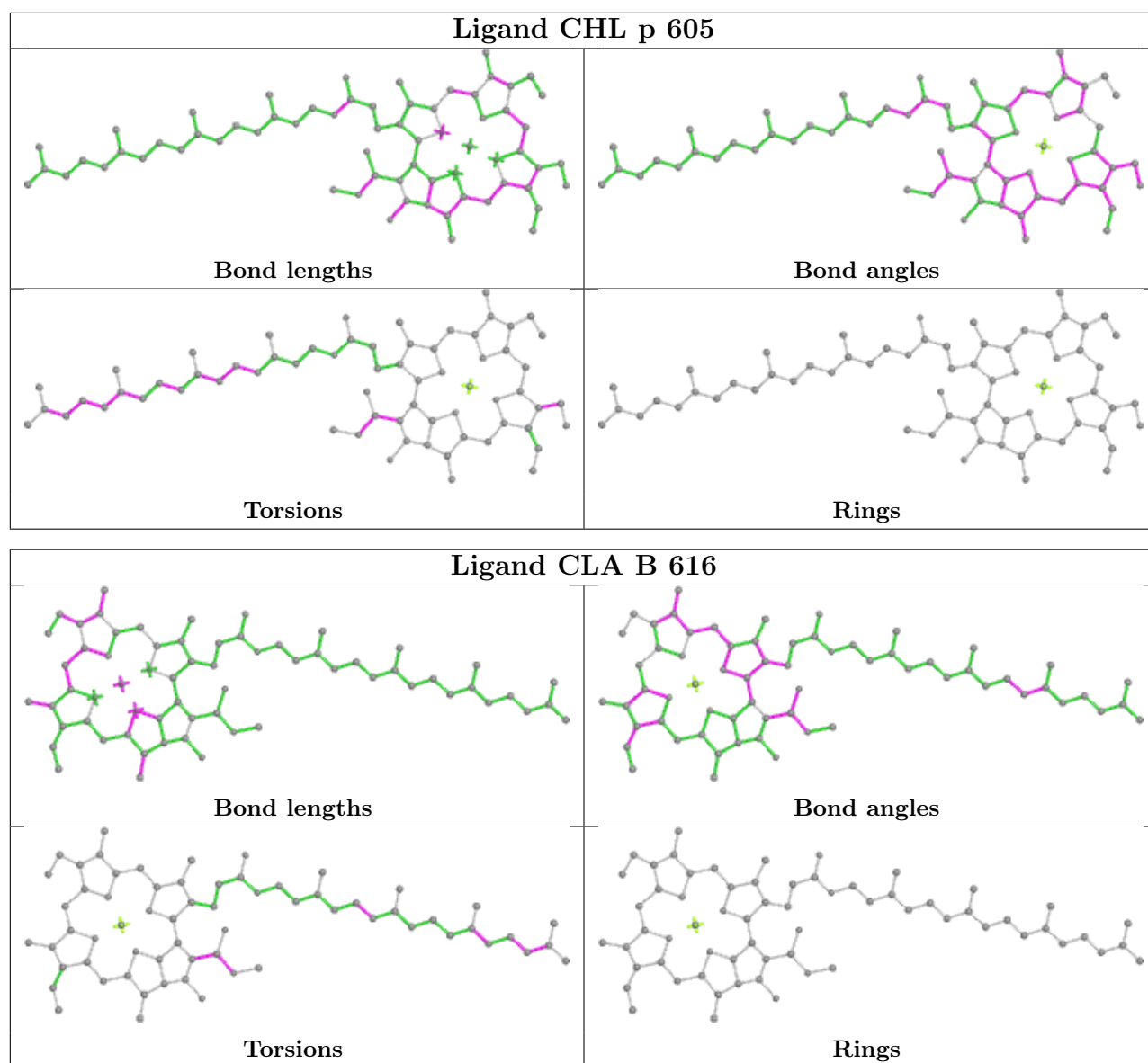
Ligand SQD b 623



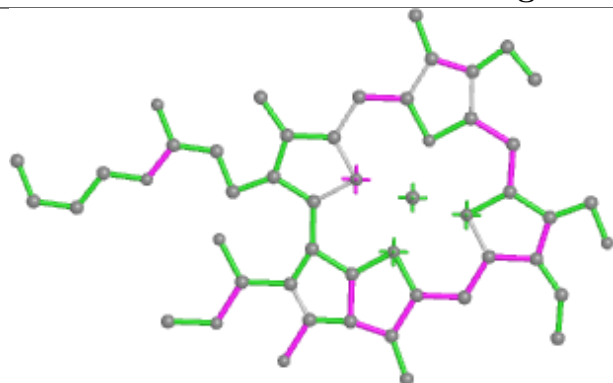
Ligand NEX R 623



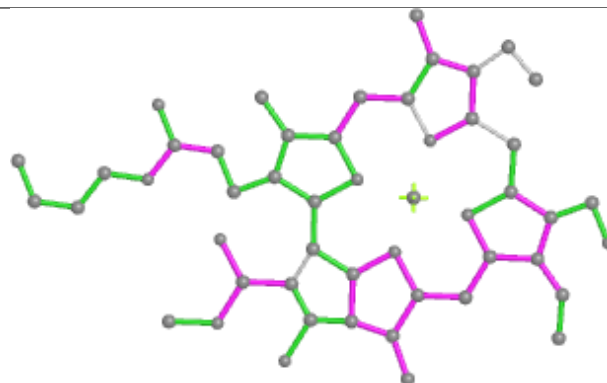




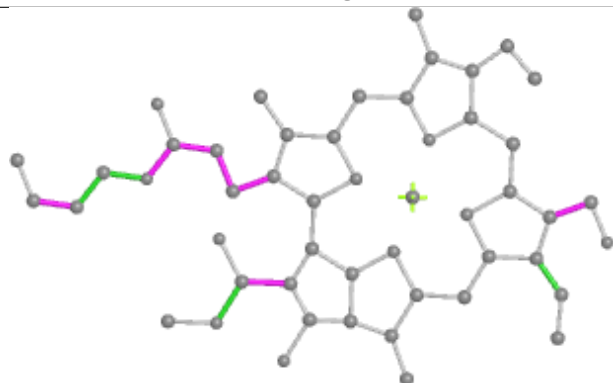
Ligand CHL 9 607



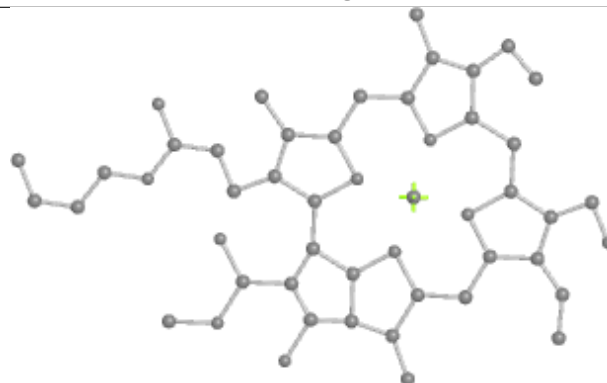
Bond lengths



Bond angles

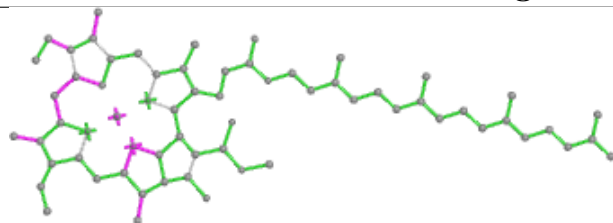


Torsions

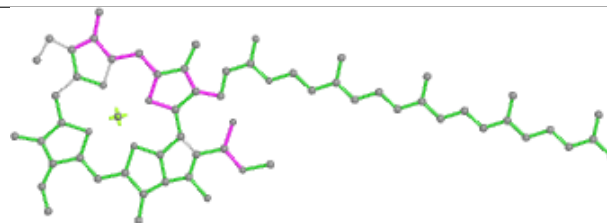


Rings

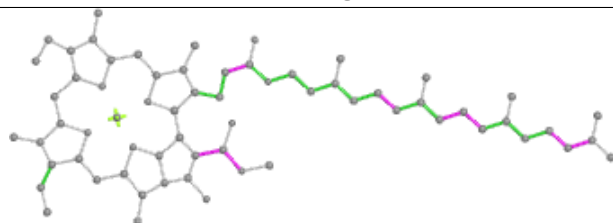
Ligand CLA B 614



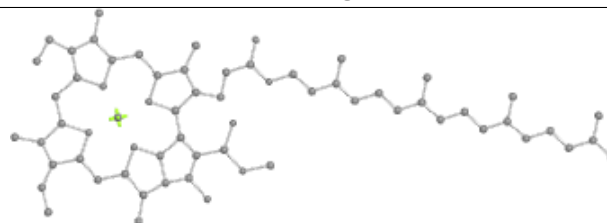
Bond lengths



Bond angles

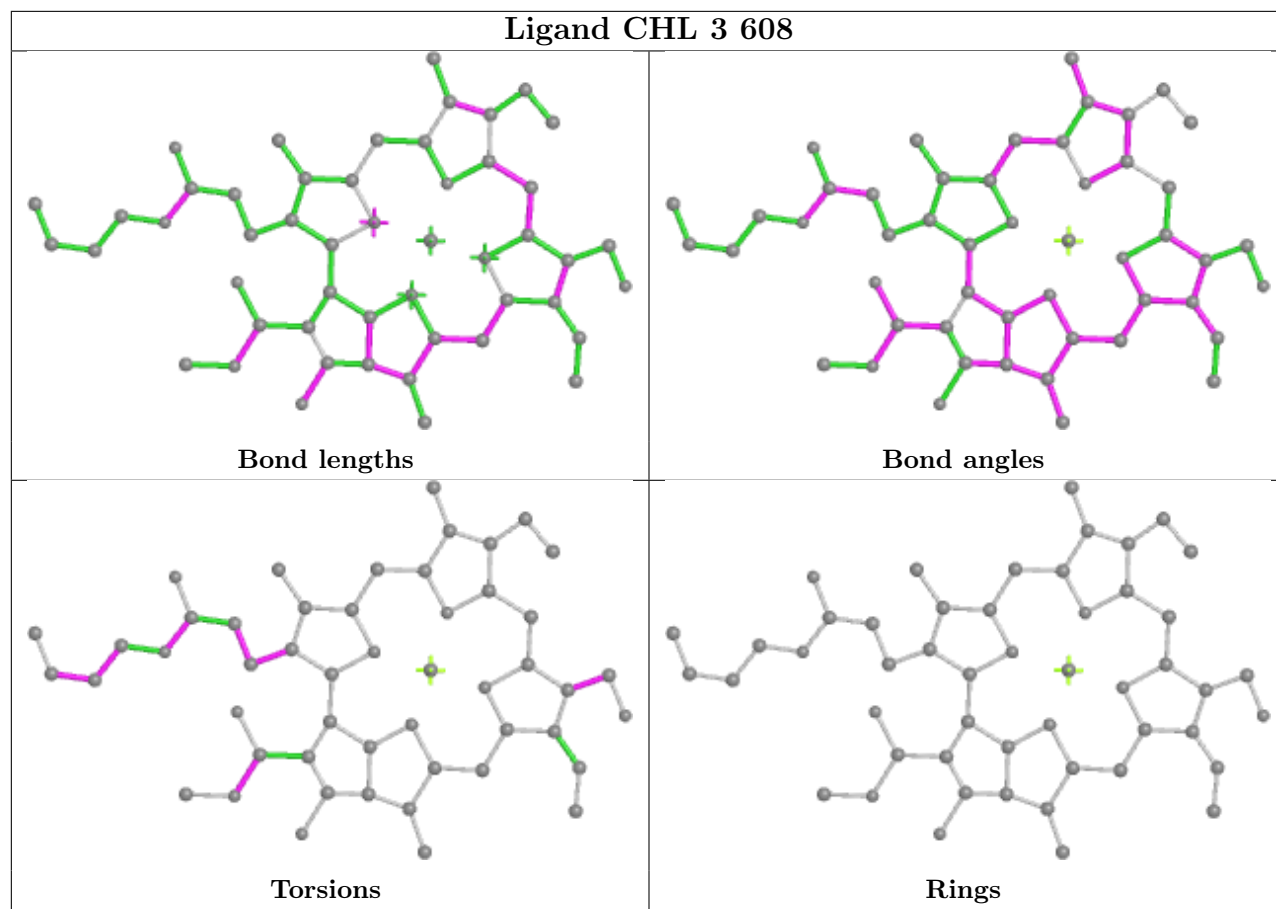


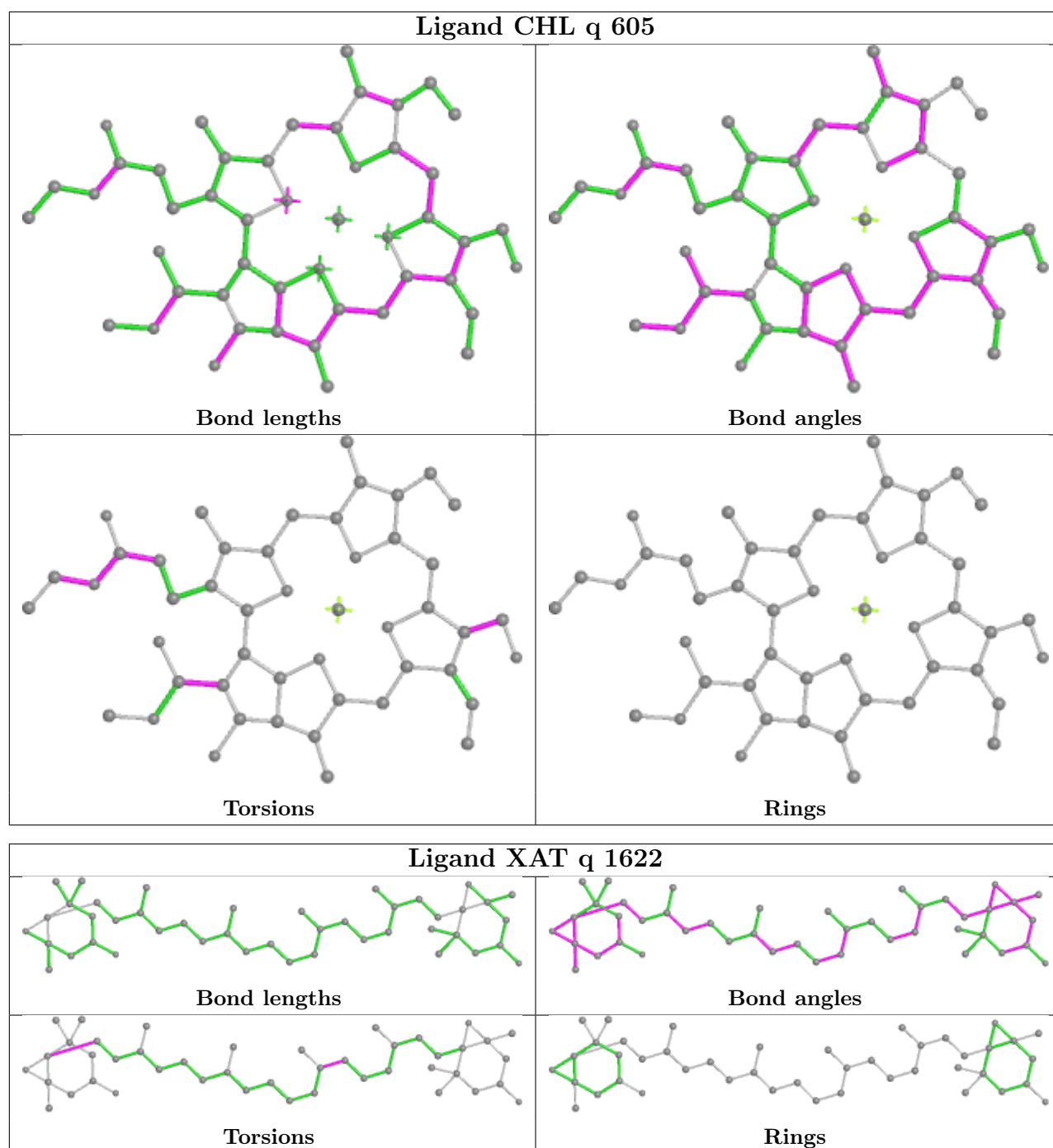
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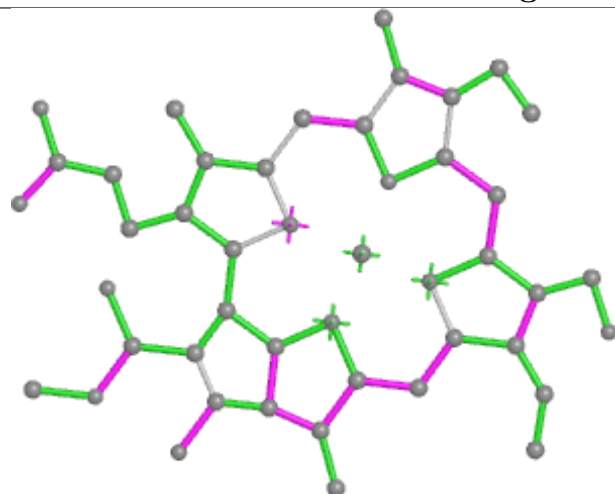
Rings

Ligand CHL 3 608

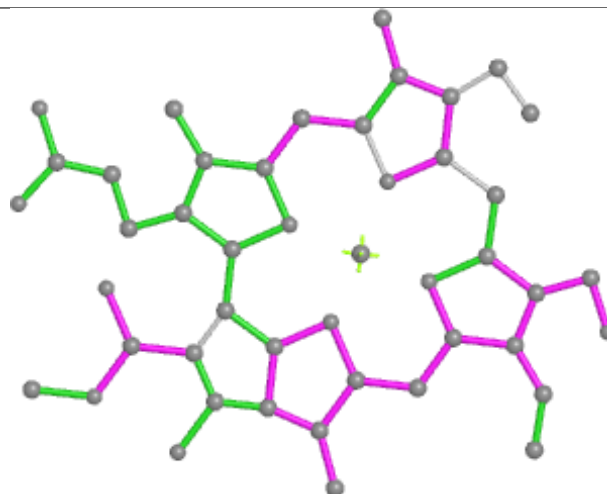




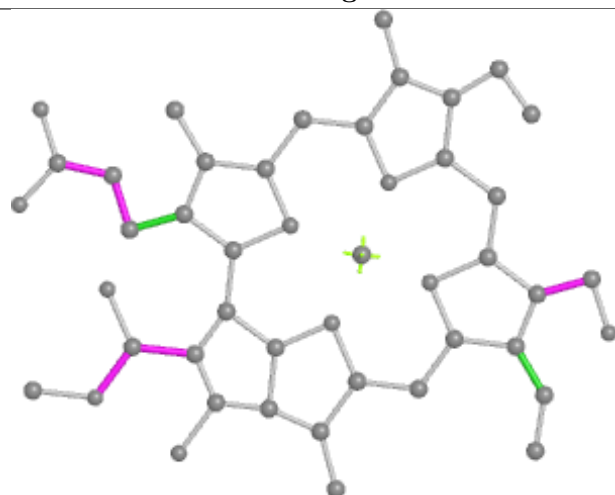
Ligand CHL 1 605



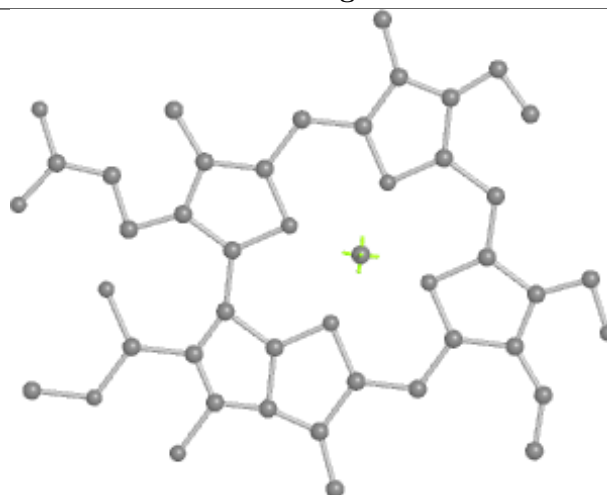
Bond lengths



Bond angles

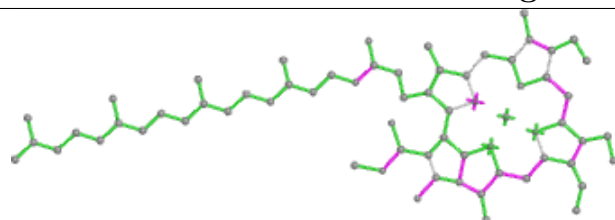


Torsions

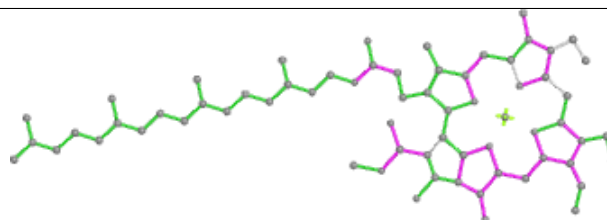


Rings

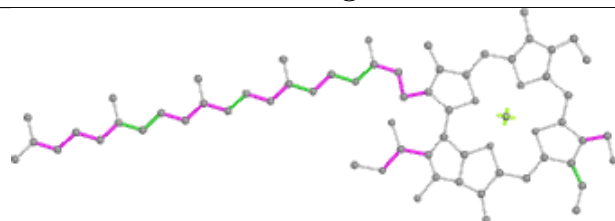
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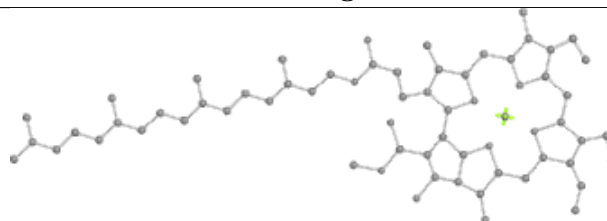
Bond lengths



Bond angles

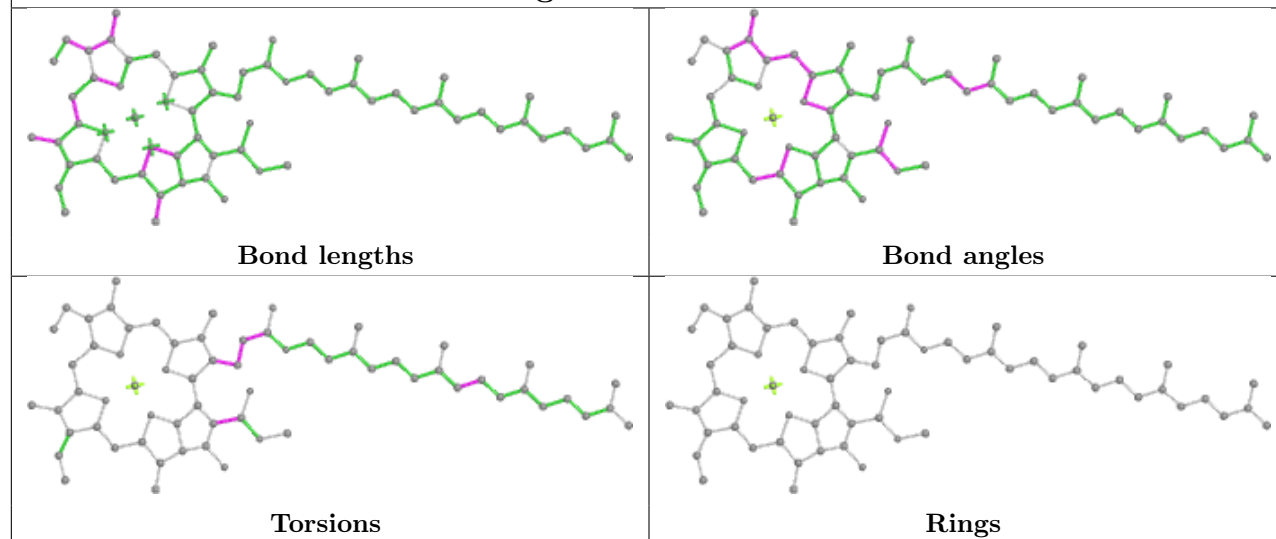


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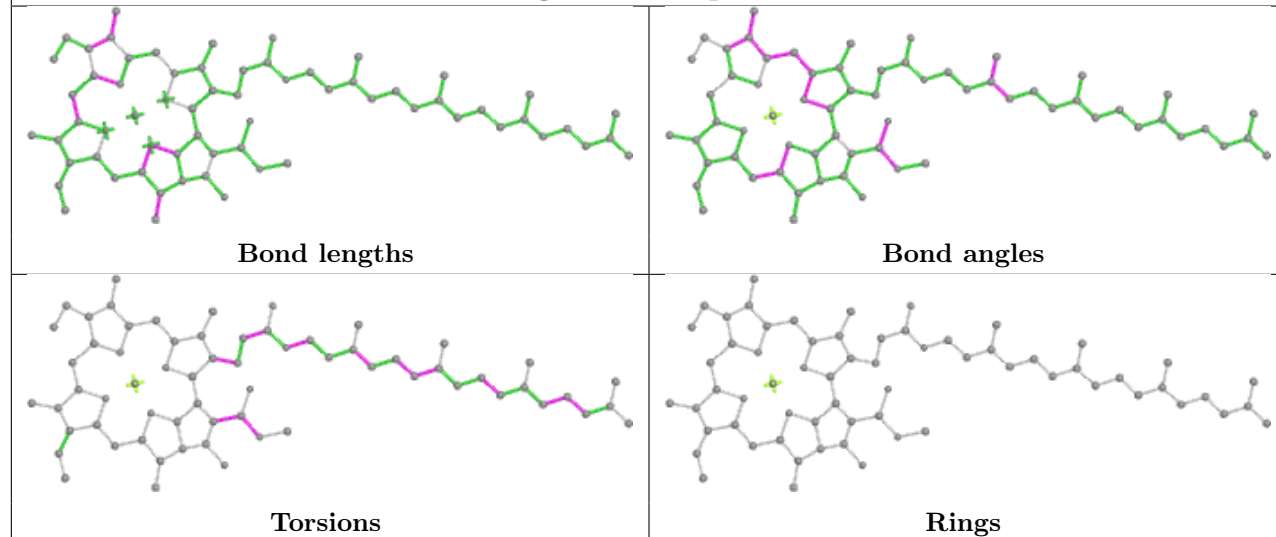


Rings

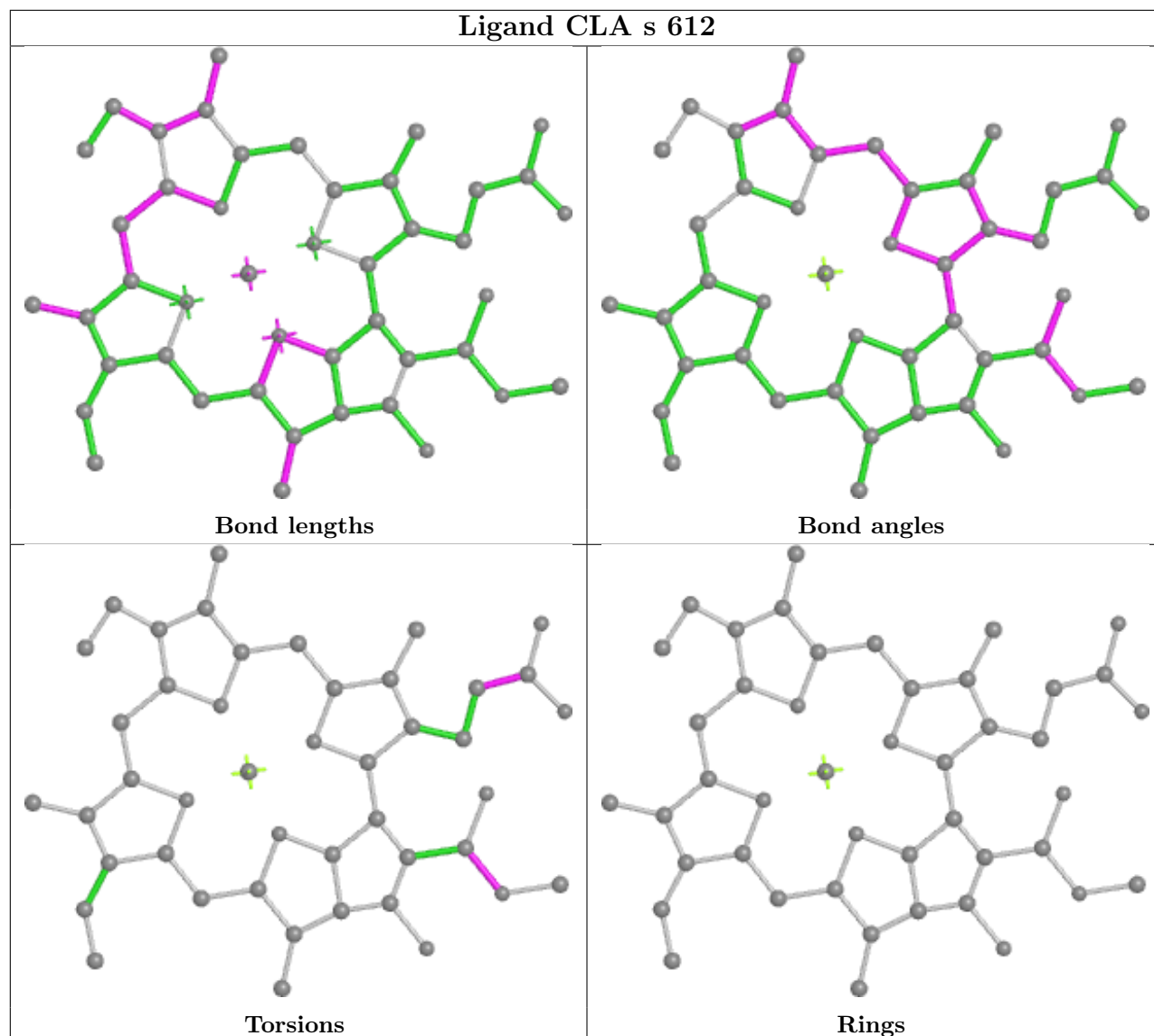
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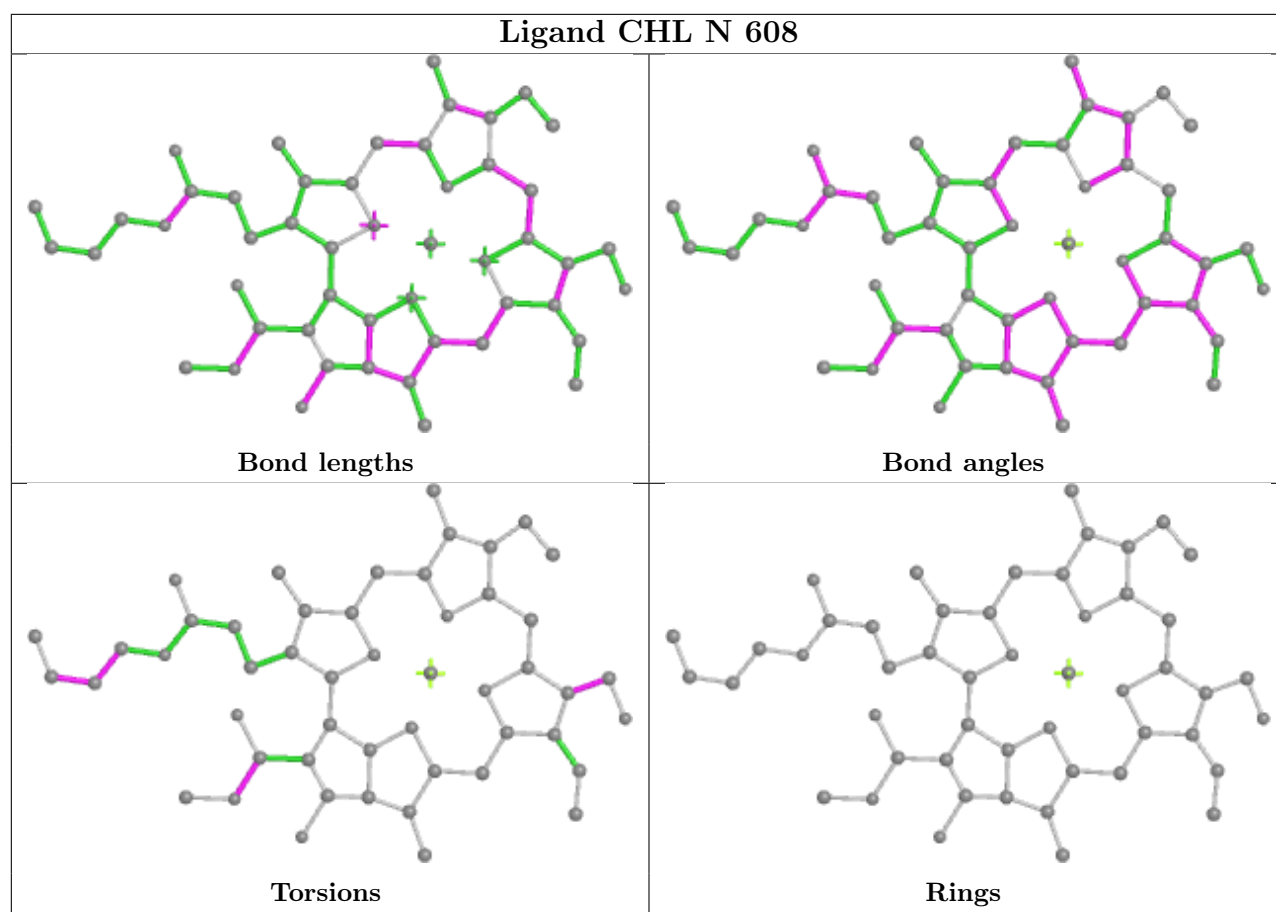


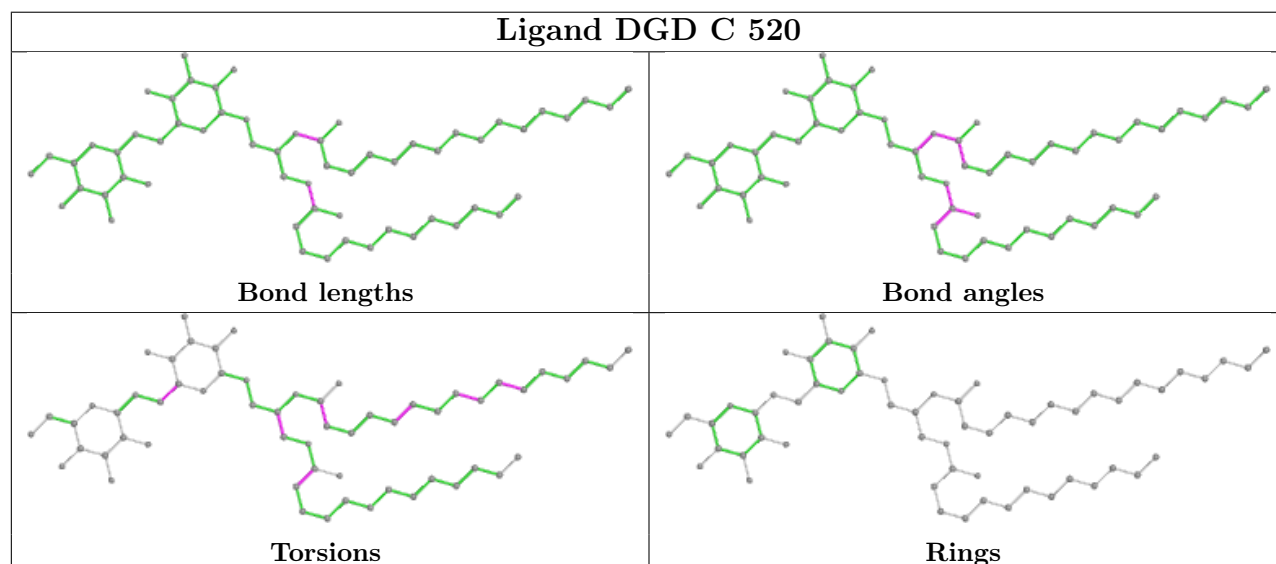
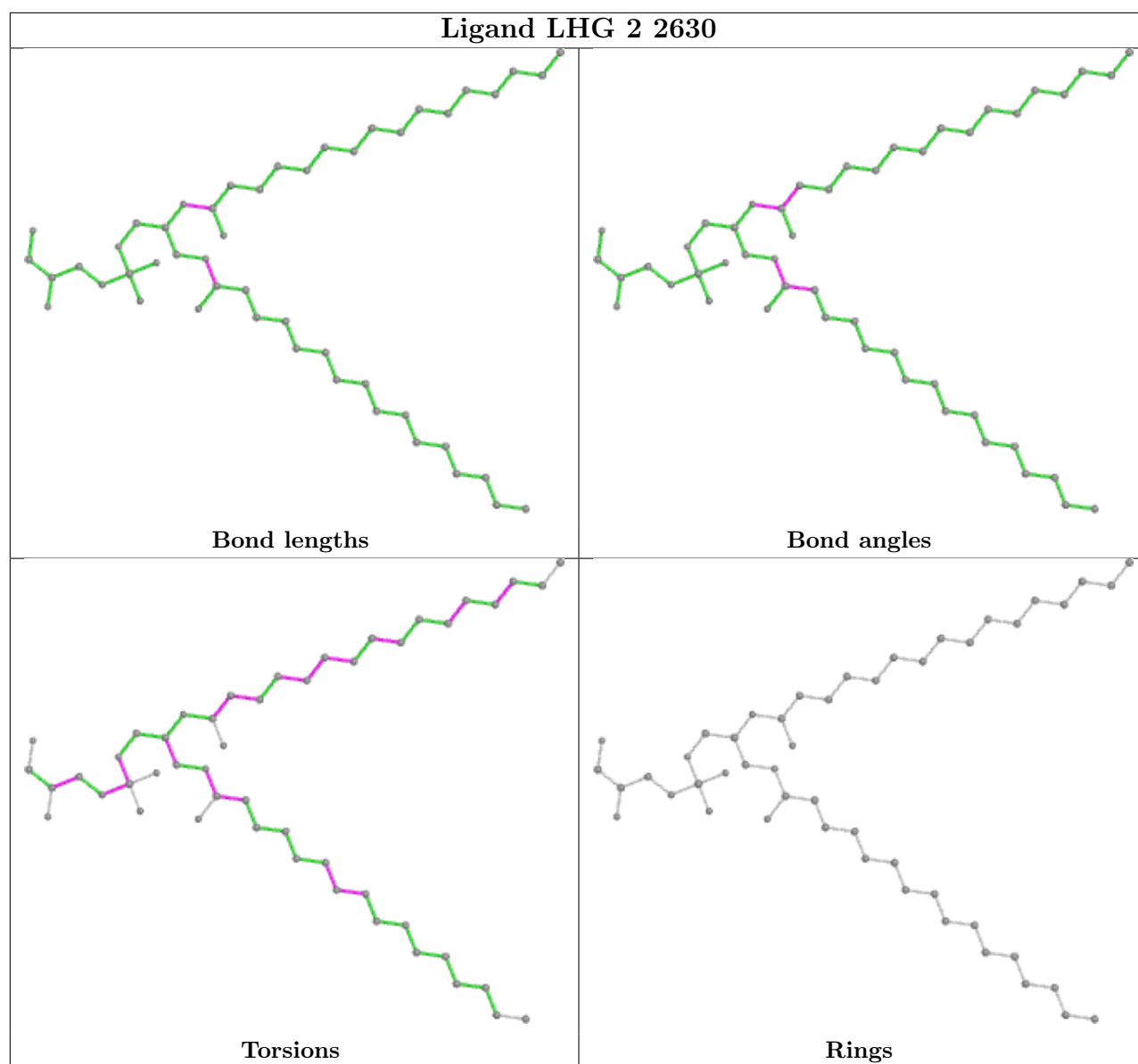
Ligand CLA p 604



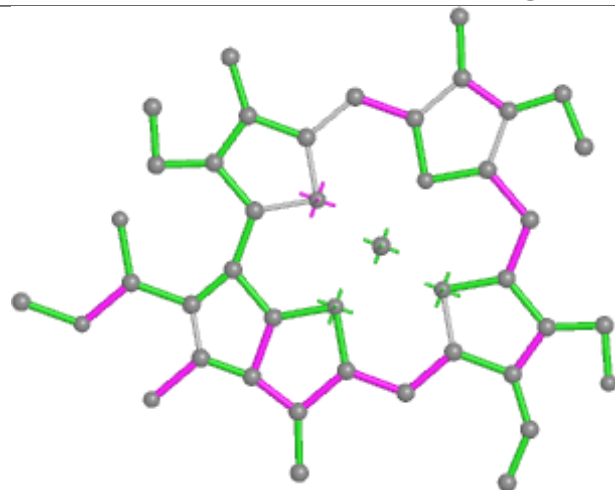
Ligand CLA s 612



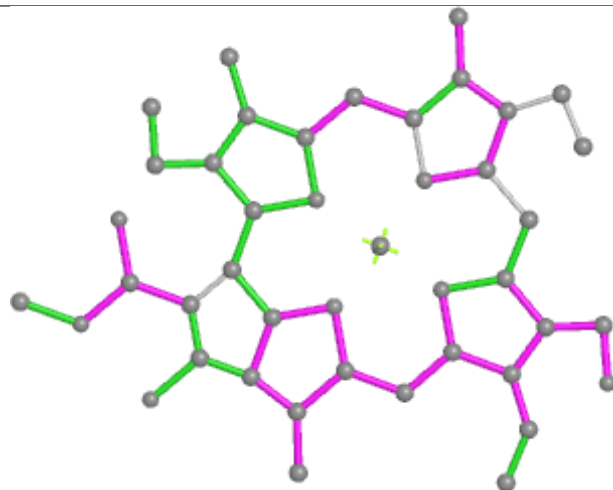




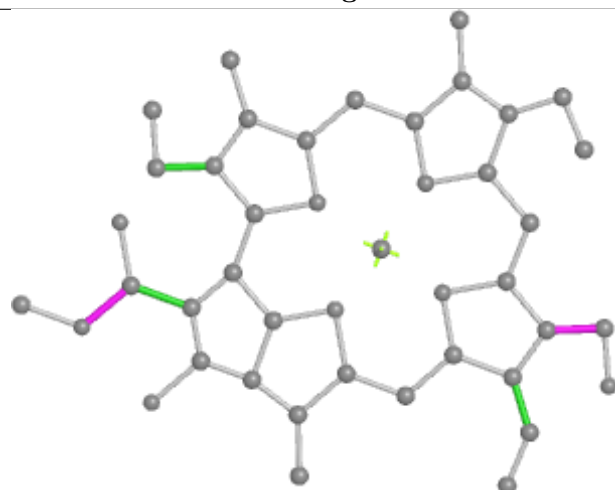
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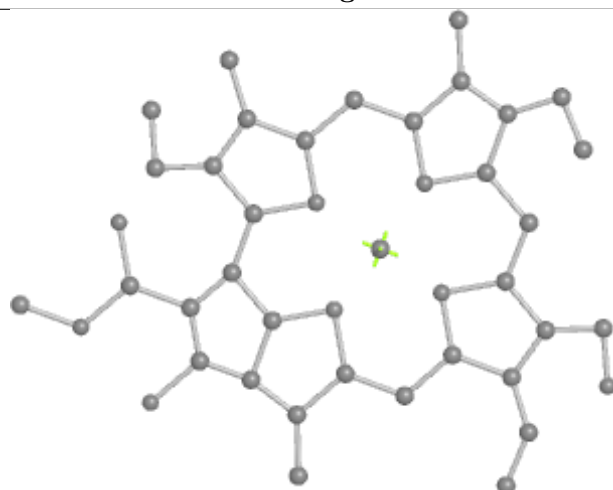
Bond lengths



Bond angles

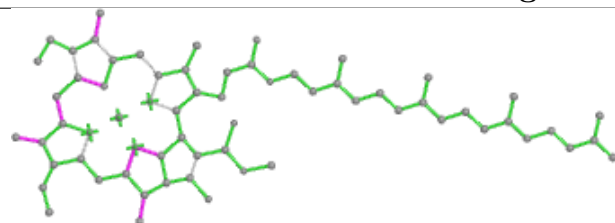


Torsions

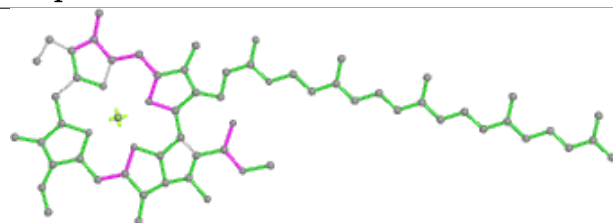


Rings

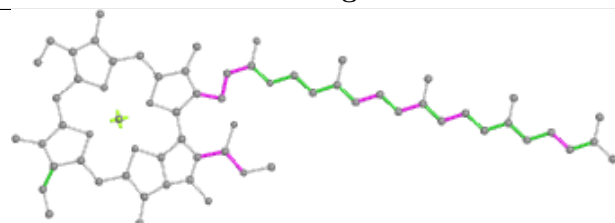
Ligand CLA p 602



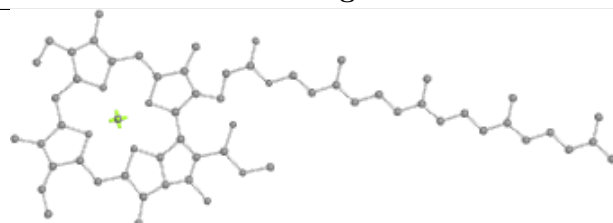
Bond lengths



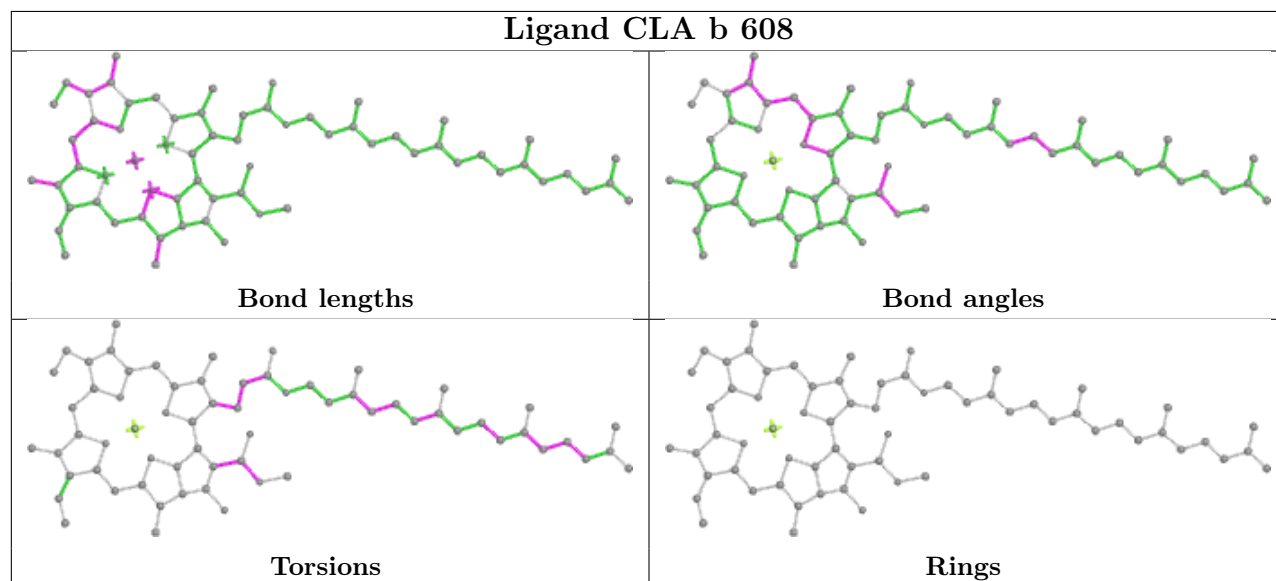
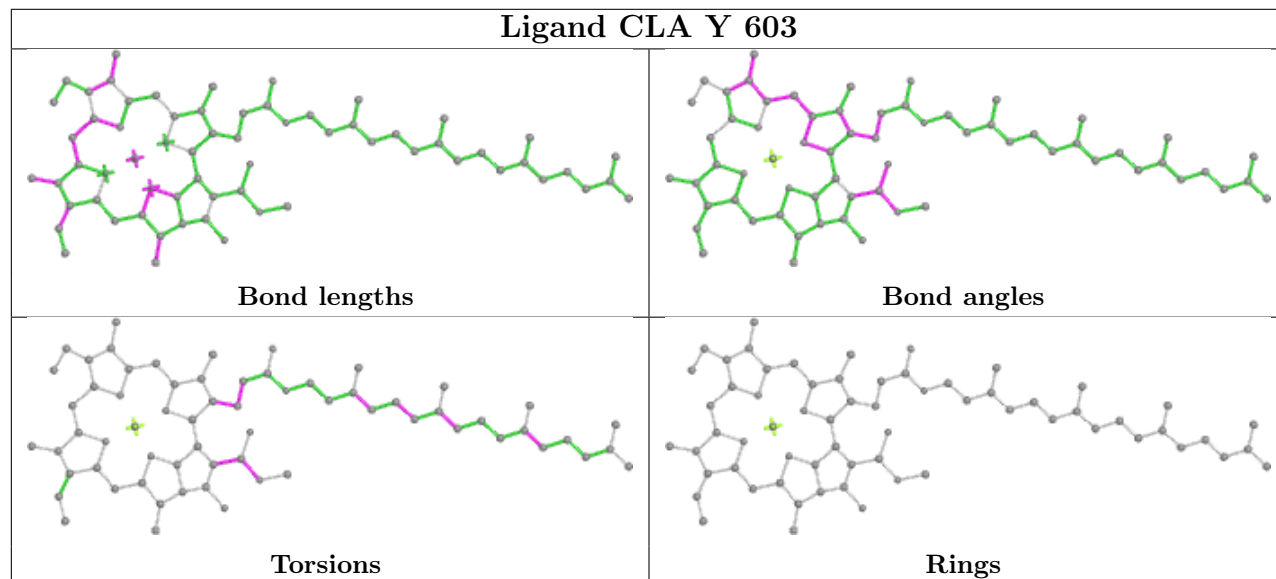
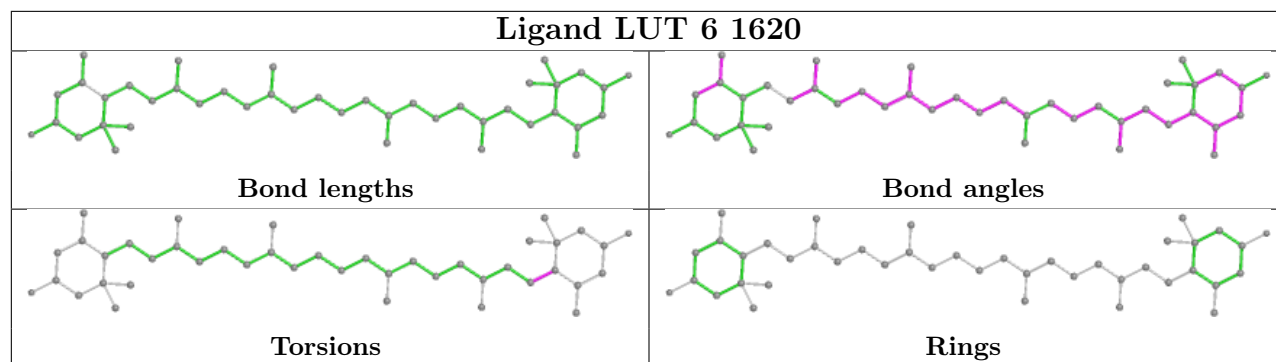
Bond angles

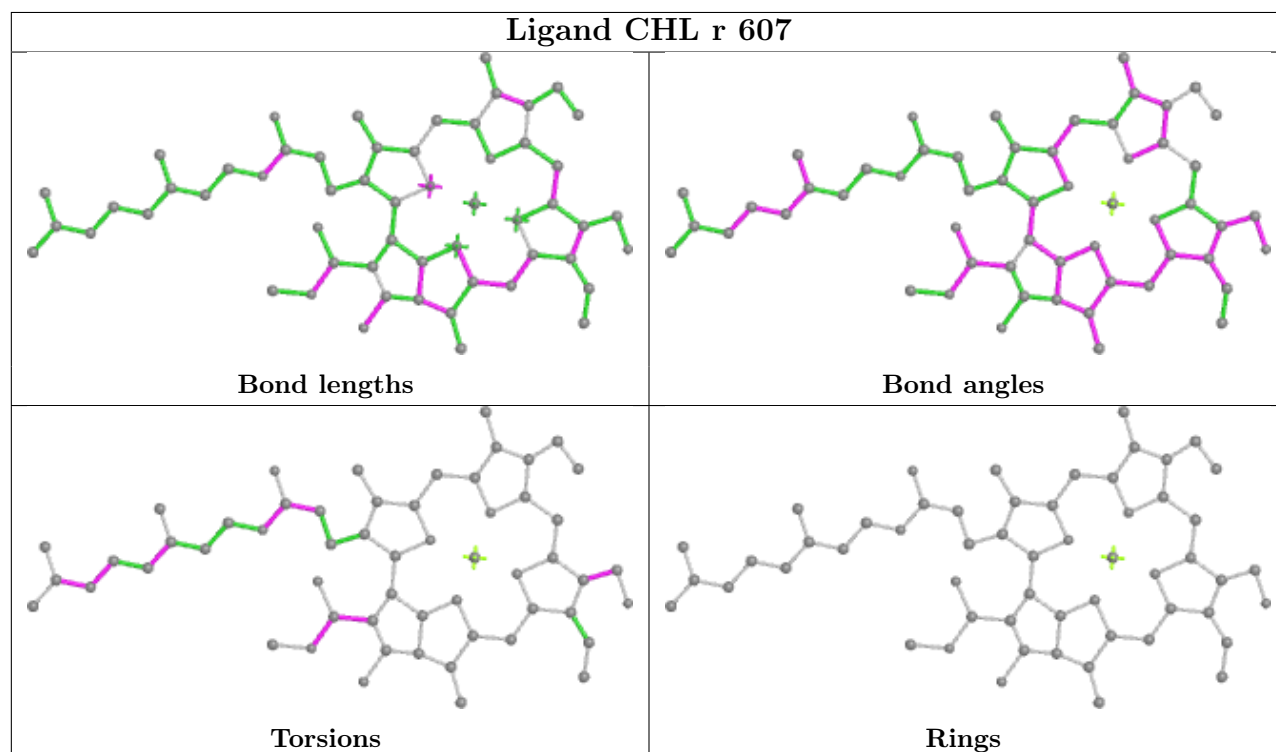
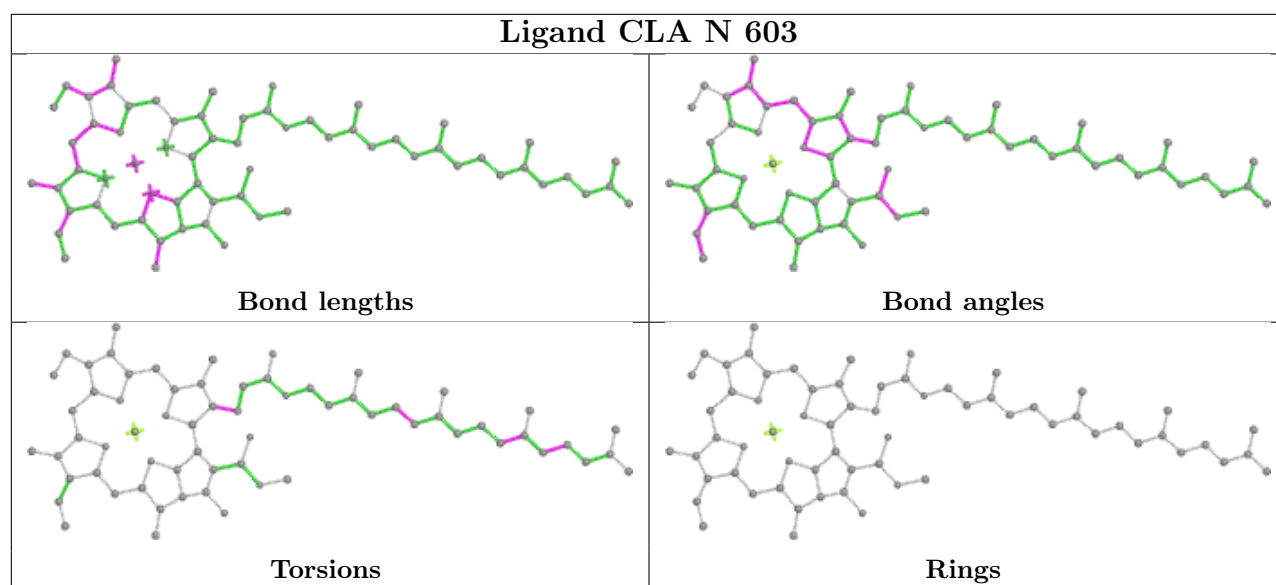


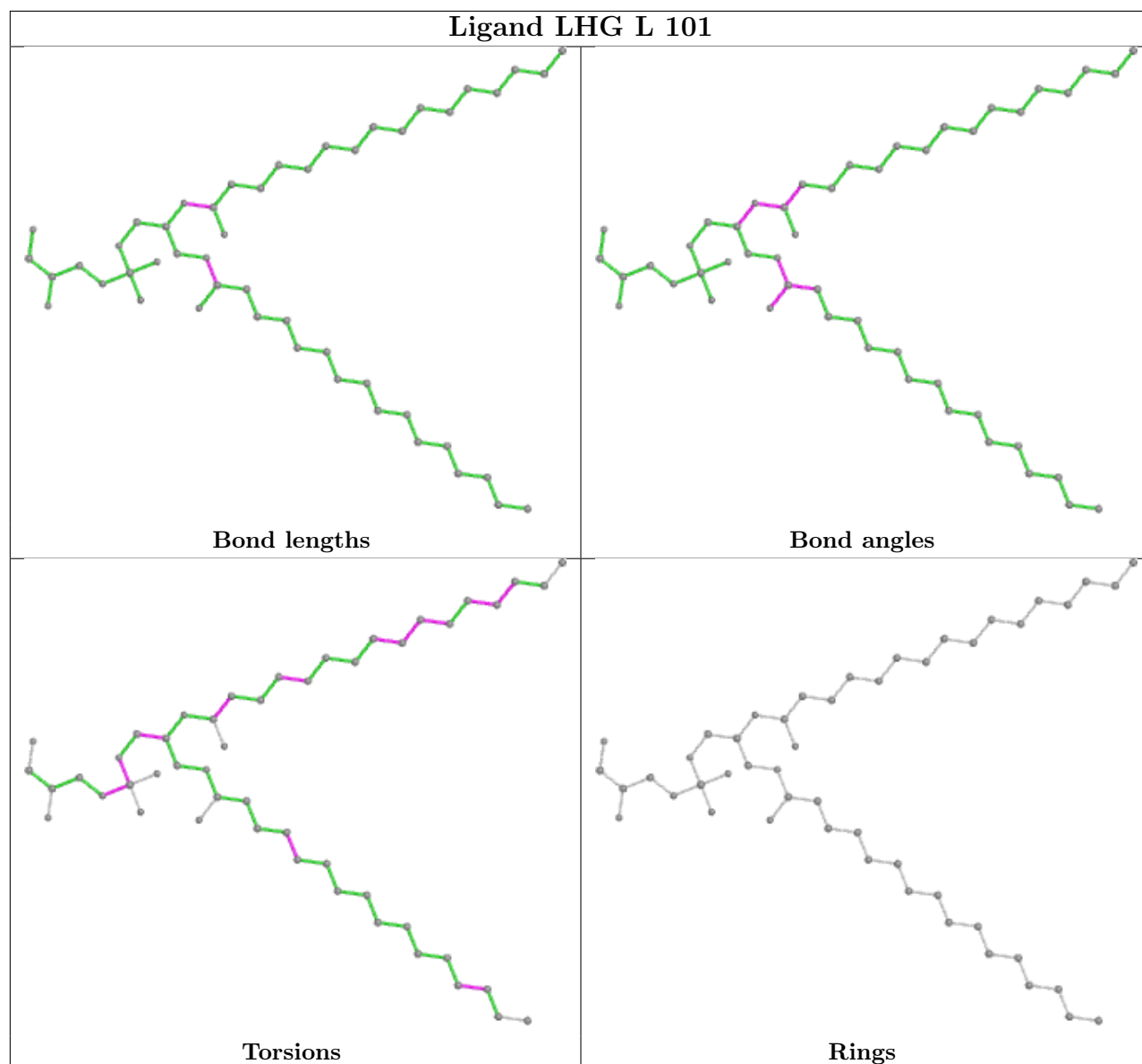
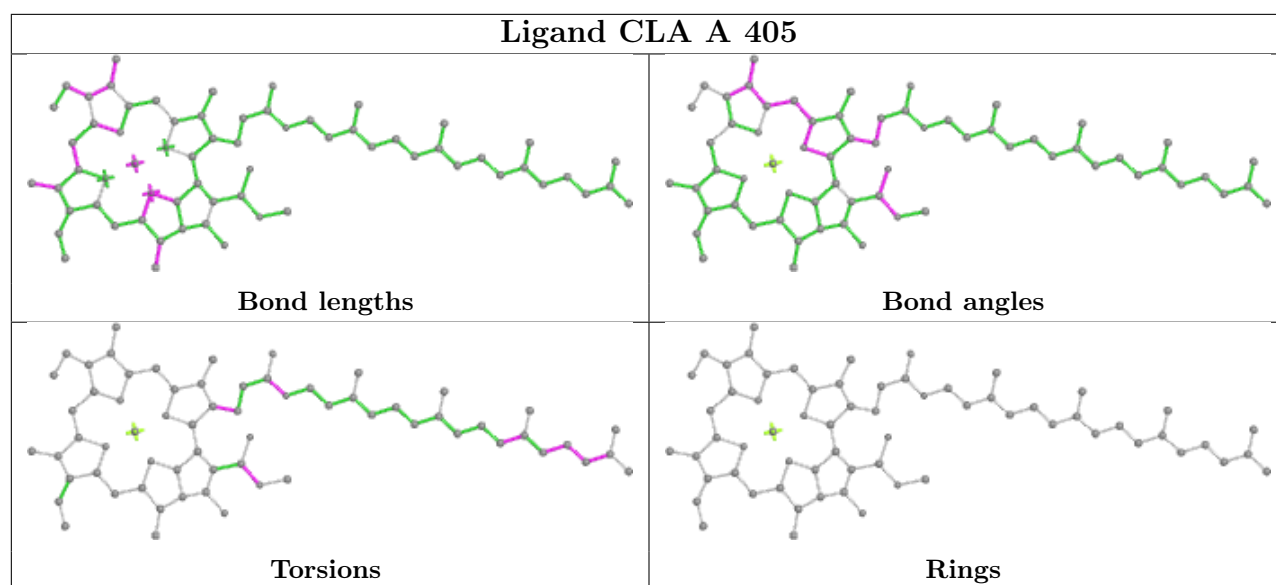
Torsions



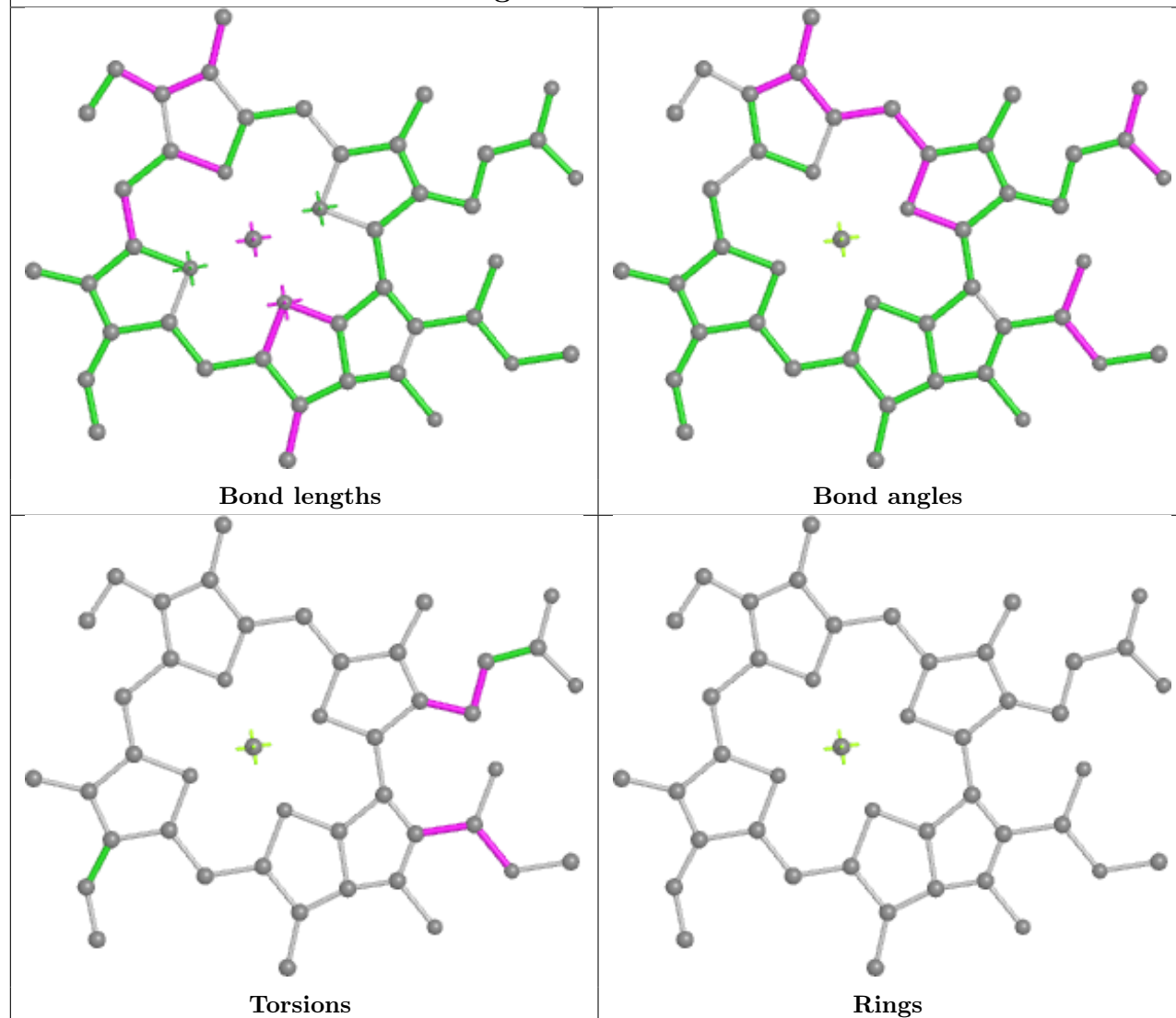
Rings



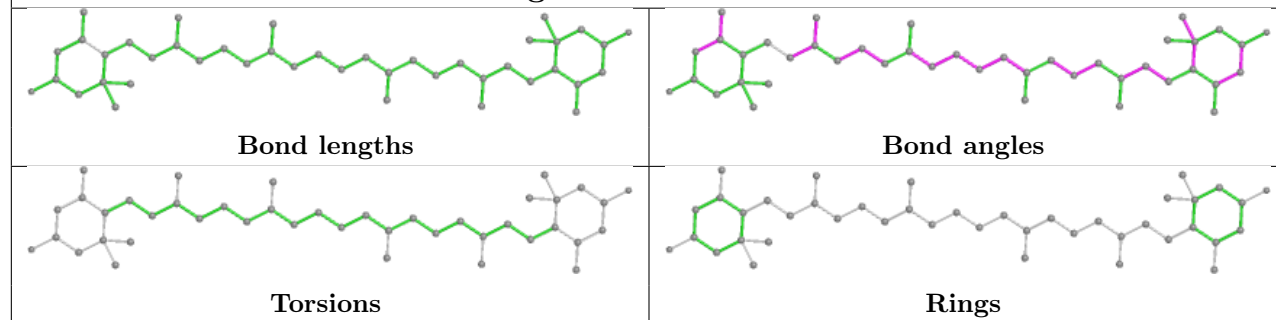


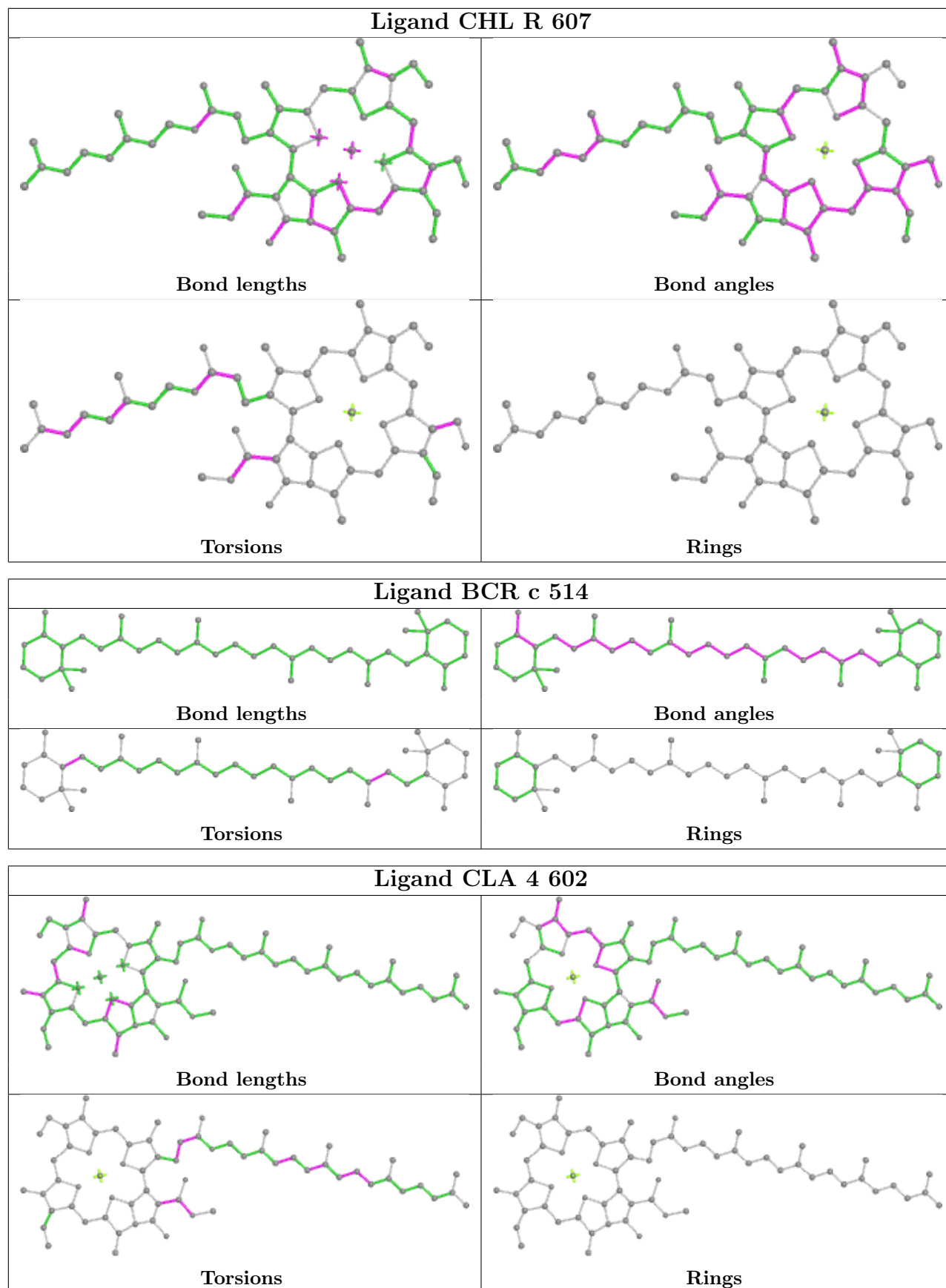


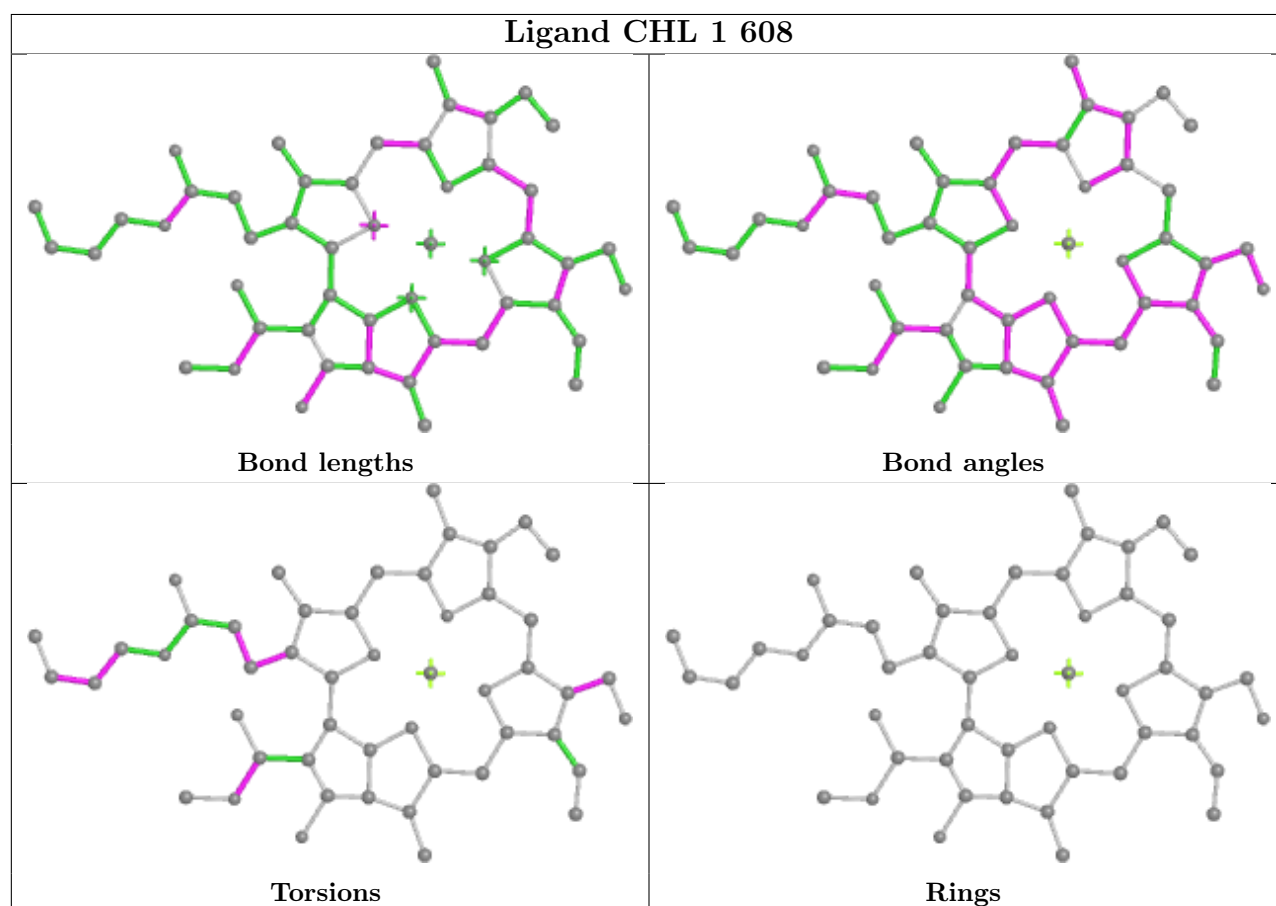
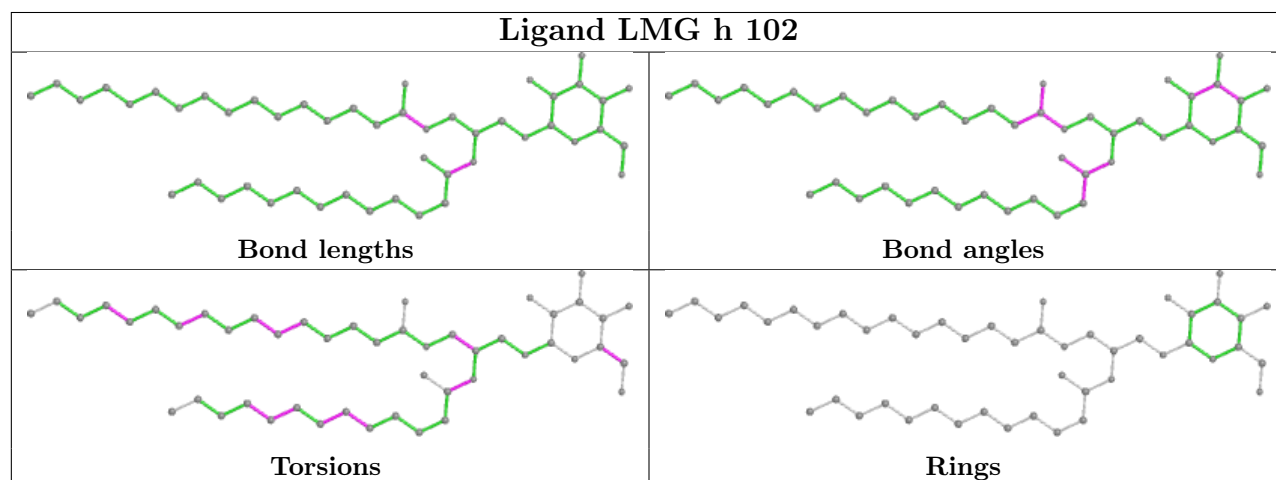
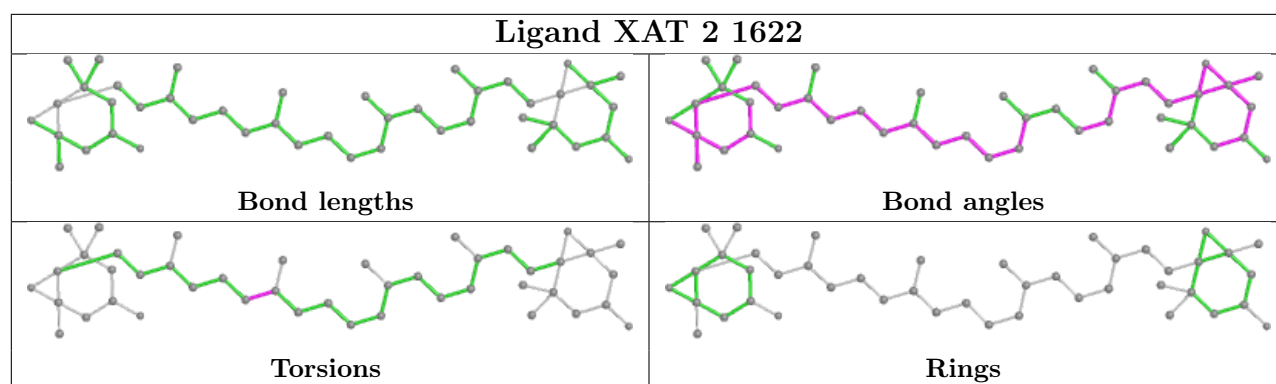
Ligand CLA 9 611

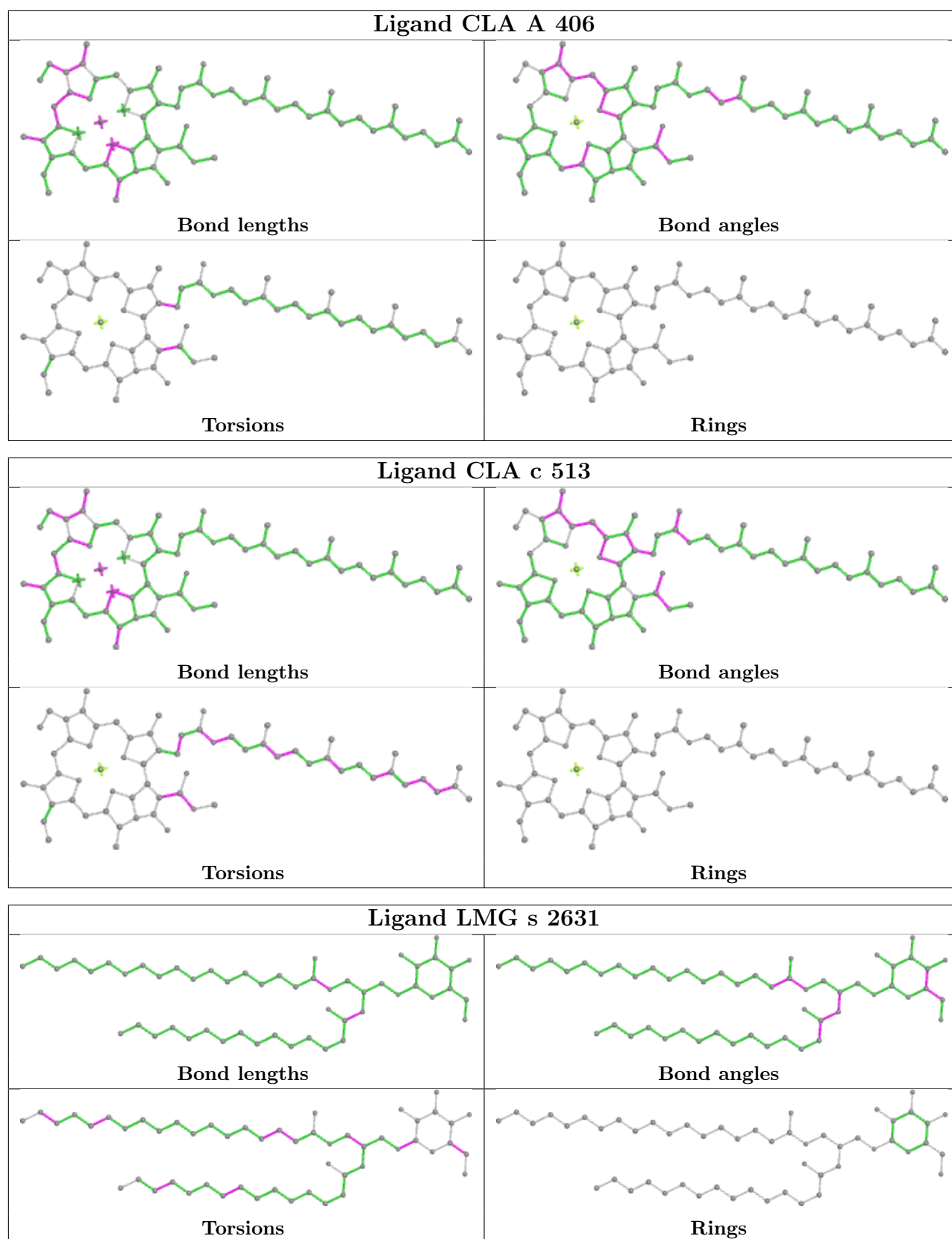


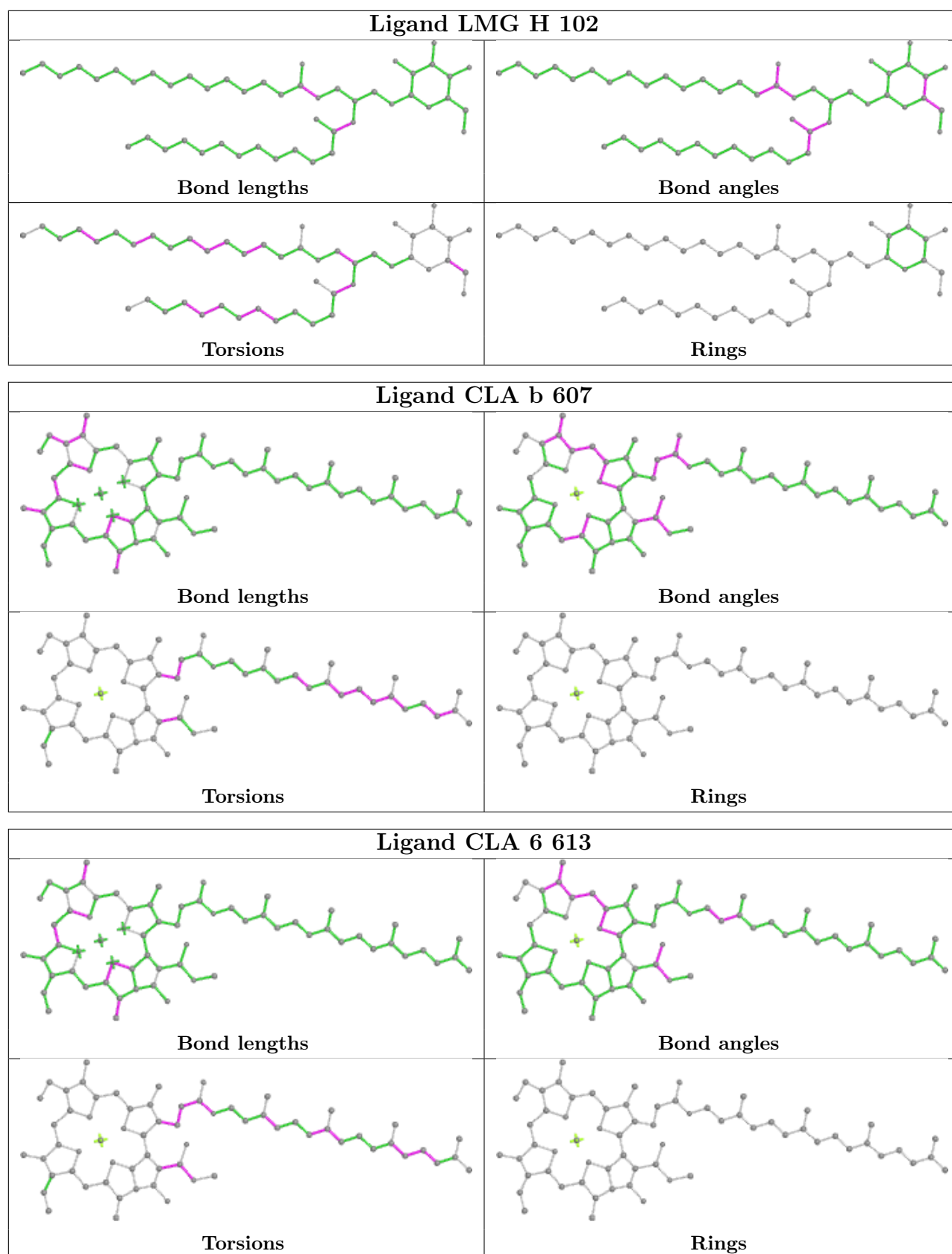
Ligand LUT 8 1621

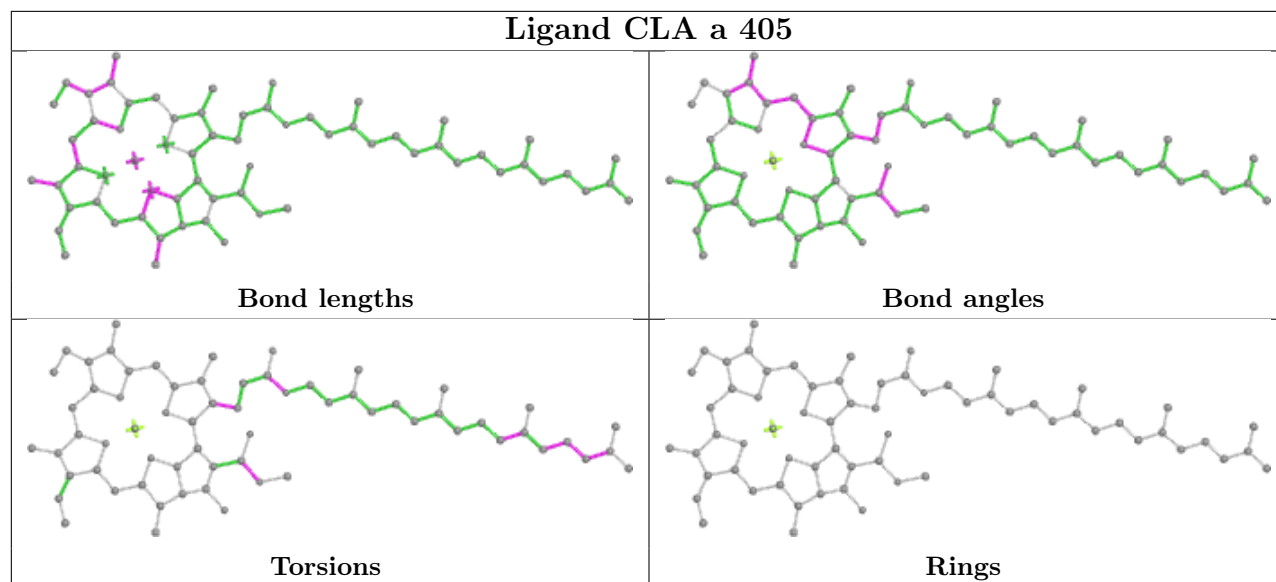
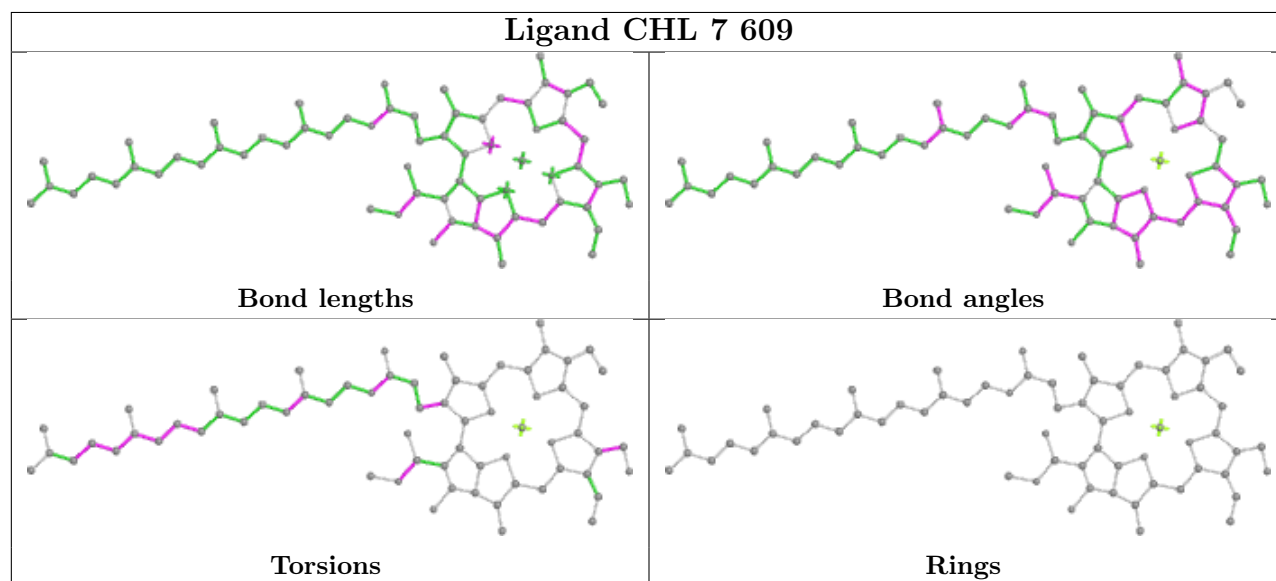




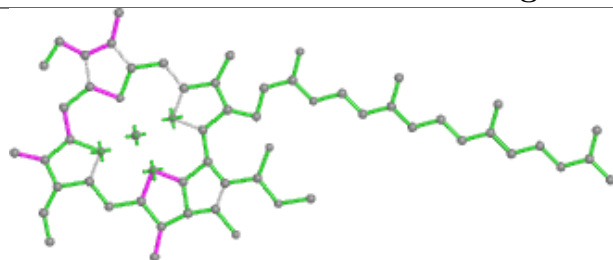




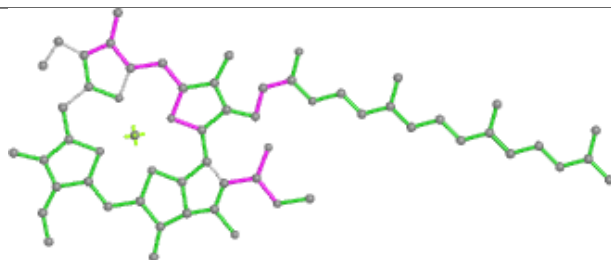


Ligand CLA a 405**Ligand CHL 7 609**

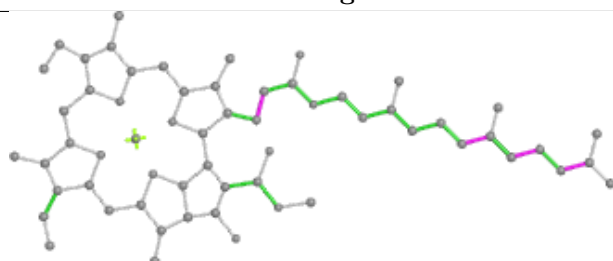
Ligand CLA r 602



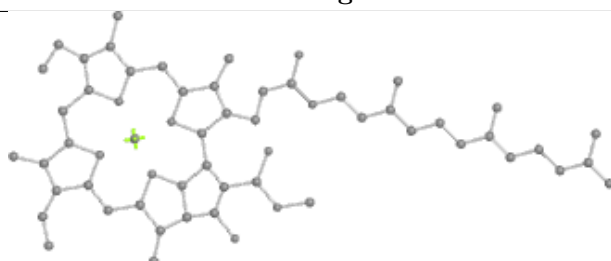
Bond lengths



Bond angles

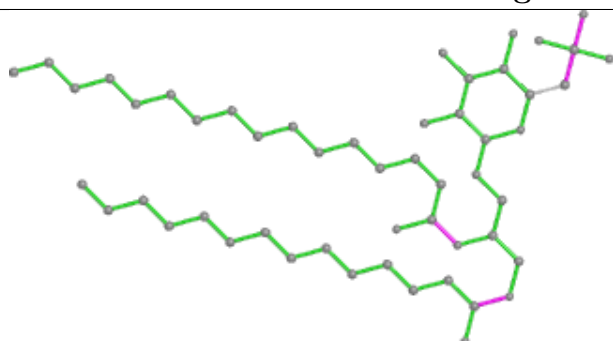


Torsions

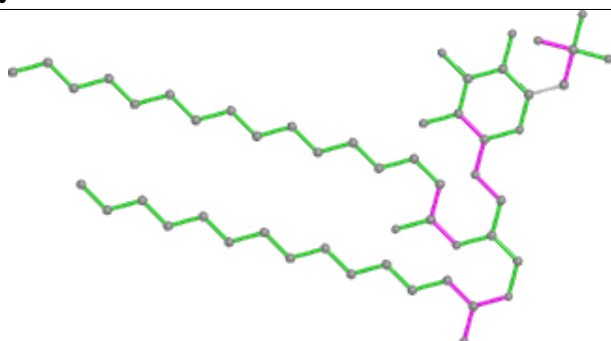


Rings

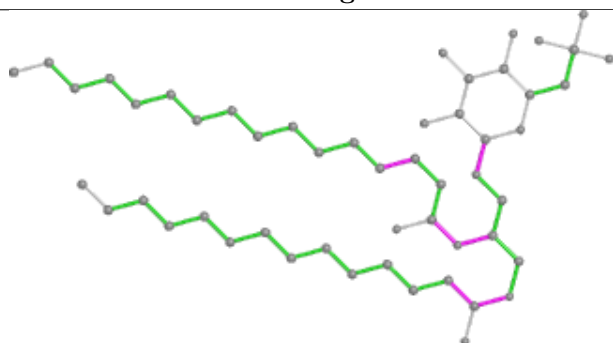
Ligand SQD D 413



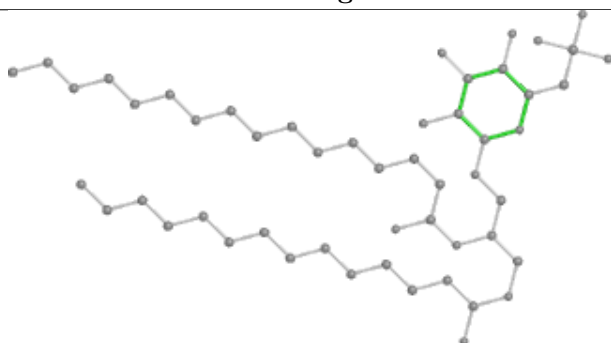
Bond lengths



Bond angles

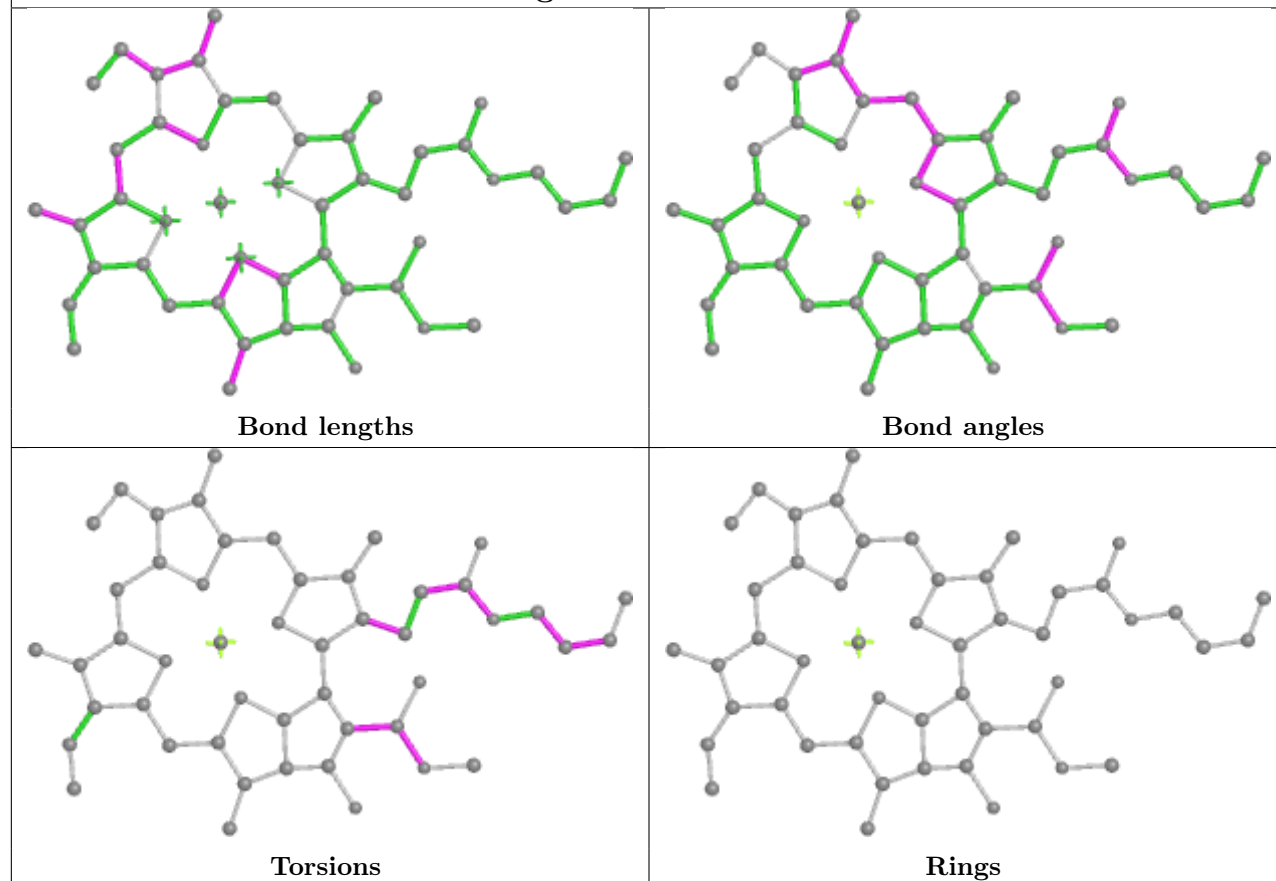


Torsions

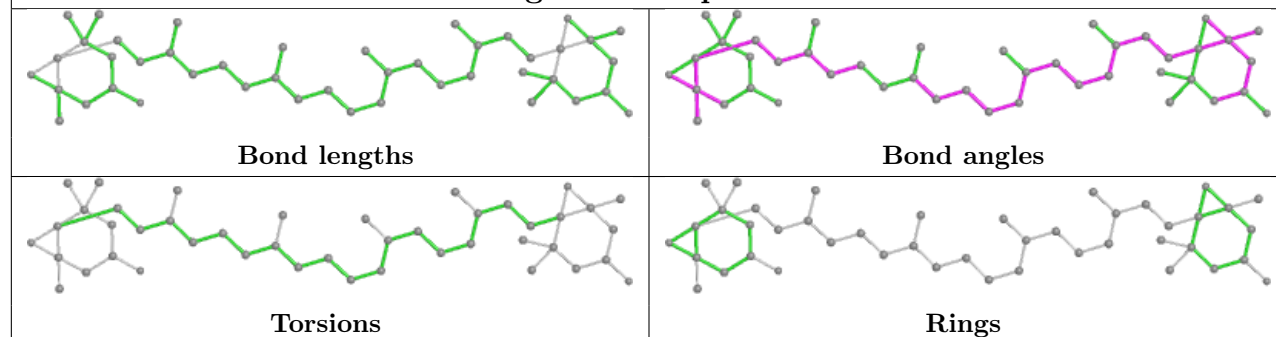


Rings

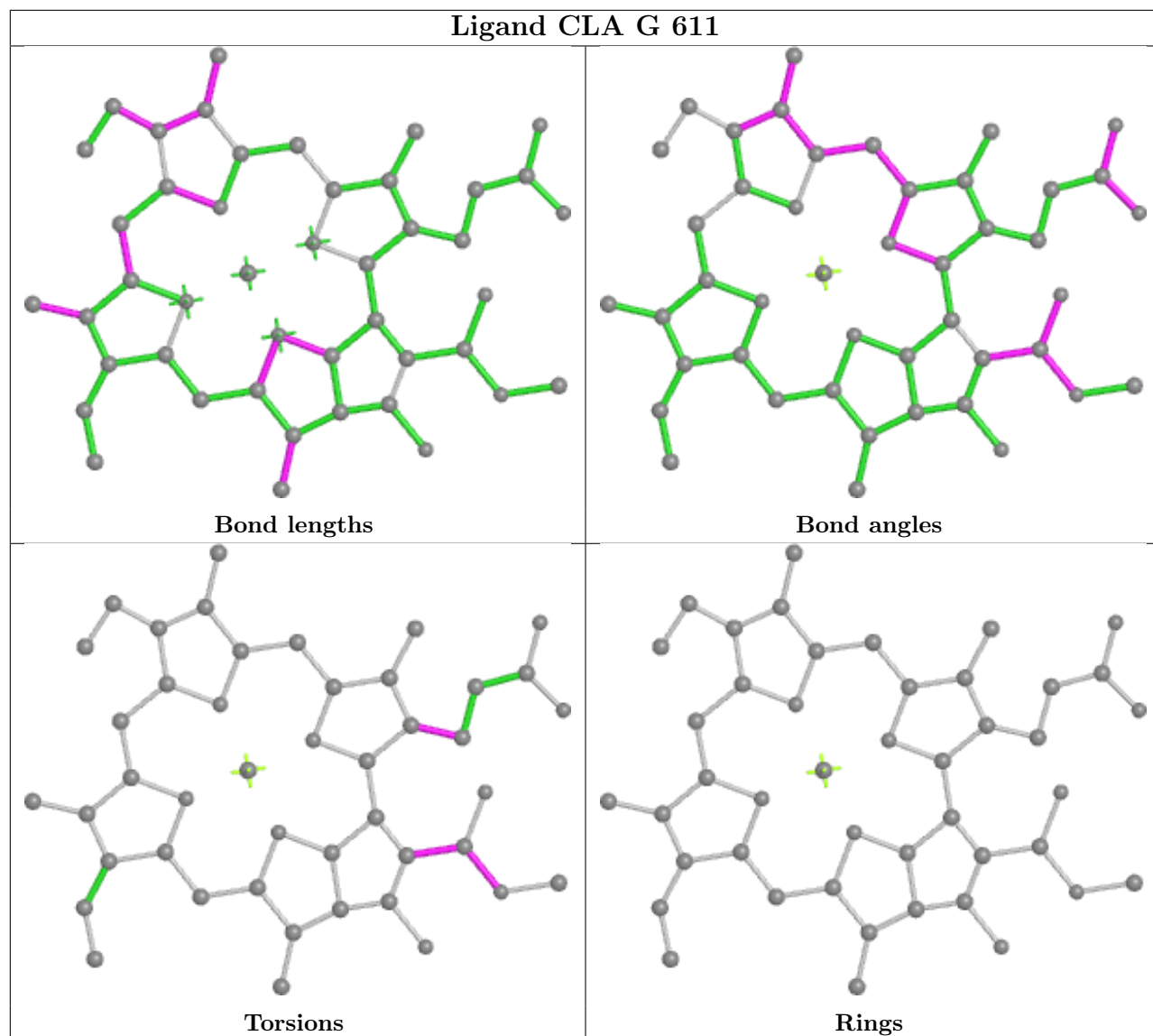
Ligand CLA 4 604

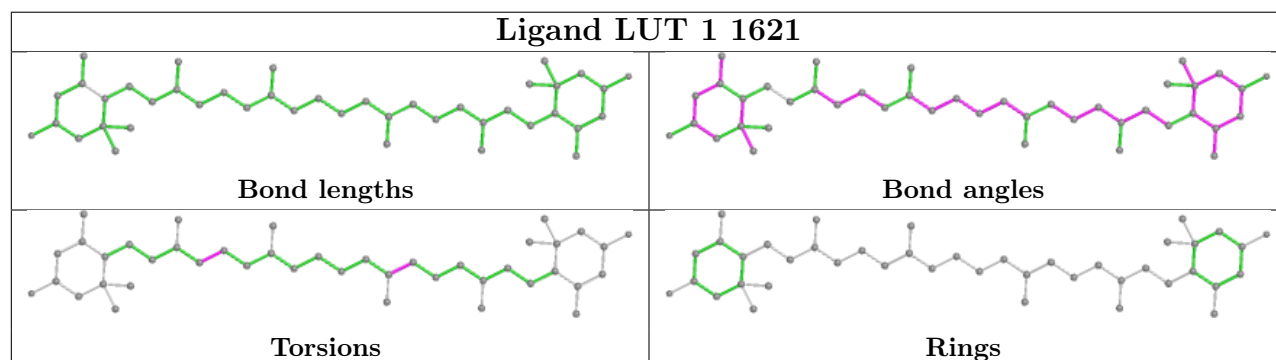
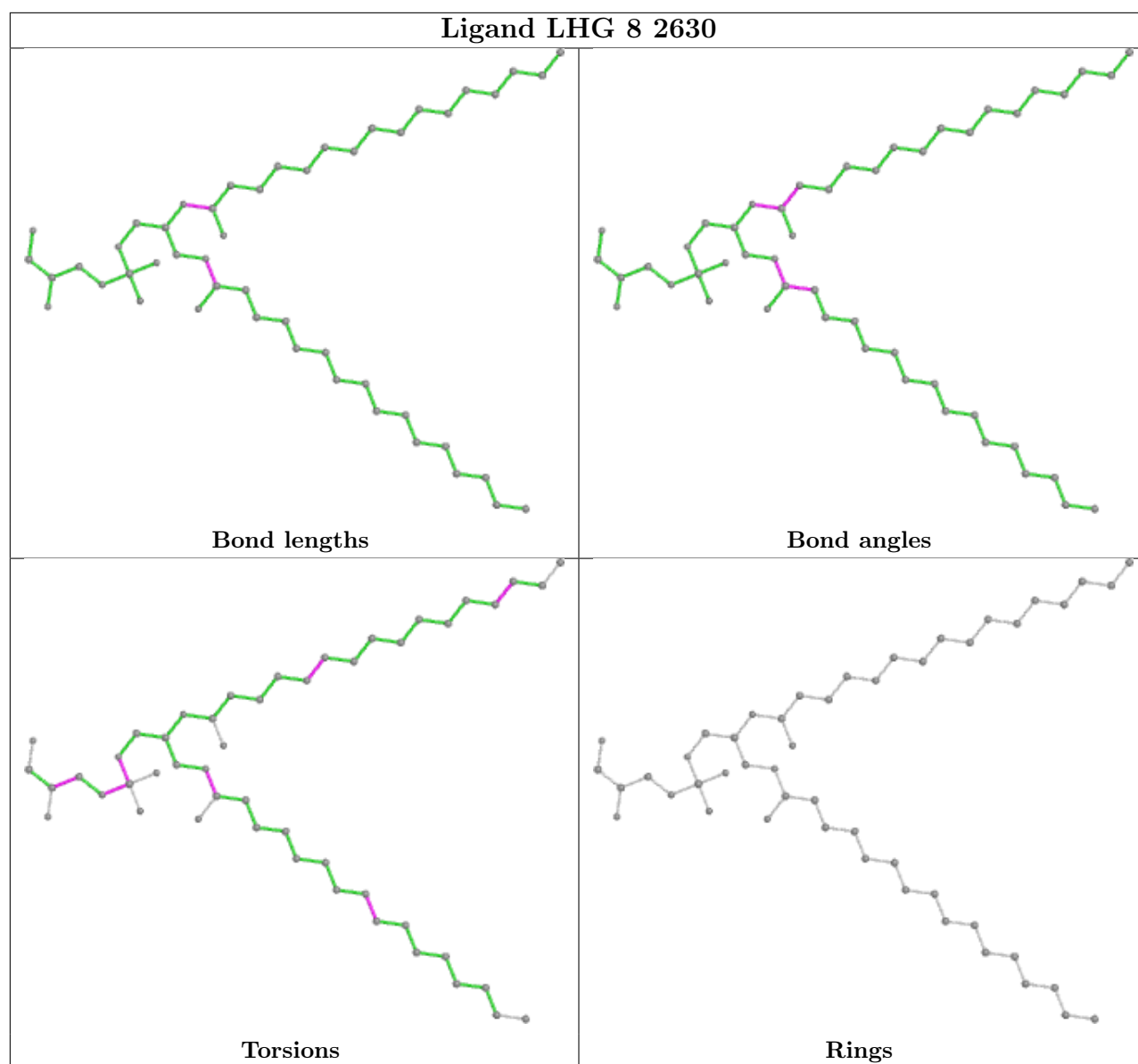


Ligand XAT p 1622

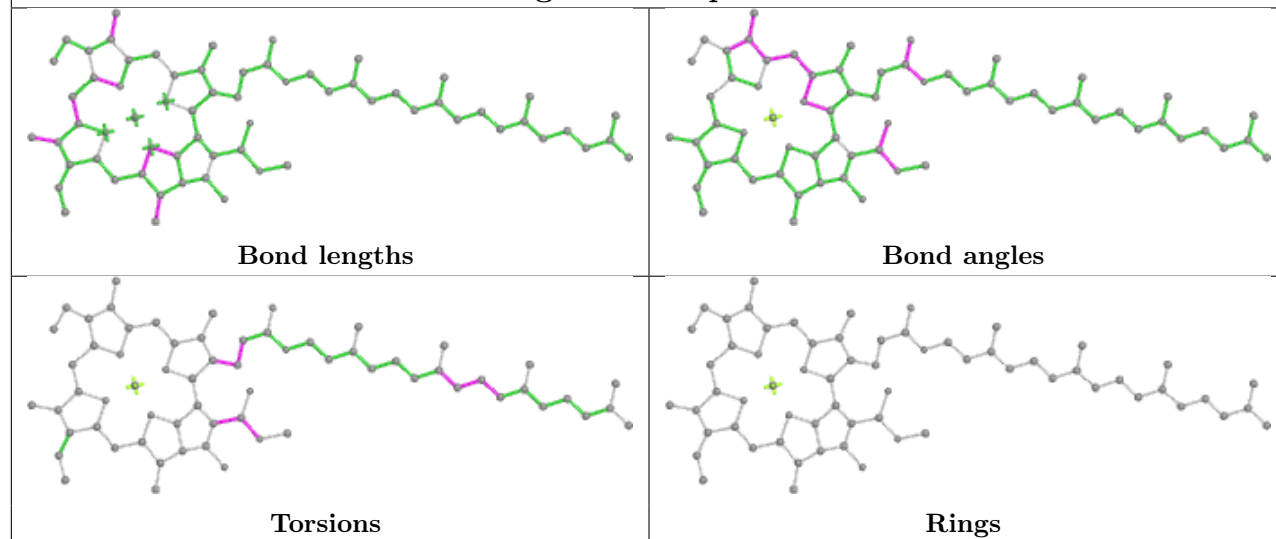


Ligand CLA G 611

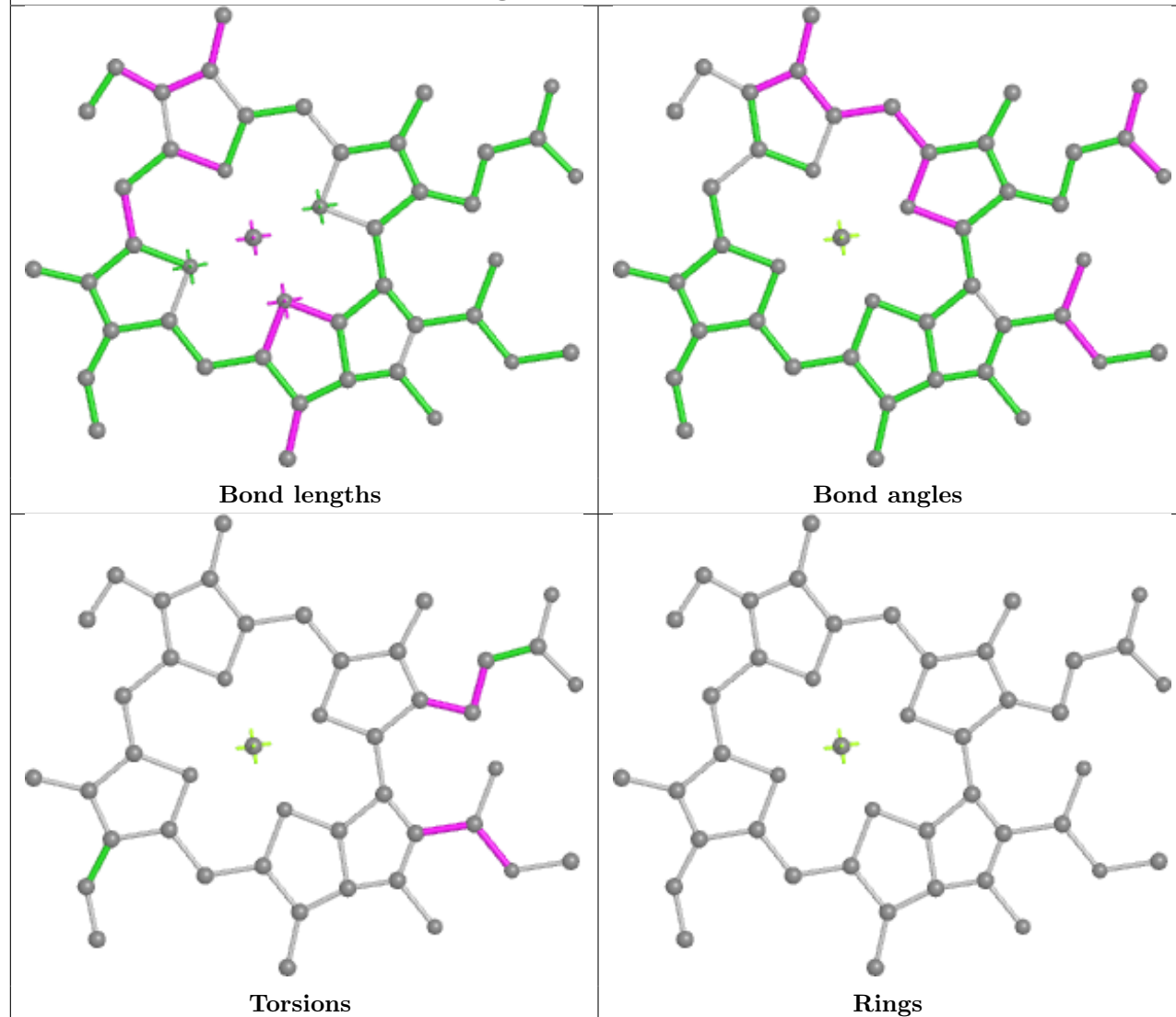




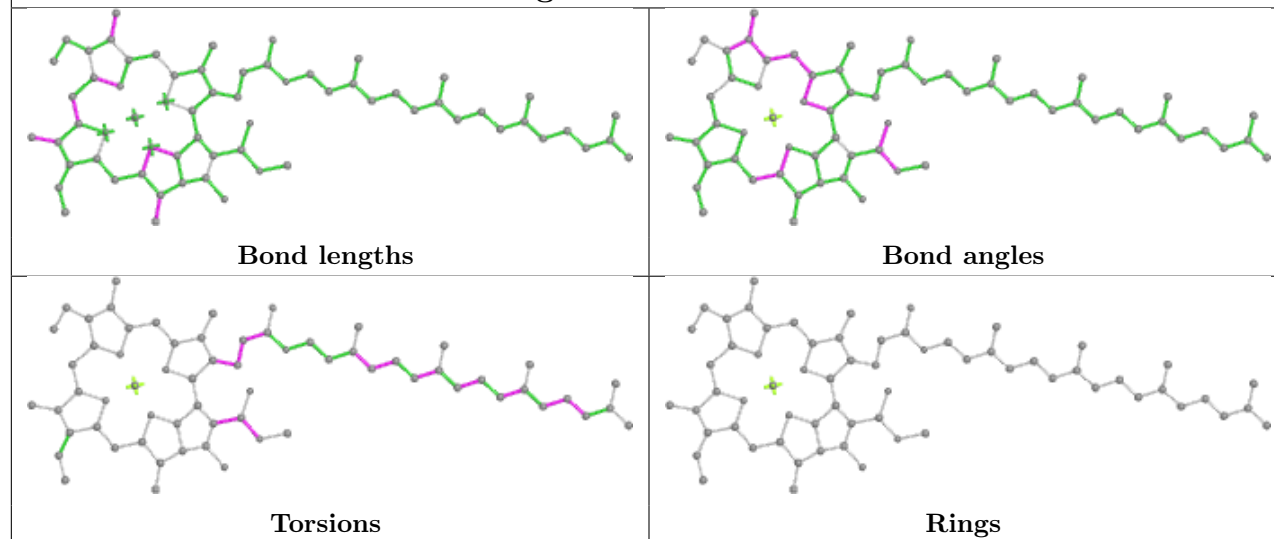
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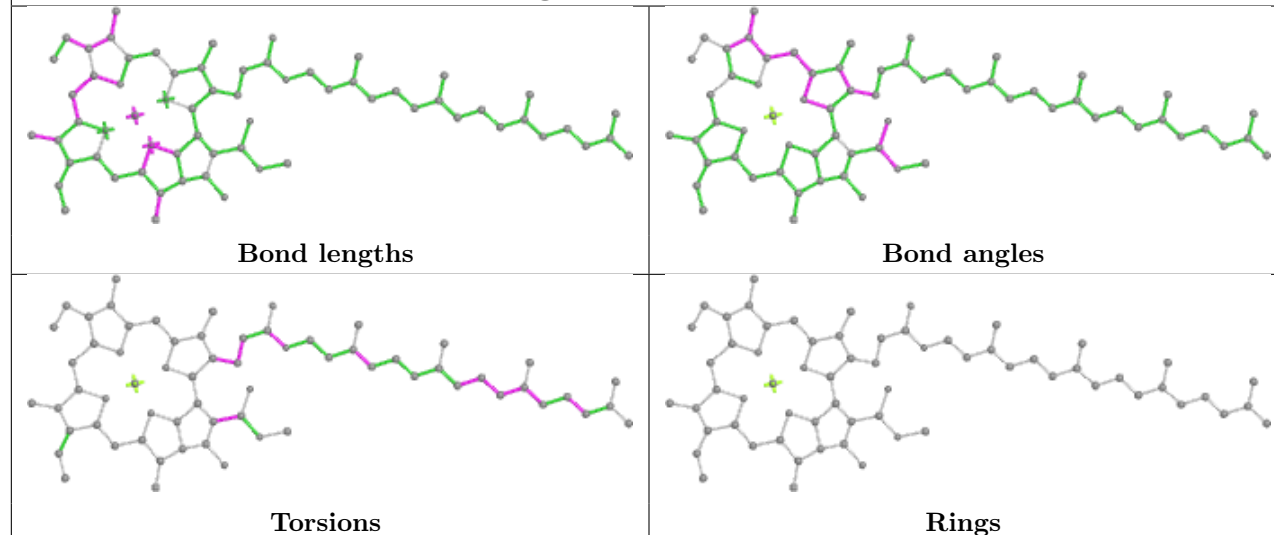
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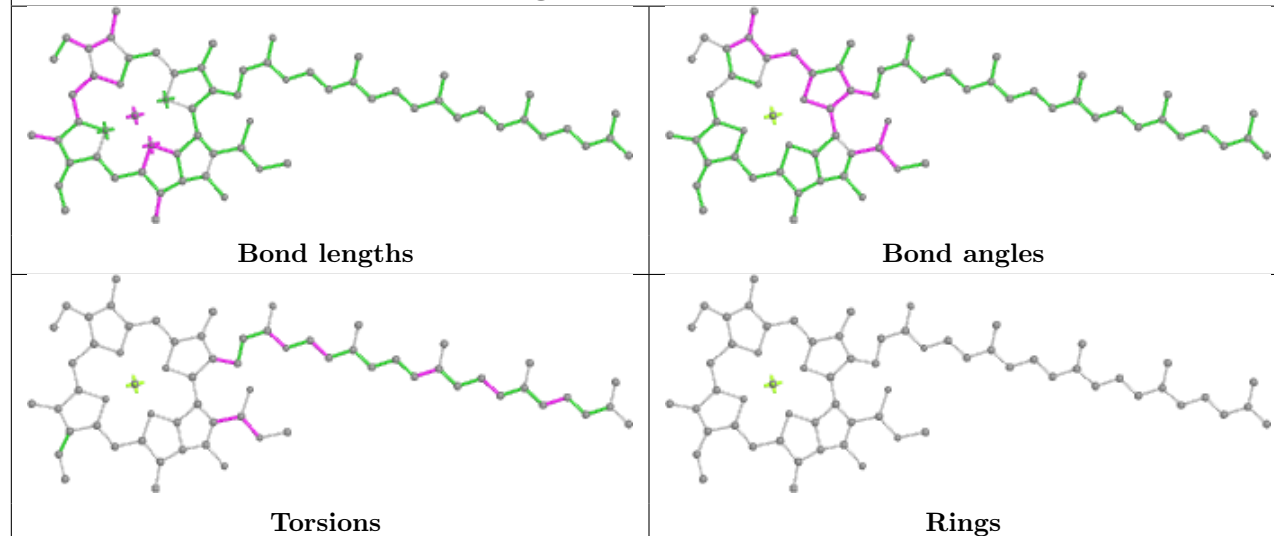
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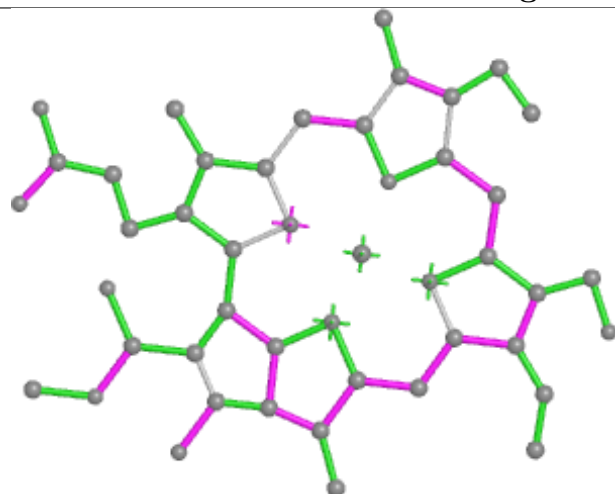
Ligand CLA 7 603



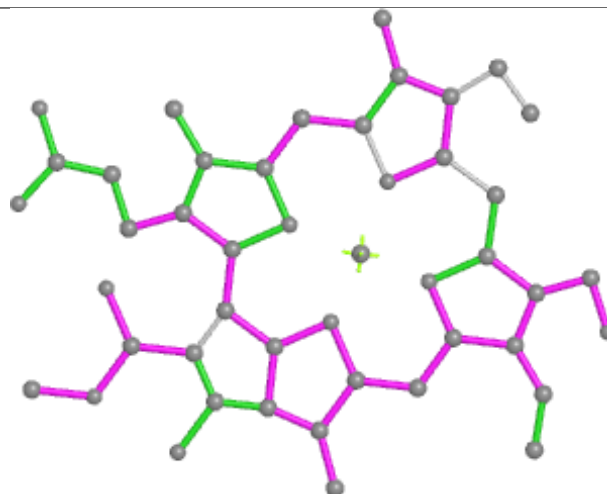
Ligand CLA B 603



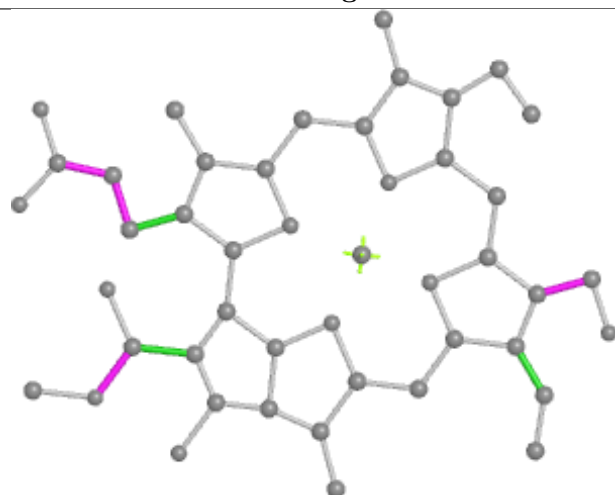
Ligand CHL 0 605



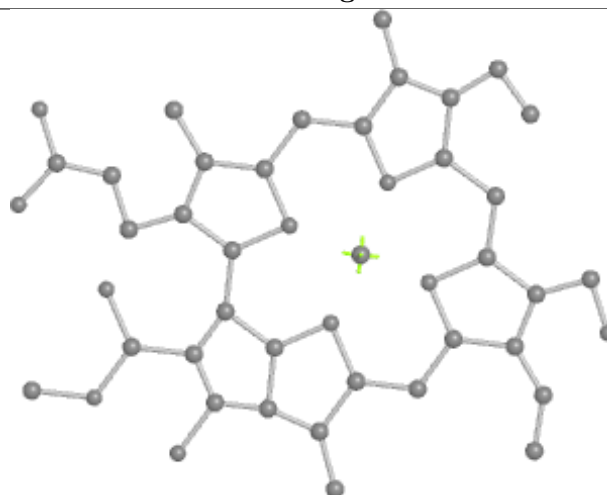
Bond lengths



Bond angles

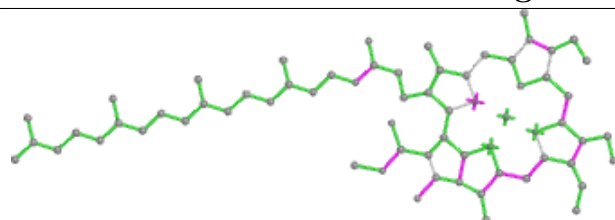


Torsions

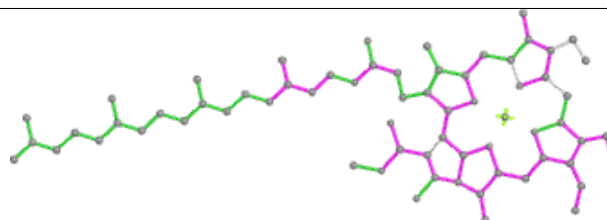


Rings

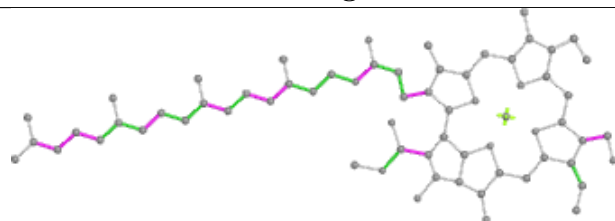
Ligand CHL G 601



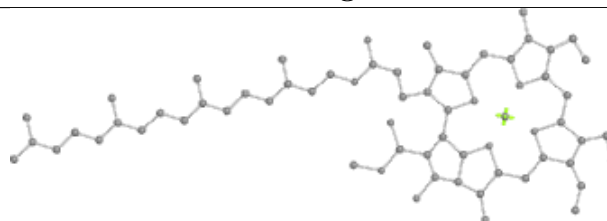
Bond lengths



Bond angles

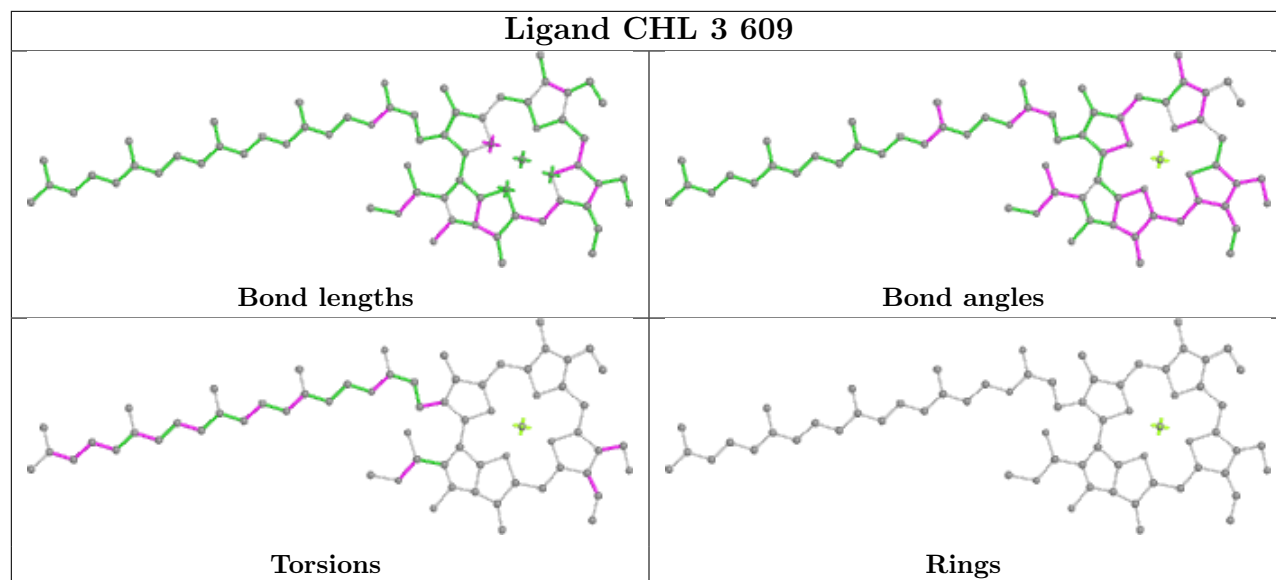


Torsions

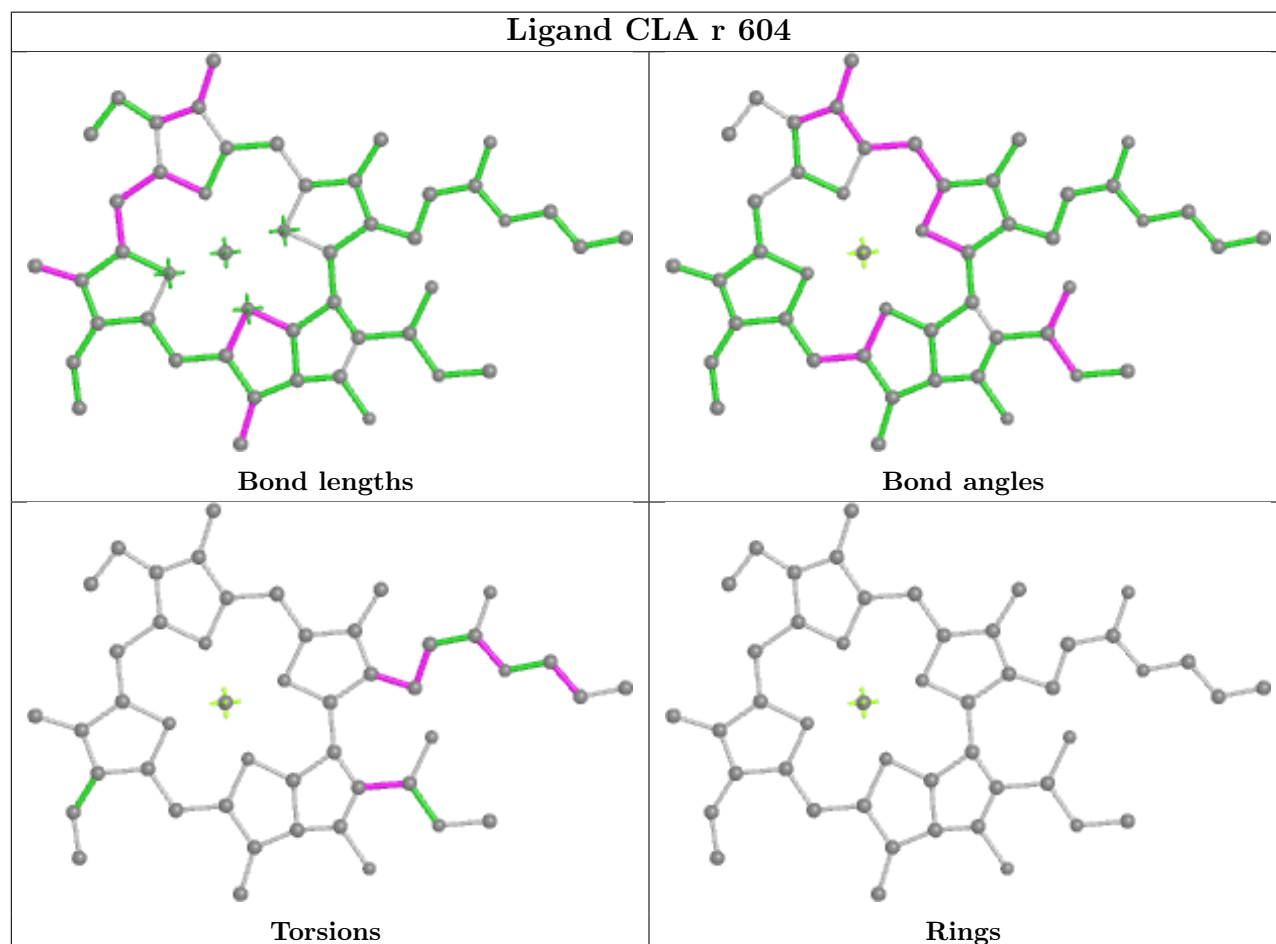


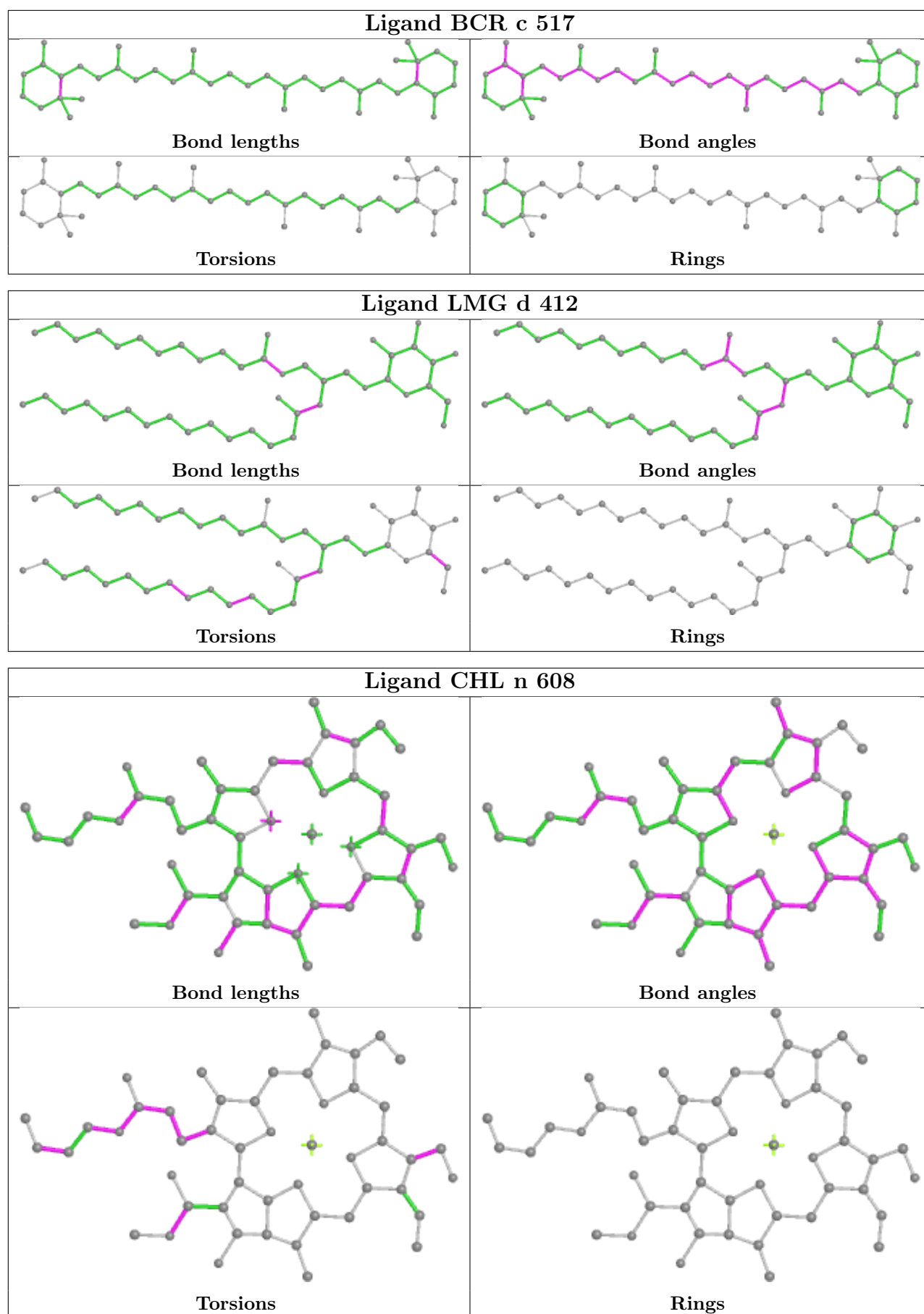
Rings

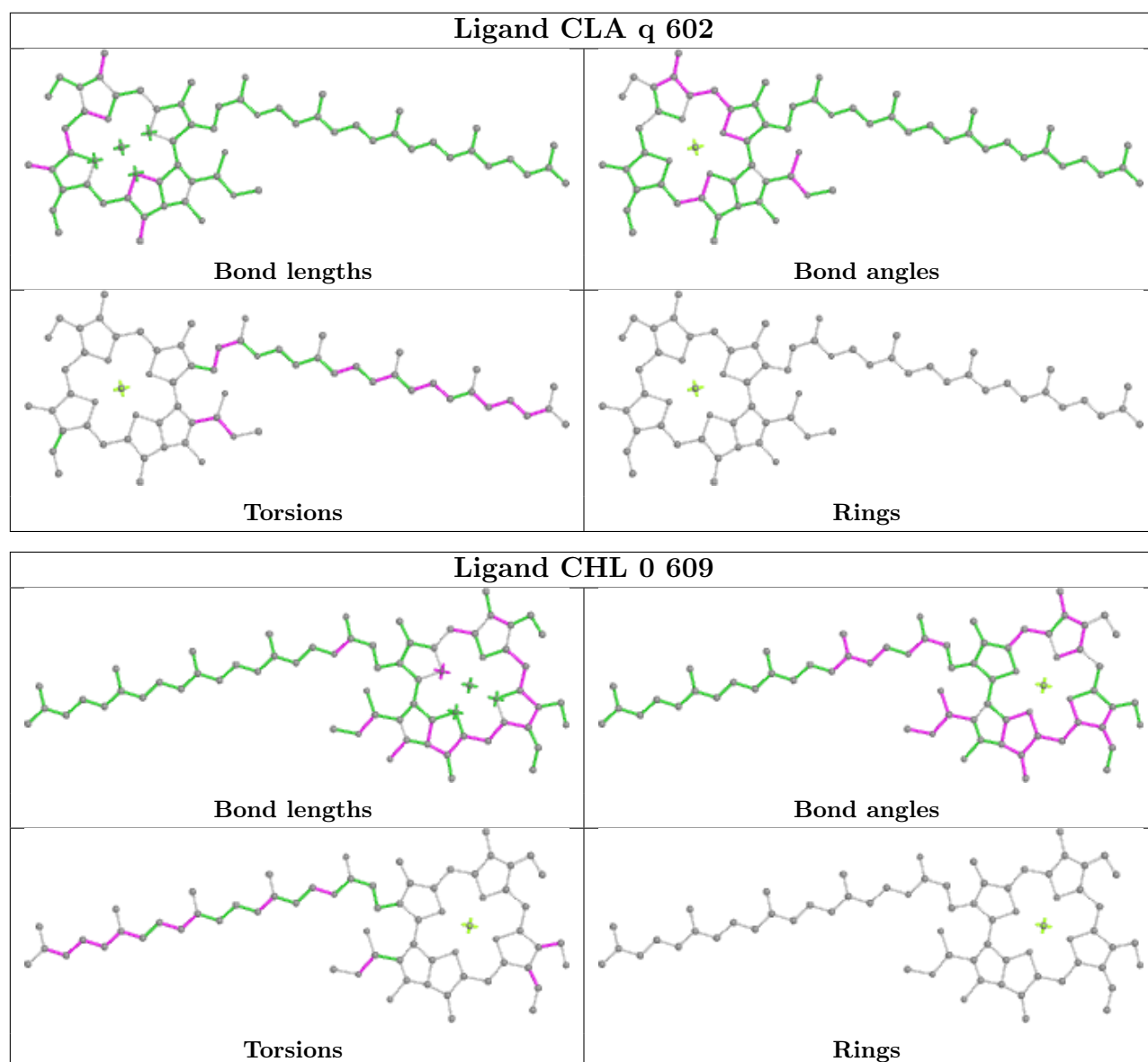
Ligand CHL 3 609

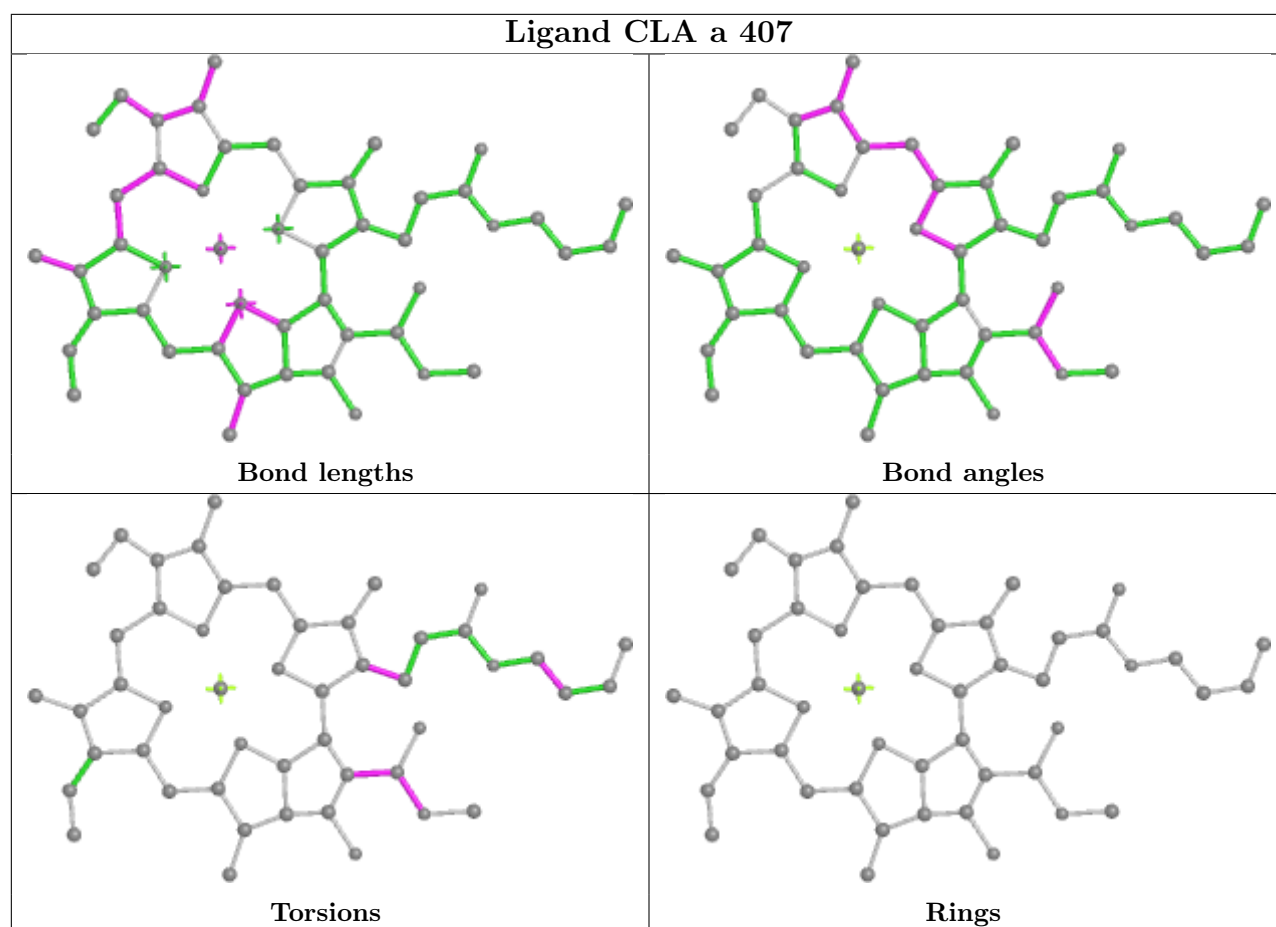


Ligand CLA r 604

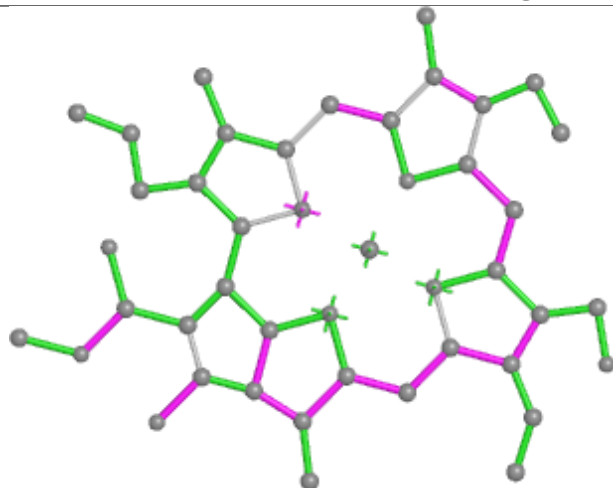




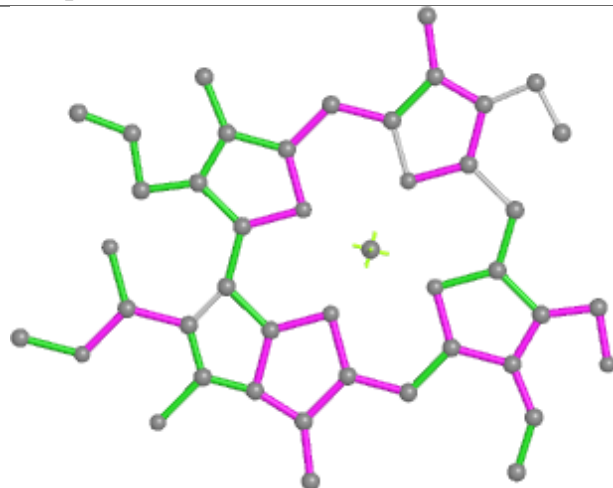




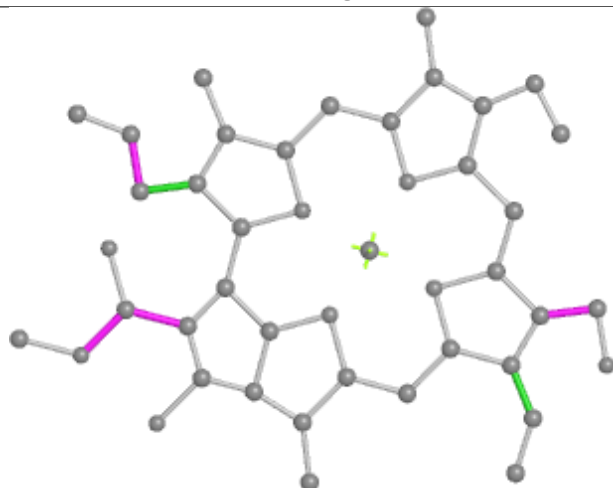
Ligand CHL q 608



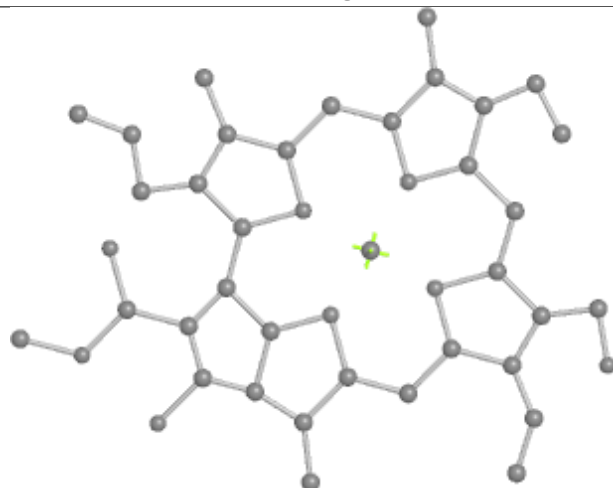
Bond lengths



Bond angles

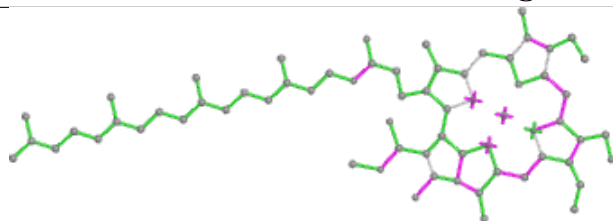


Torsions

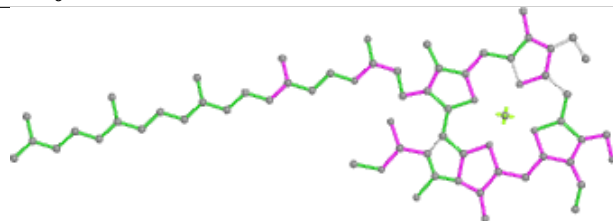


Rings

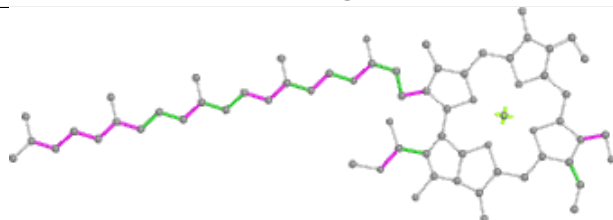
Ligand CHL y 606



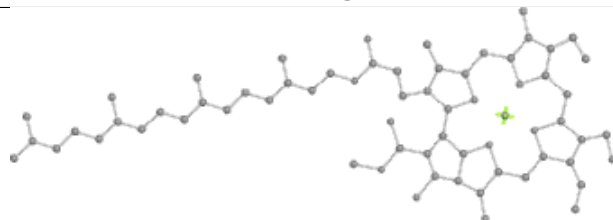
Bond lengths



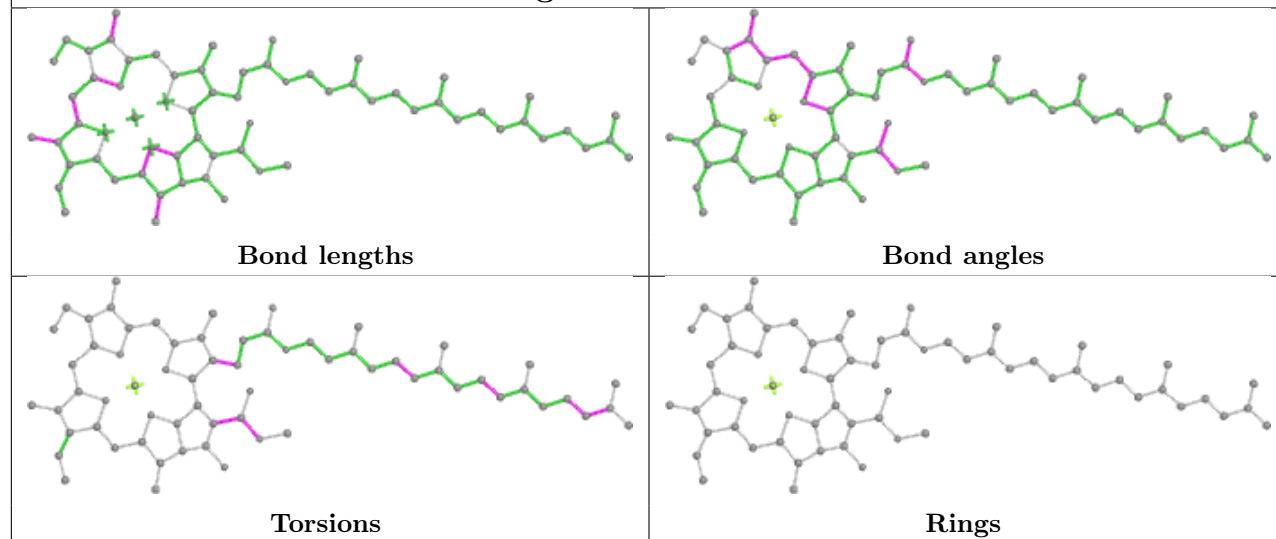
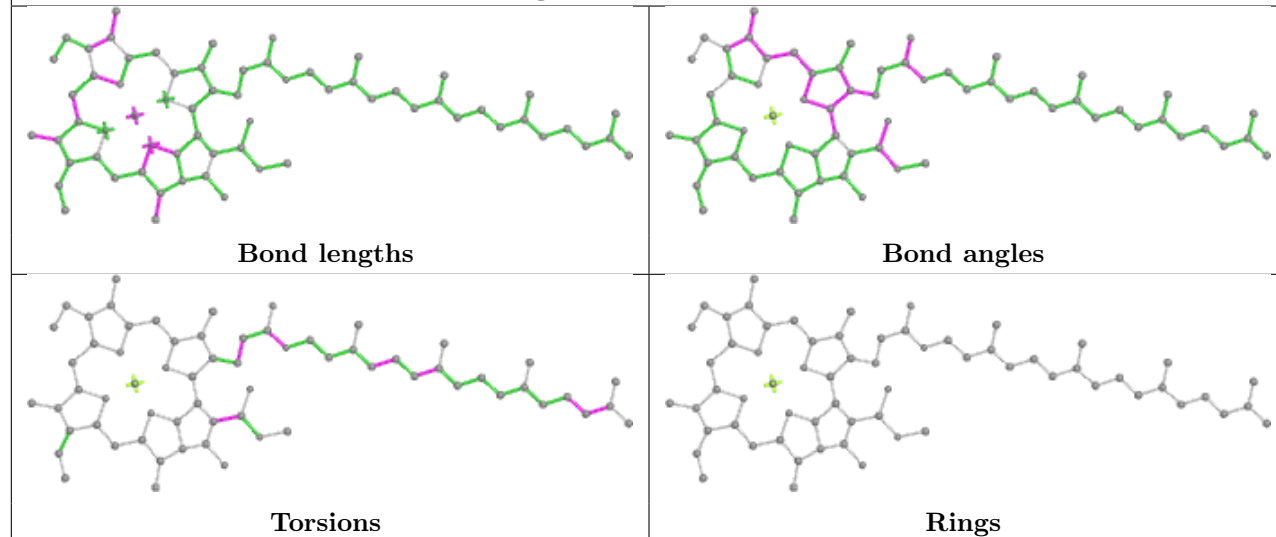
Bond angles



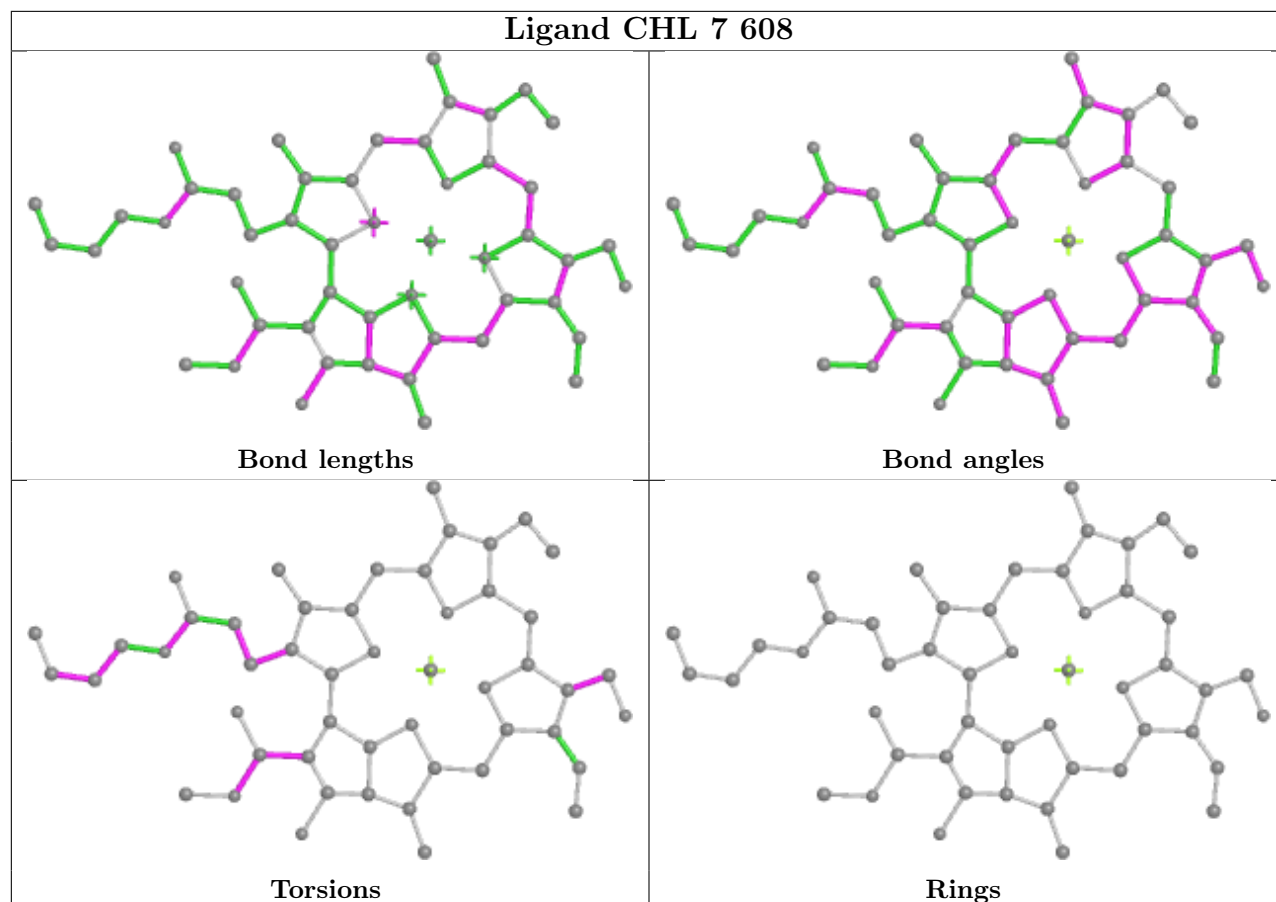
Torsions



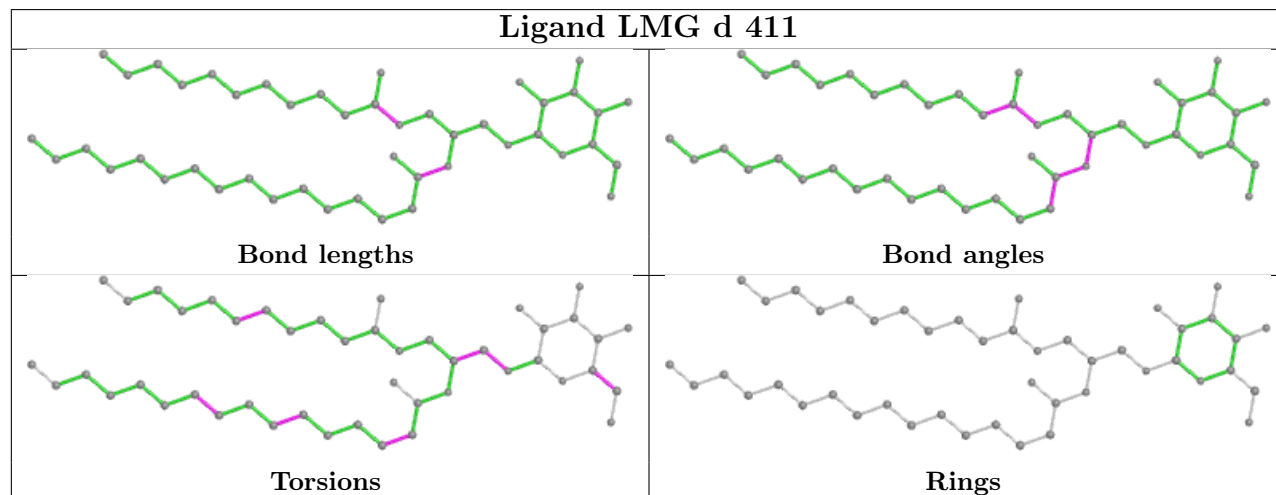
Rings

Ligand CLA 8 610**Ligand CLA B 617**

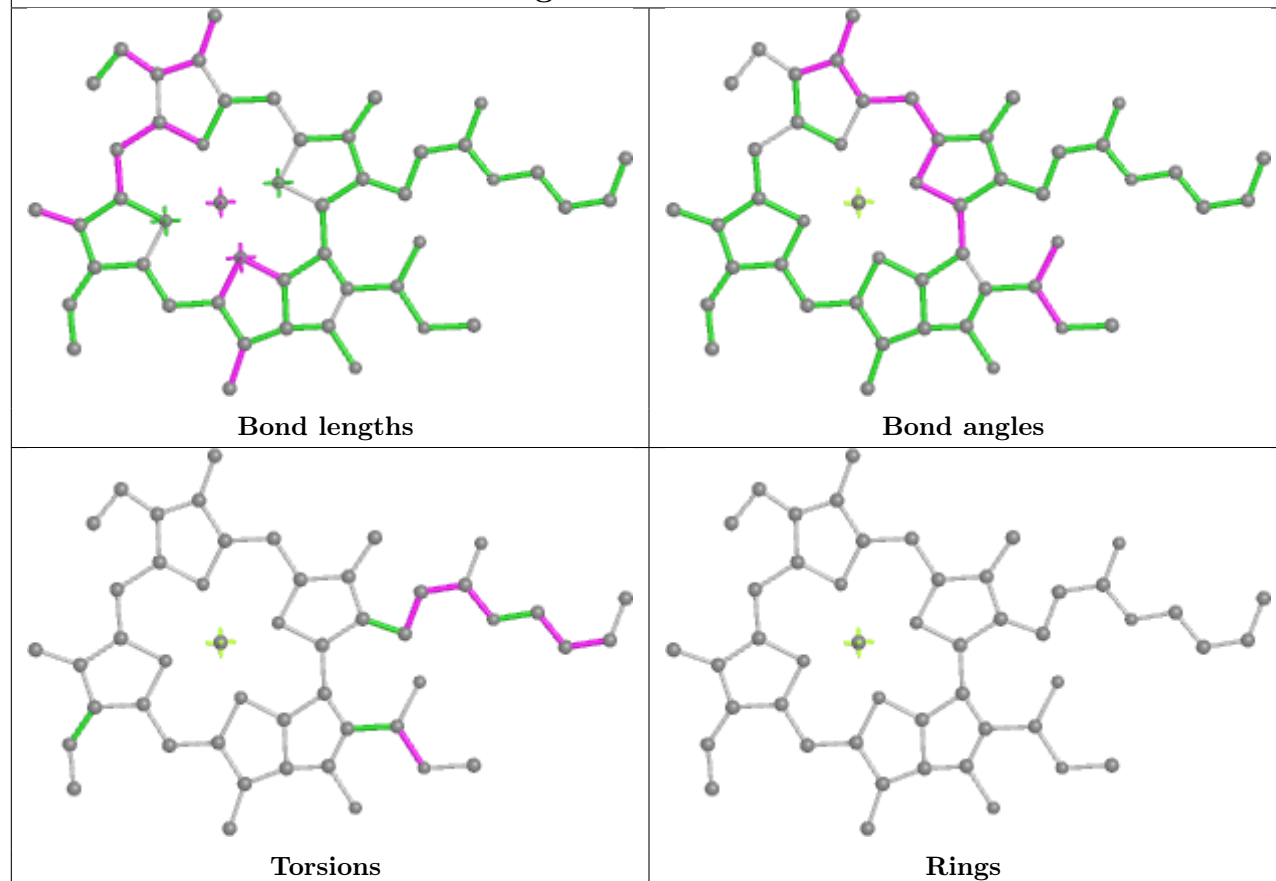
Ligand CHL 7 608



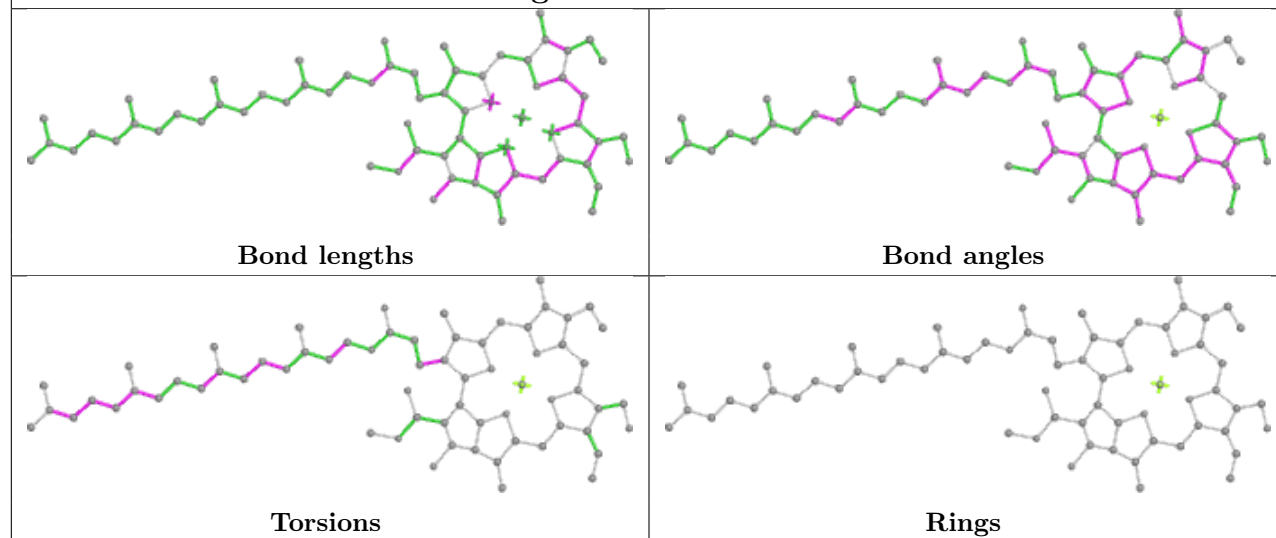
Ligand LMG d 411

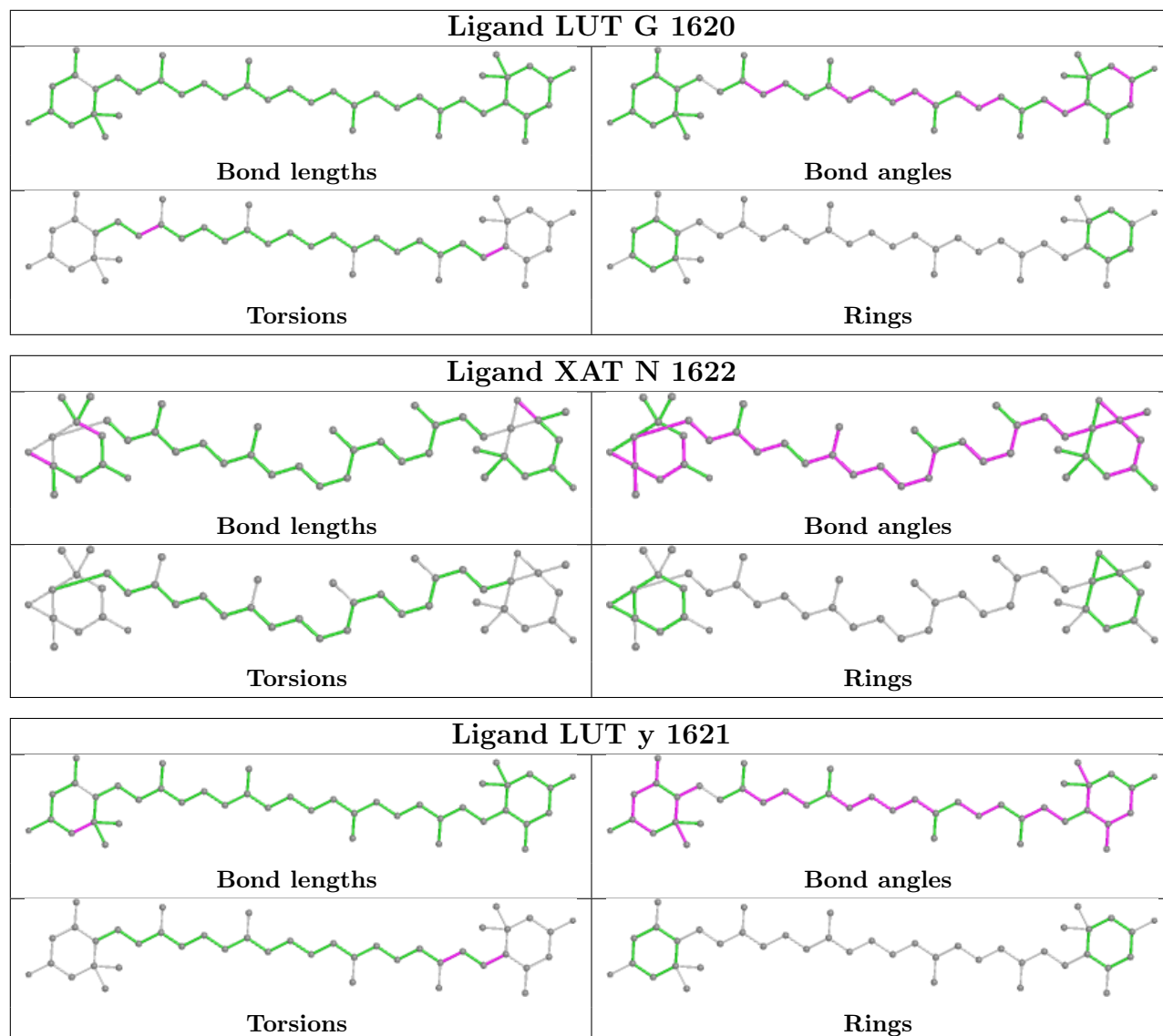


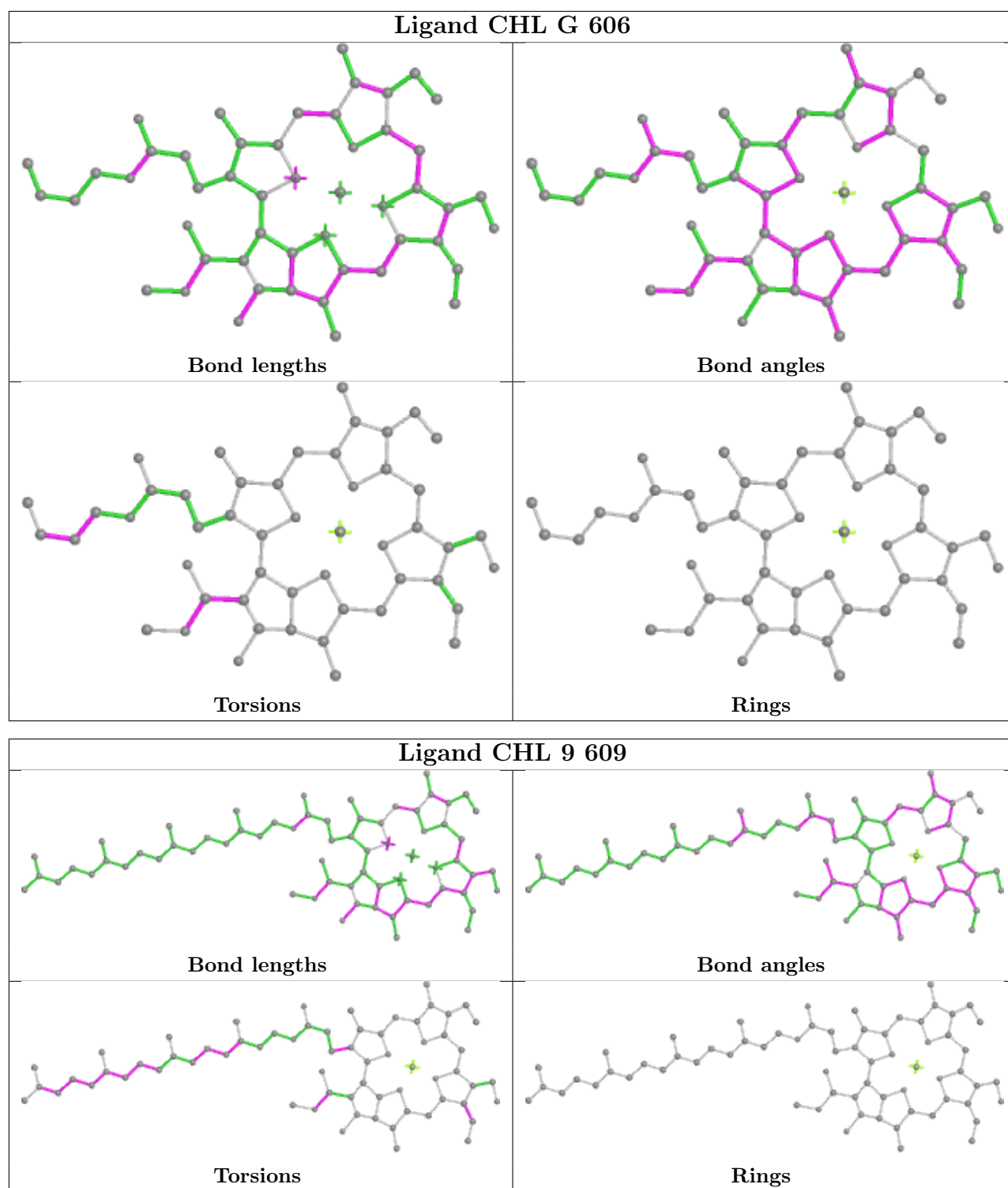
Ligand CLA S 613



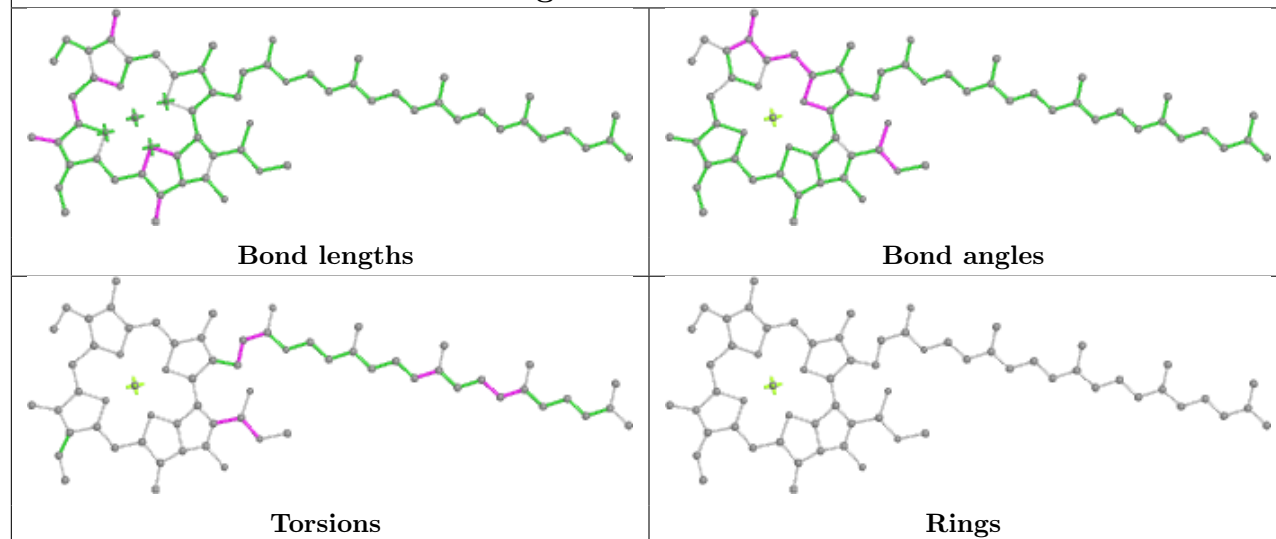
Ligand CHL Y 601



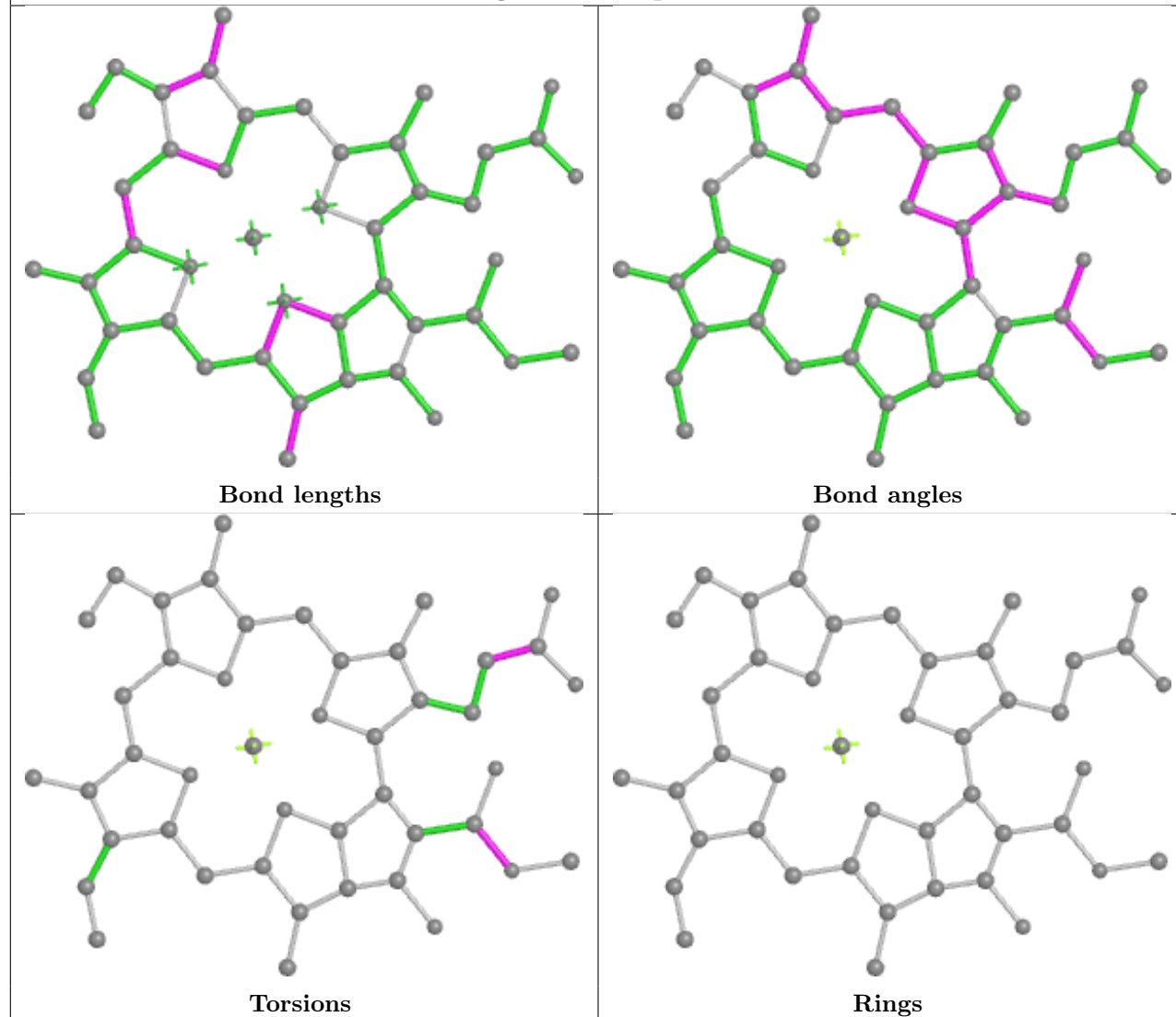


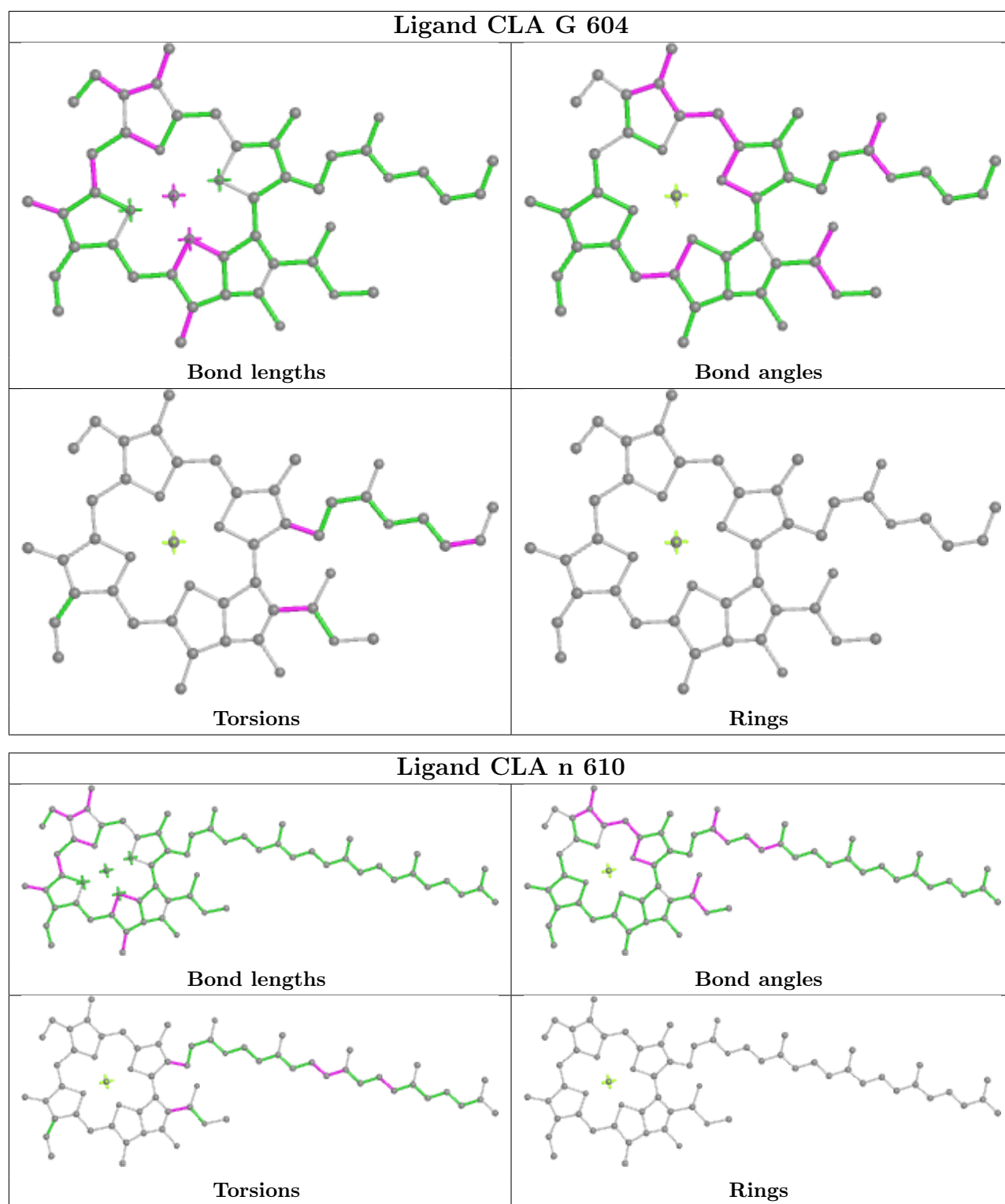


Ligand CLA 8 602

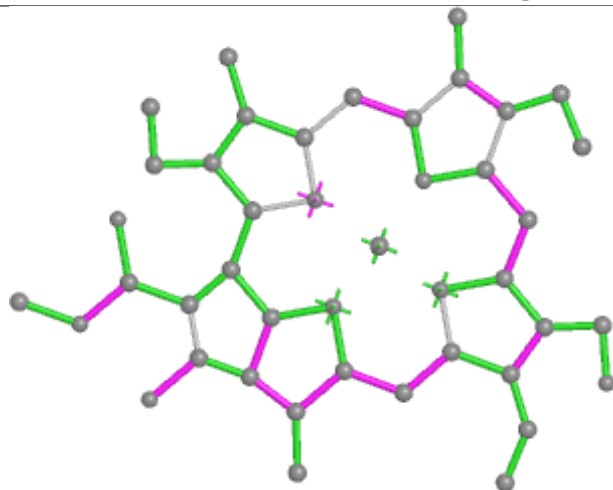


Ligand CLA p 612

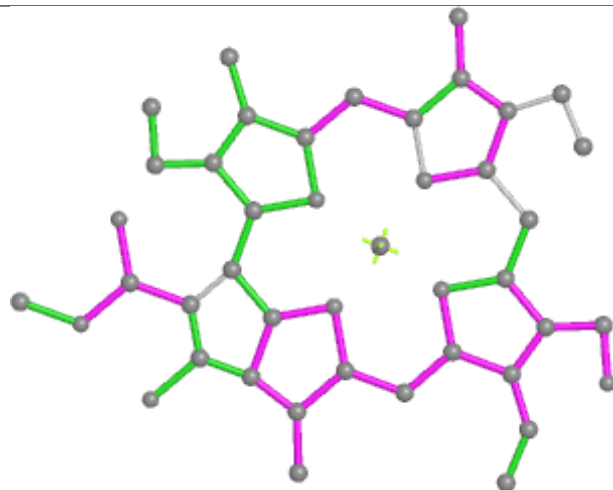




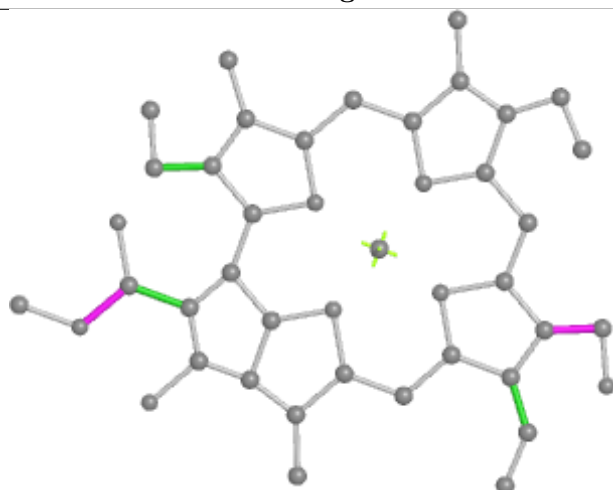
Ligand CHL S 607



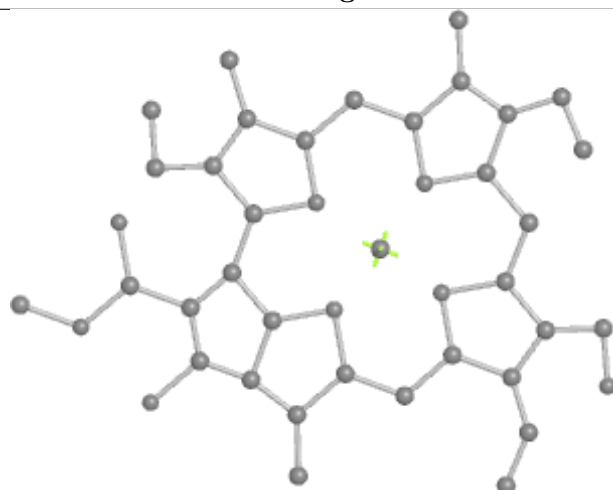
Bond lengths



Bond angles

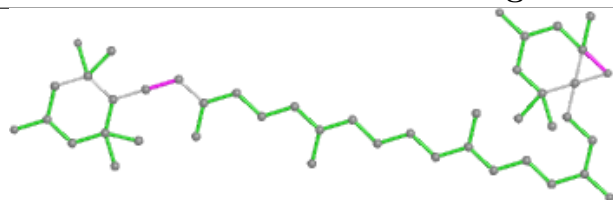


Torsions

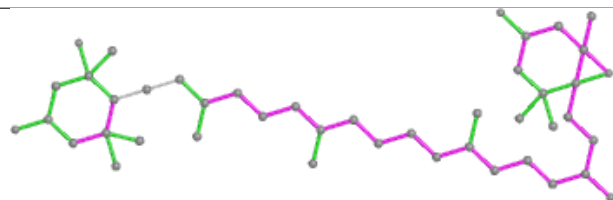


Rings

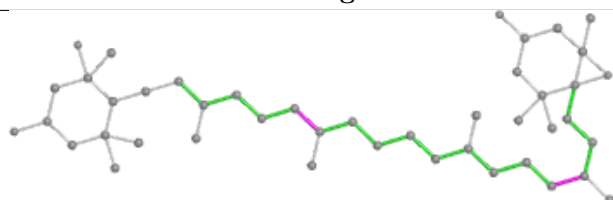
Ligand NEX S 1623



Bond lengths



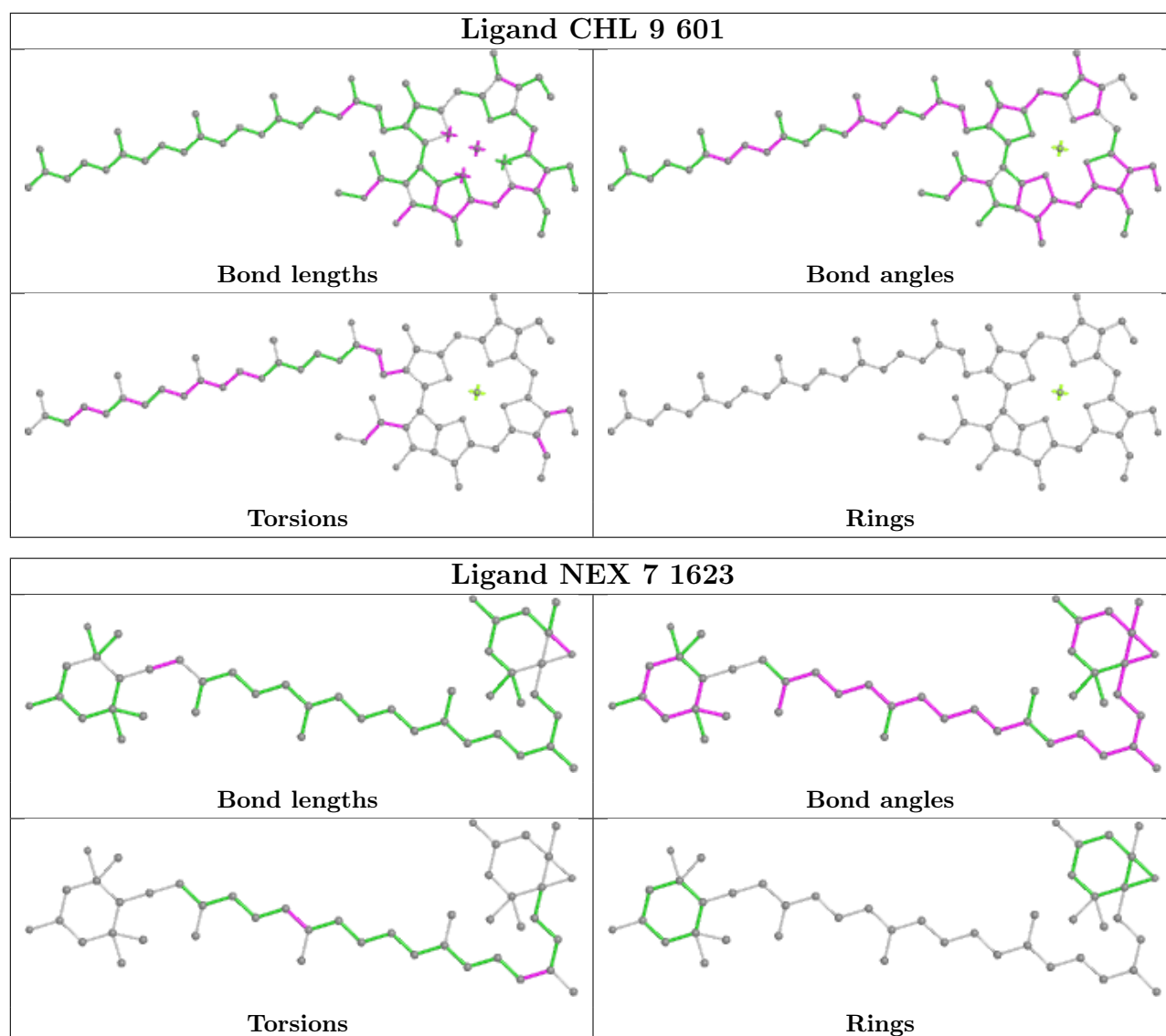
Bond angles



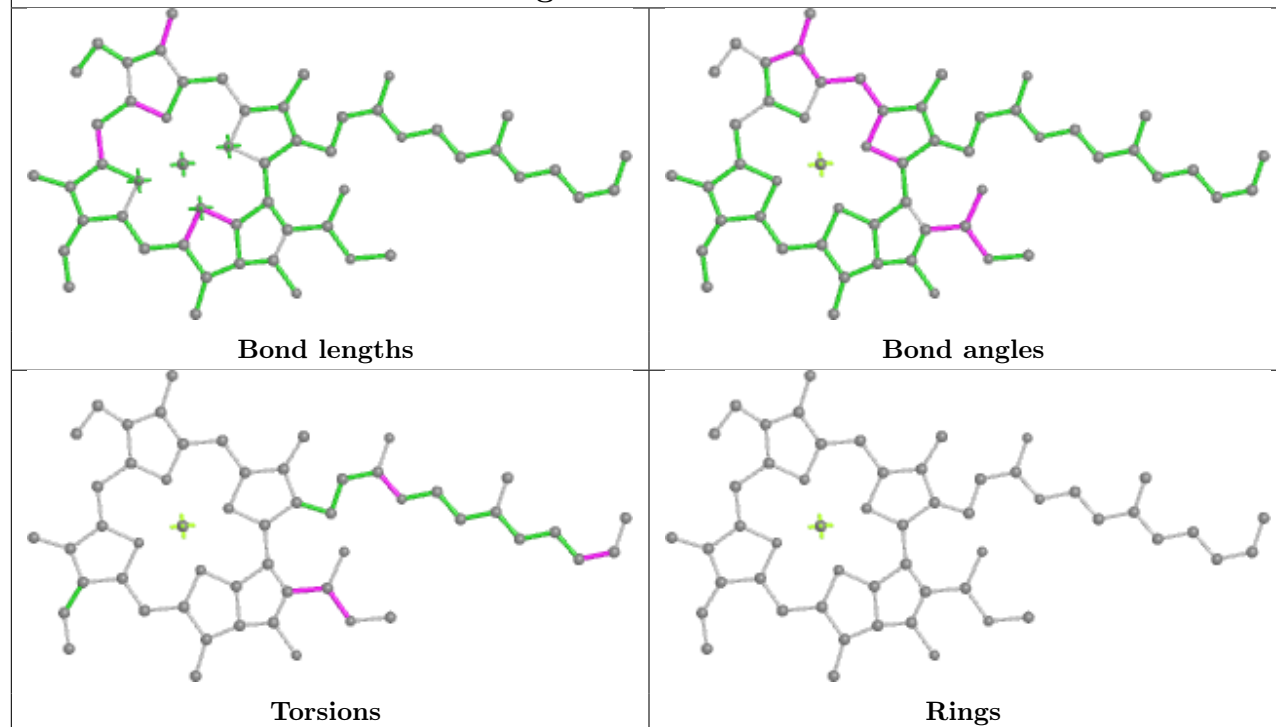
Torsions



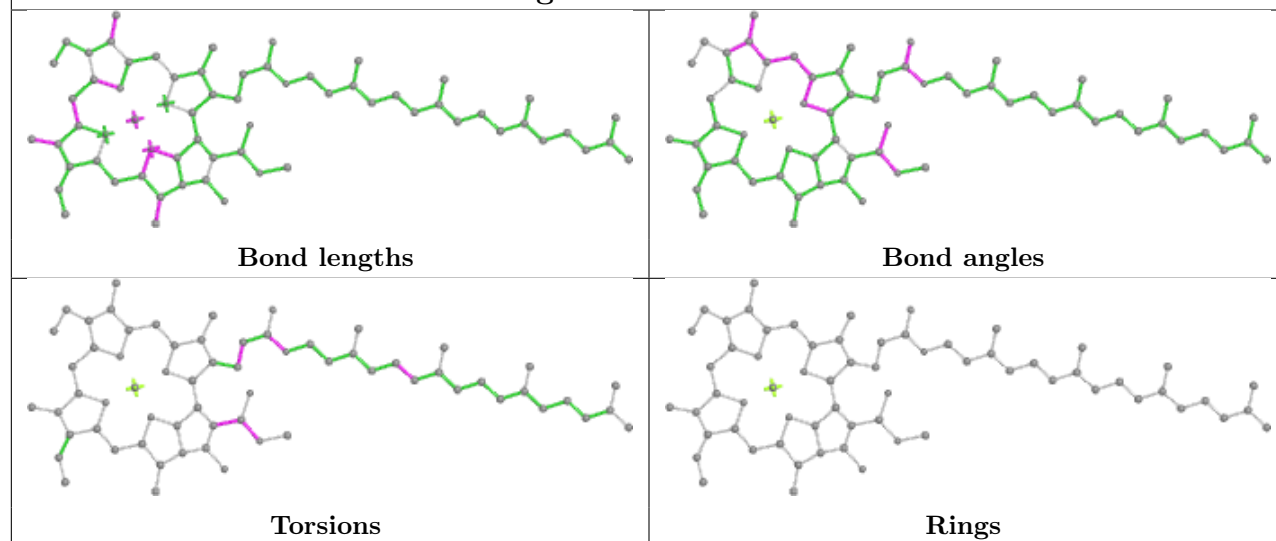
Rings

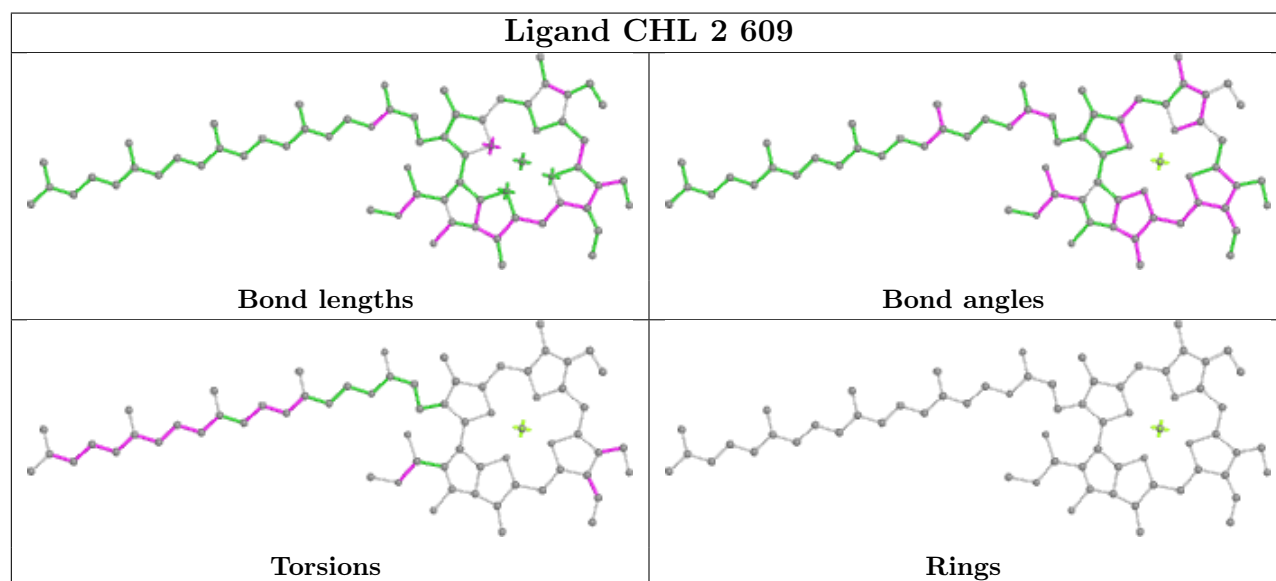
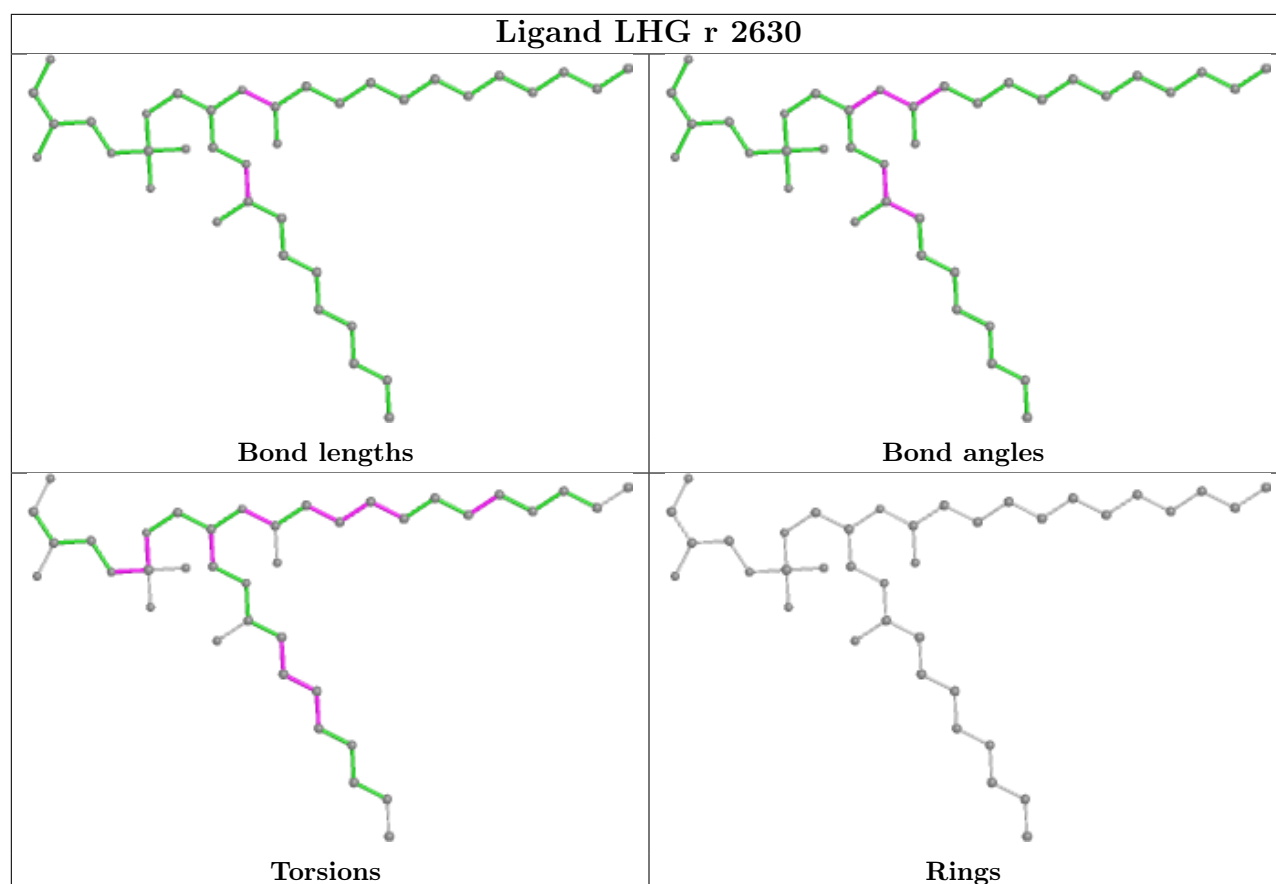


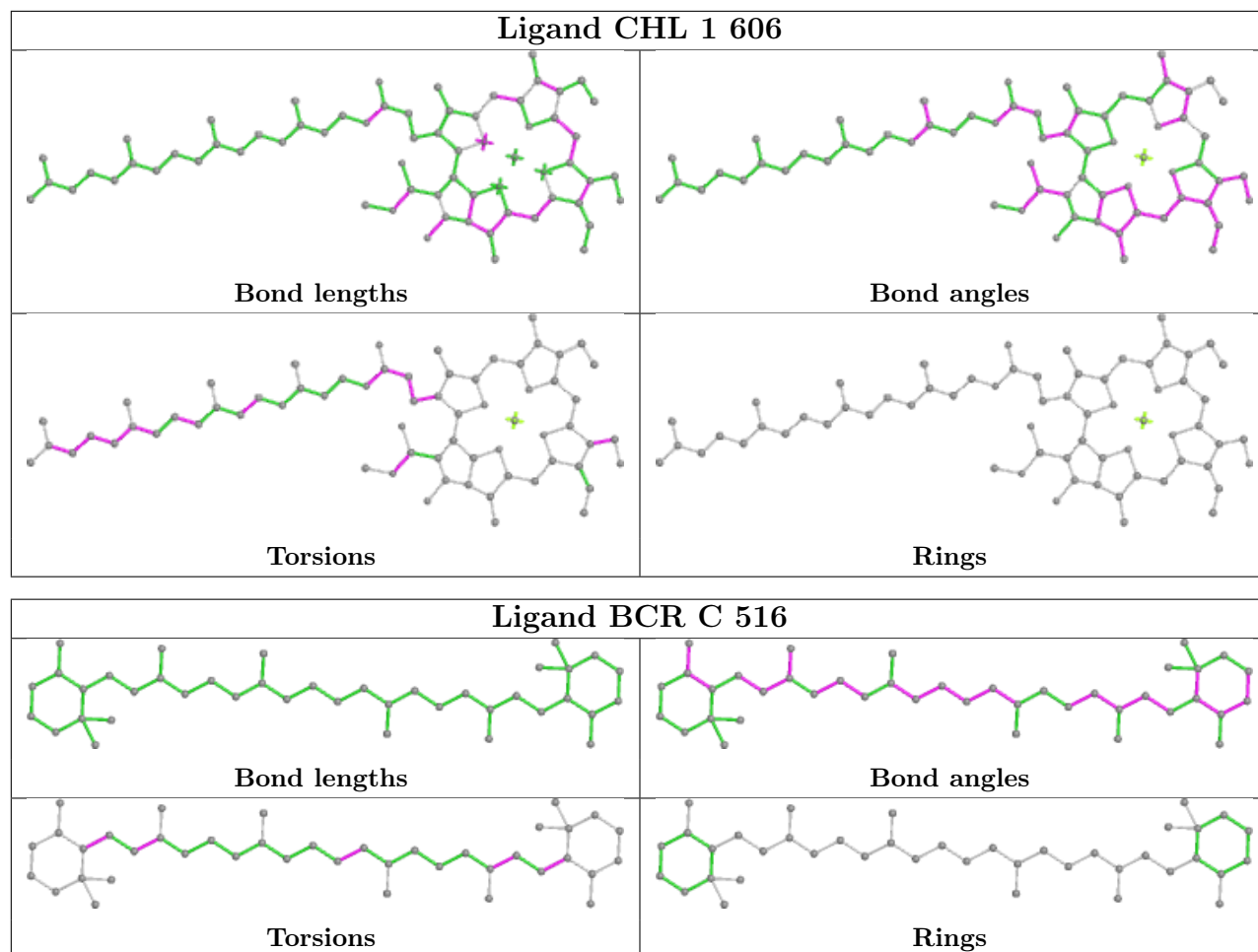
Ligand CLA 0 614

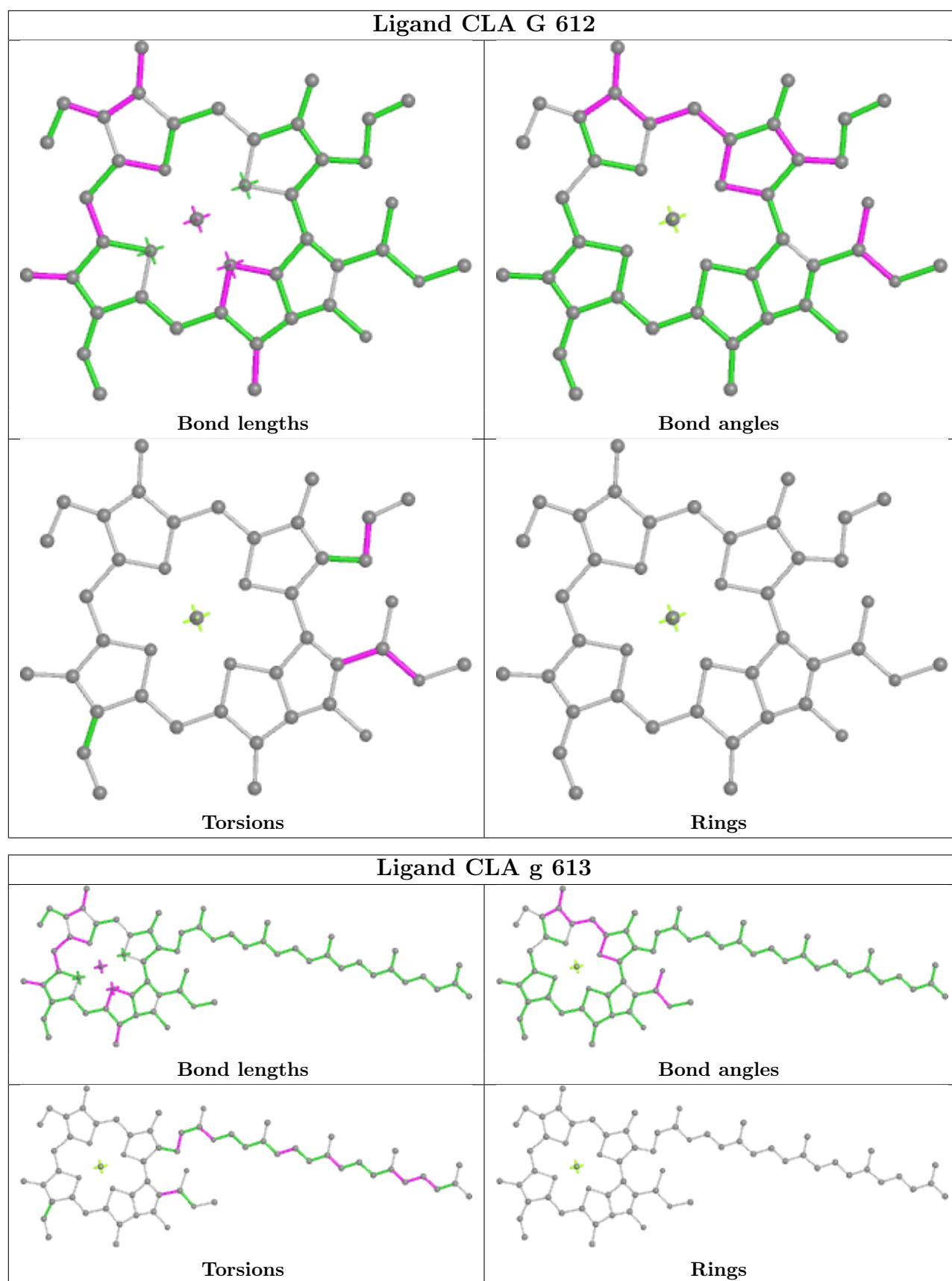


Ligand CLA 2 613

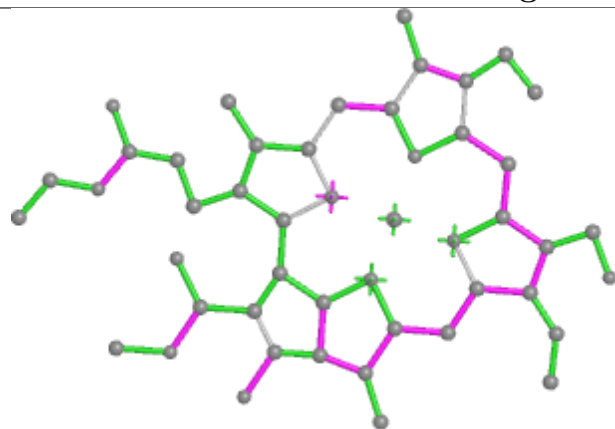




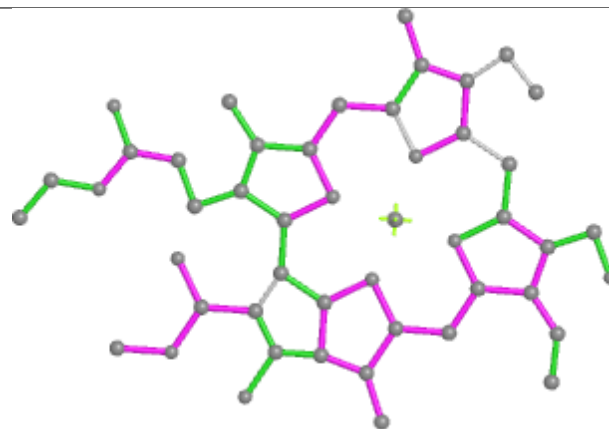




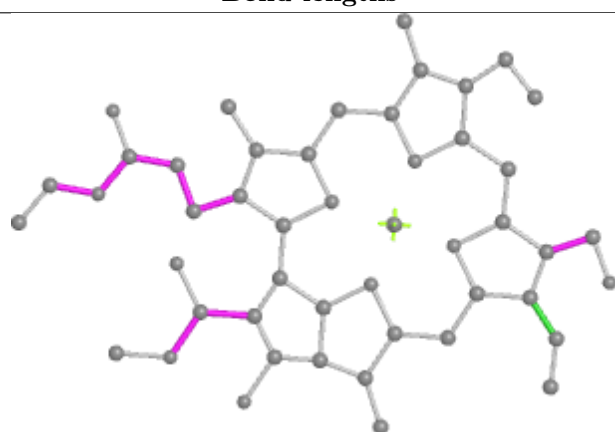
Ligand CHL 4 605



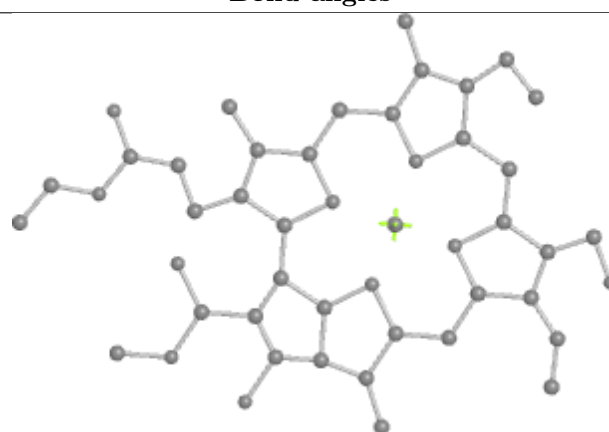
Bond lengths



Bond angles

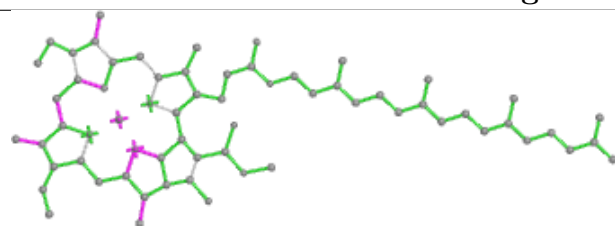


Torsions

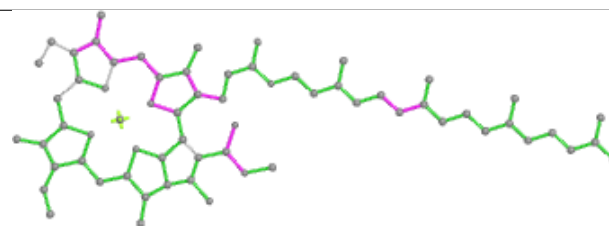


Rings

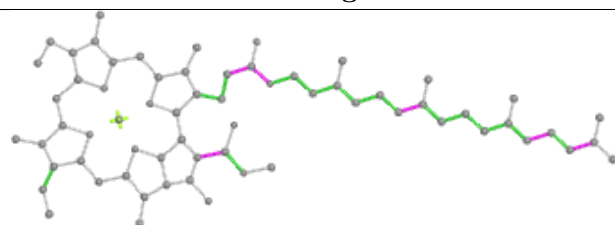
Ligand CLA c 510



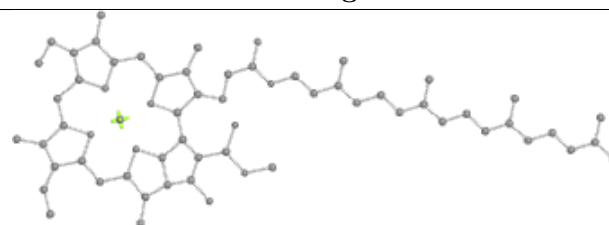
Bond lengths



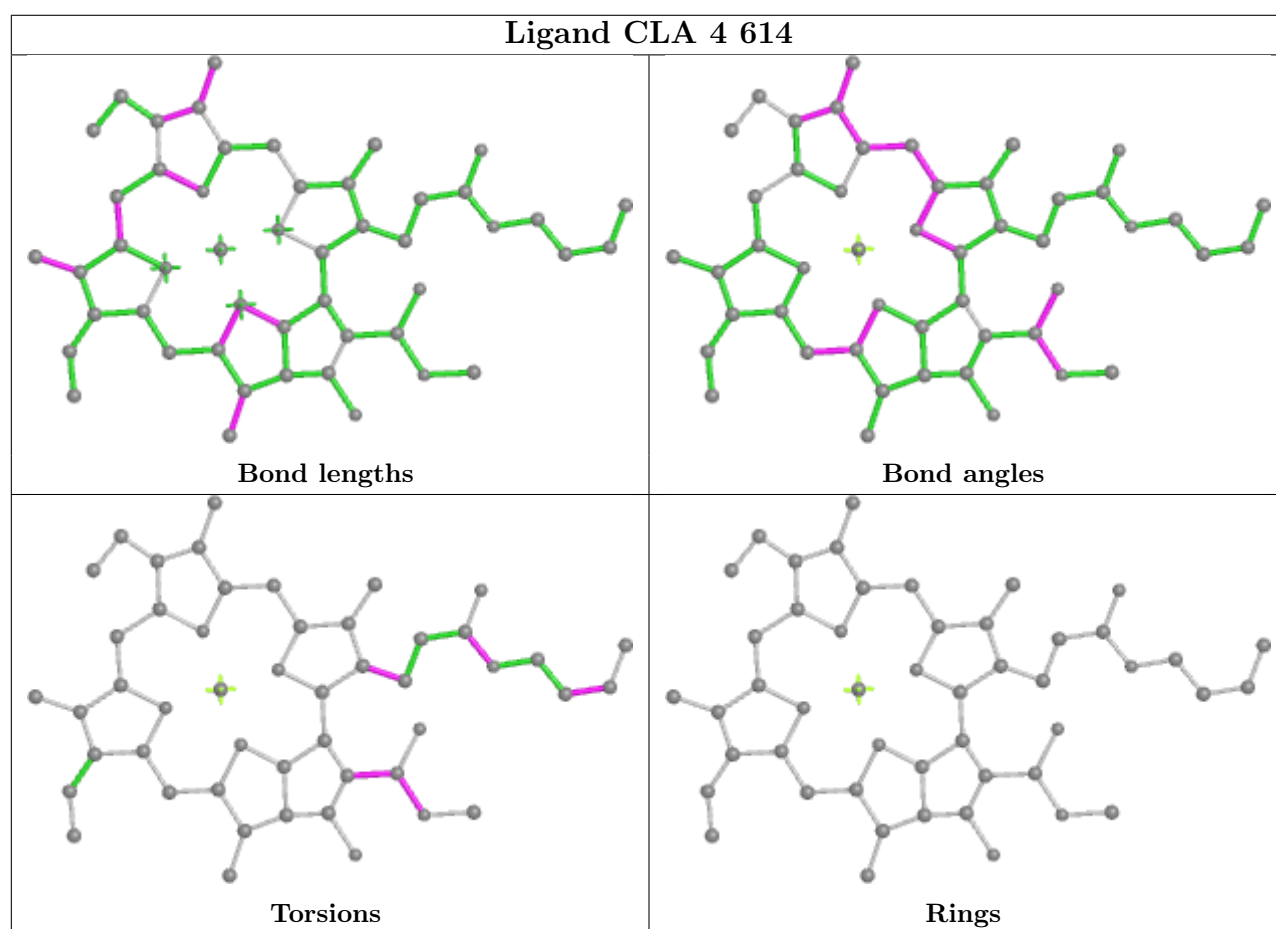
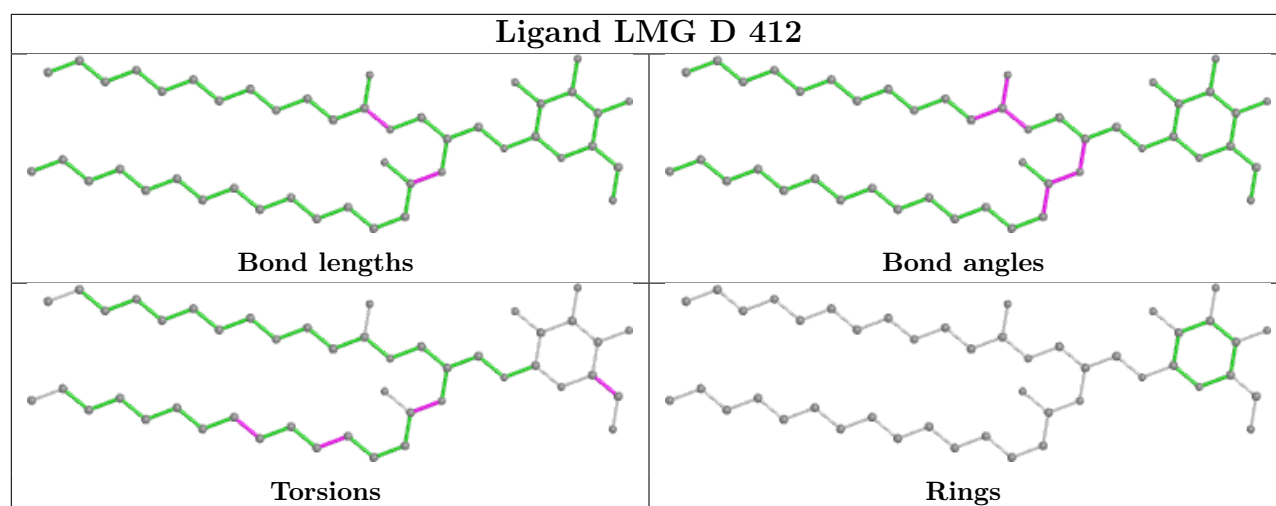
Bond angles

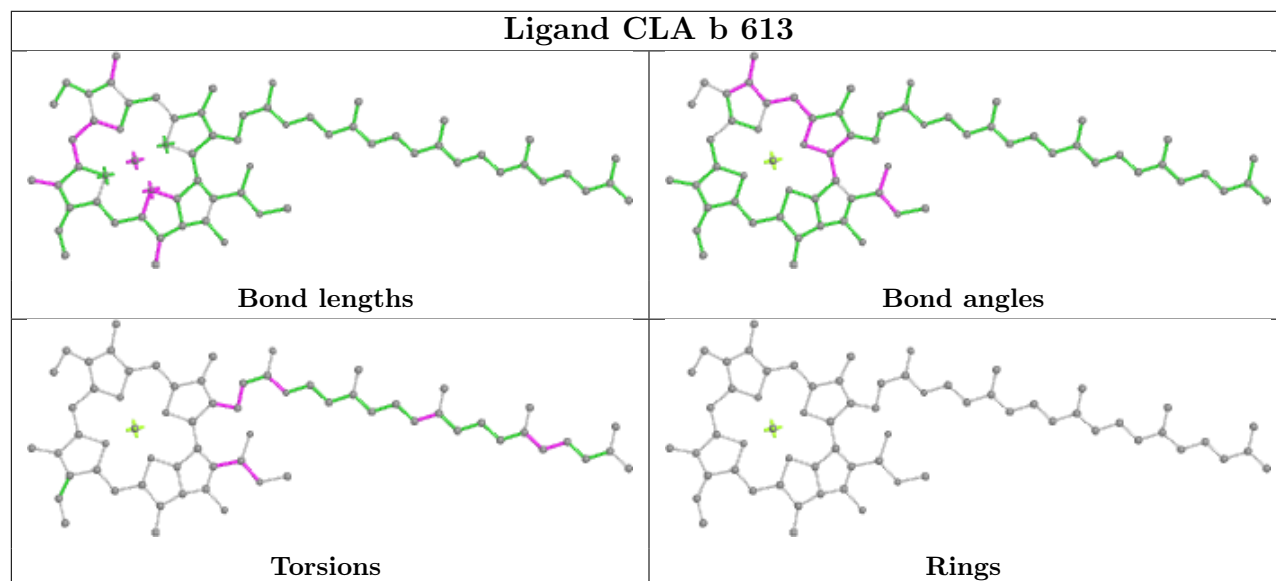
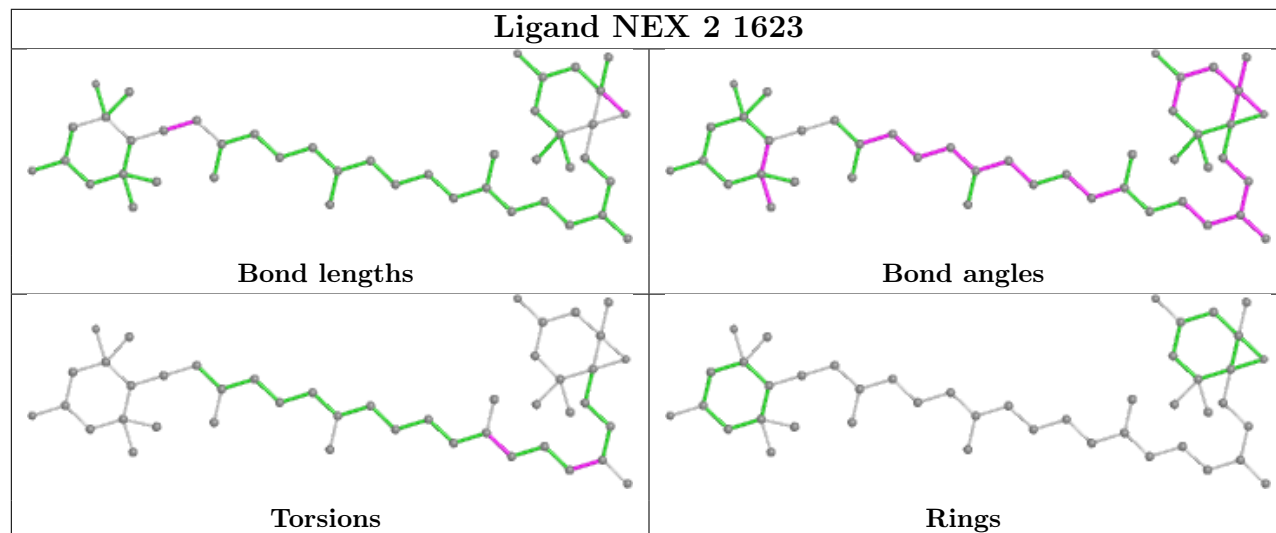
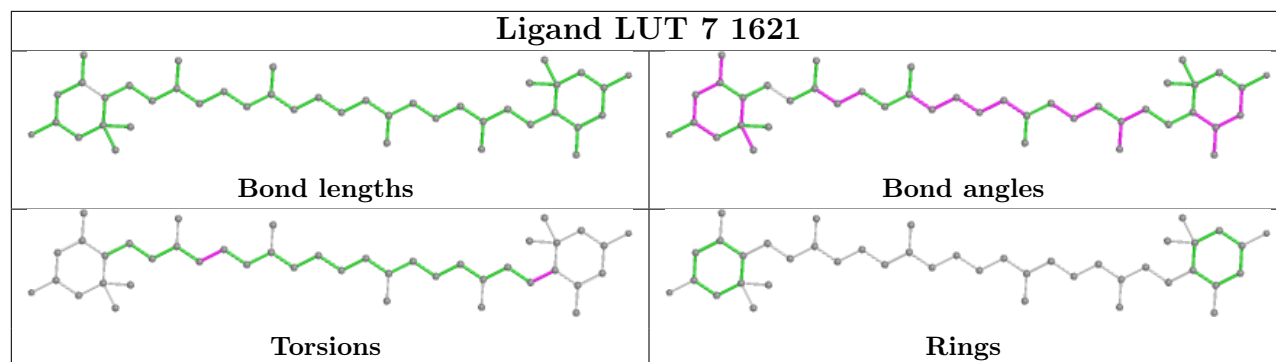


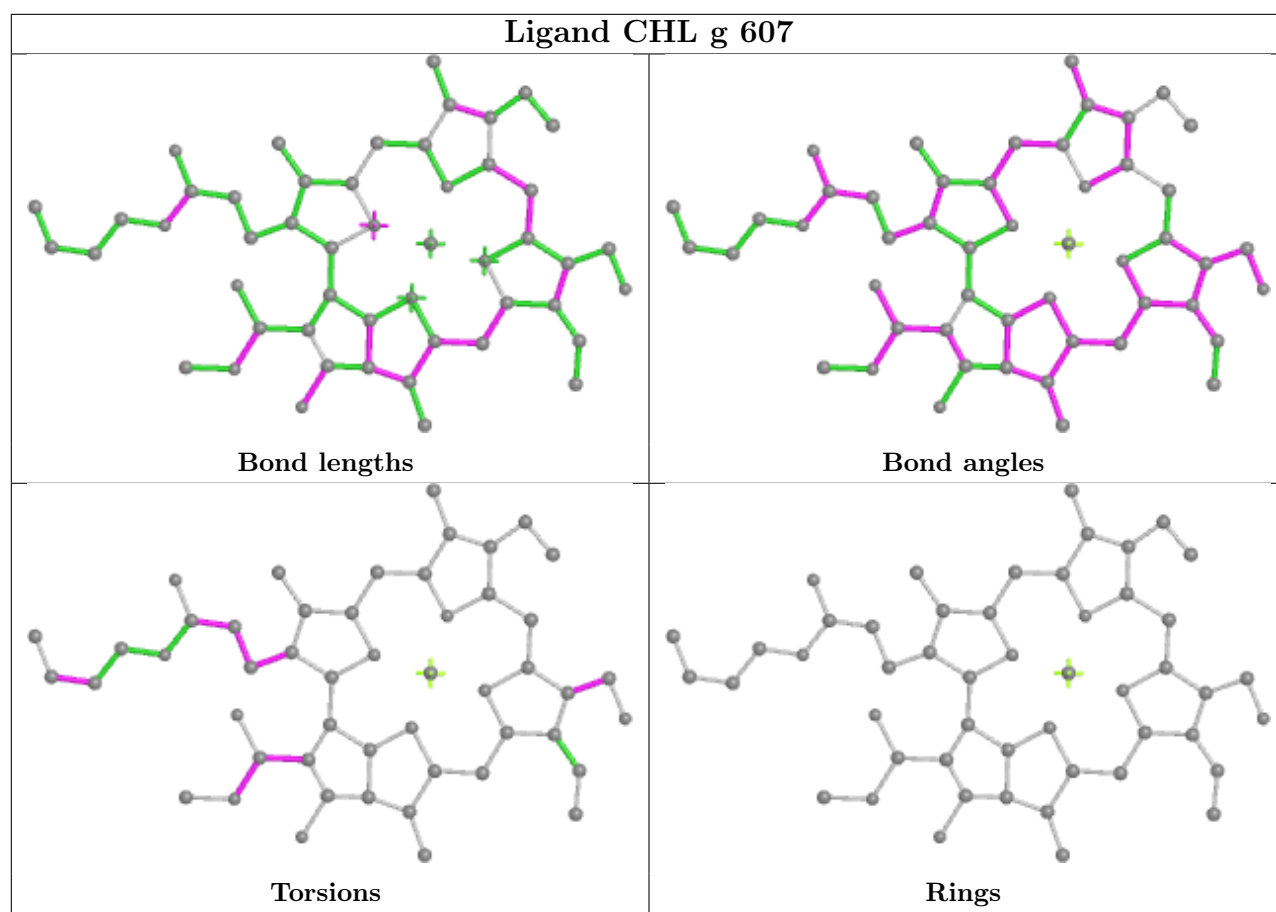
Torsions



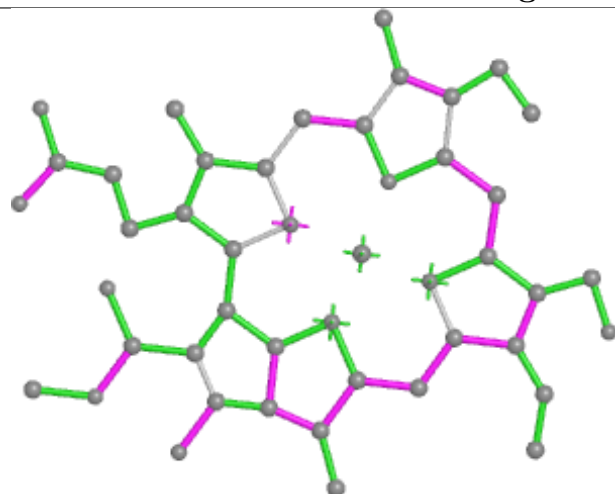
Rings



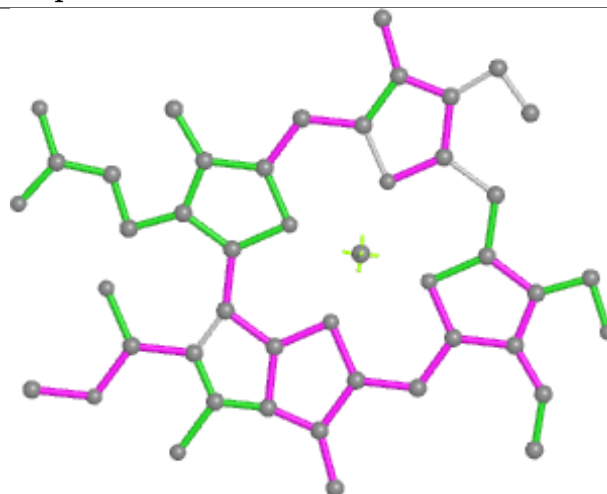




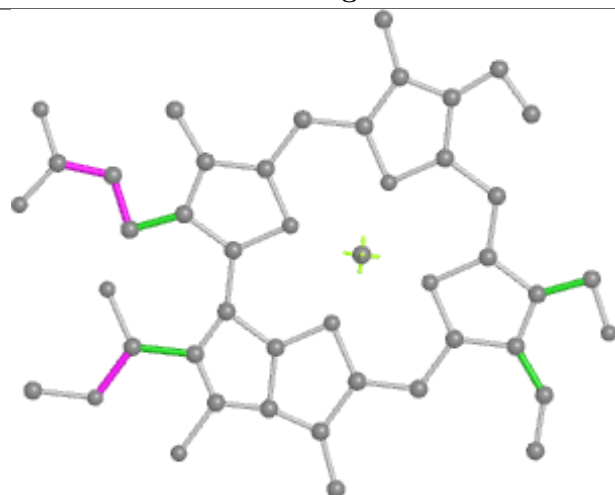
Ligand CHL p 606



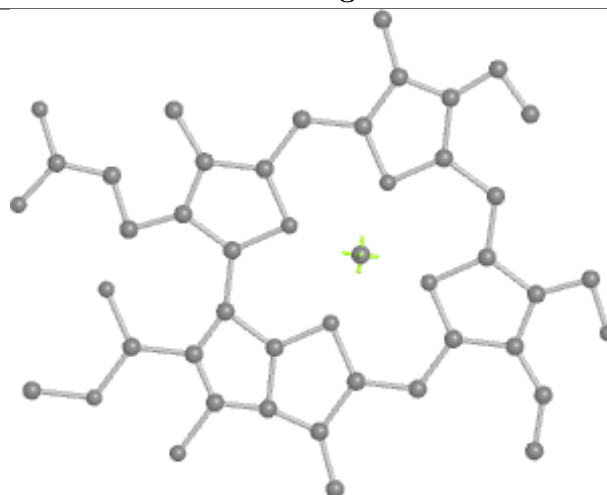
Bond lengths



Bond angles

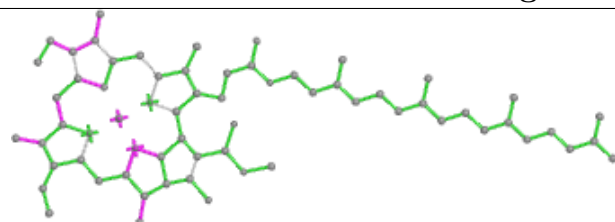


Torsions

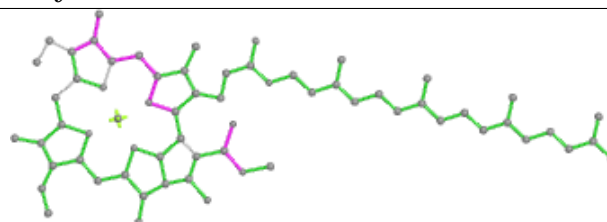


Rings

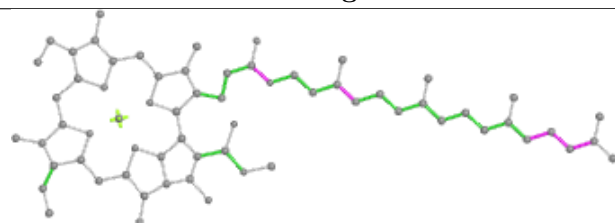
Ligand CLA y 611



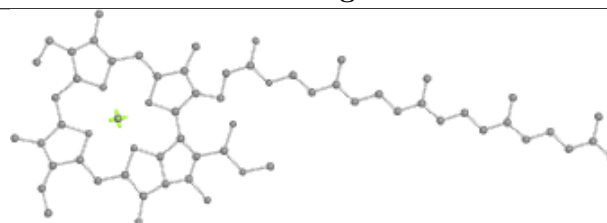
Bond lengths



Bond angles

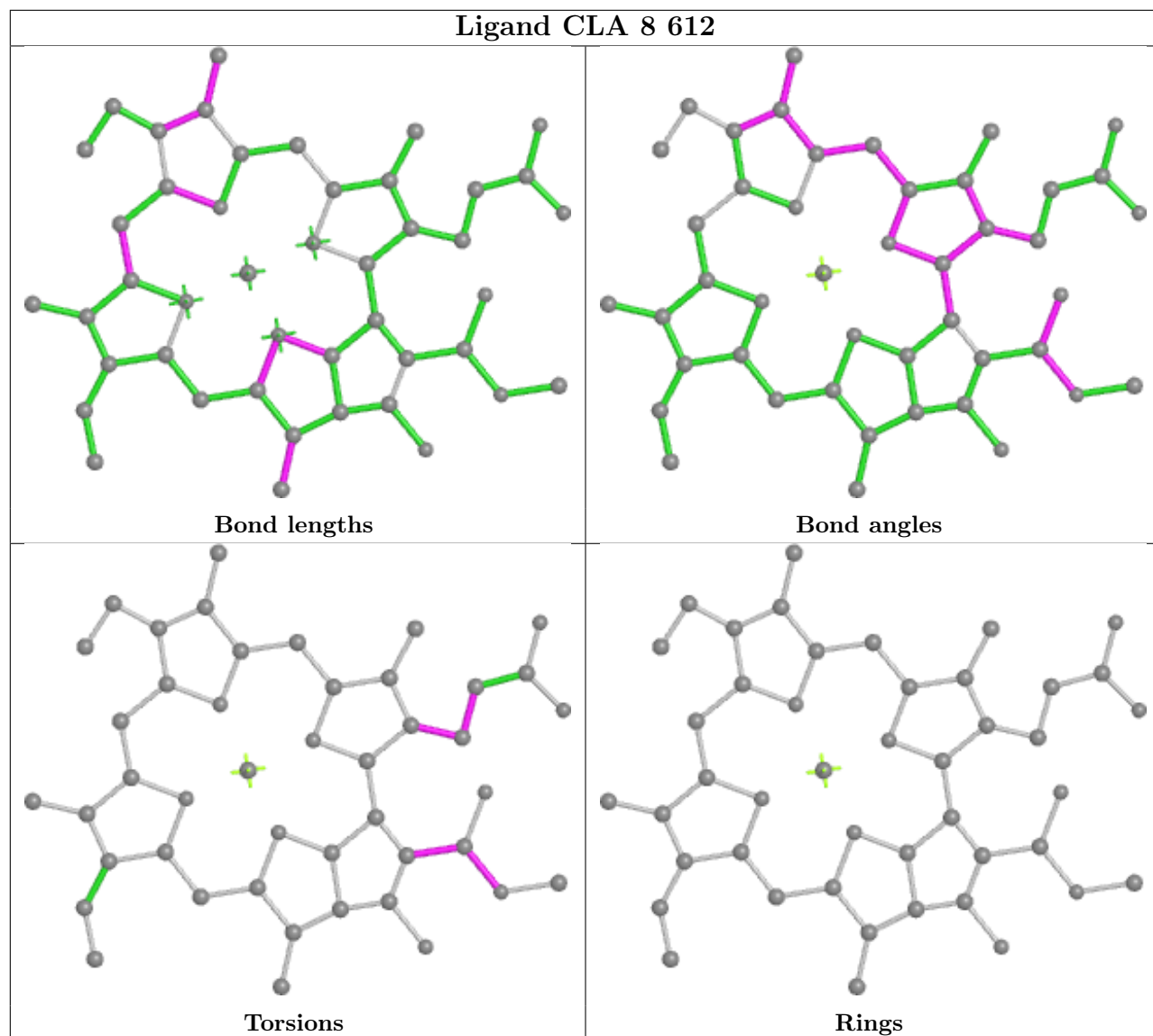


Torsions

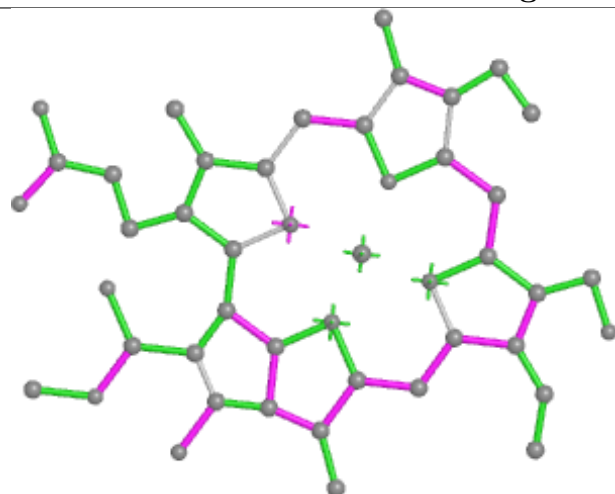


Rings

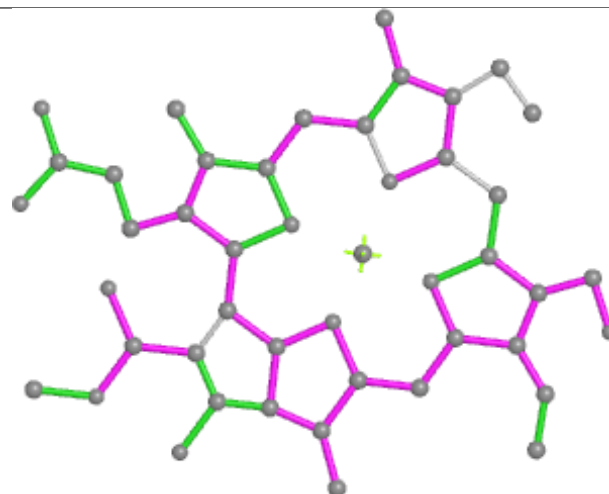
Ligand CLA 8 612



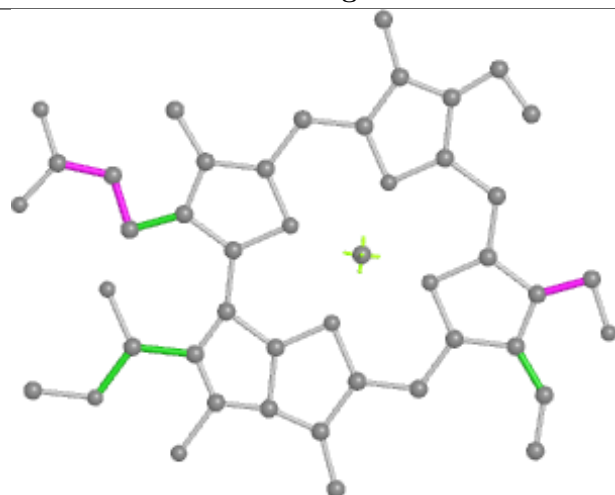
Ligand CHL 6 605



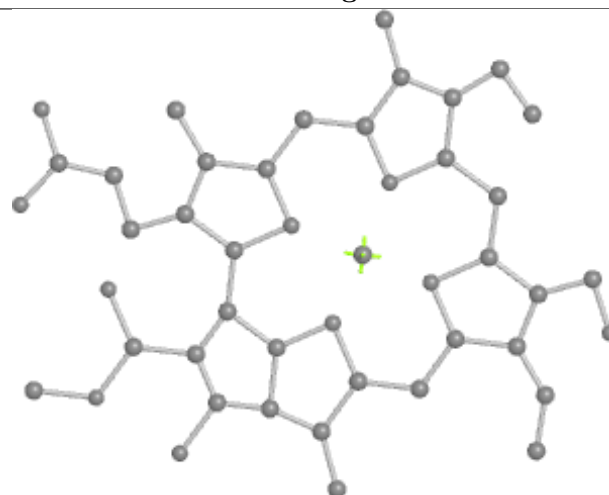
Bond lengths



Bond angles

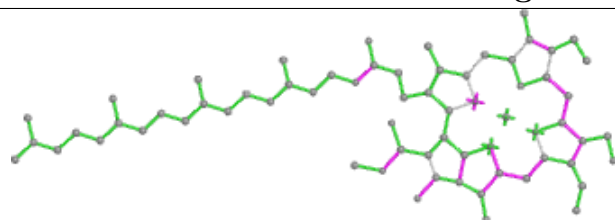


Torsions

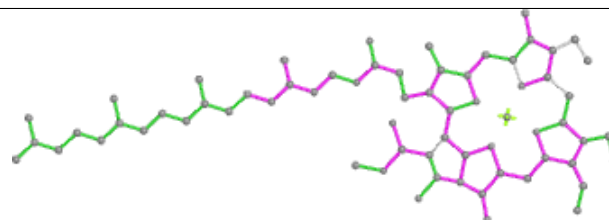


Rings

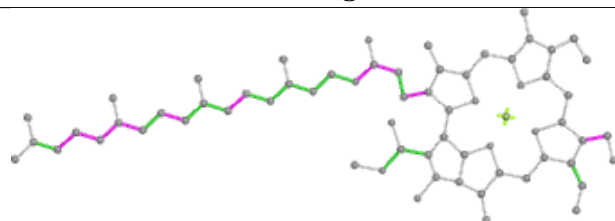
Ligand CHL N 607



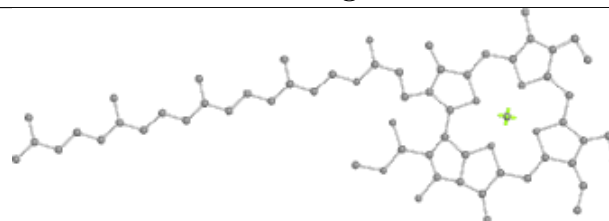
Bond lengths



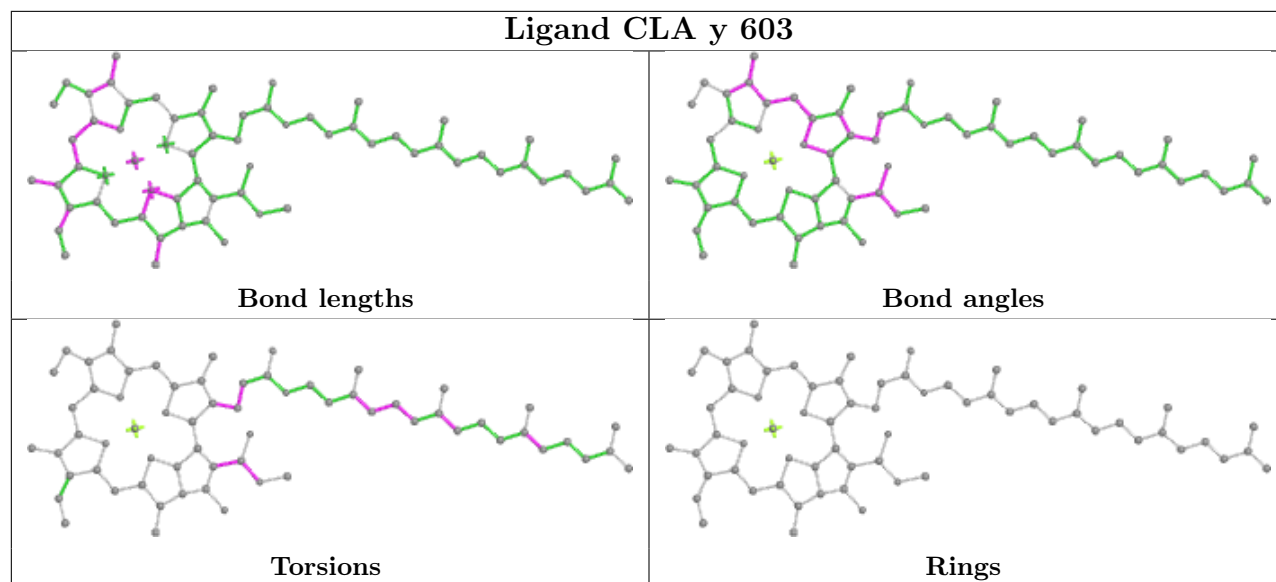
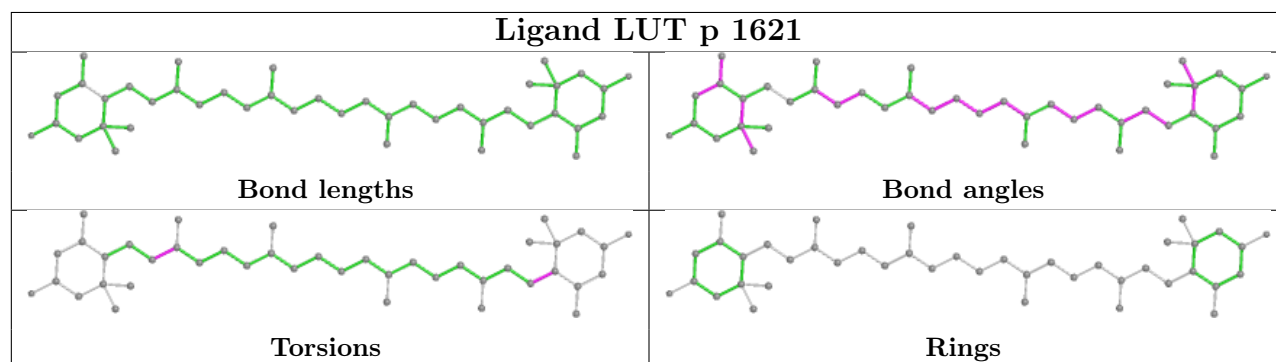
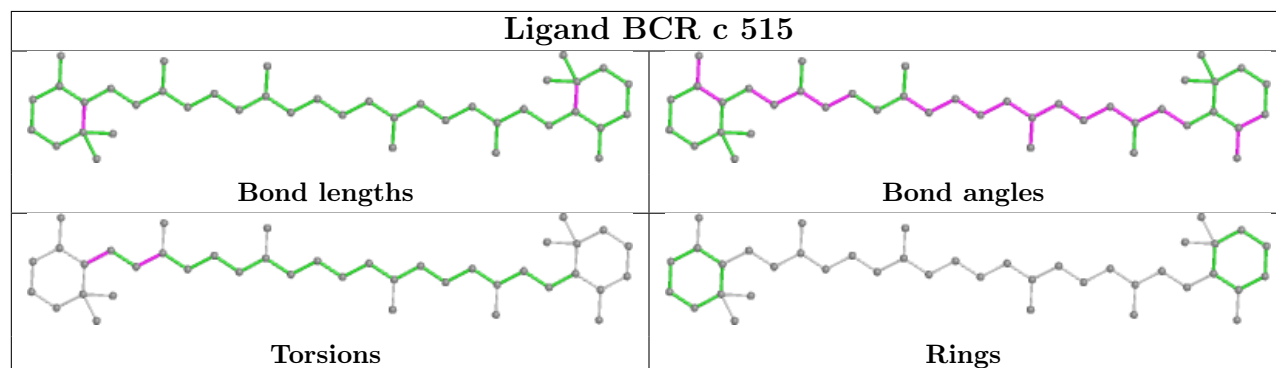
Bond angles

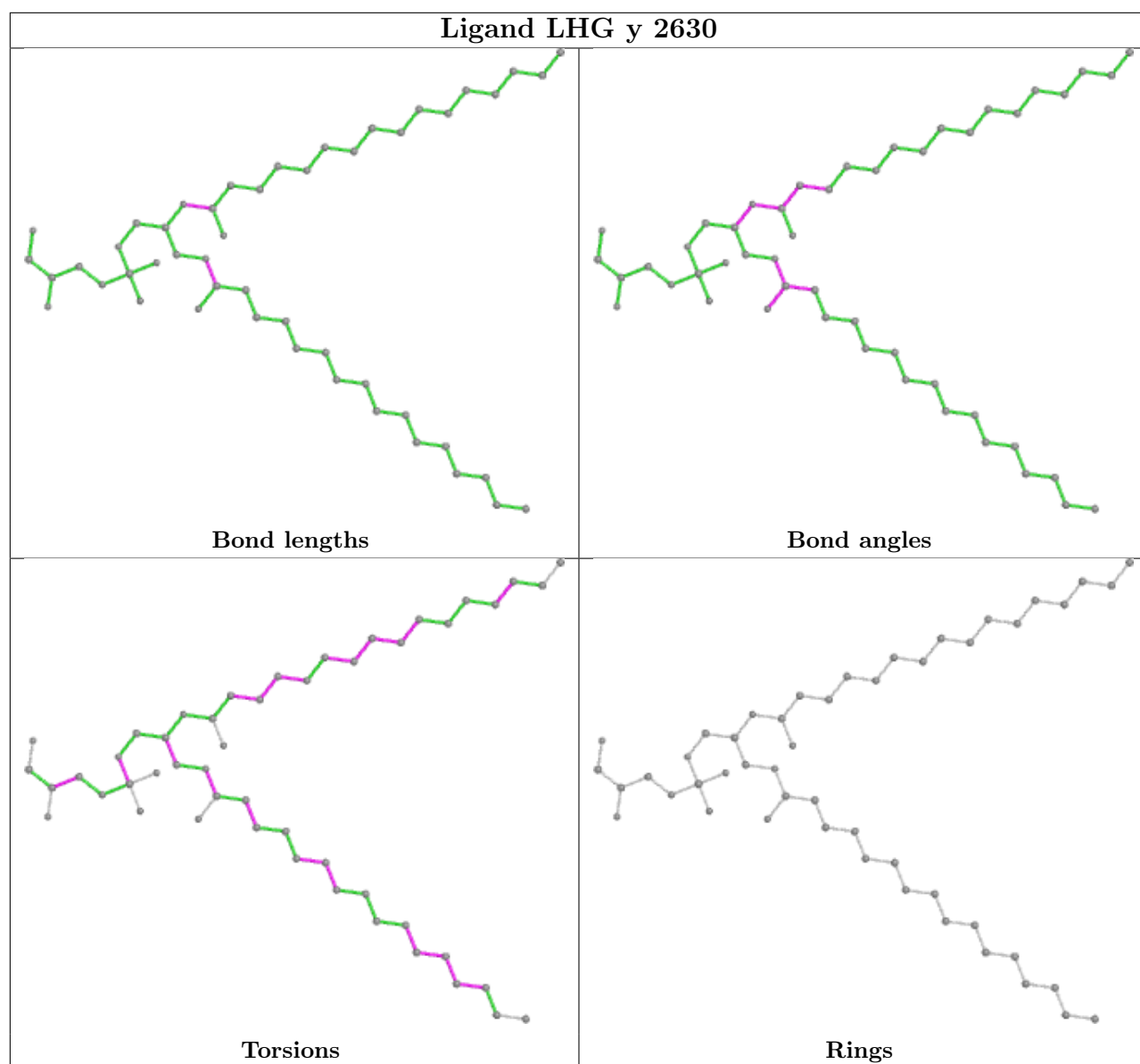


Torsions

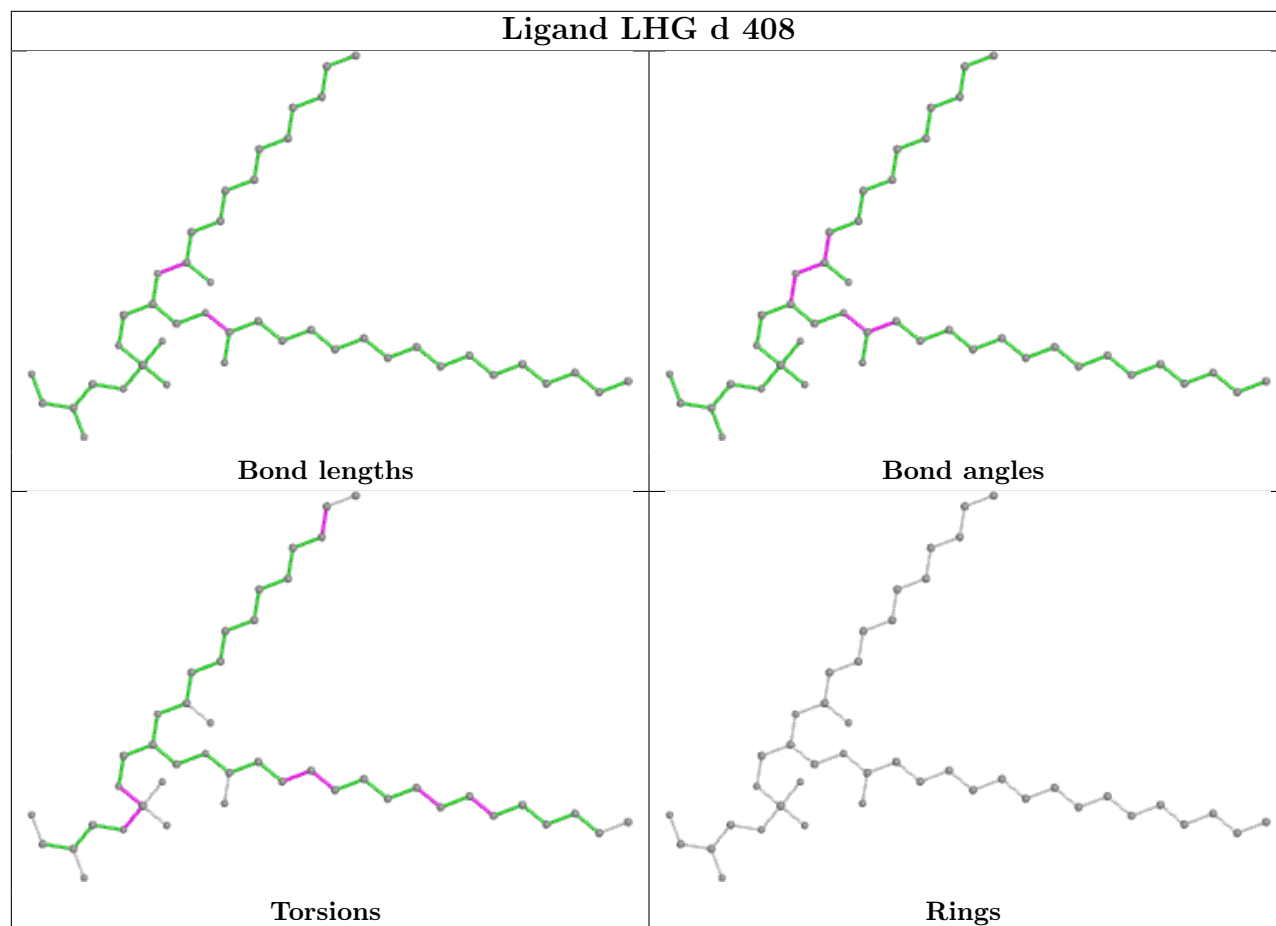


Rings

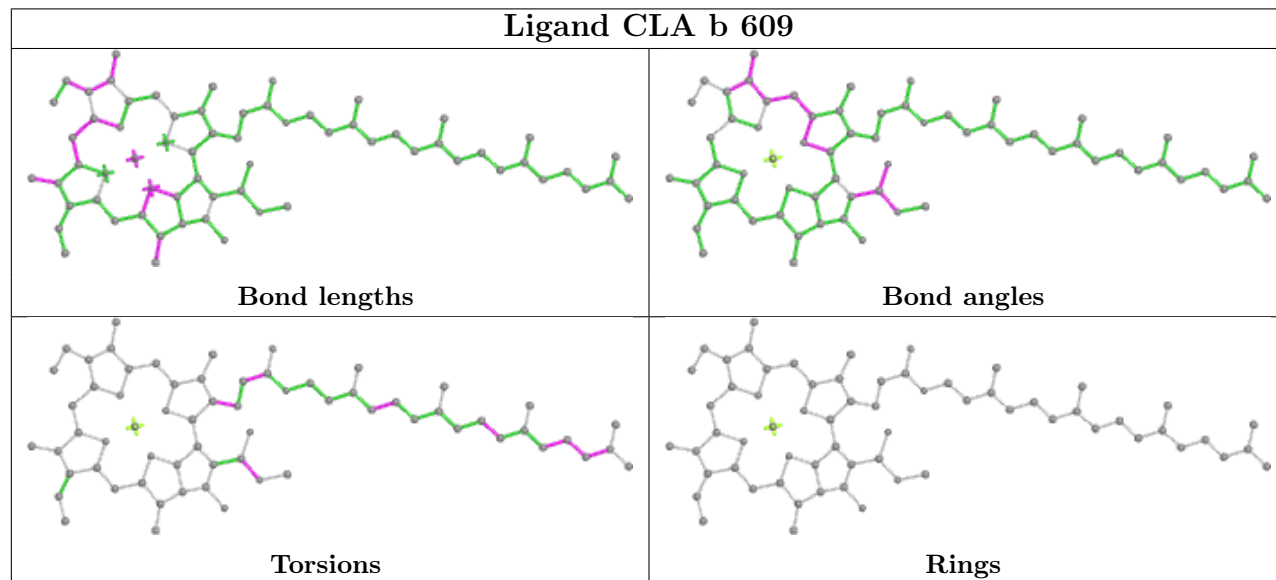
Ligand CLA y 603**Ligand LUT p 1621****Ligand BCR c 515**



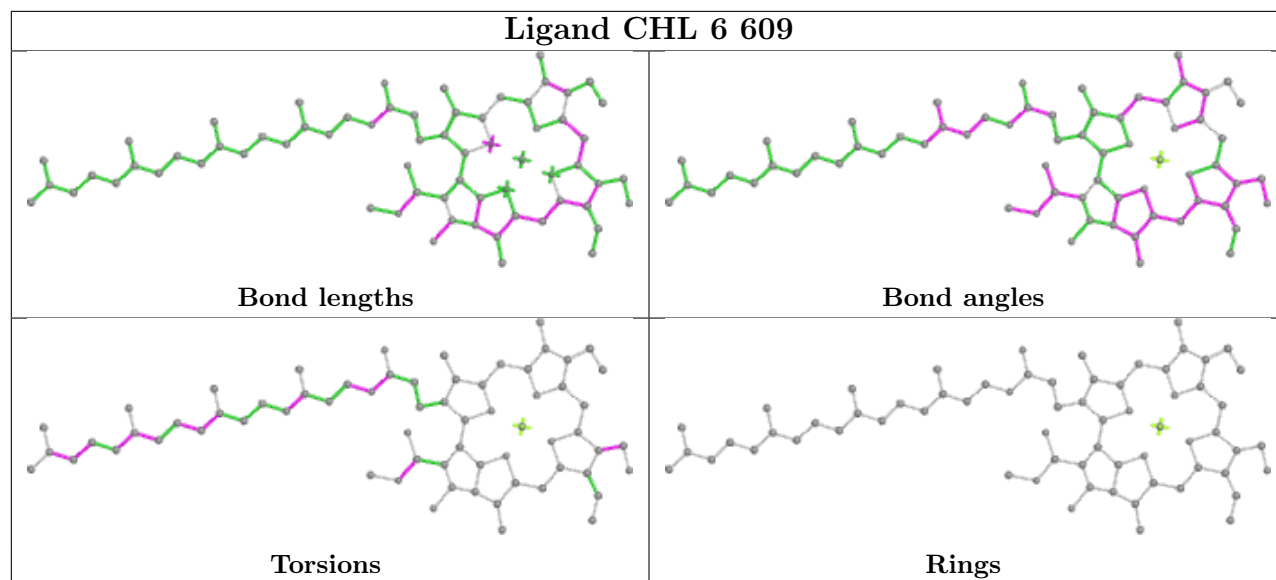
Ligand LHG d 408



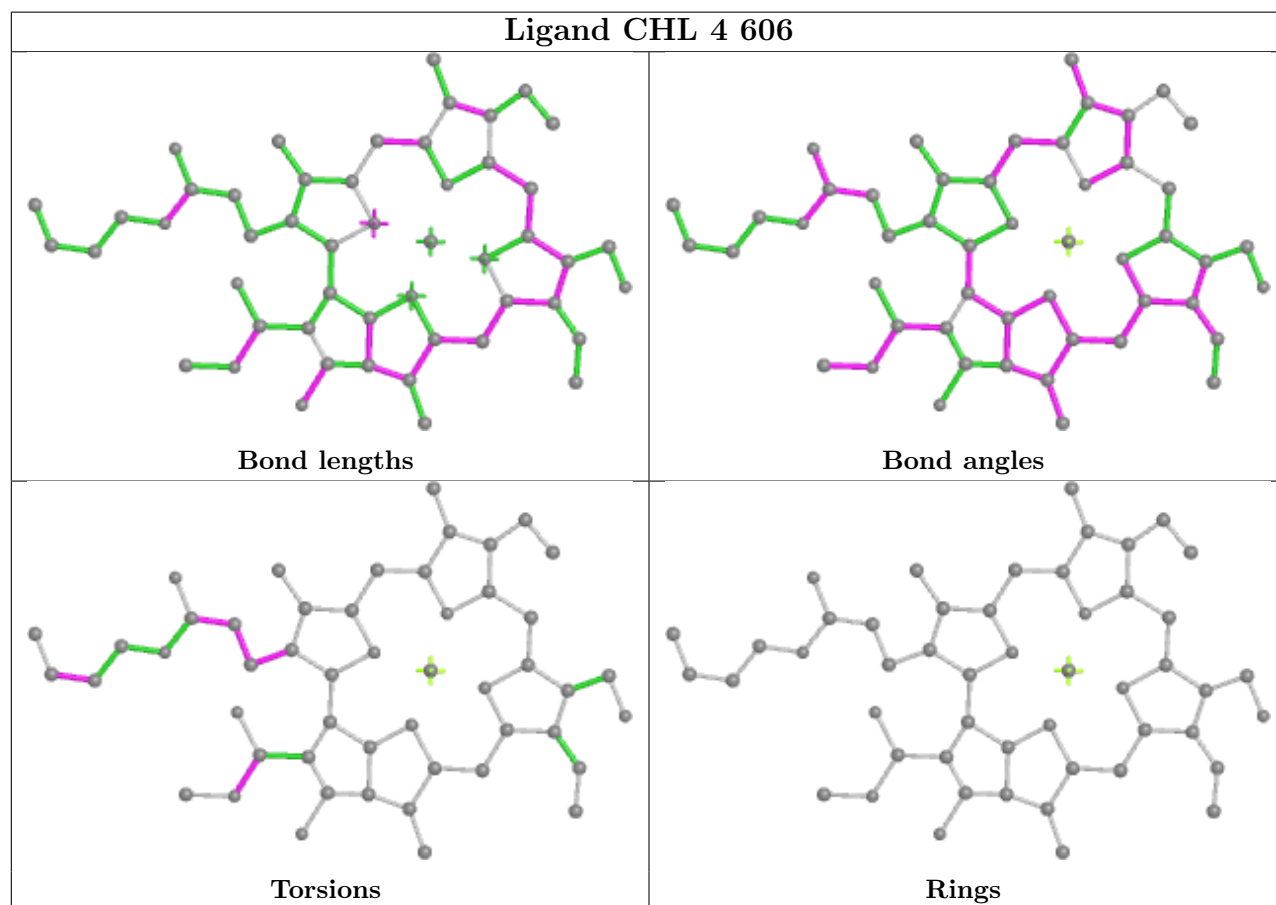
Ligand CLA b 609

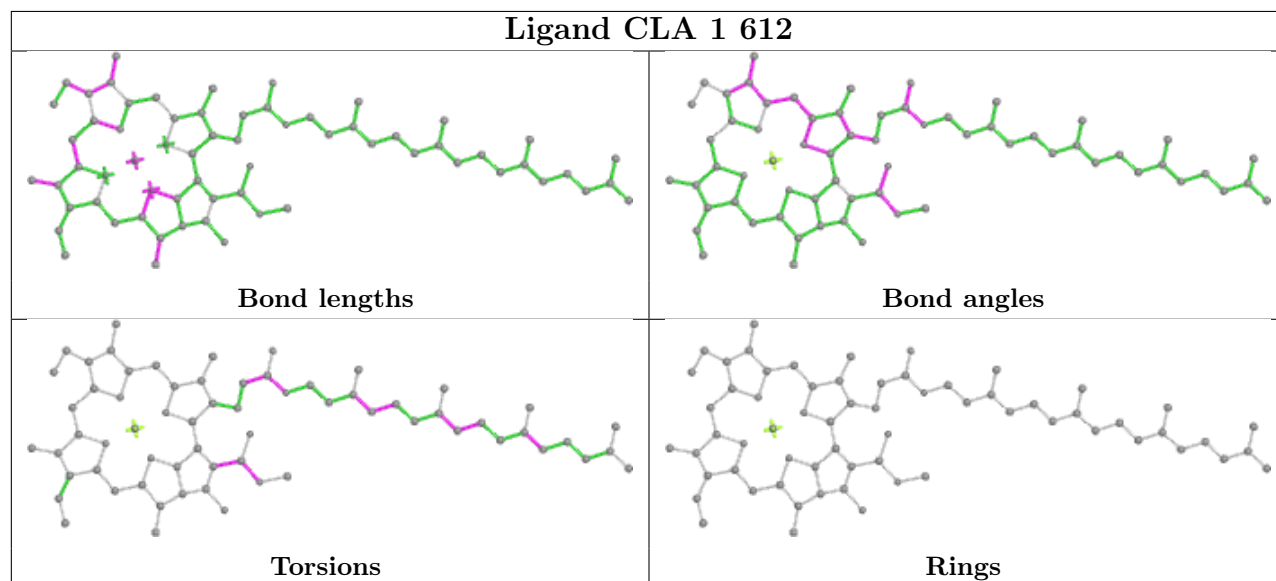
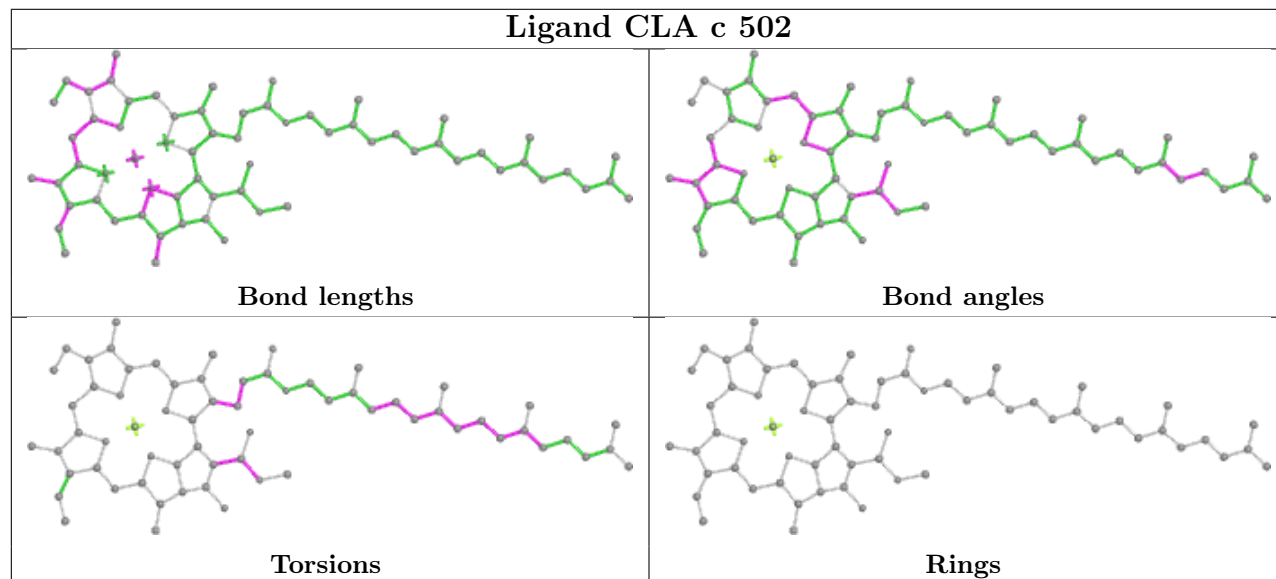
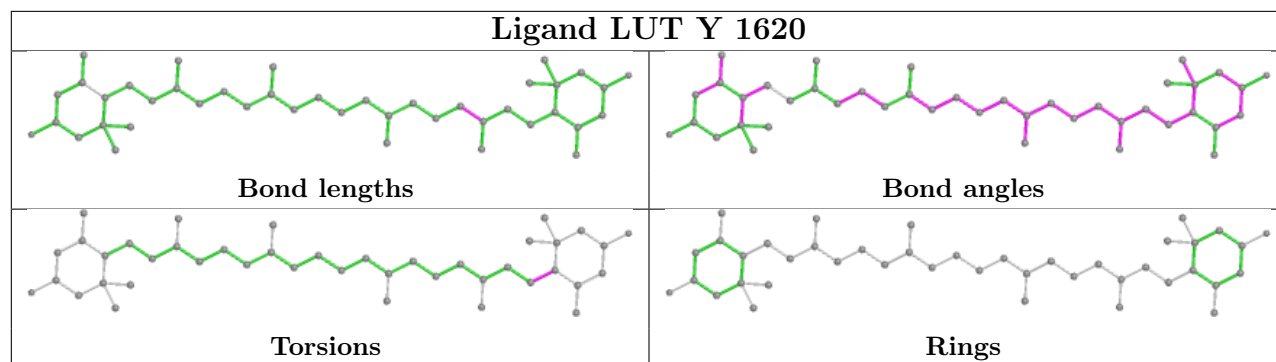


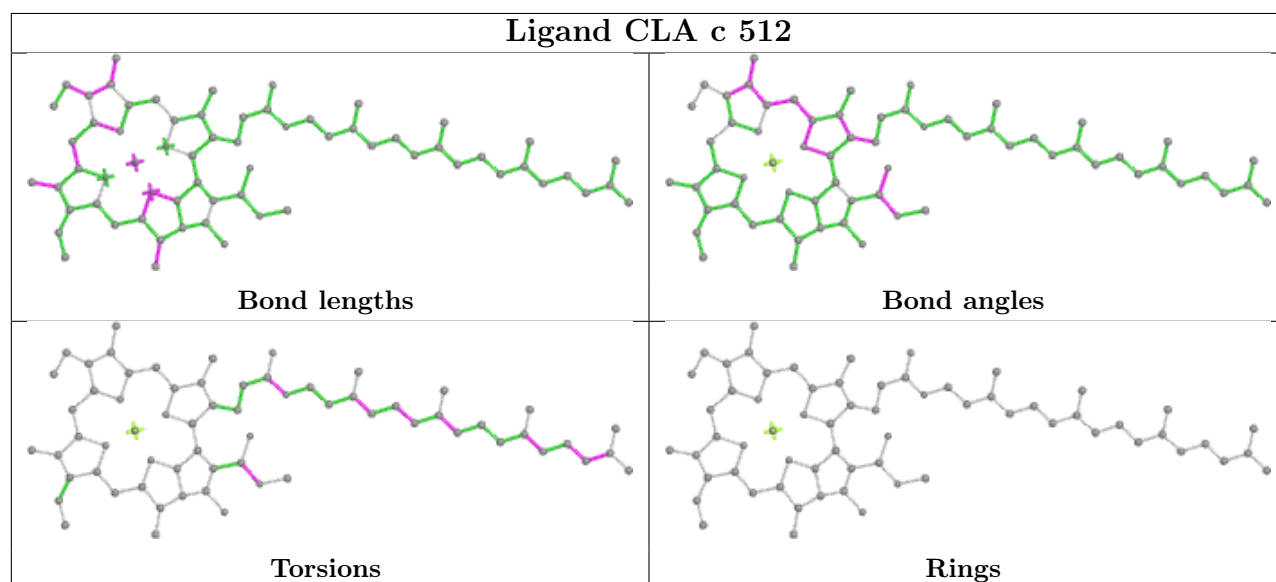
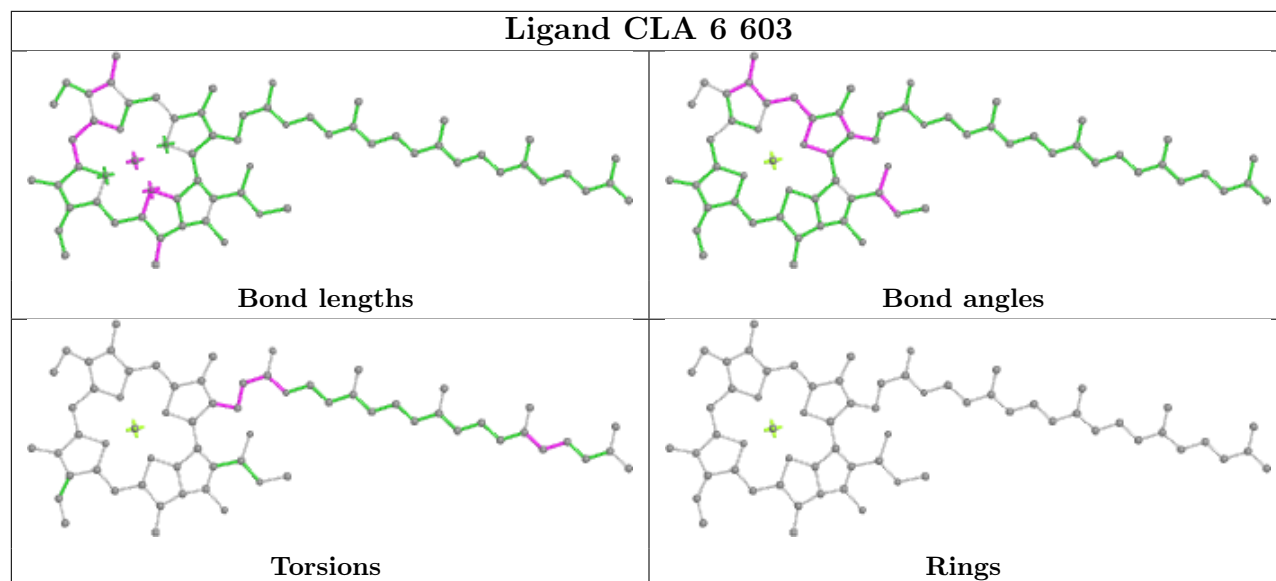
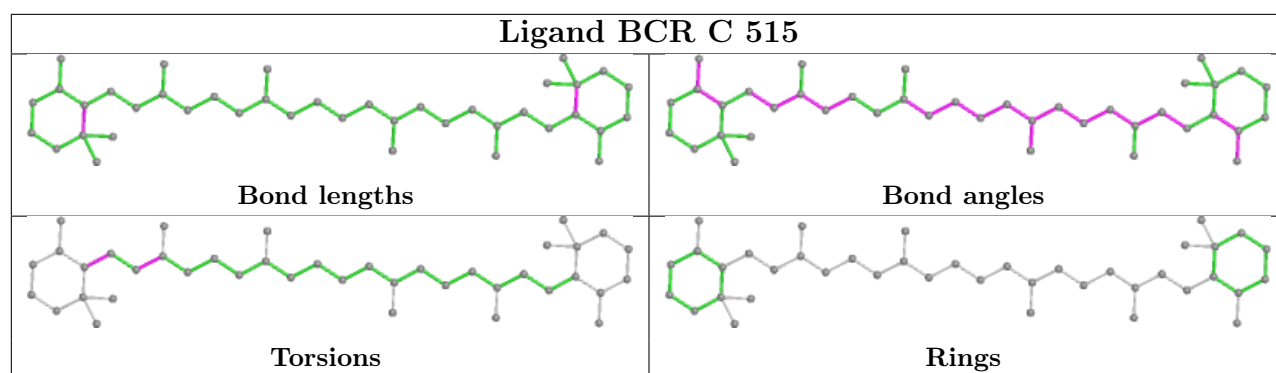
Ligand CHL 6 609

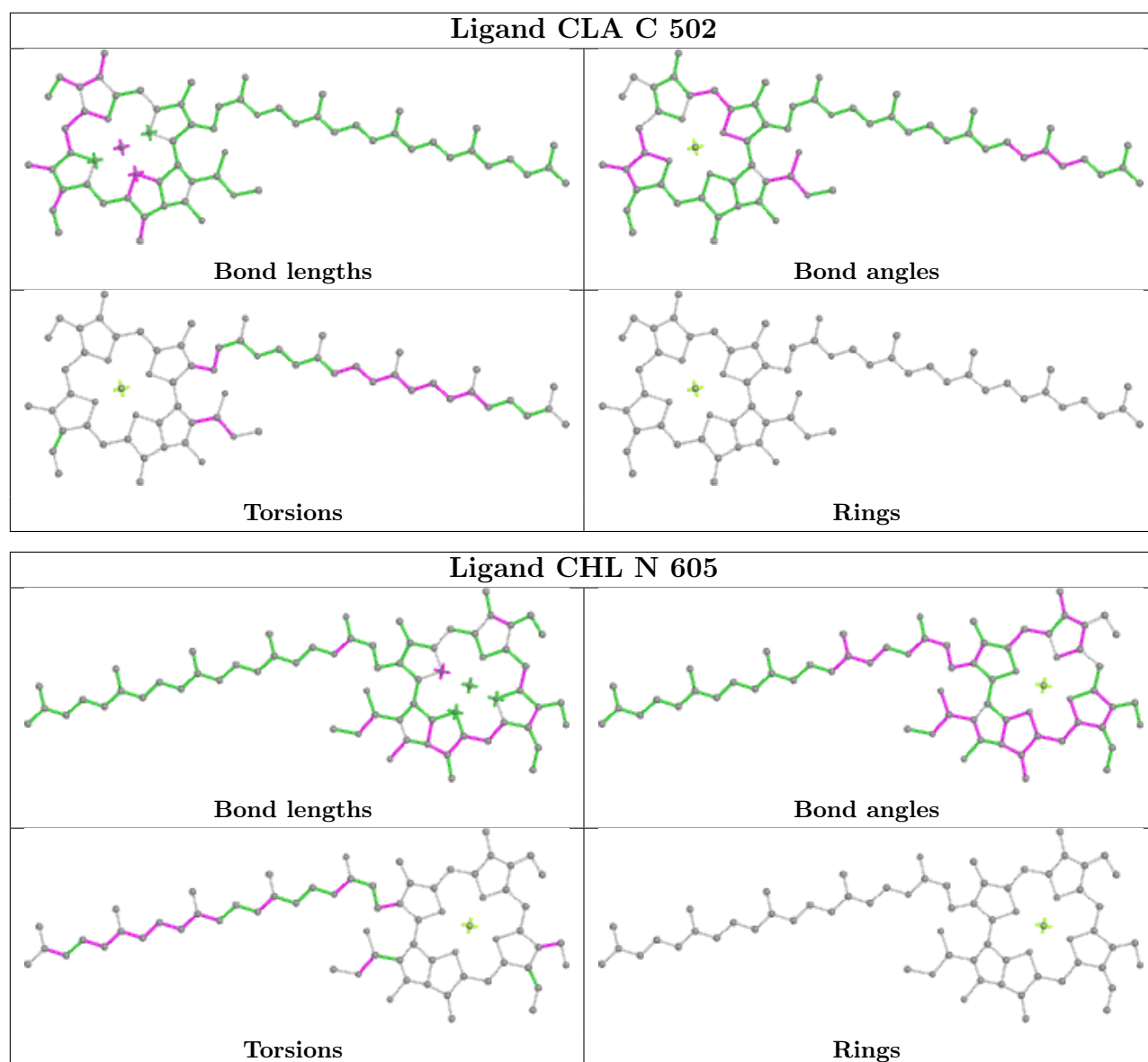


Ligand CHL 4 606

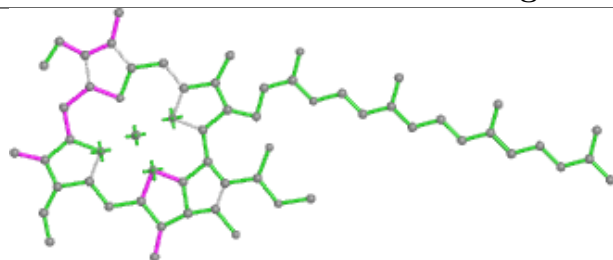




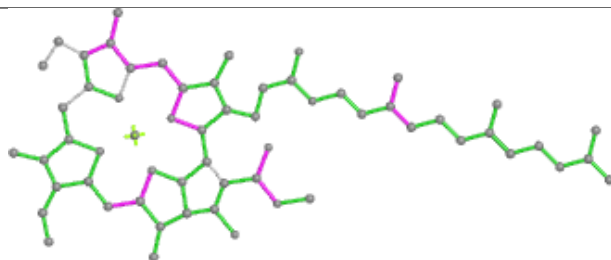




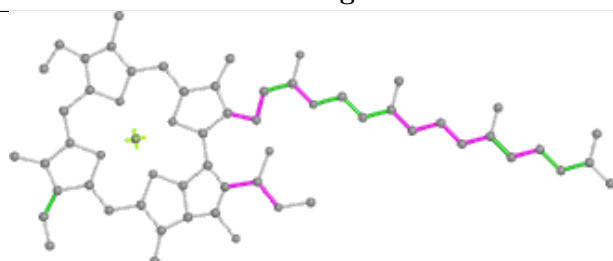
Ligand CLA r 613



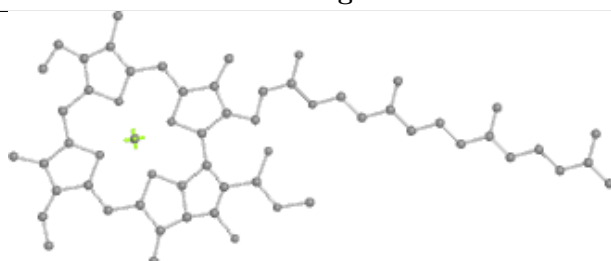
Bond lengths



Bond angles

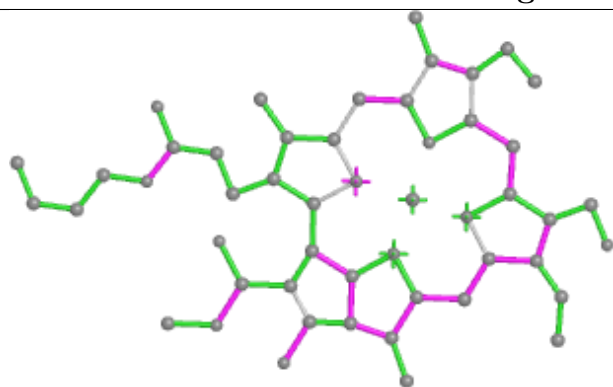


Torsions

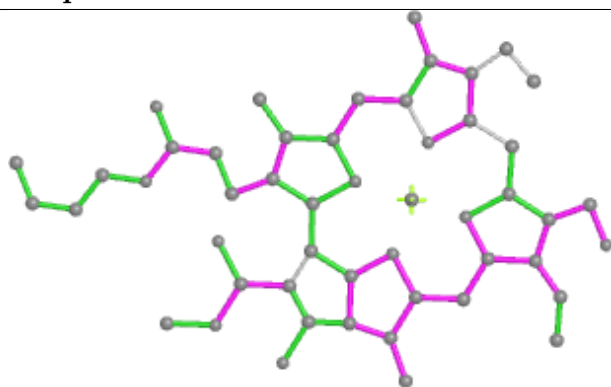


Rings

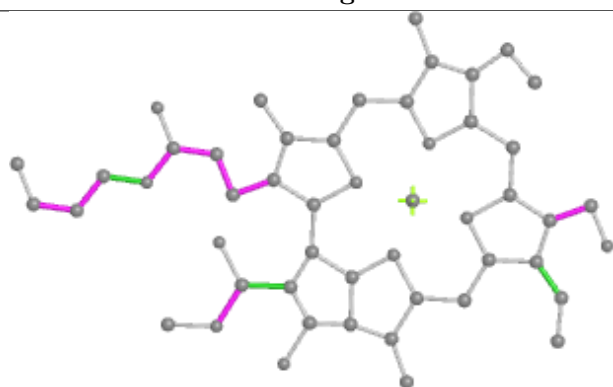
Ligand CHL q 607



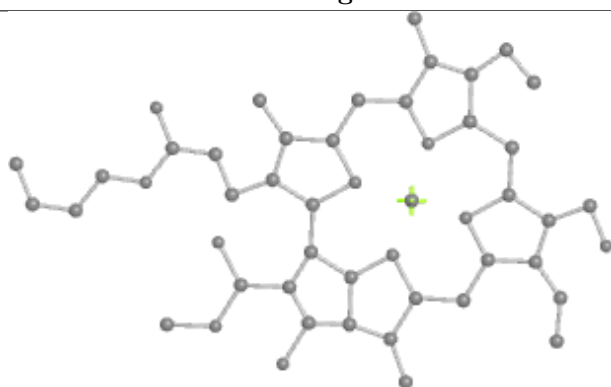
Bond lengths



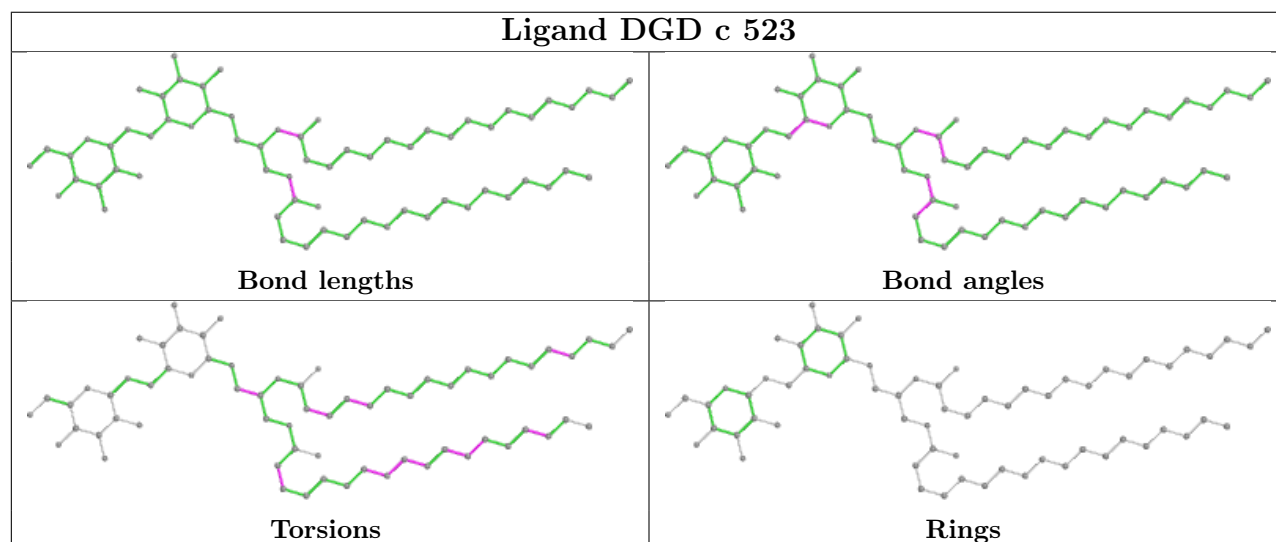
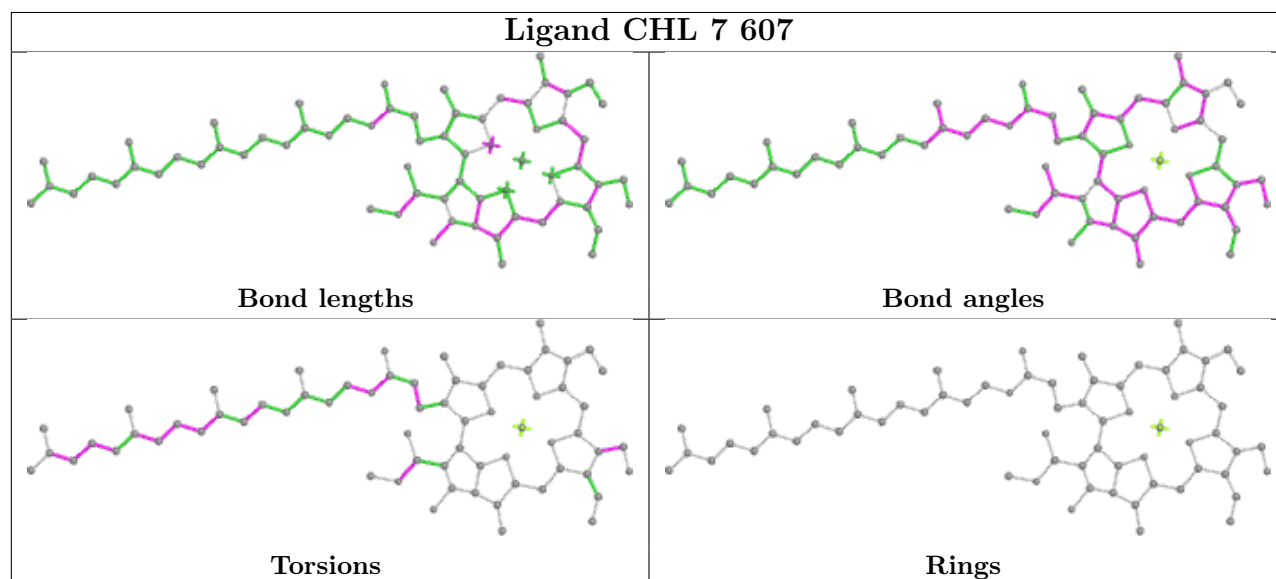
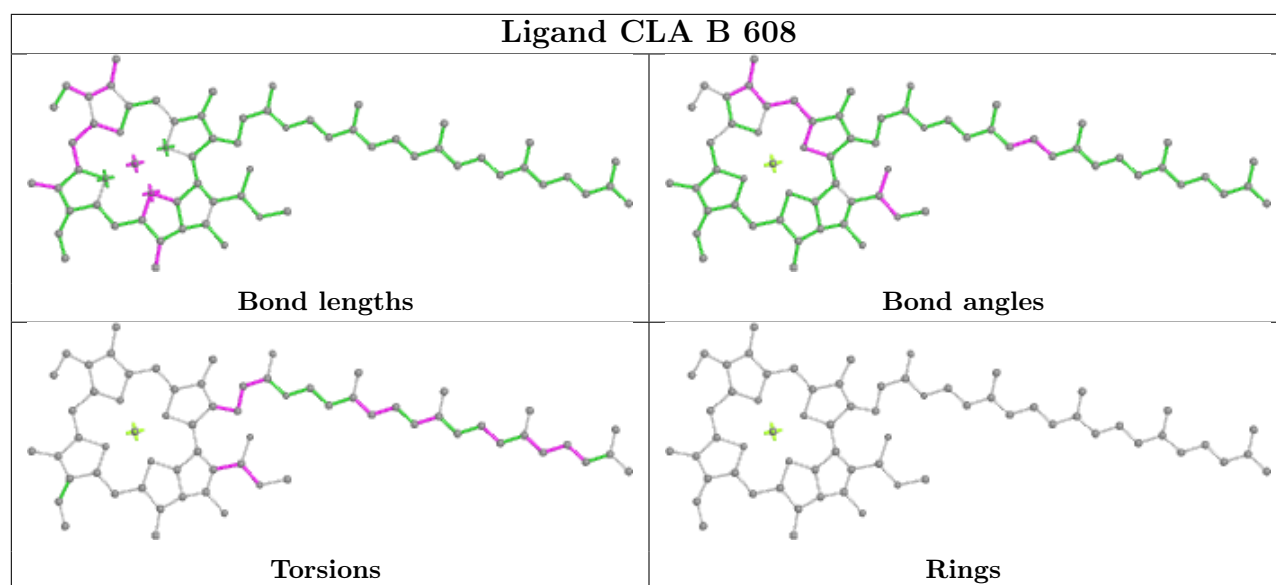
Bond angles

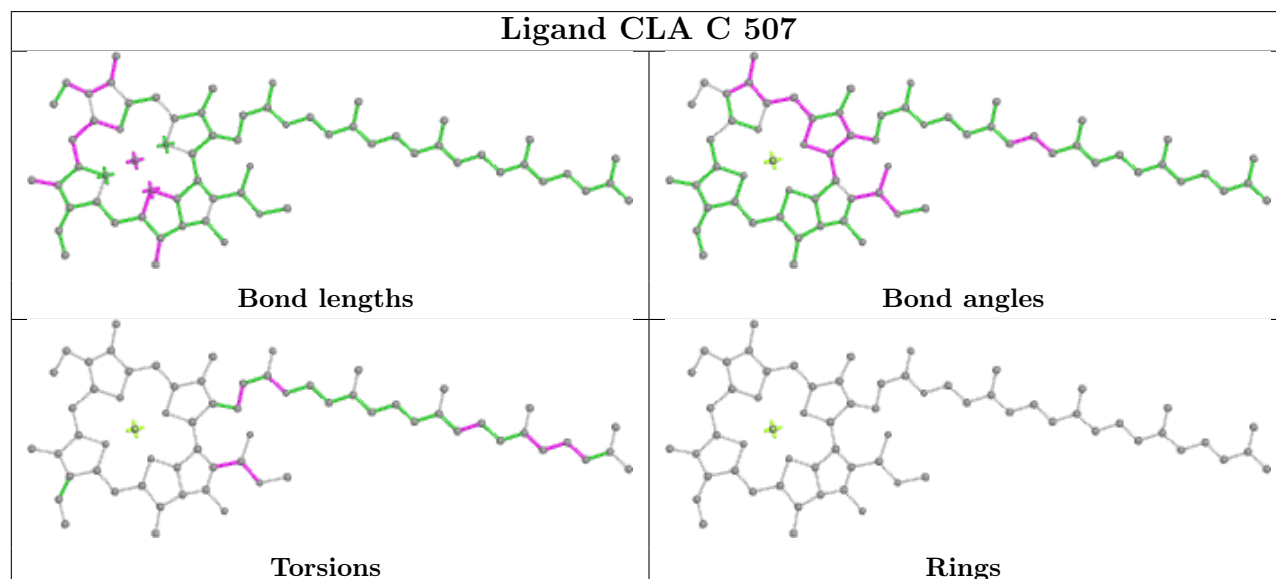
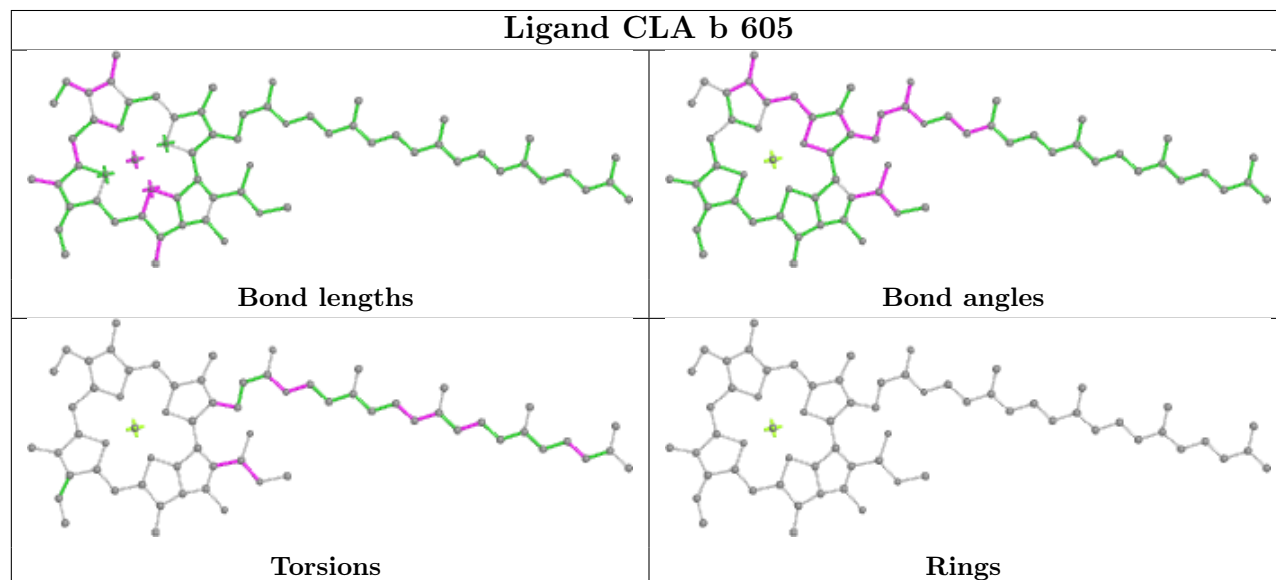
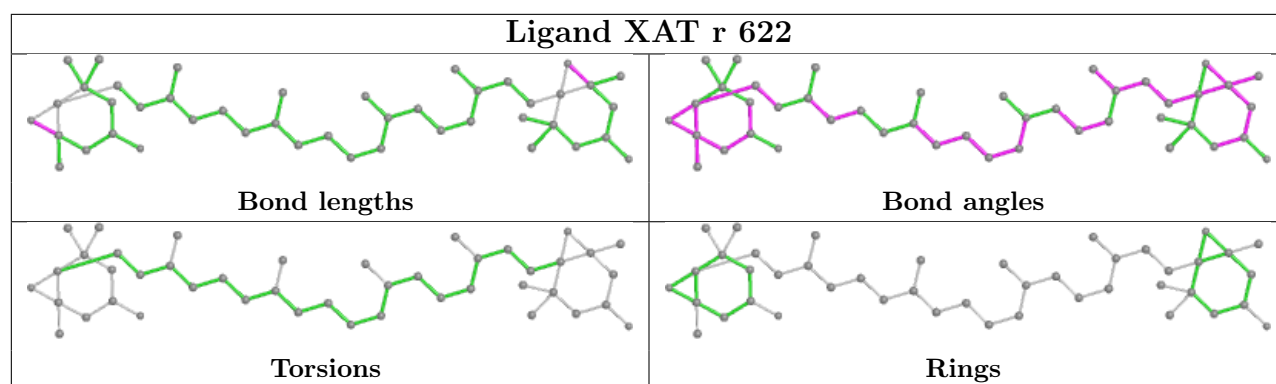


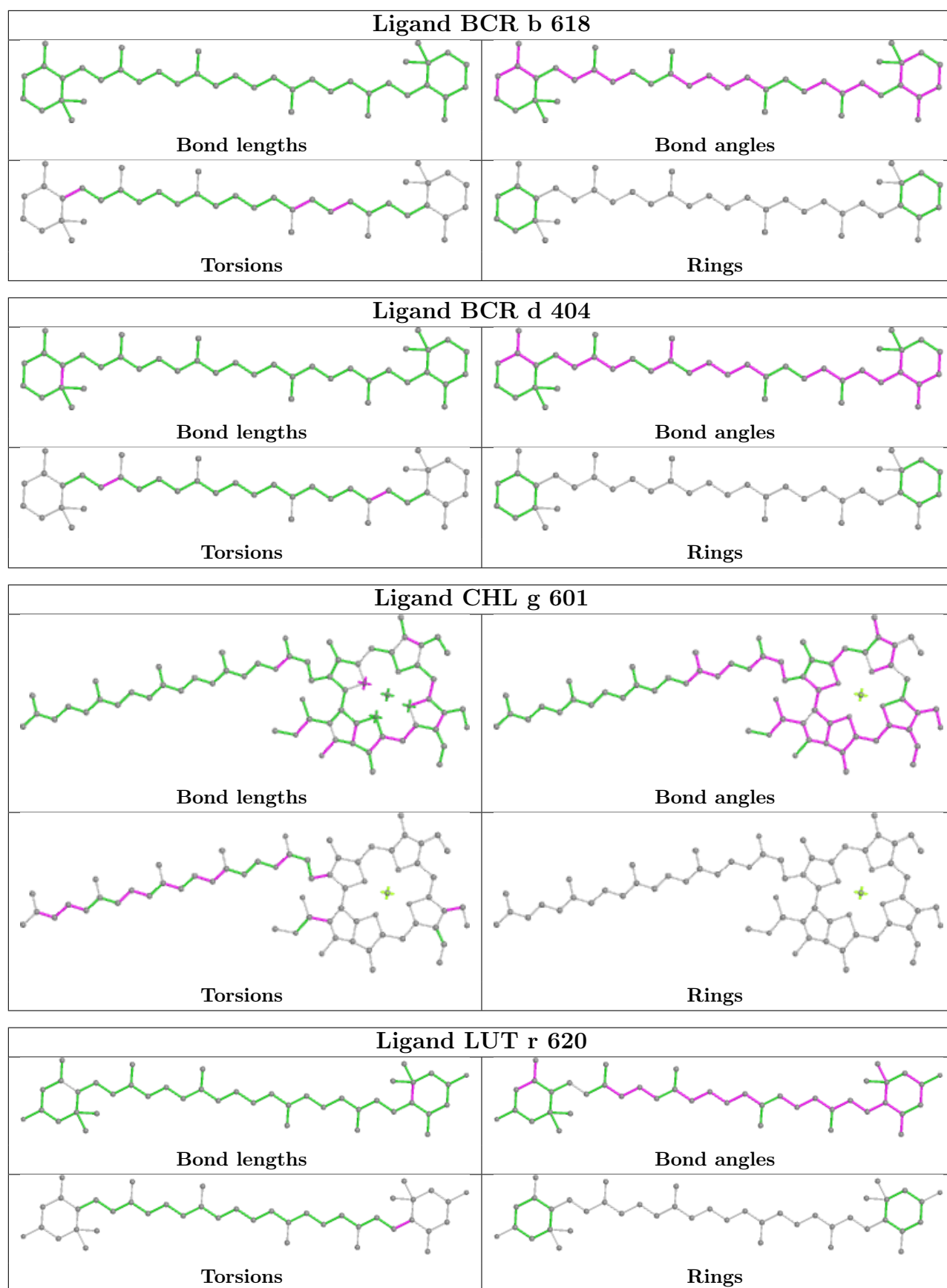
Torsions



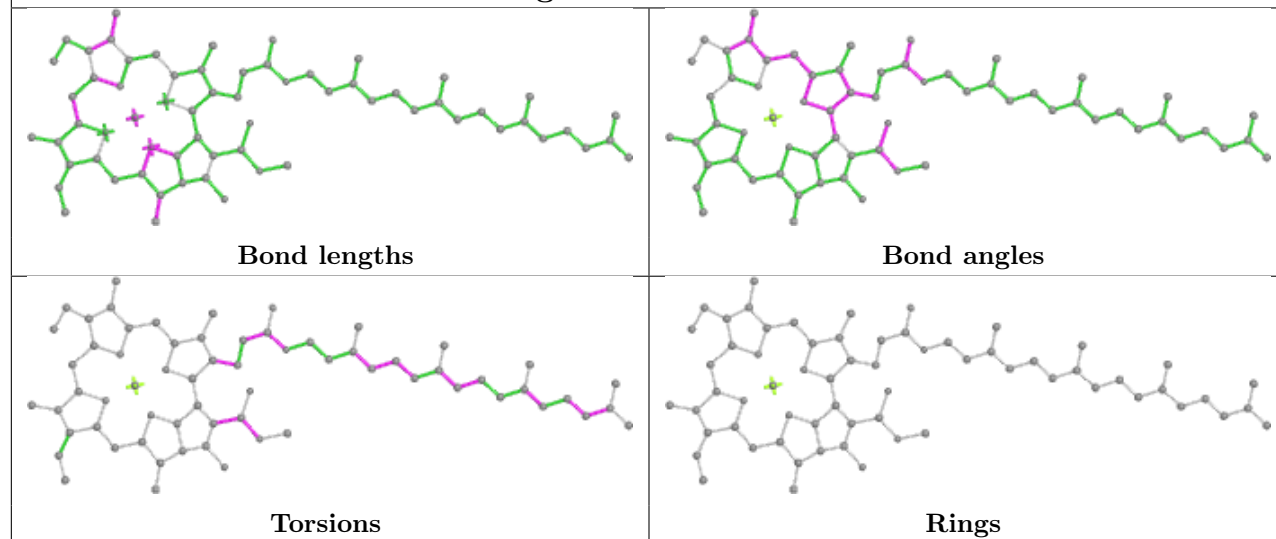
Rings



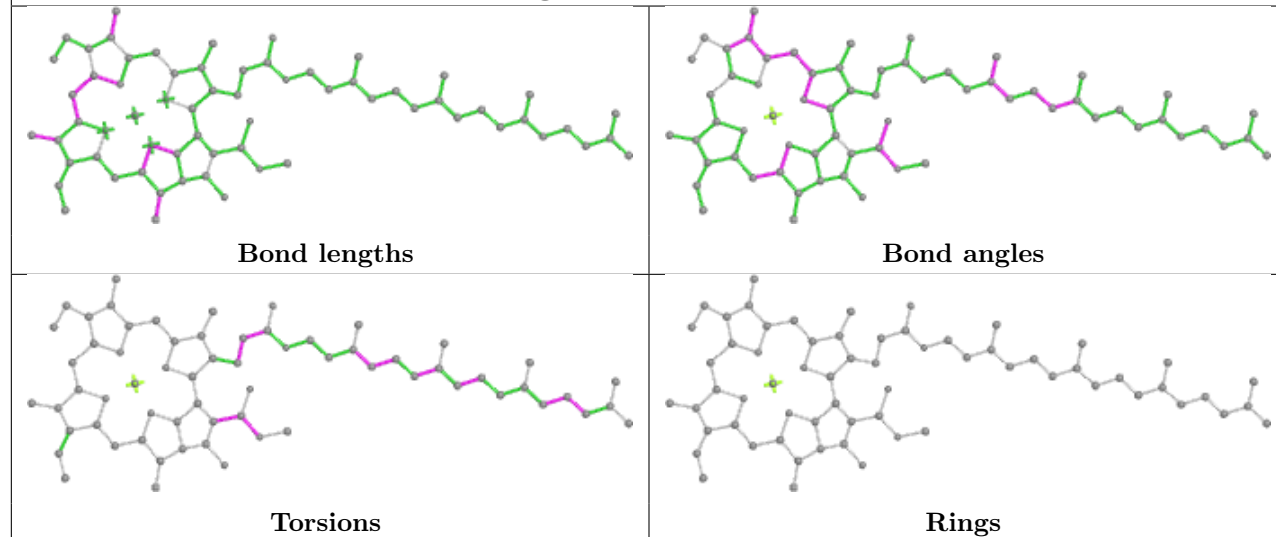


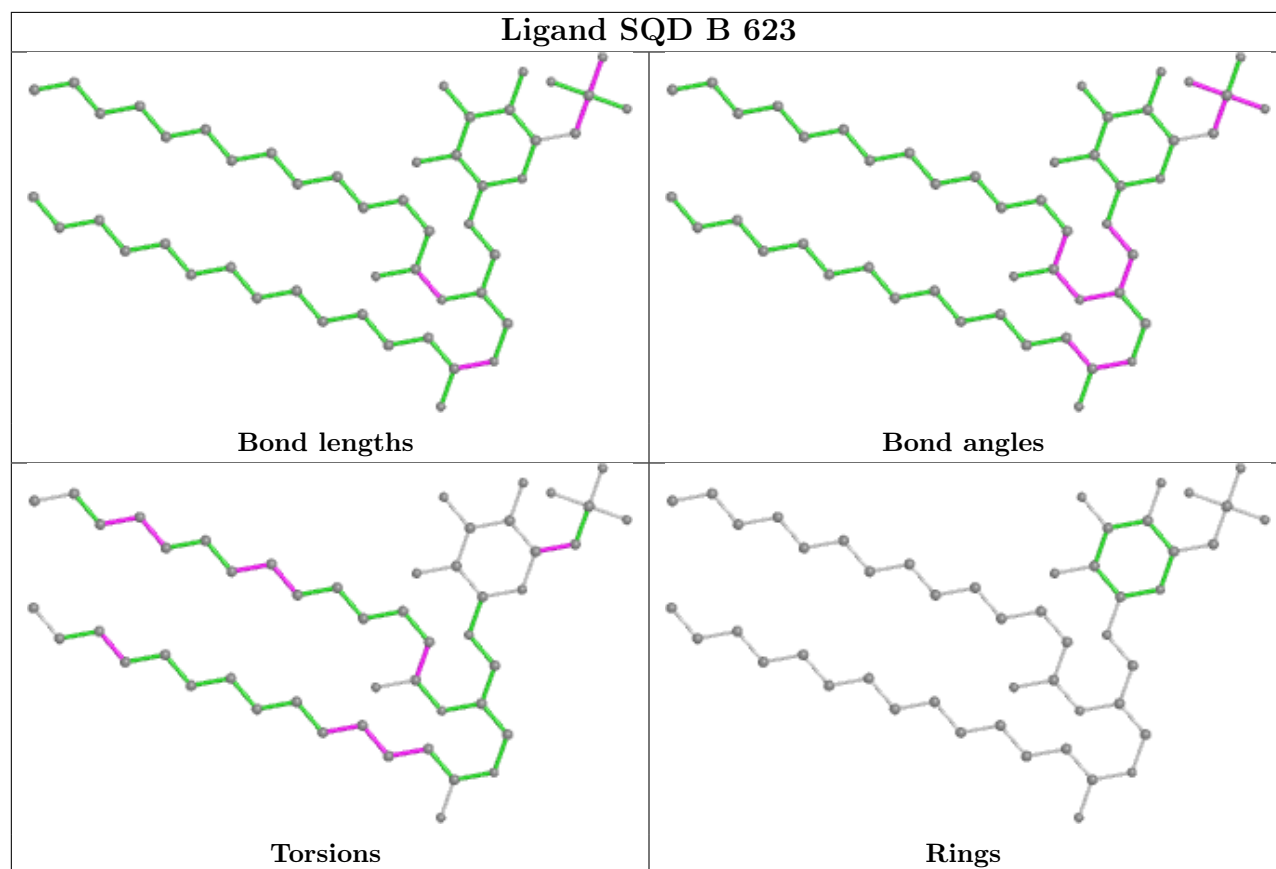
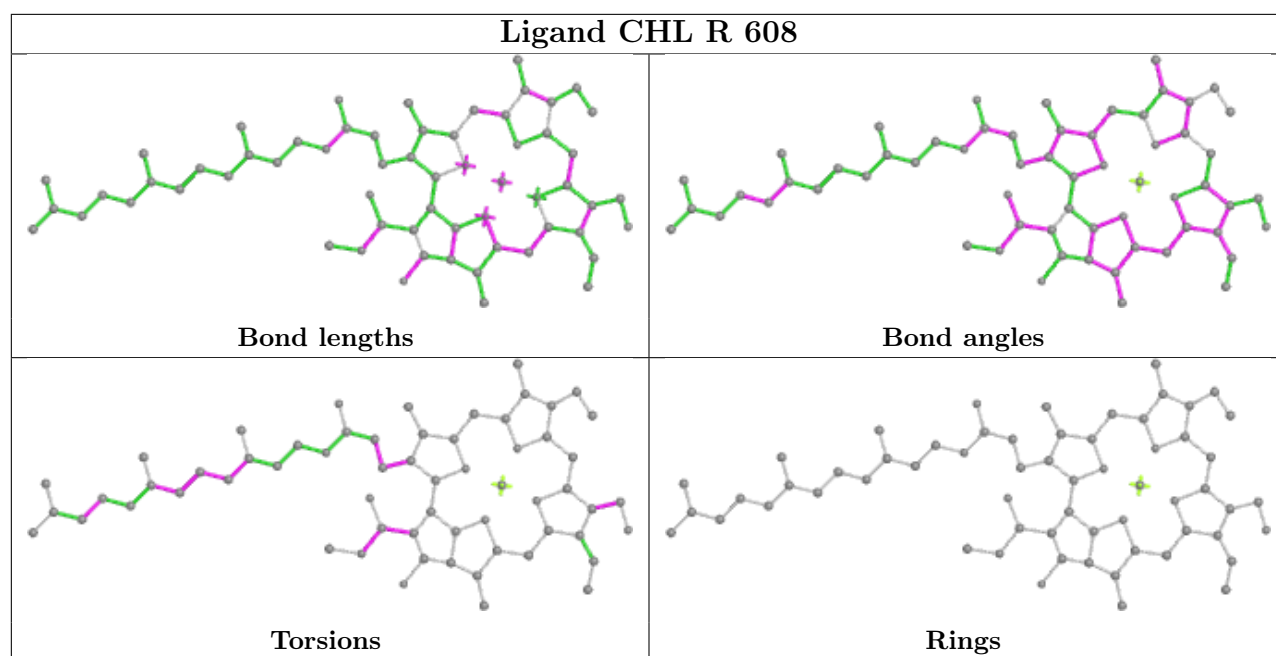


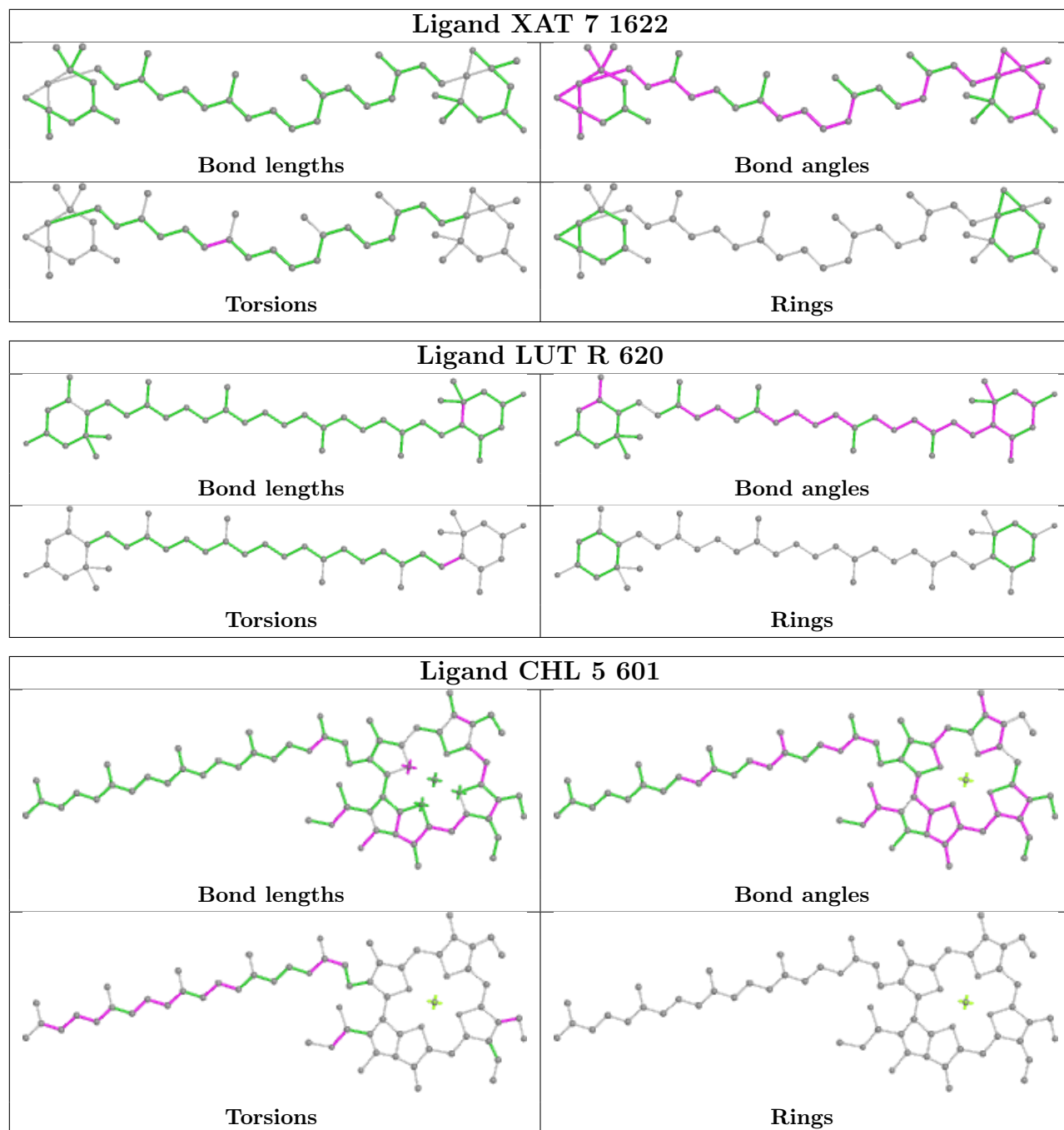
Ligand CLA 2 603



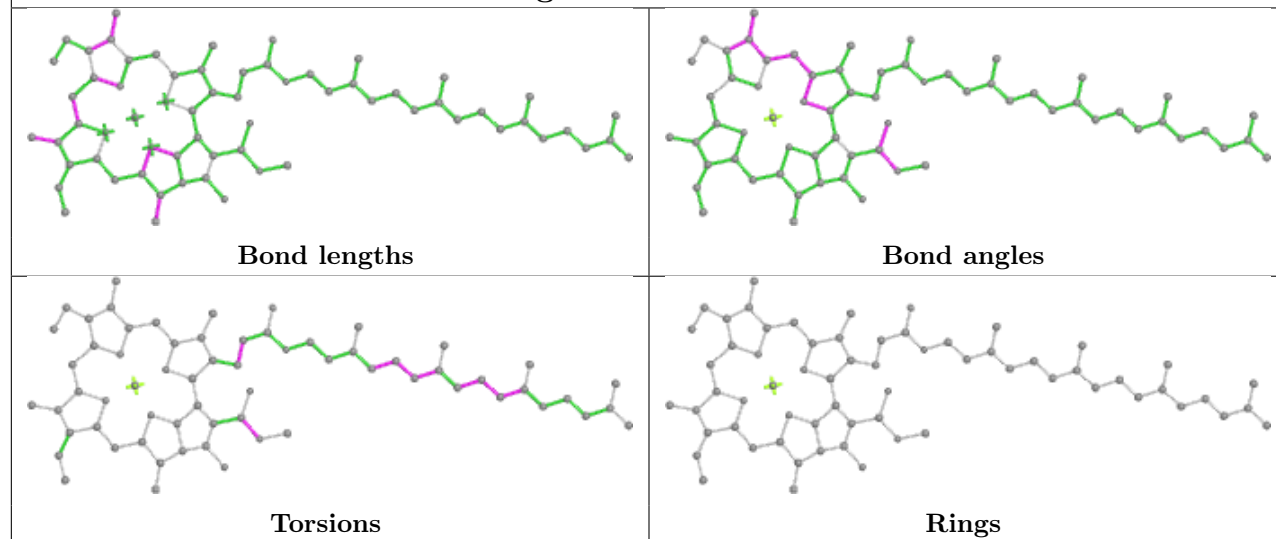
Ligand CLA 9 602



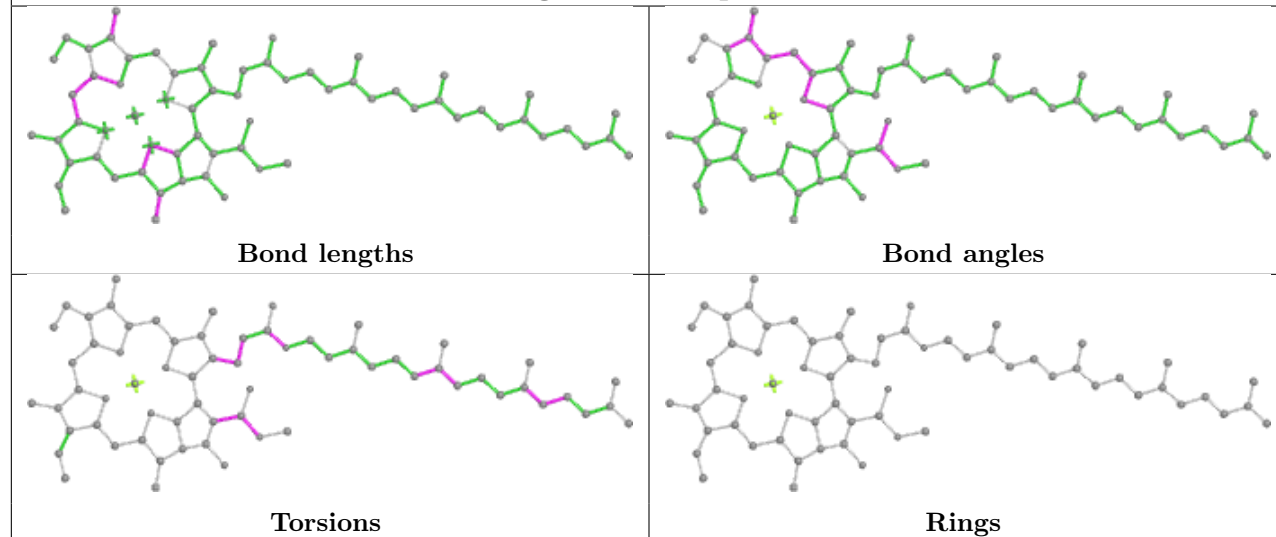




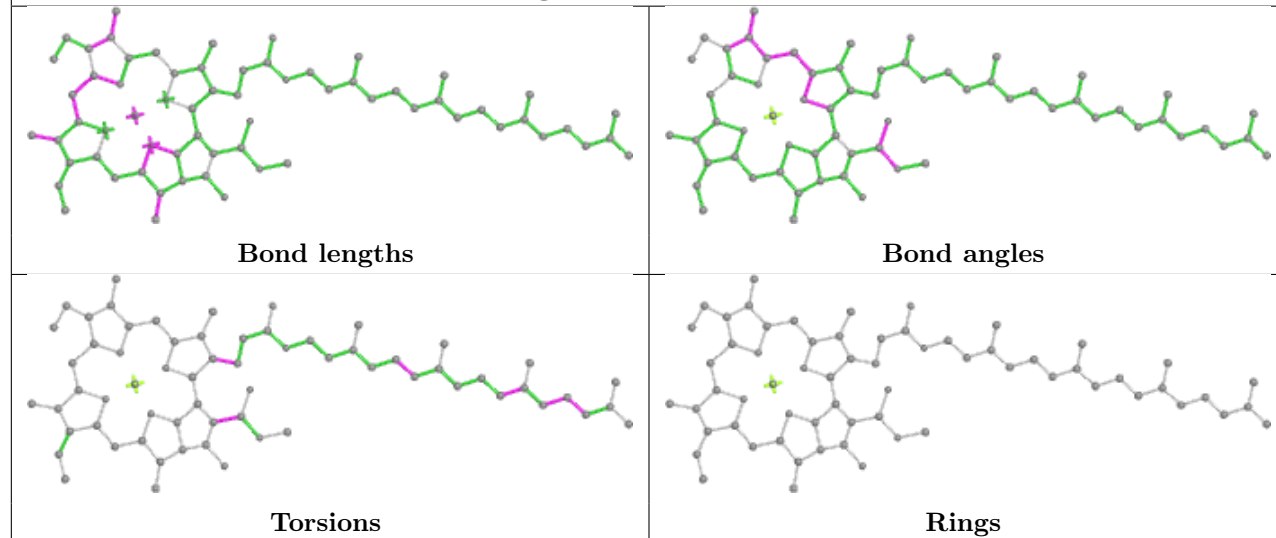
Ligand CLA 0 602

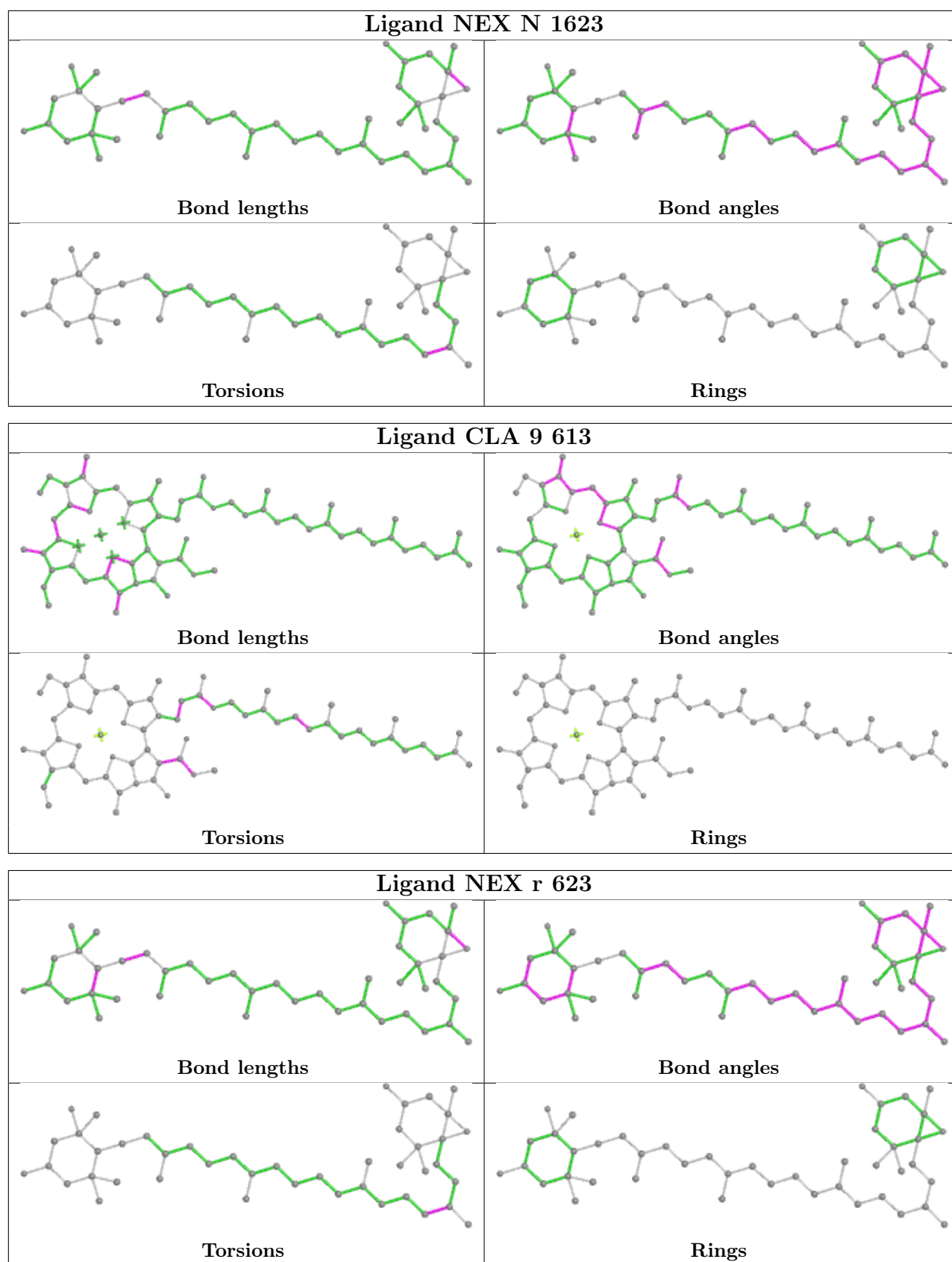


Ligand CLA q 613

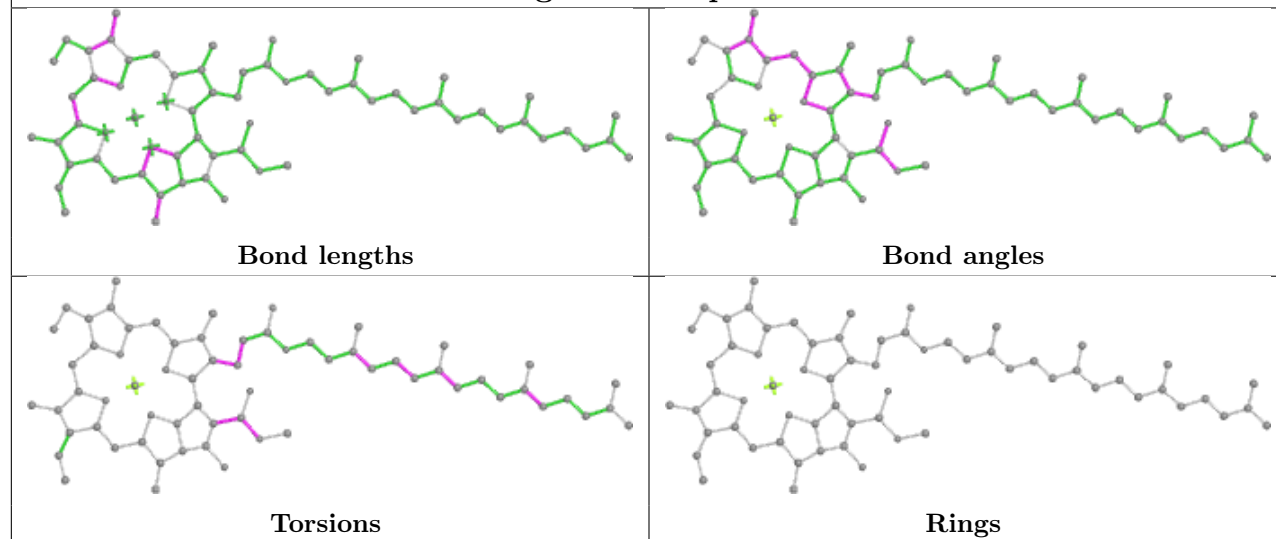


Ligand CLA b 610

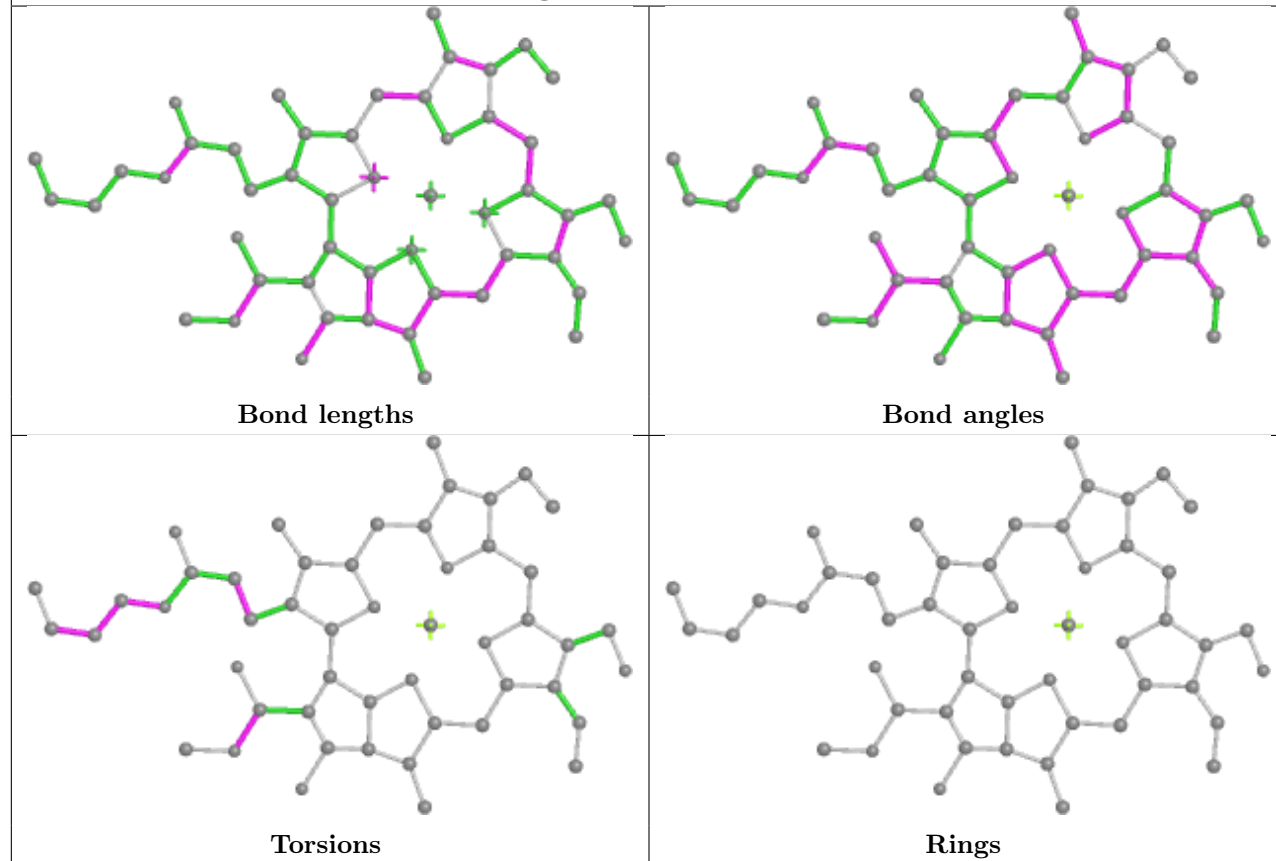


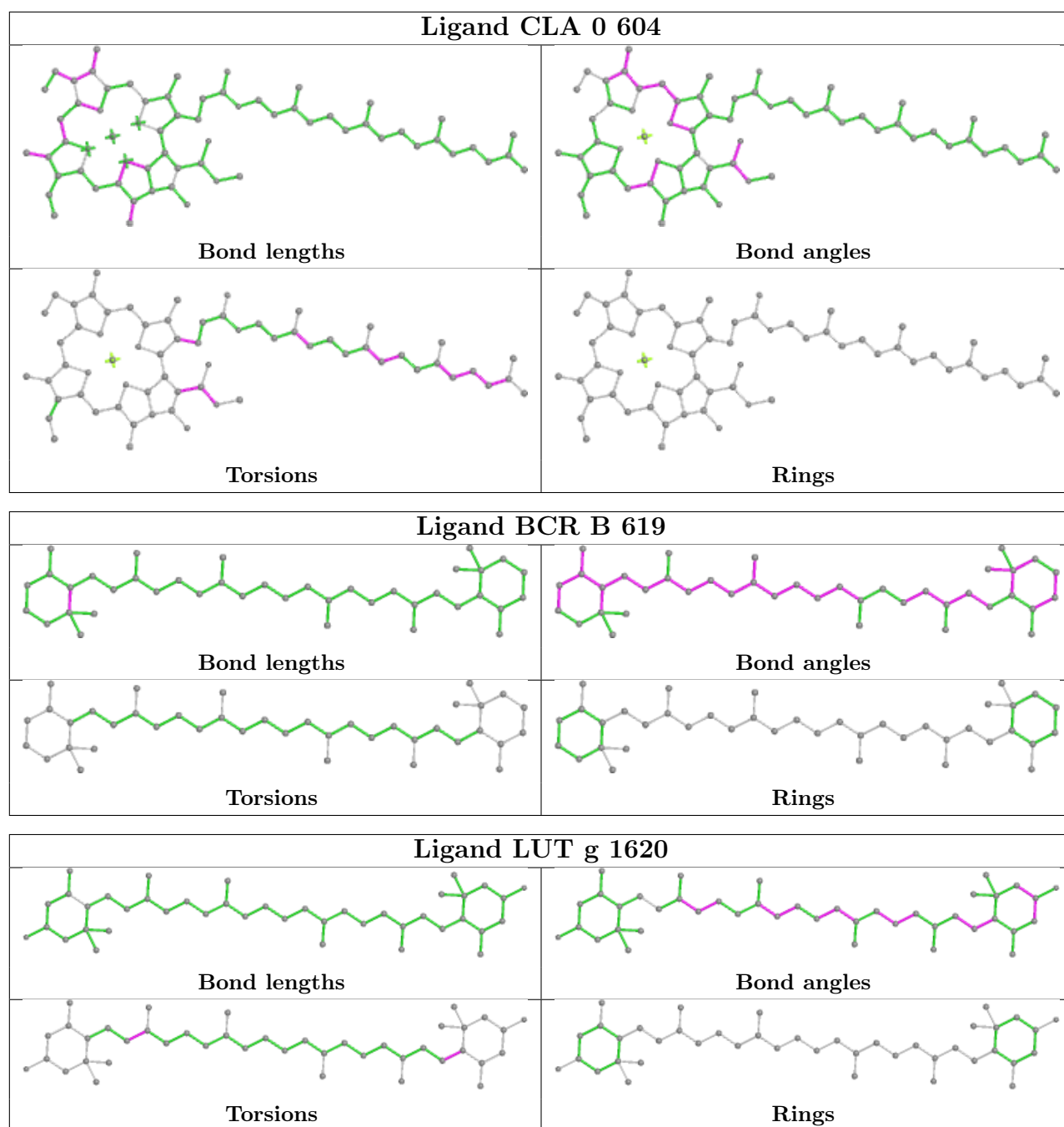


Ligand CLA p 603

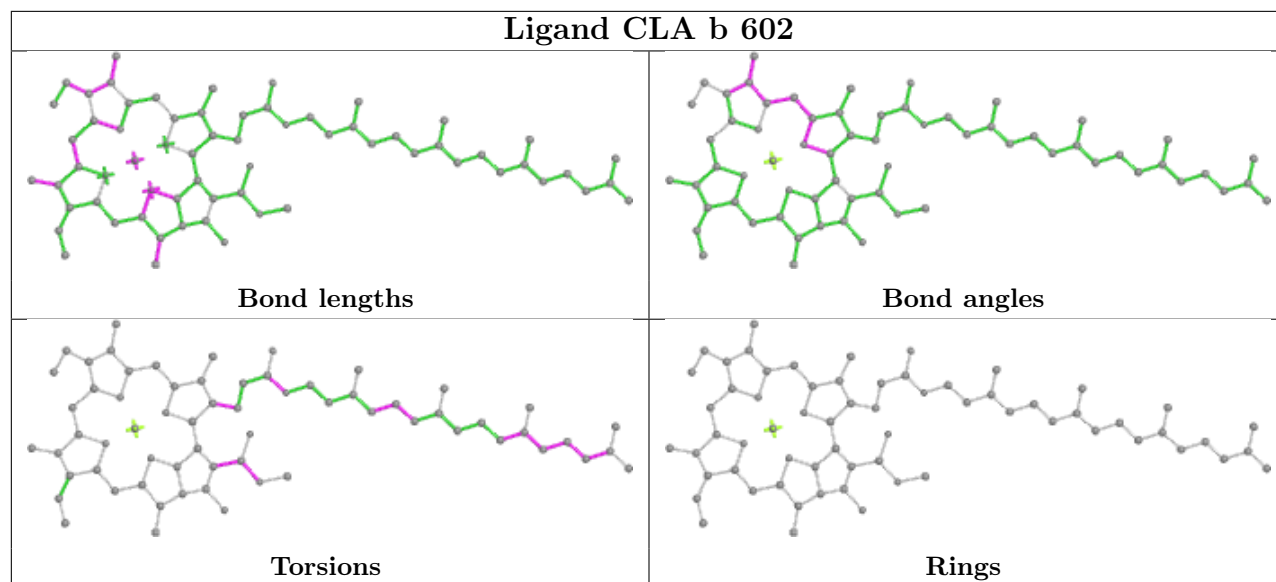


Ligand CHL 0 608

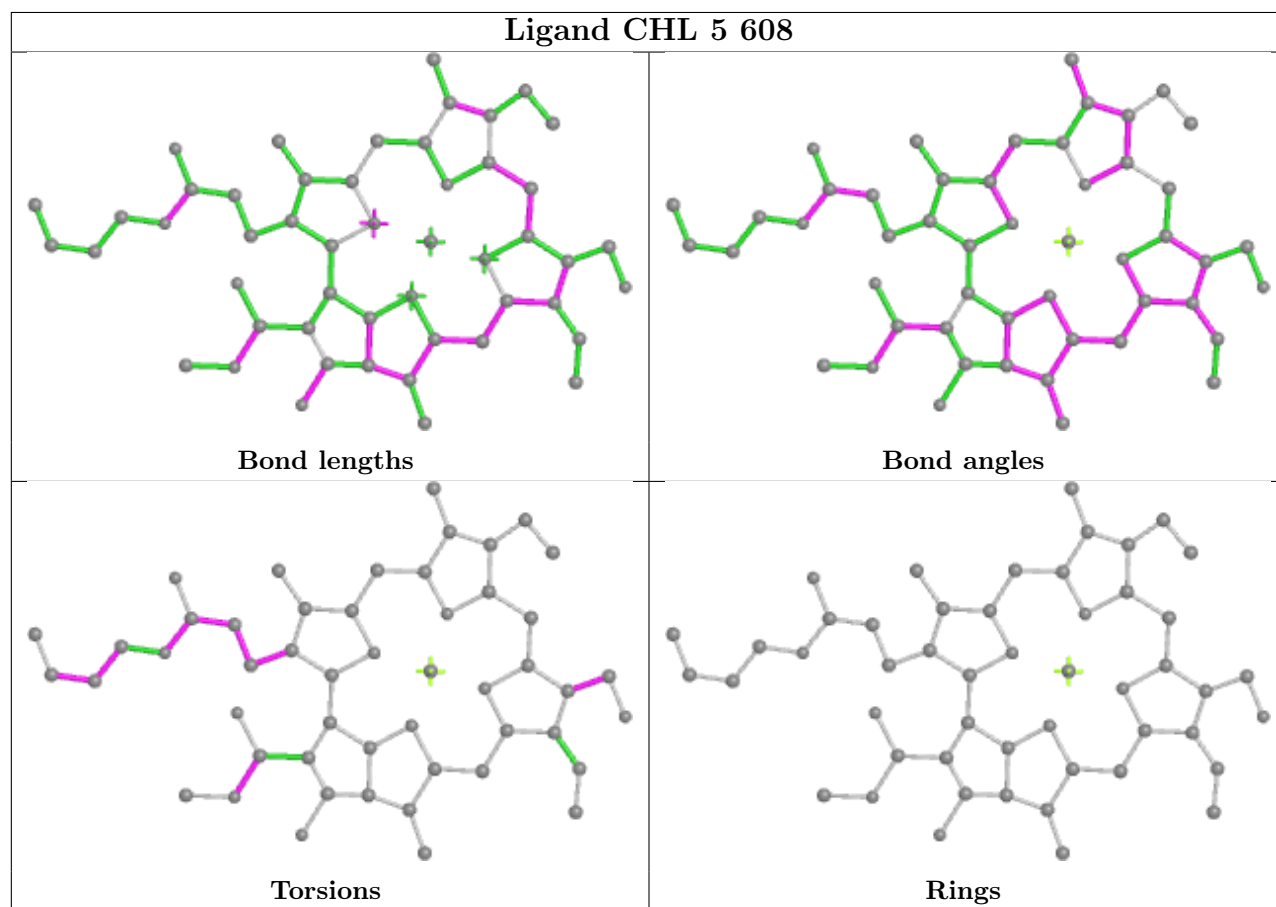


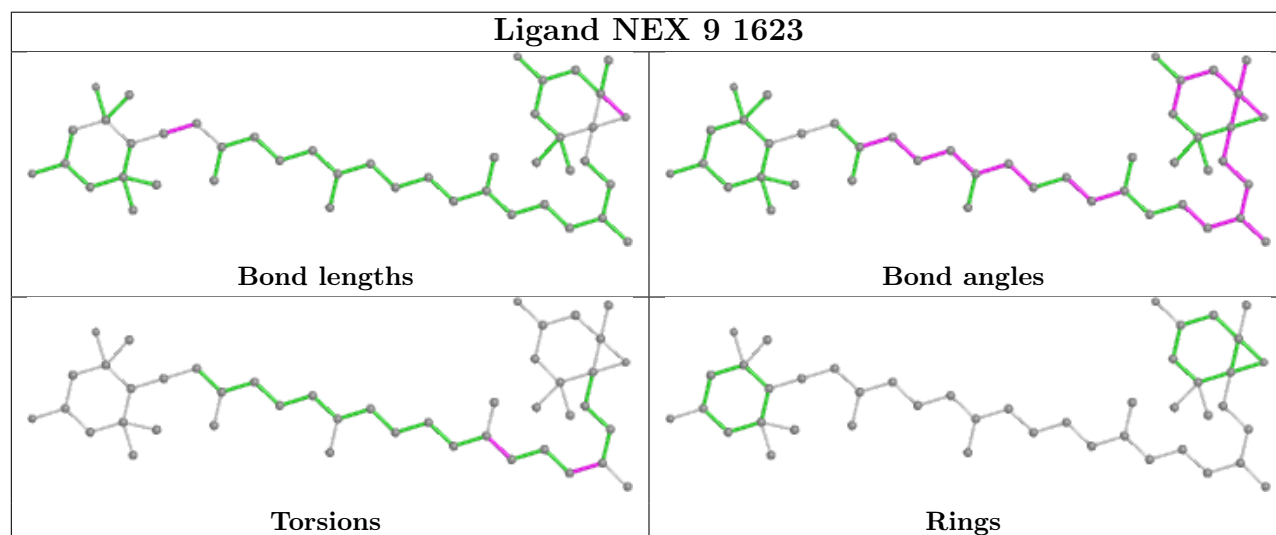
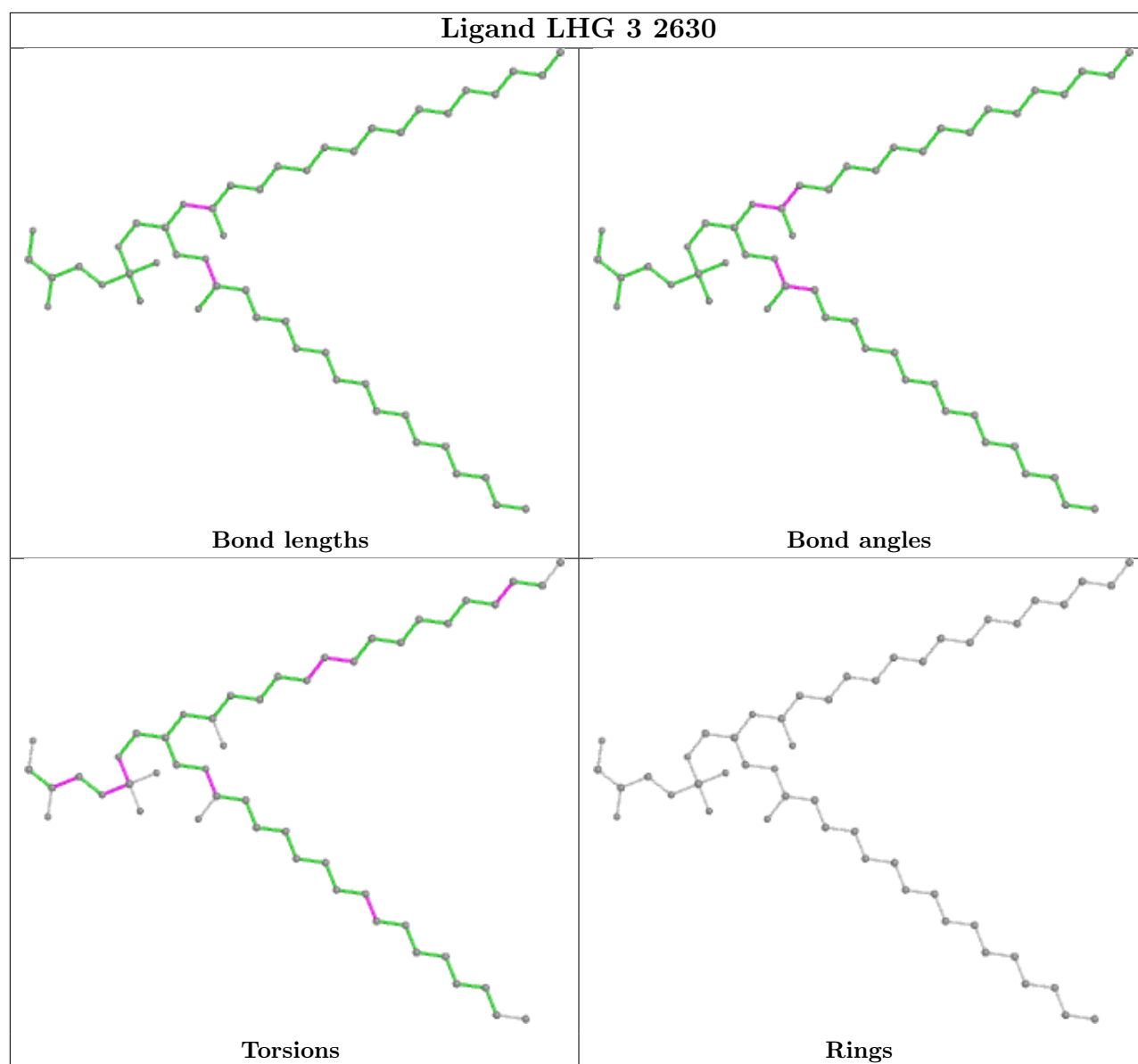


Ligand CLA b 602

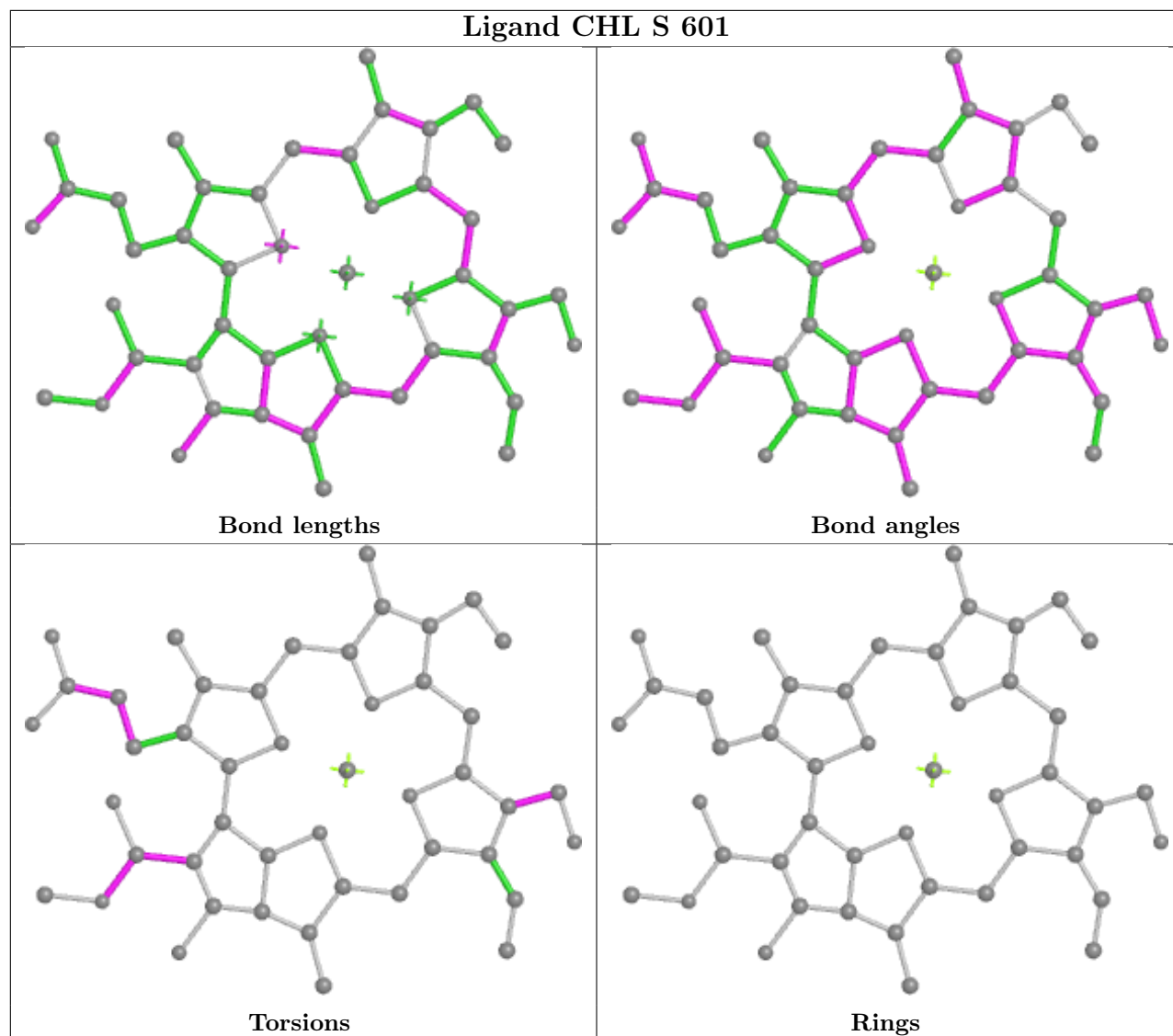


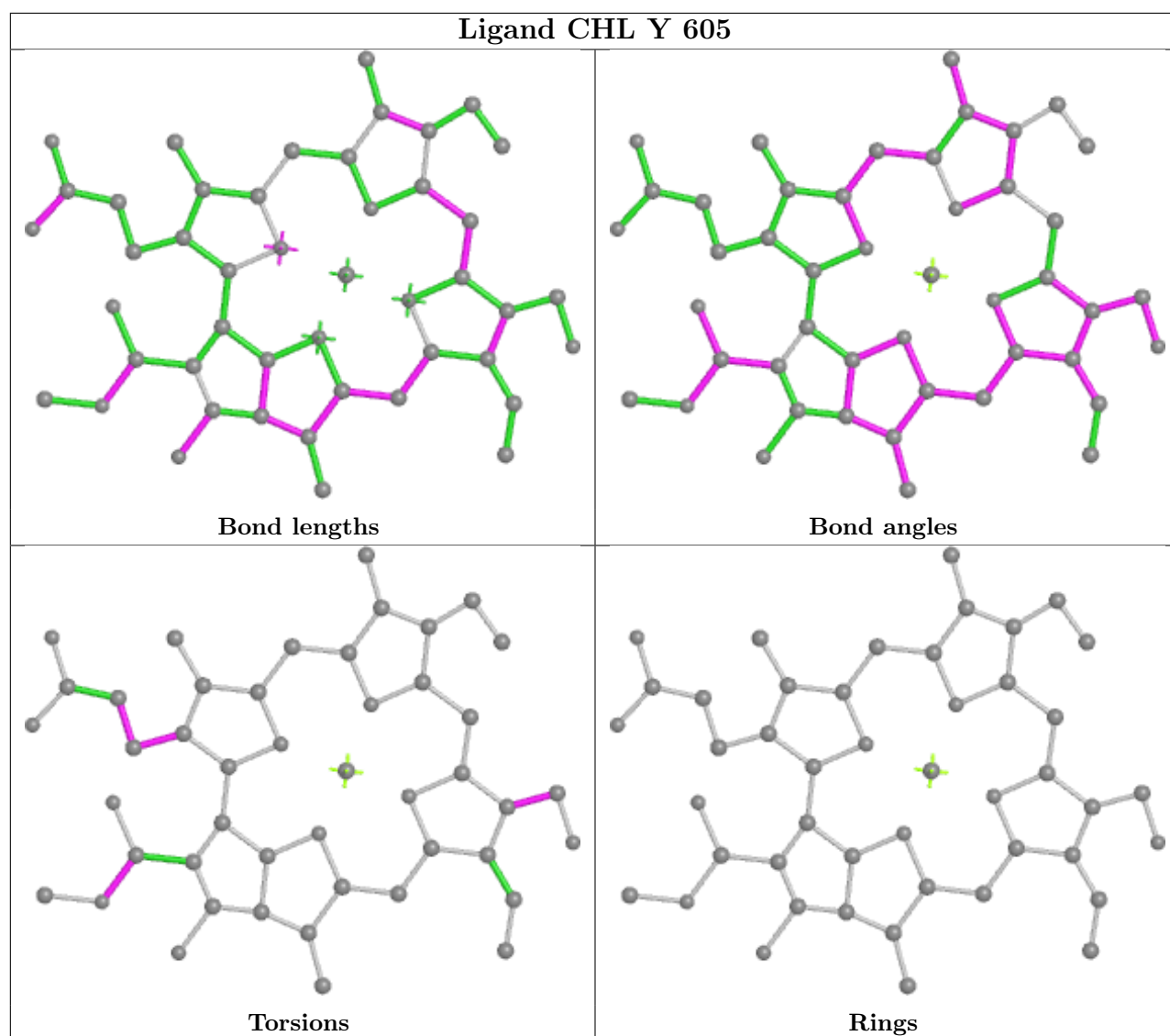
Ligand CHL 5 608

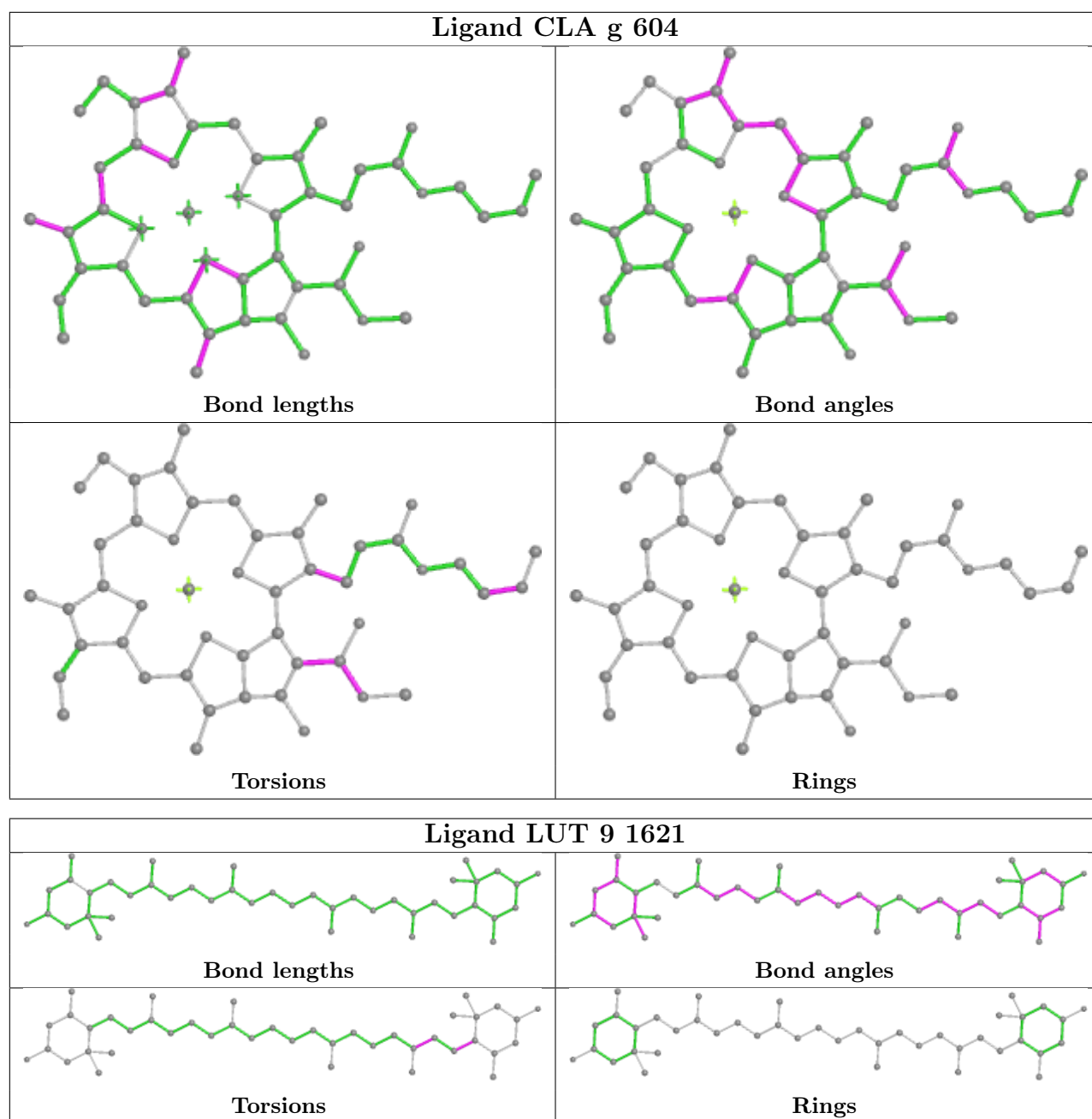


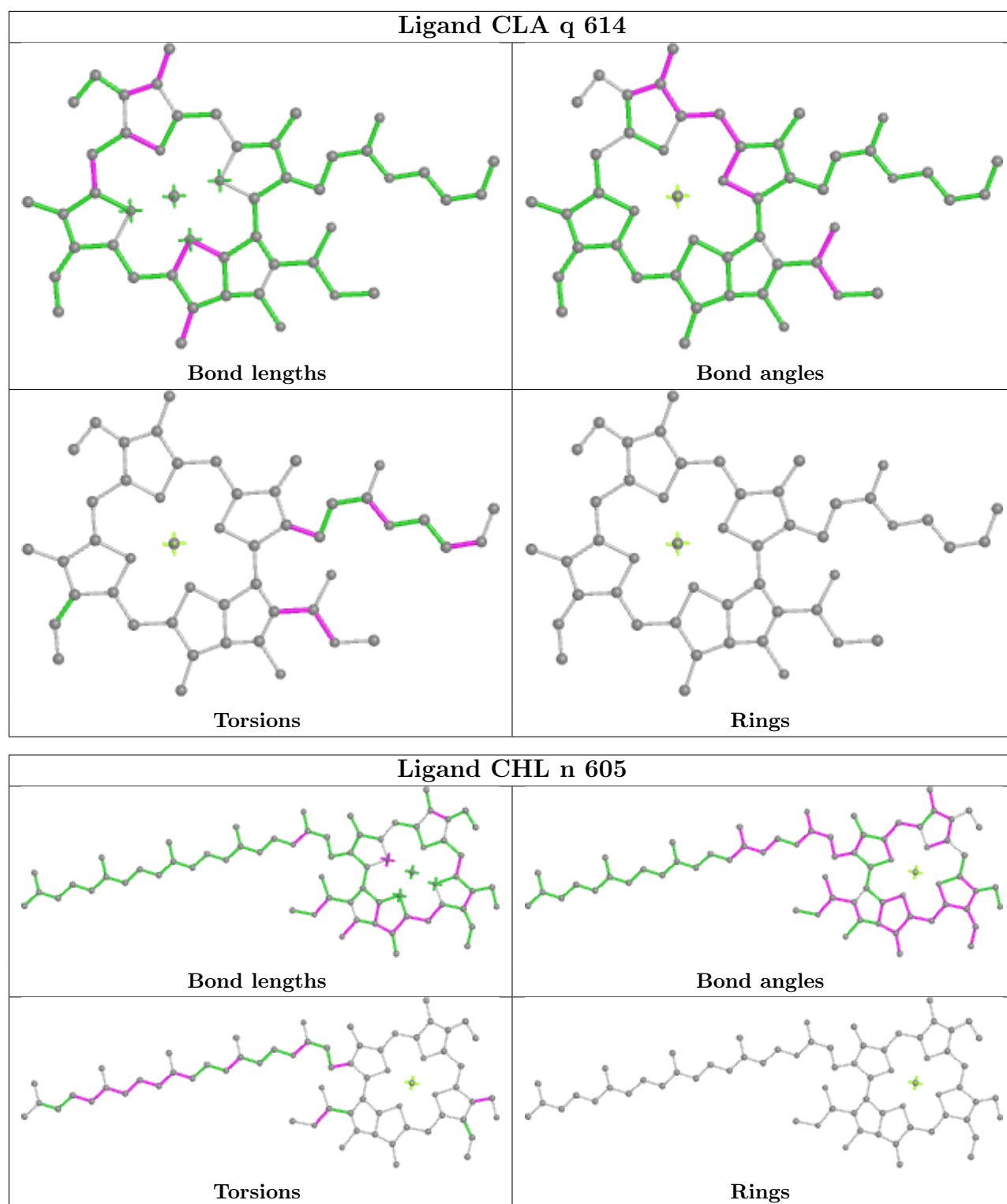


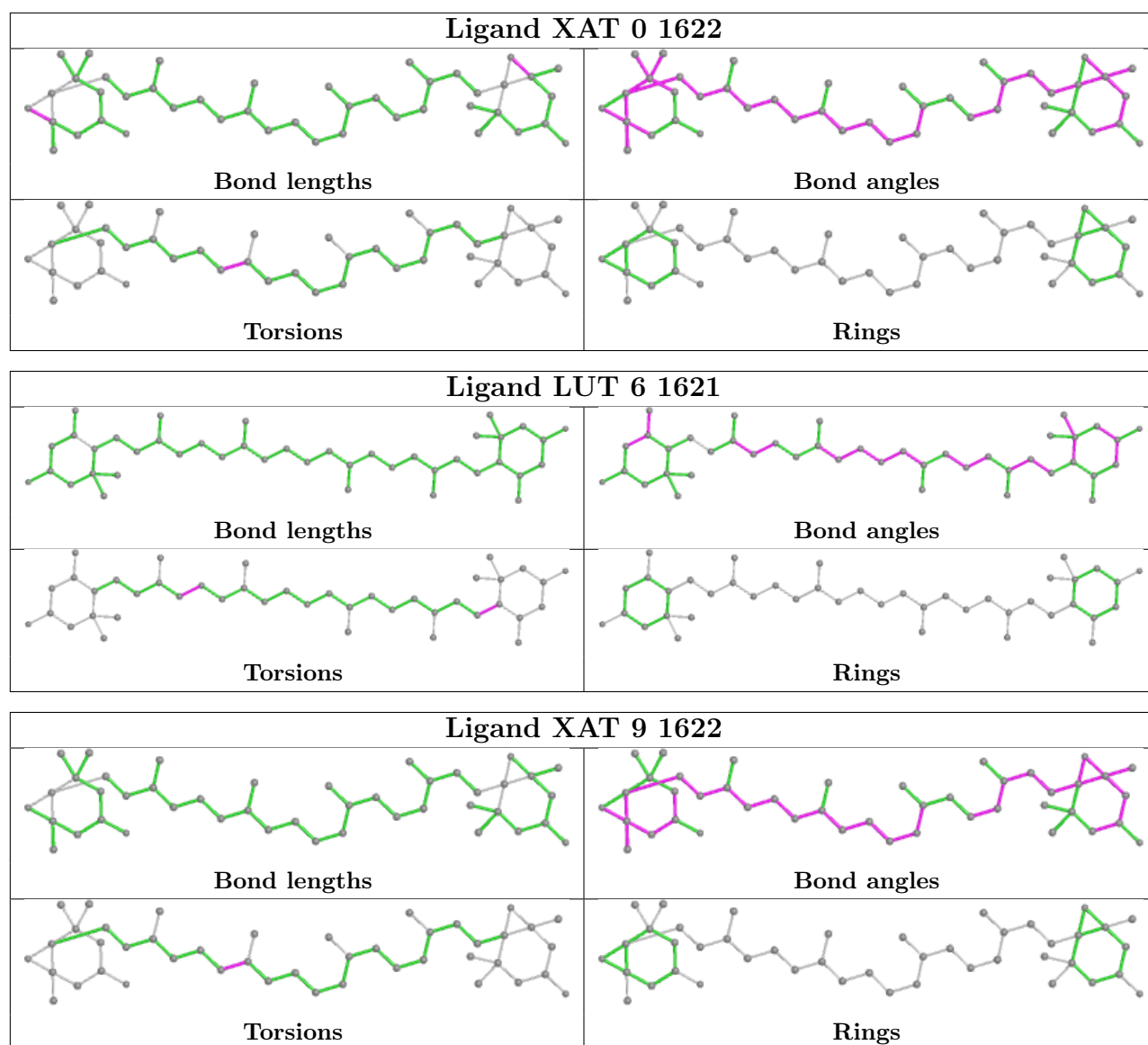
Ligand CHL S 601



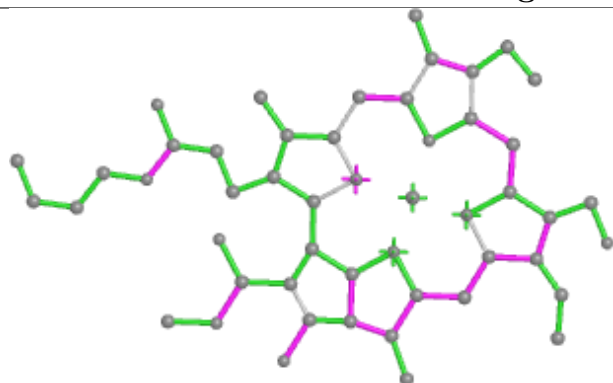




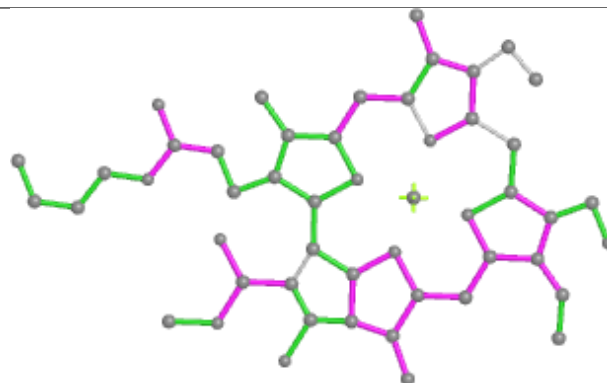




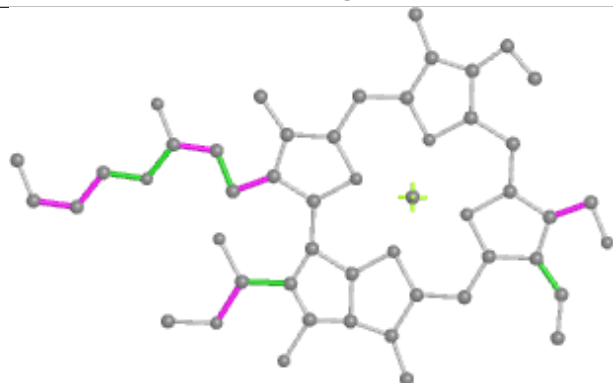
Ligand CHL 2 606



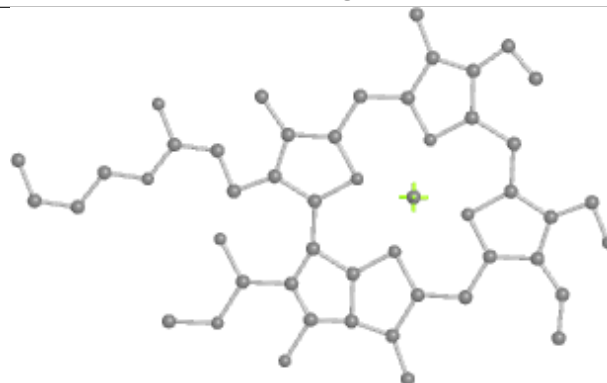
Bond lengths



Bond angles

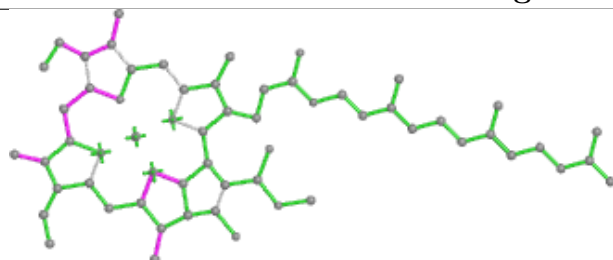


Torsions

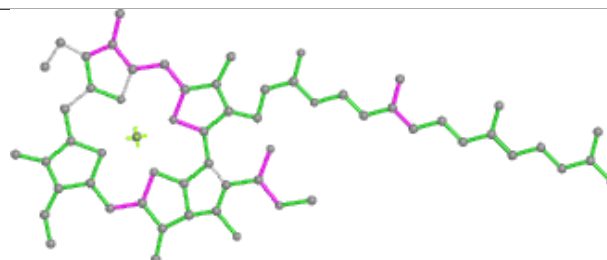


Rings

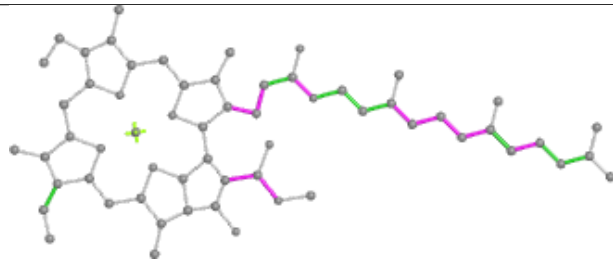
Ligand CLA R 613



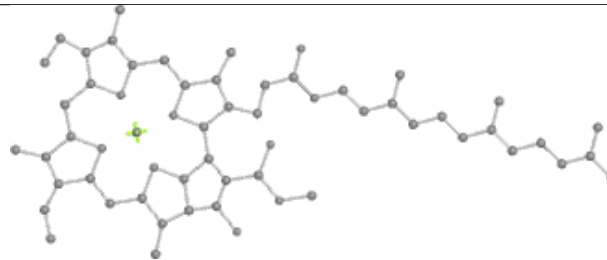
Bond lengths



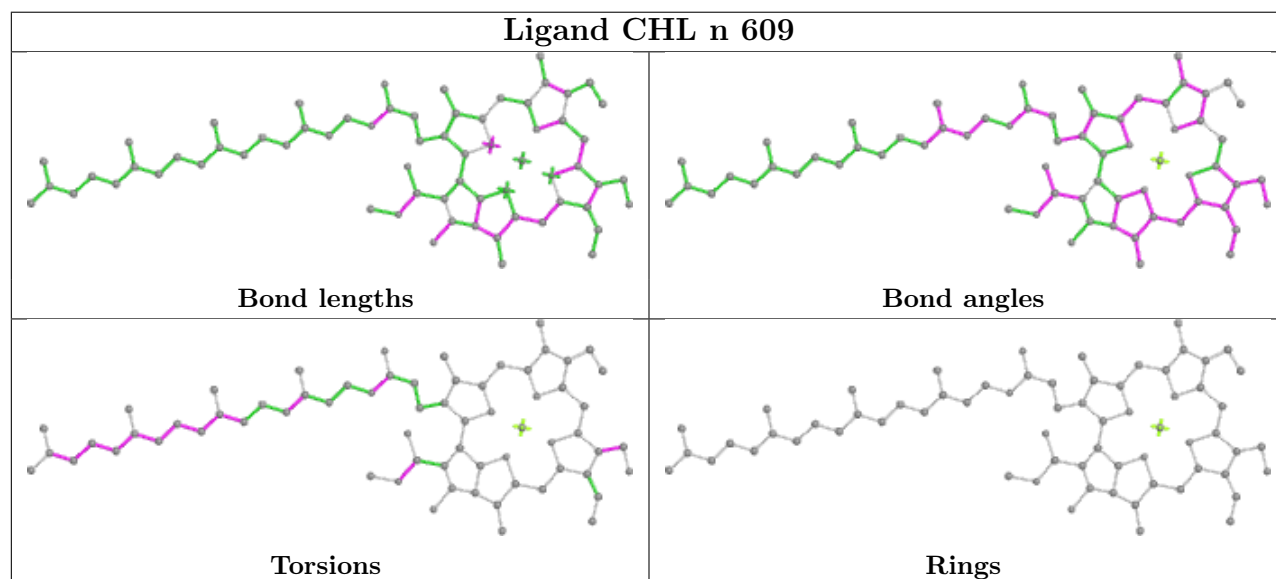
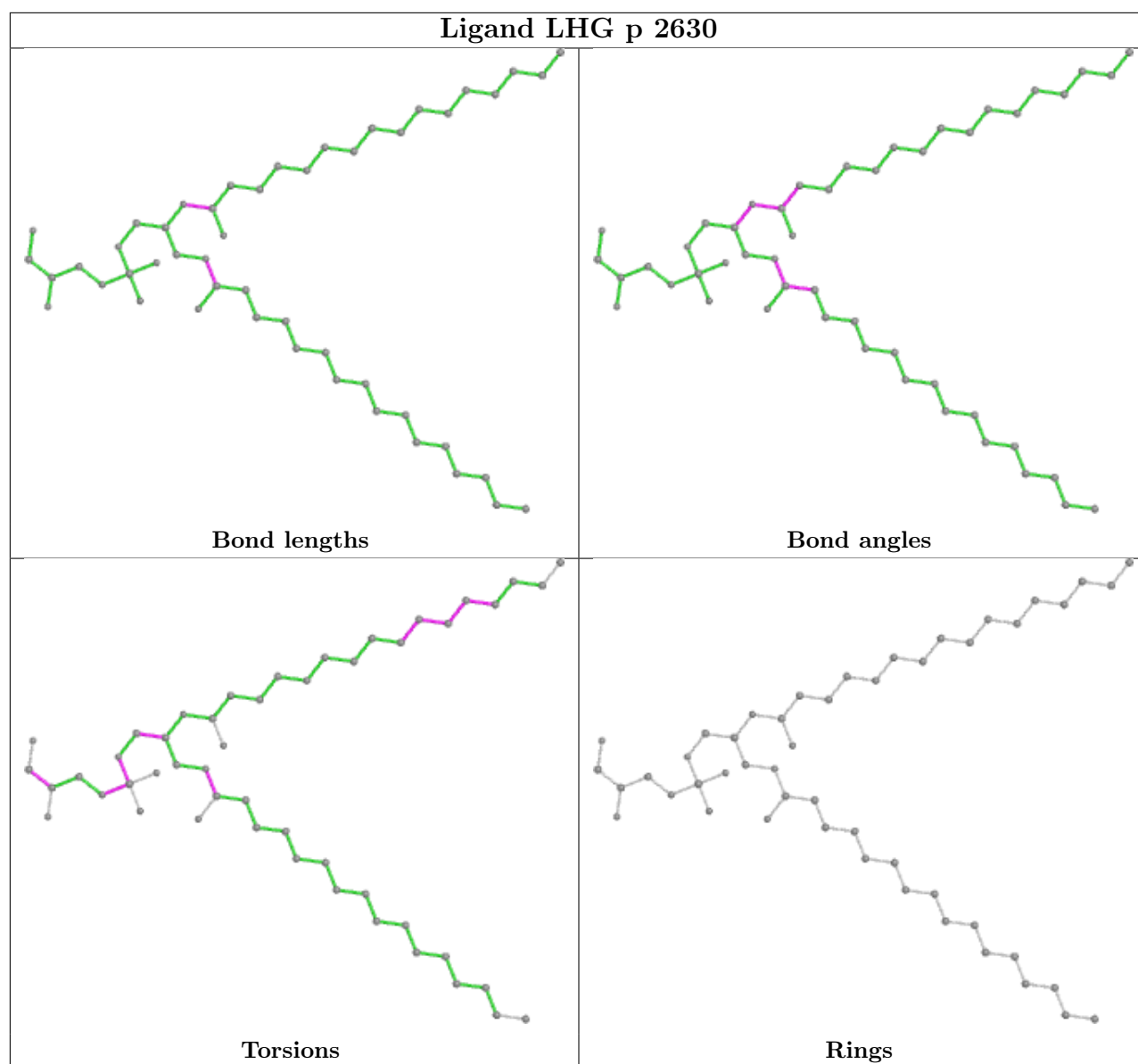
Bond angles

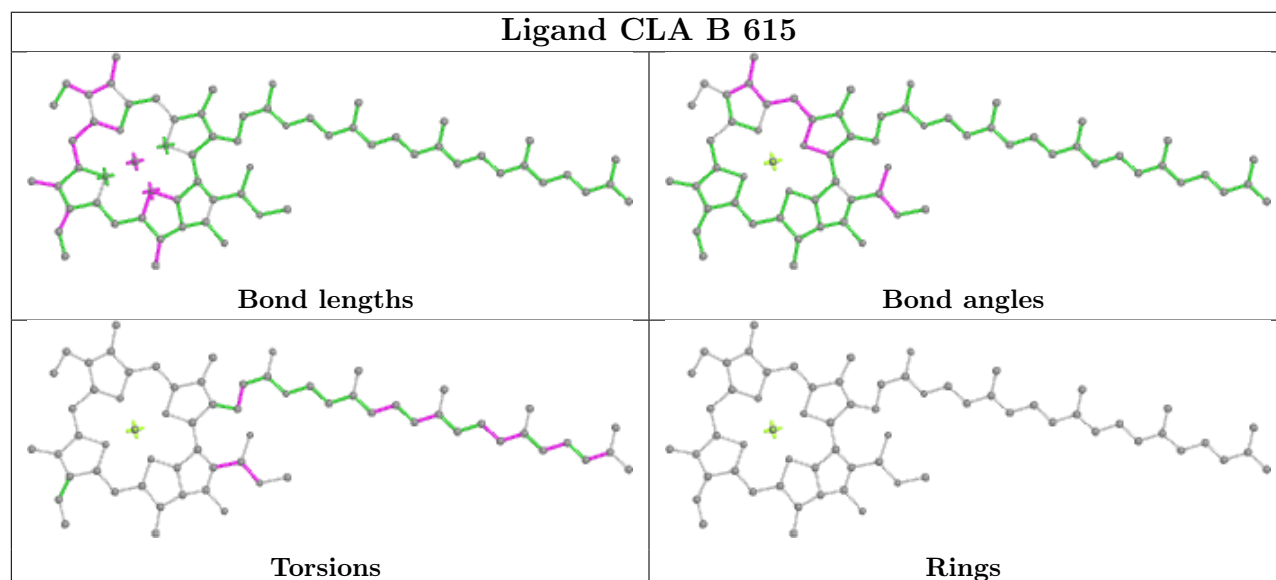
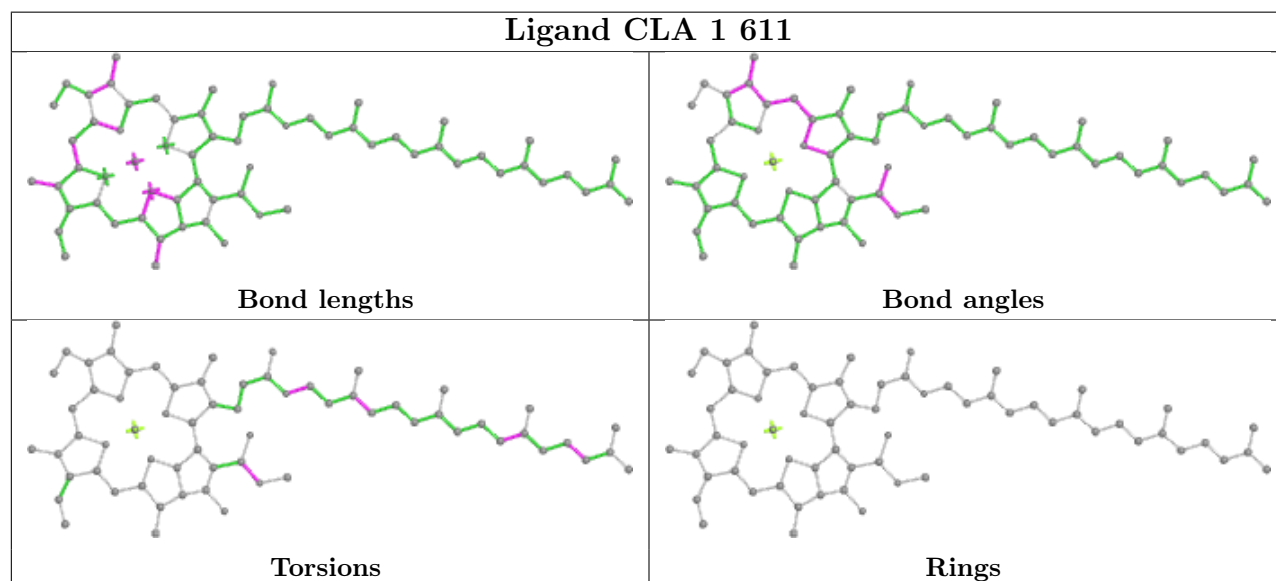
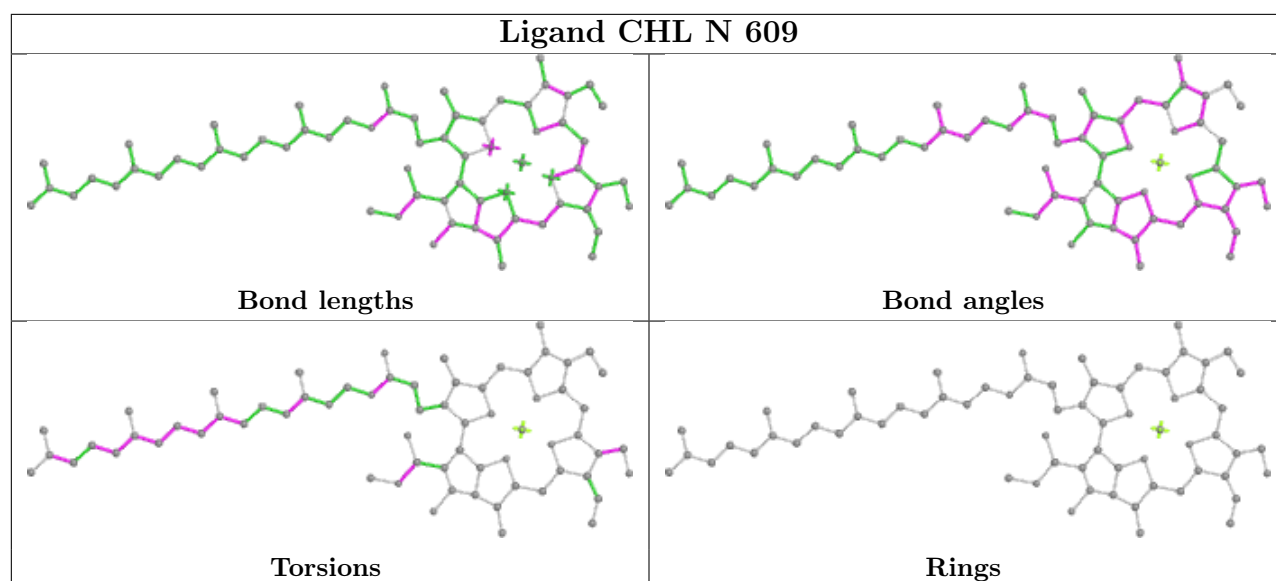


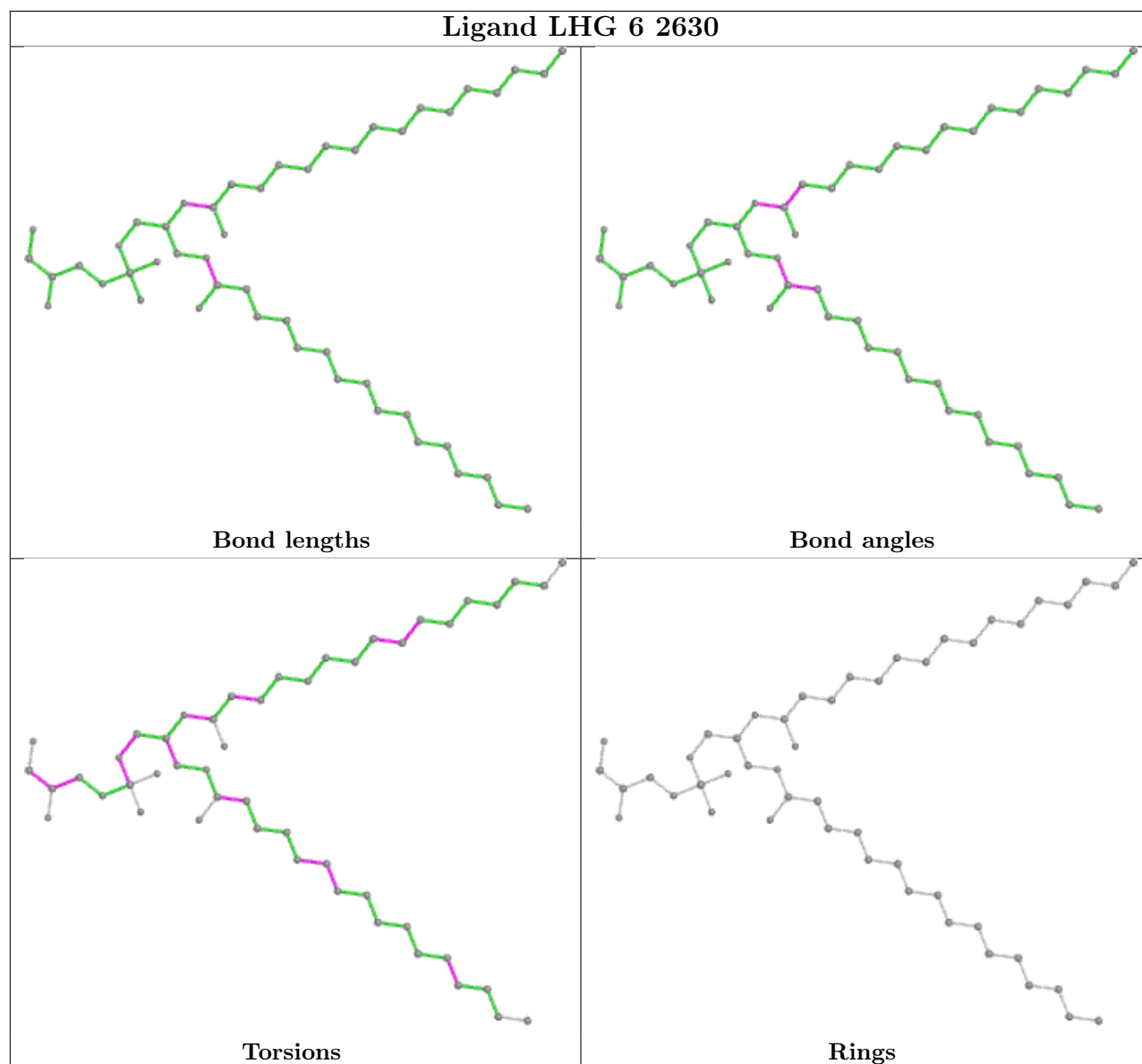
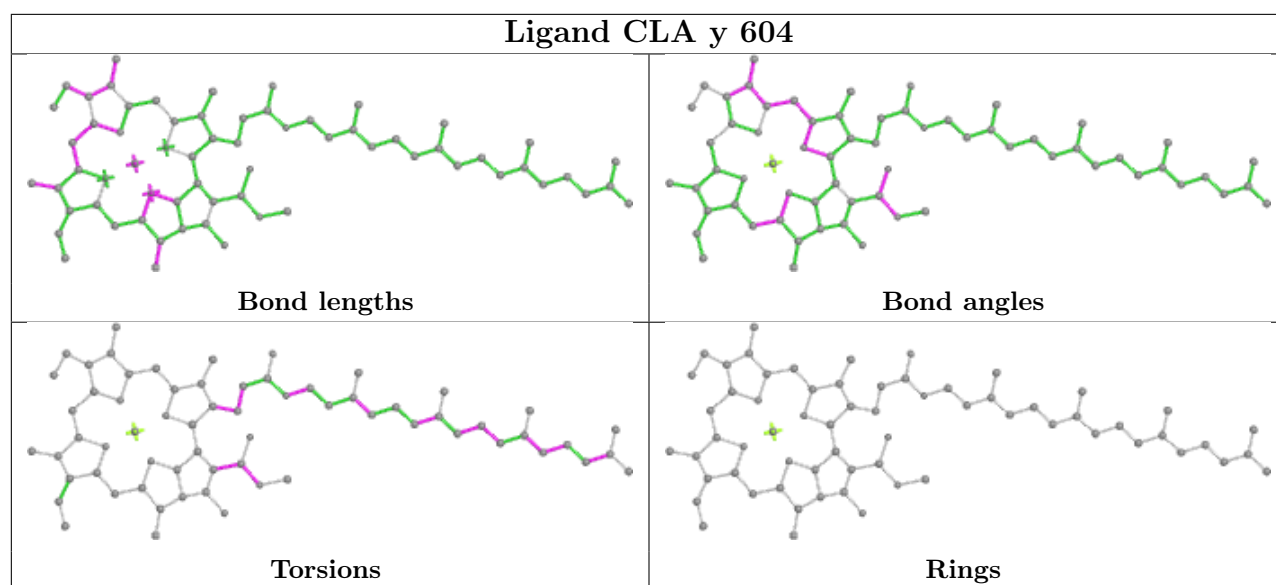
Torsions

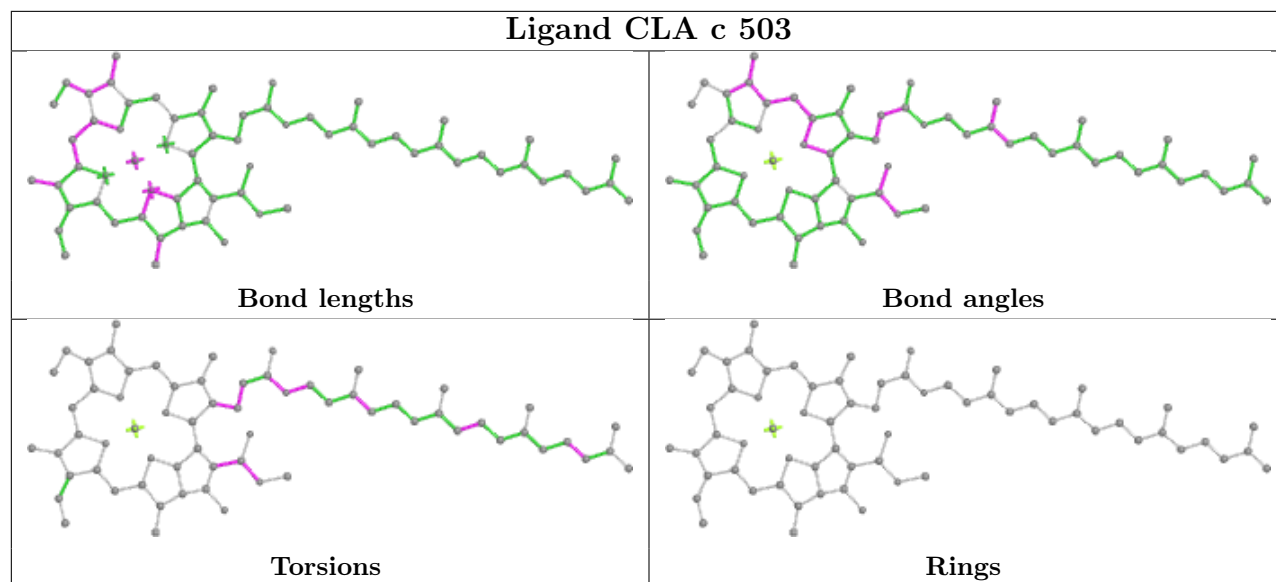
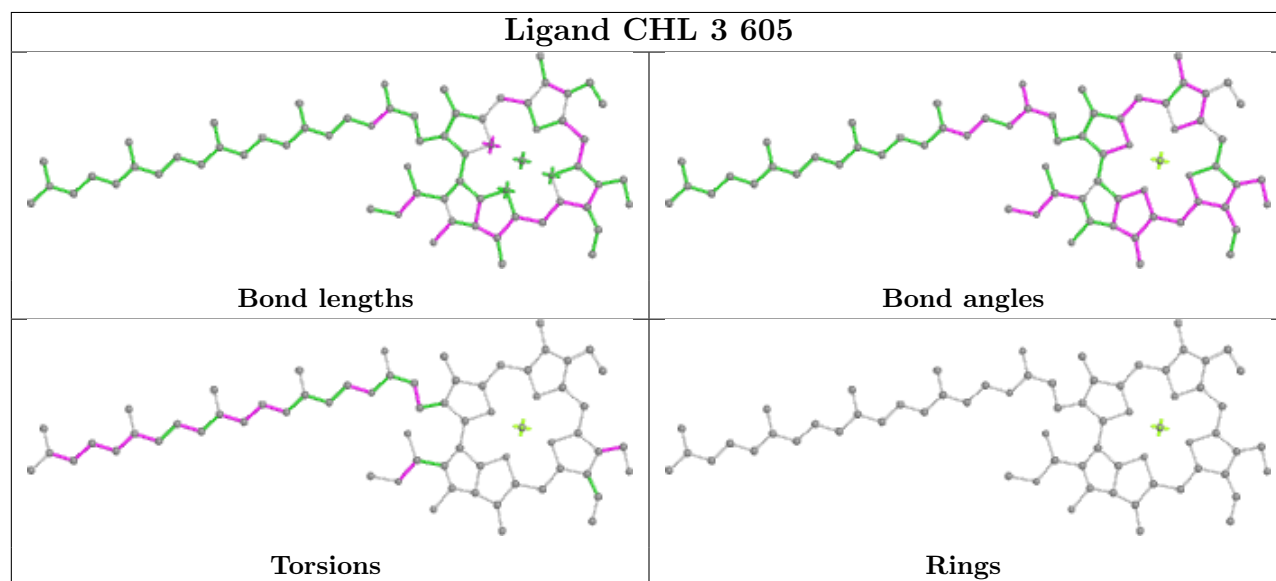


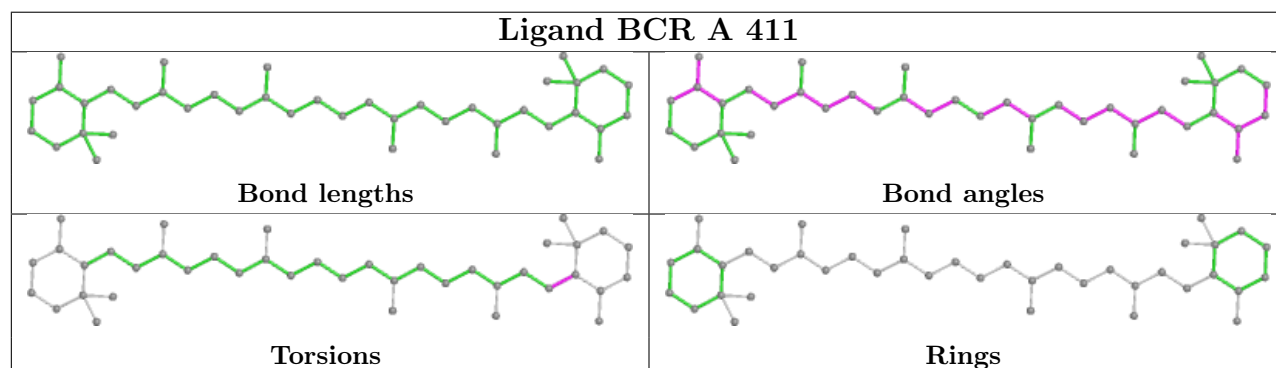
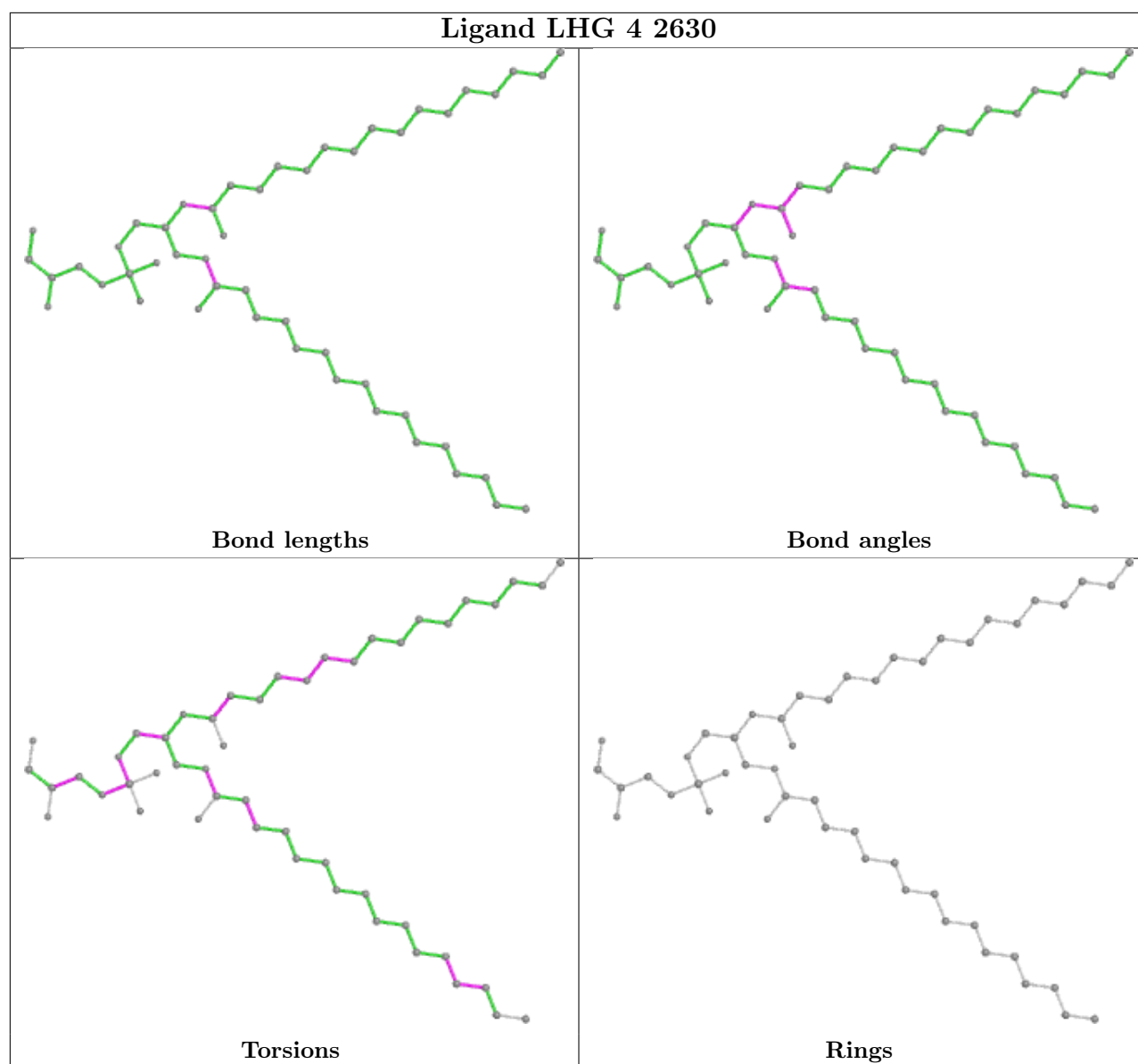
Rings

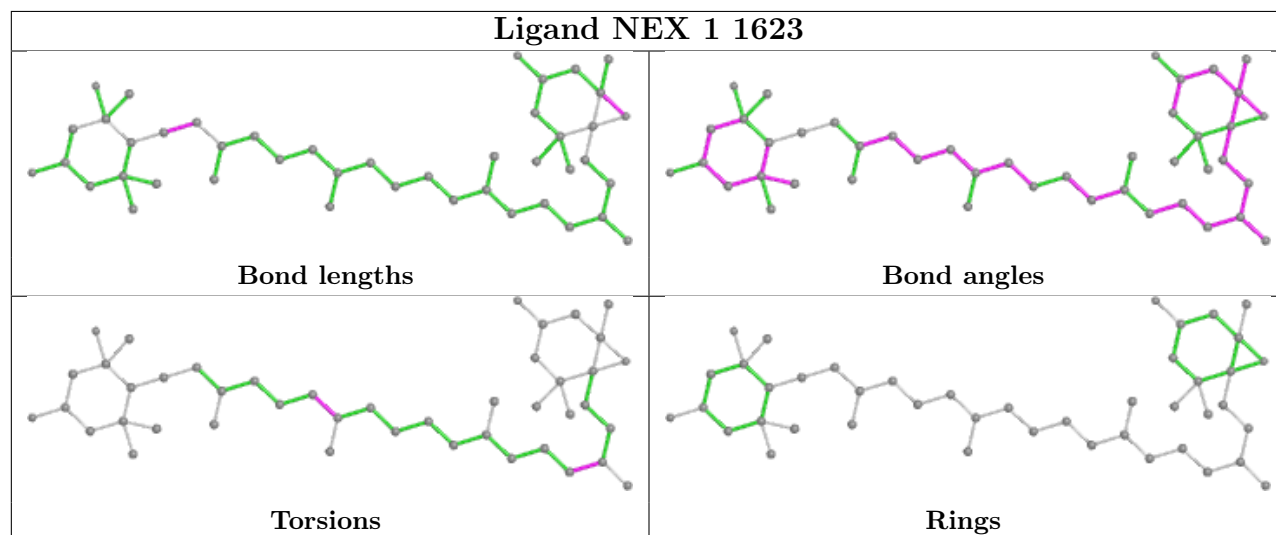
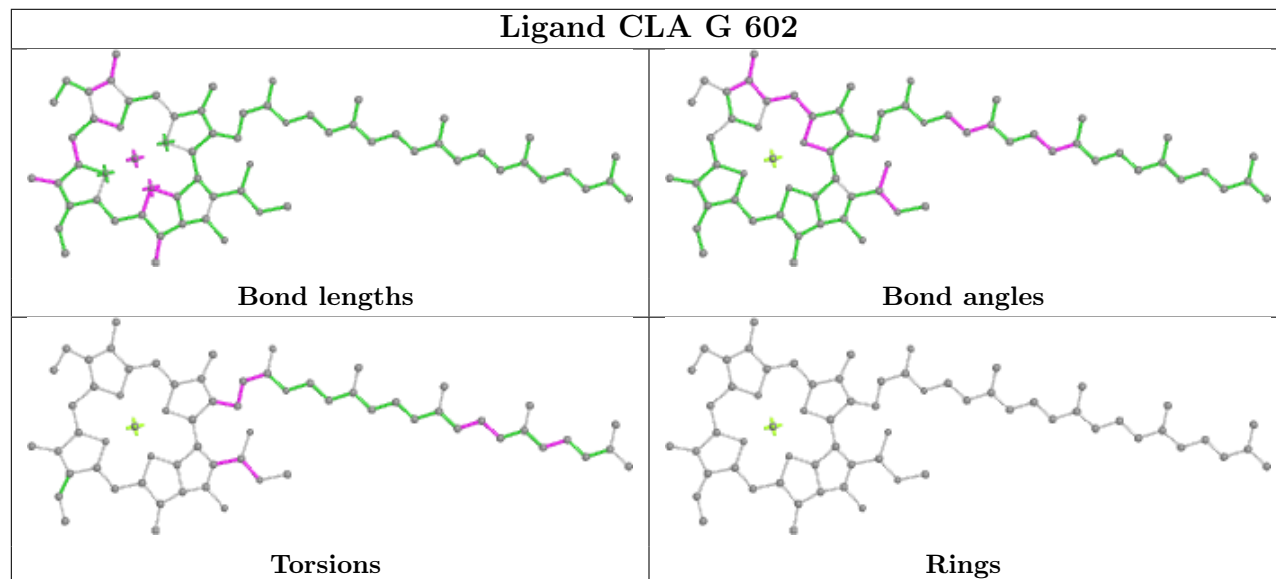
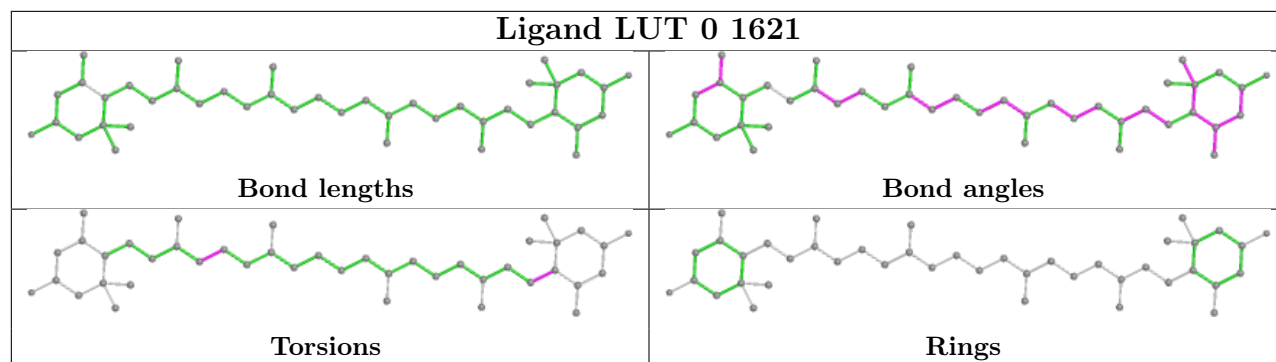




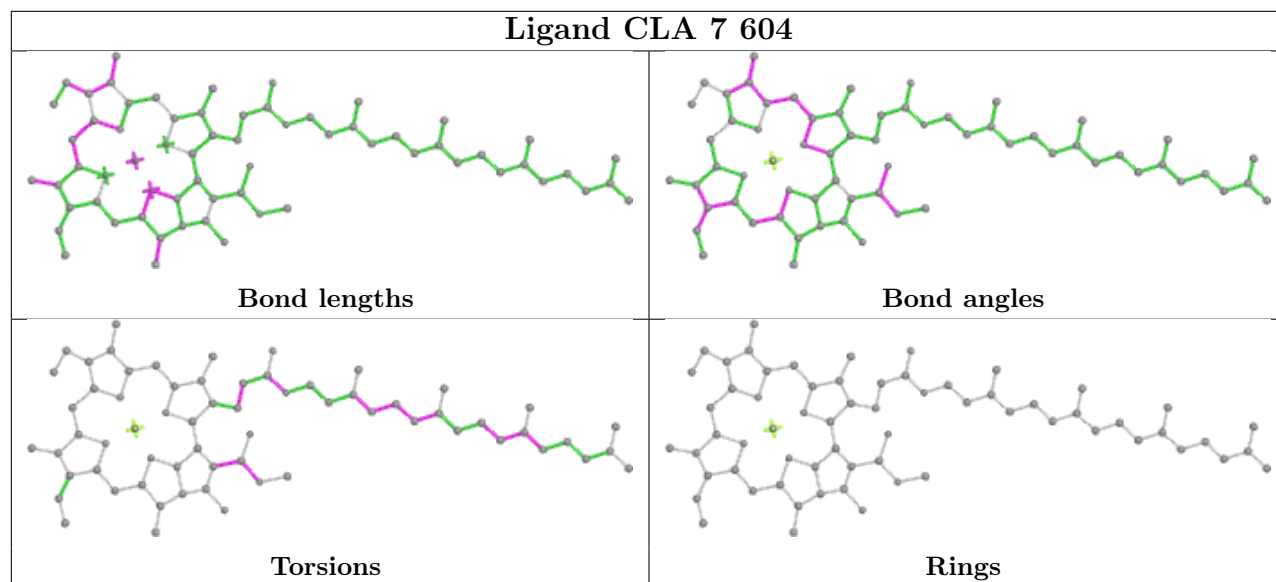


Ligand CLA c 503**Ligand CHL 3 605**

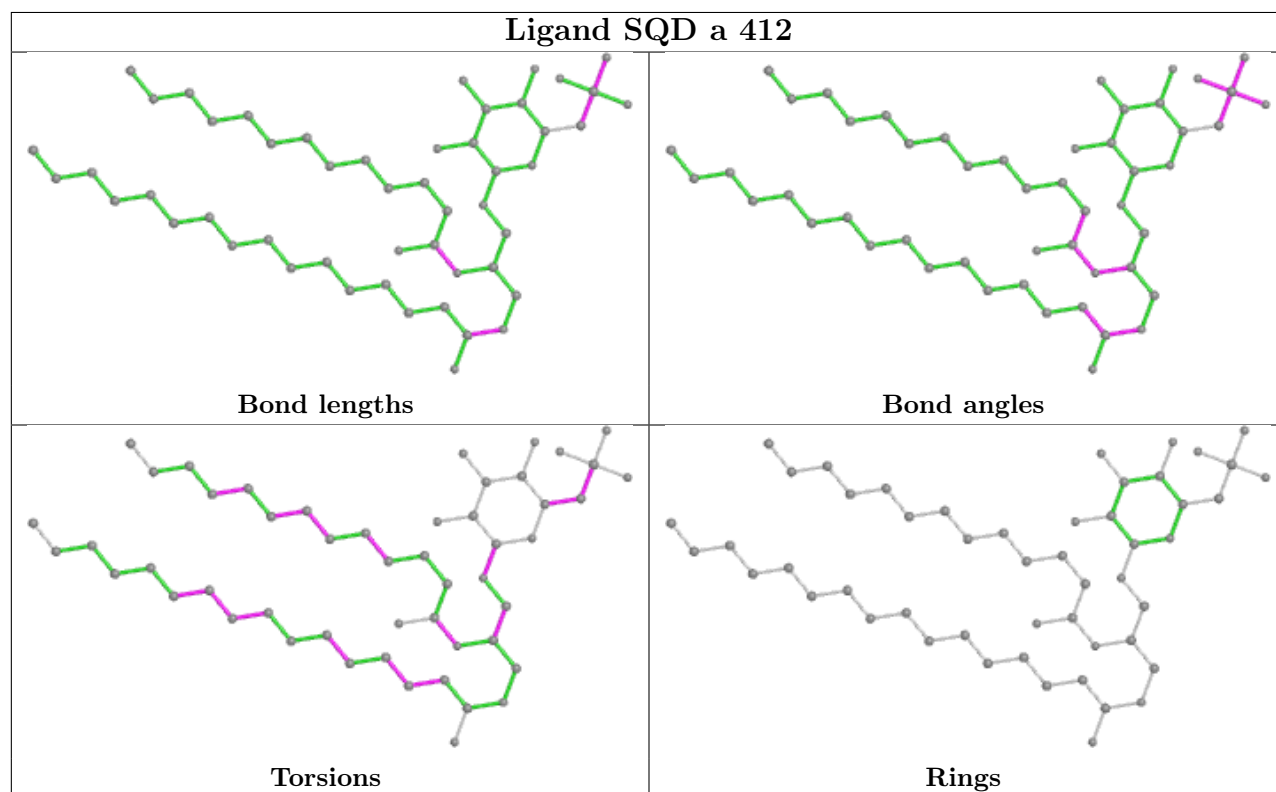


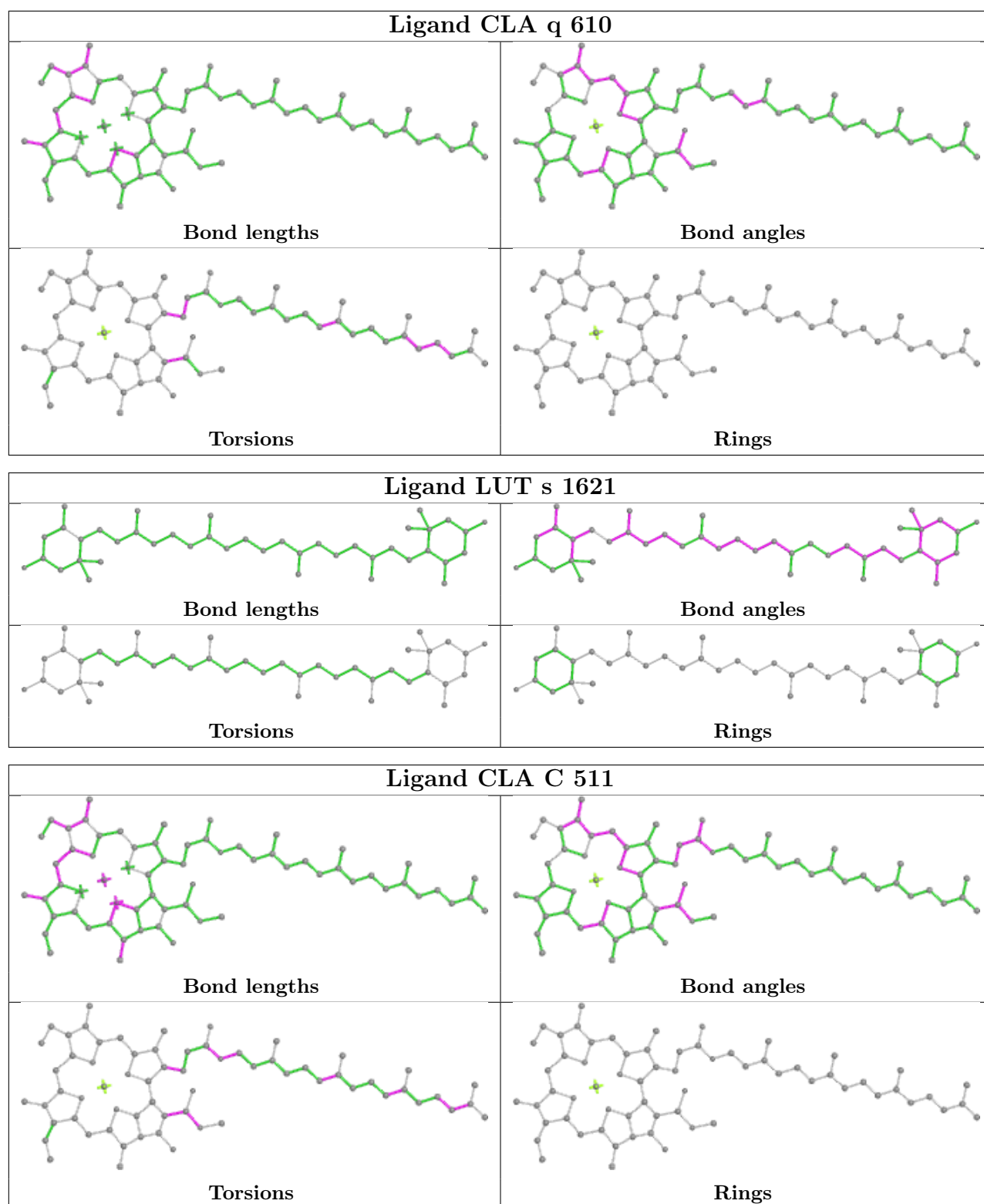


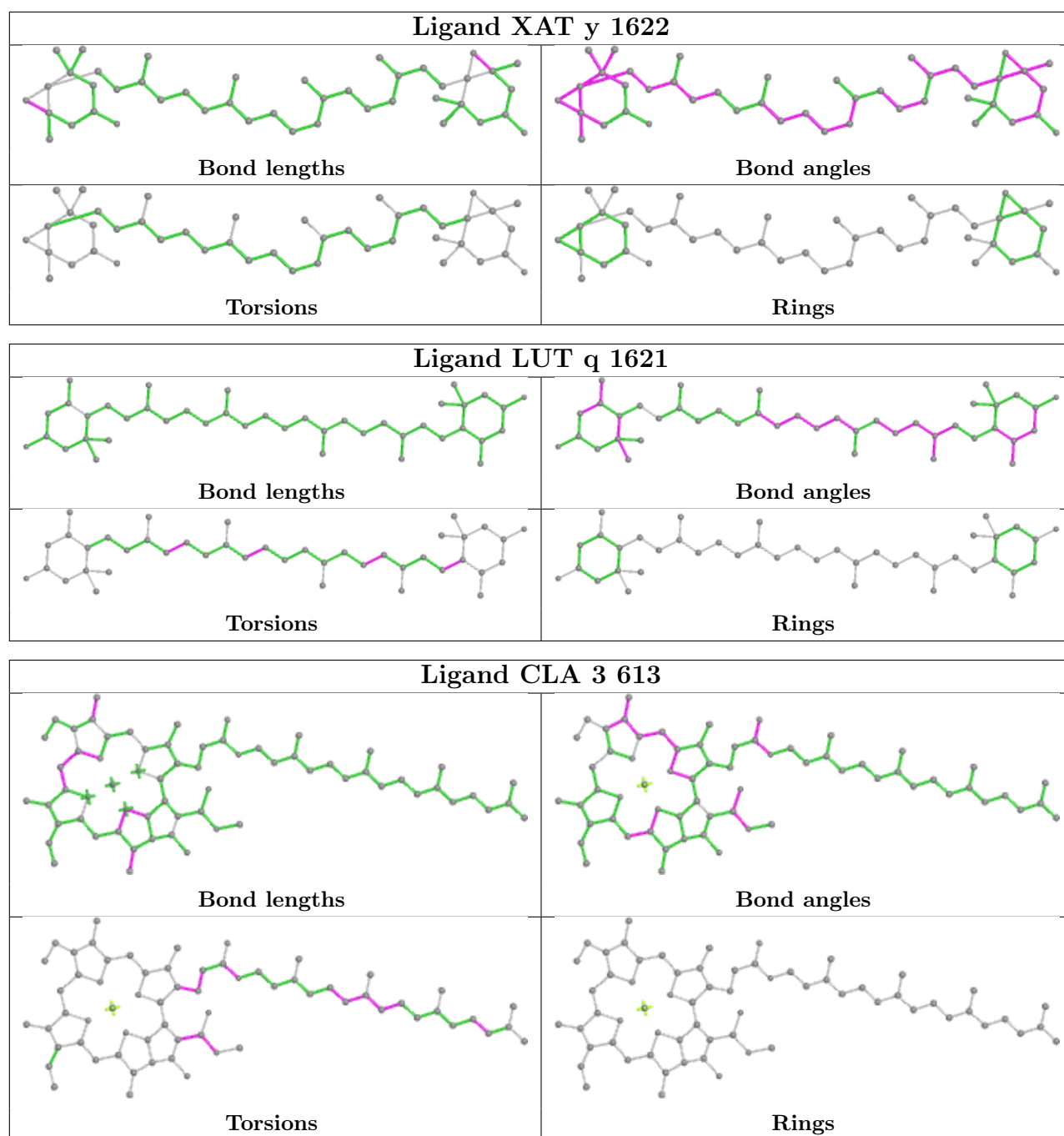
Ligand CLA 7 604

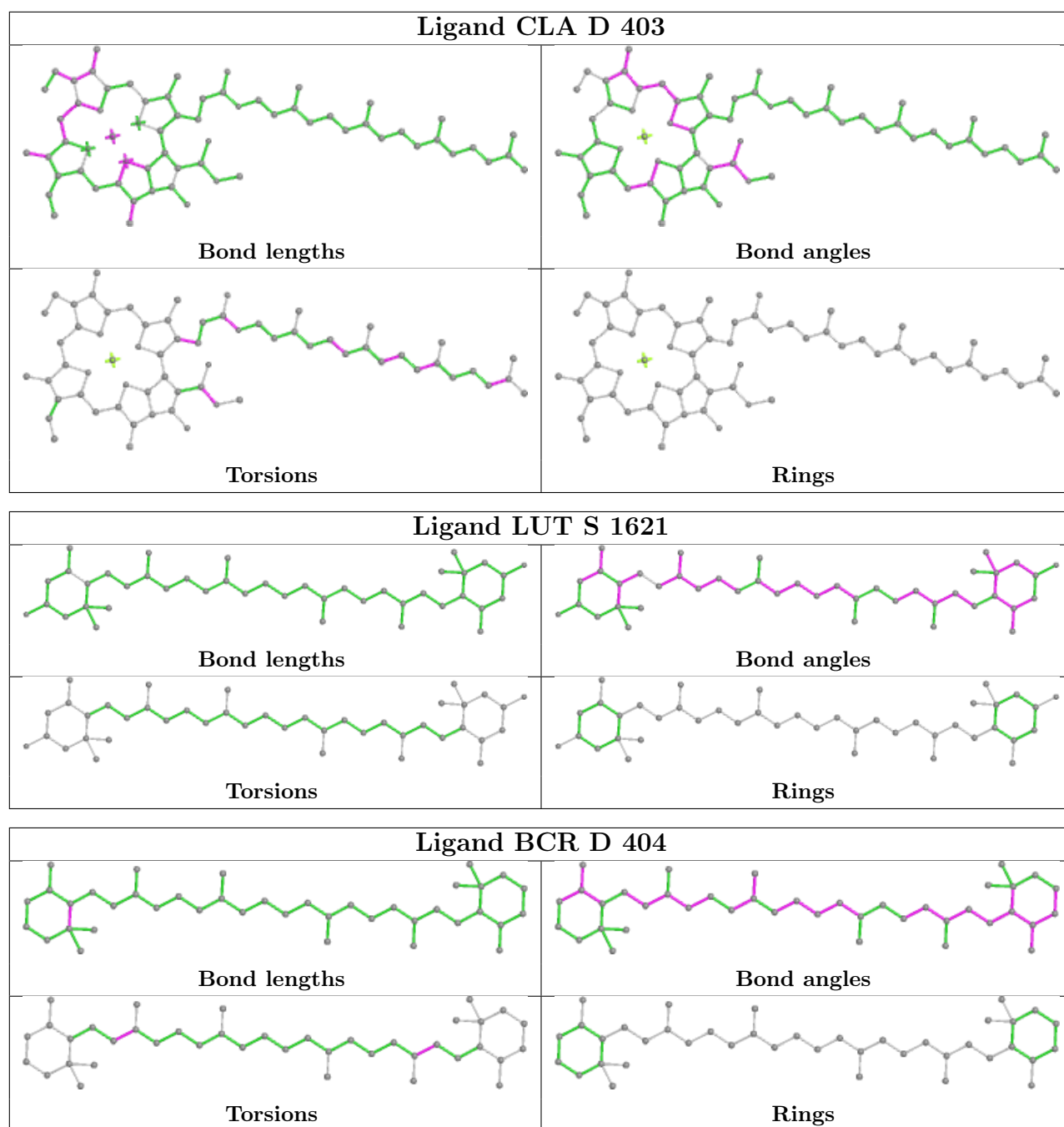


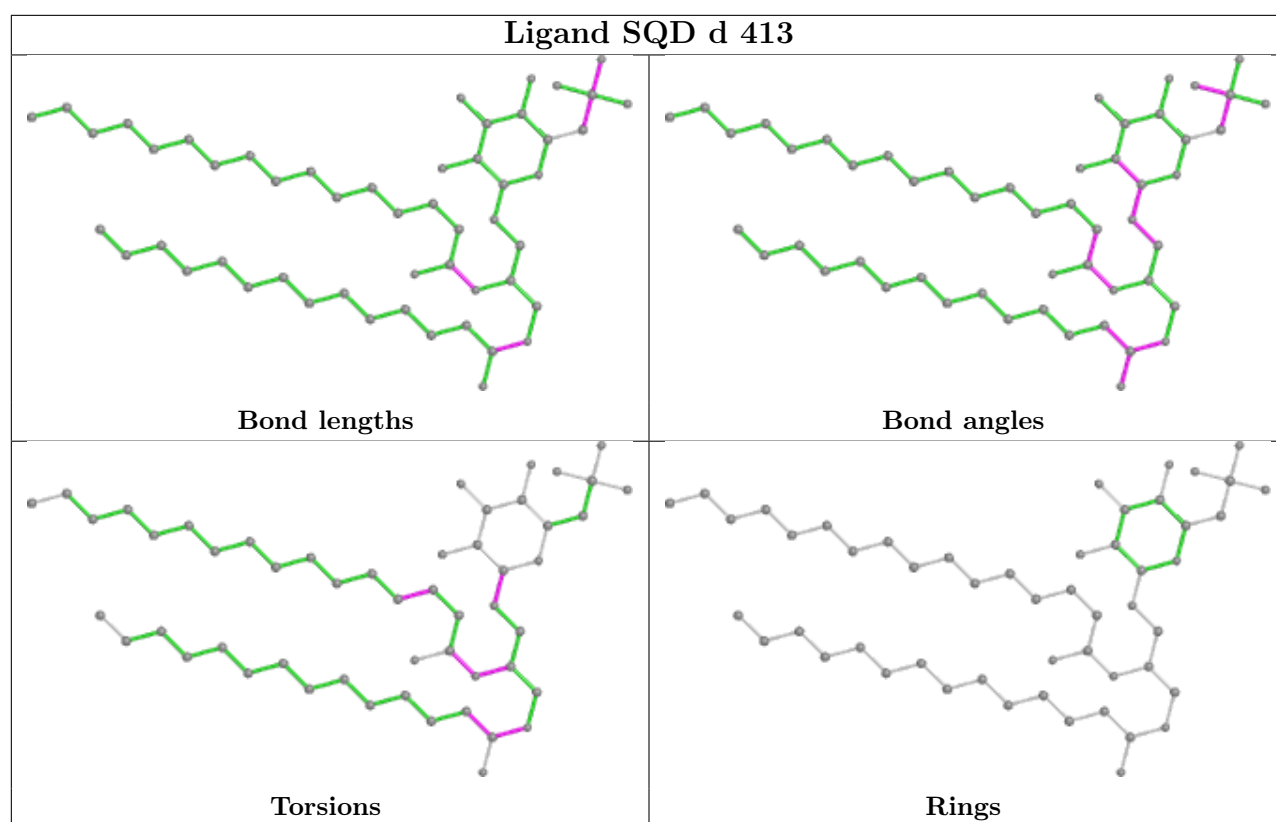
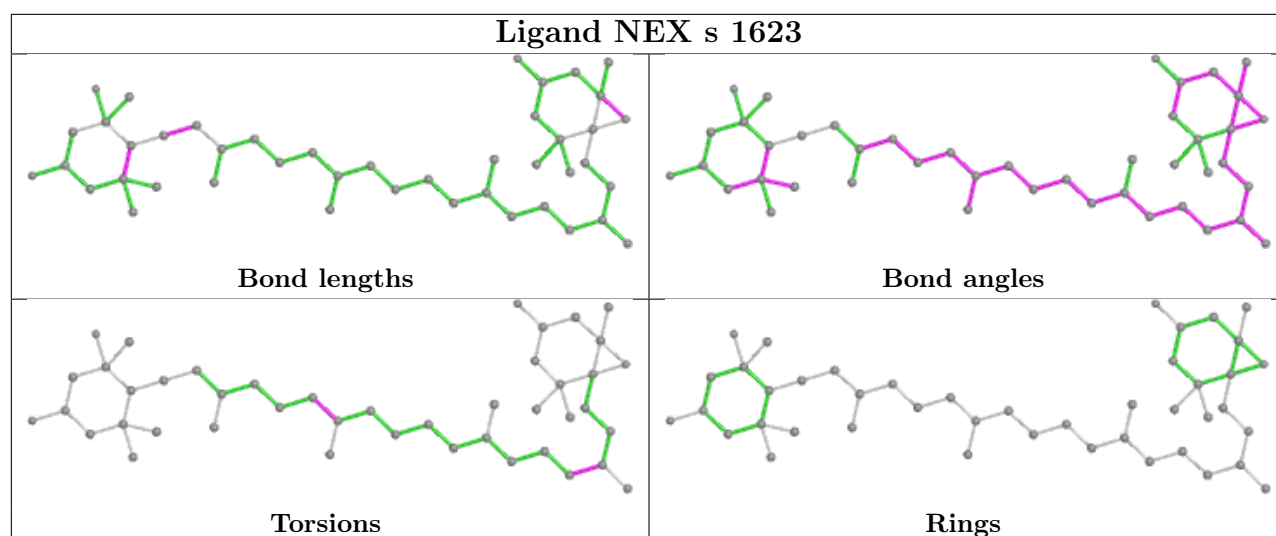
Ligand SQD a 412



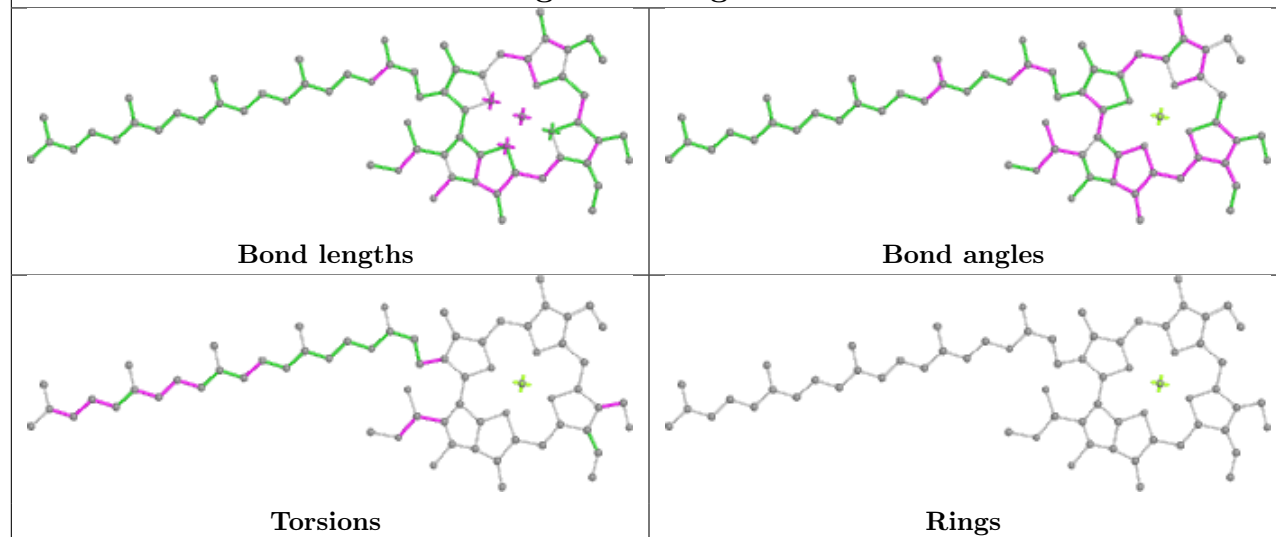




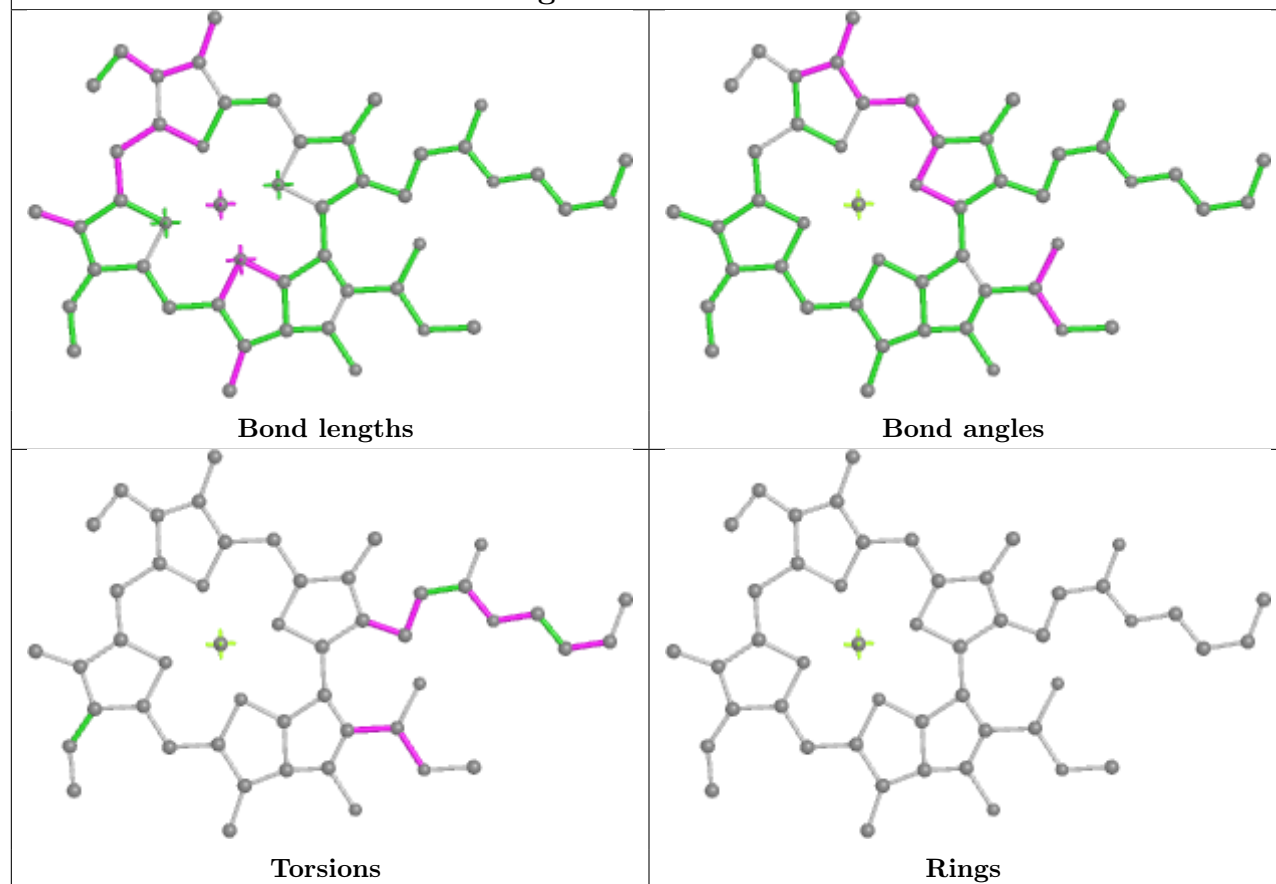


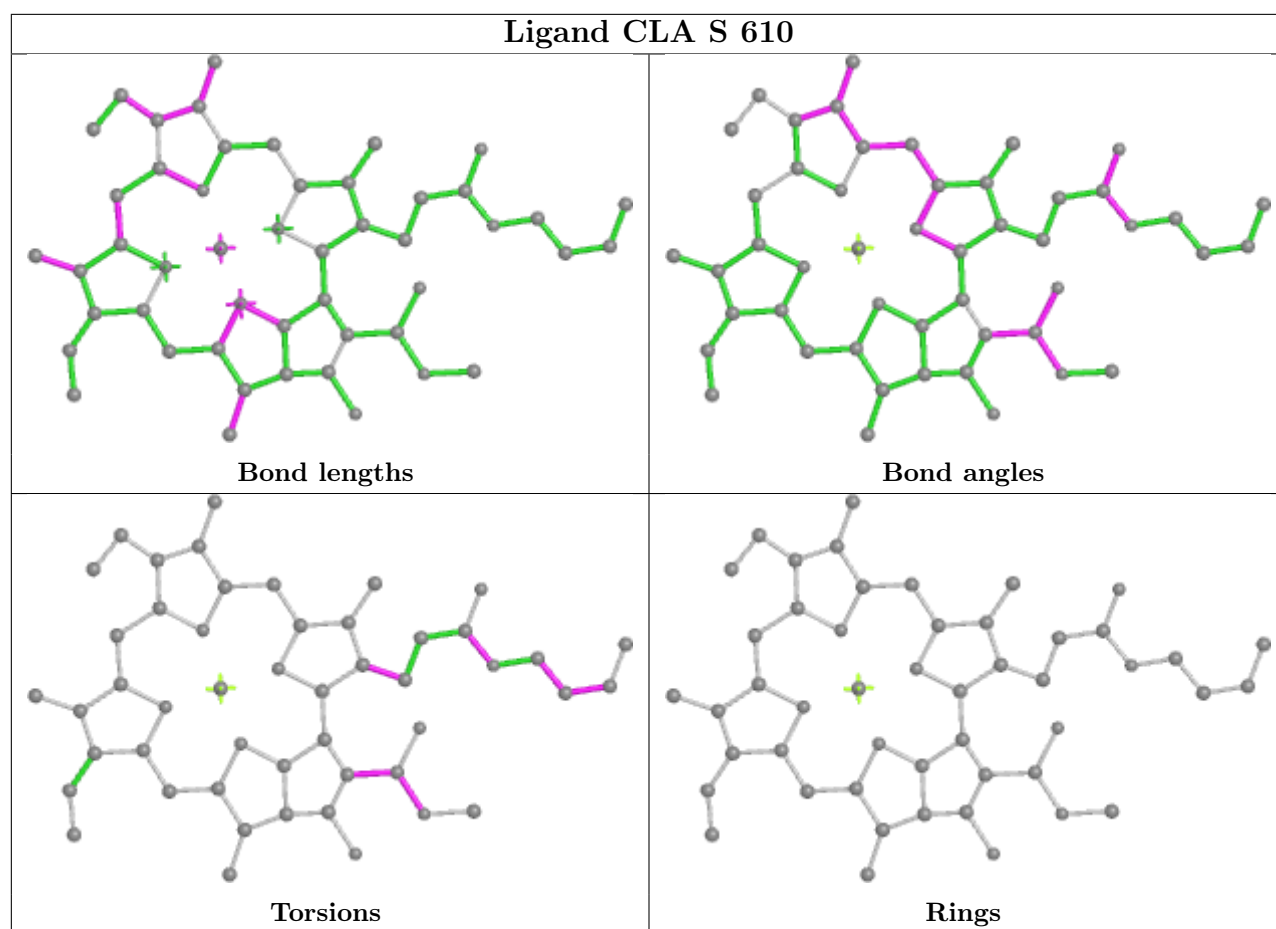


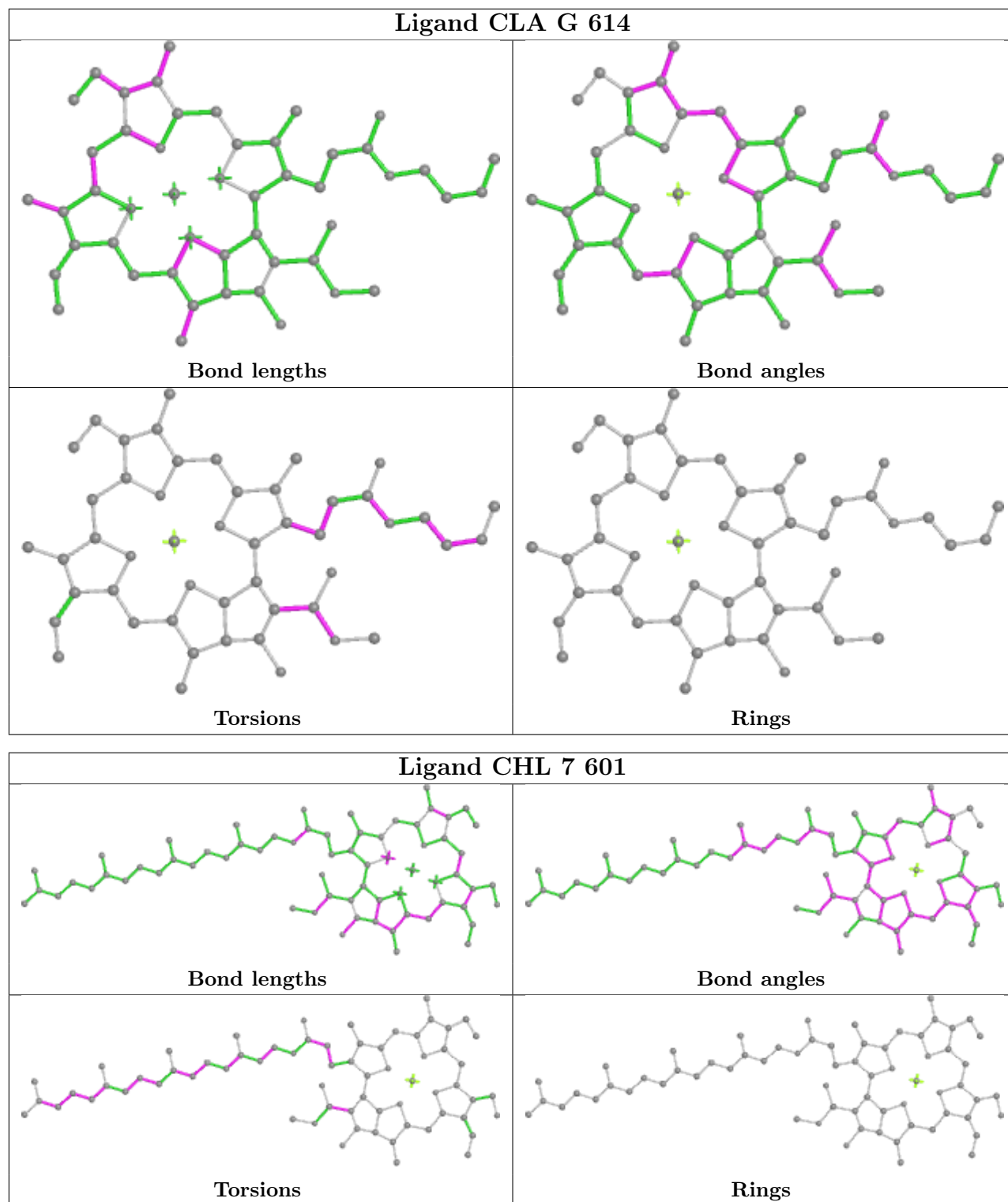
Ligand CHL g 609

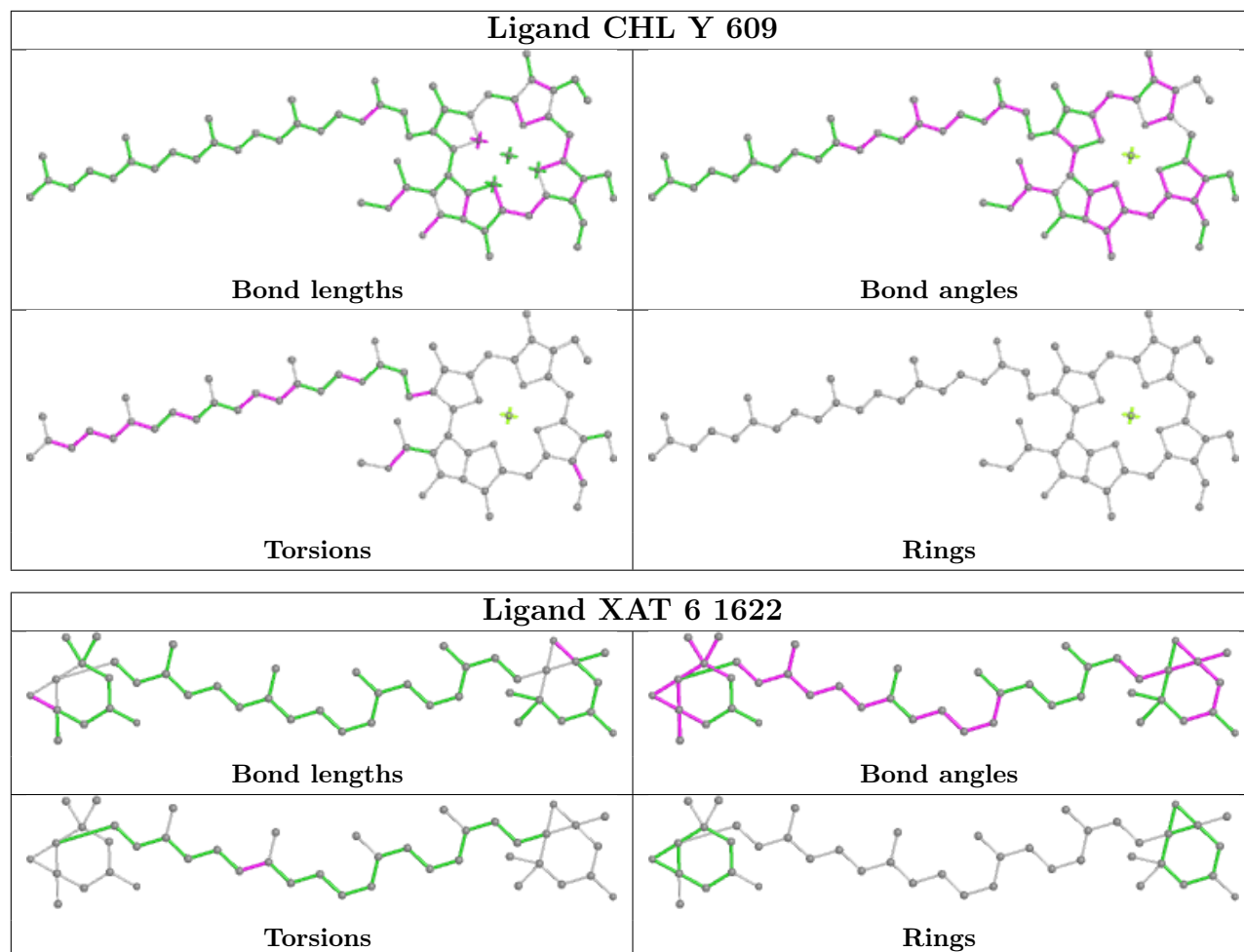


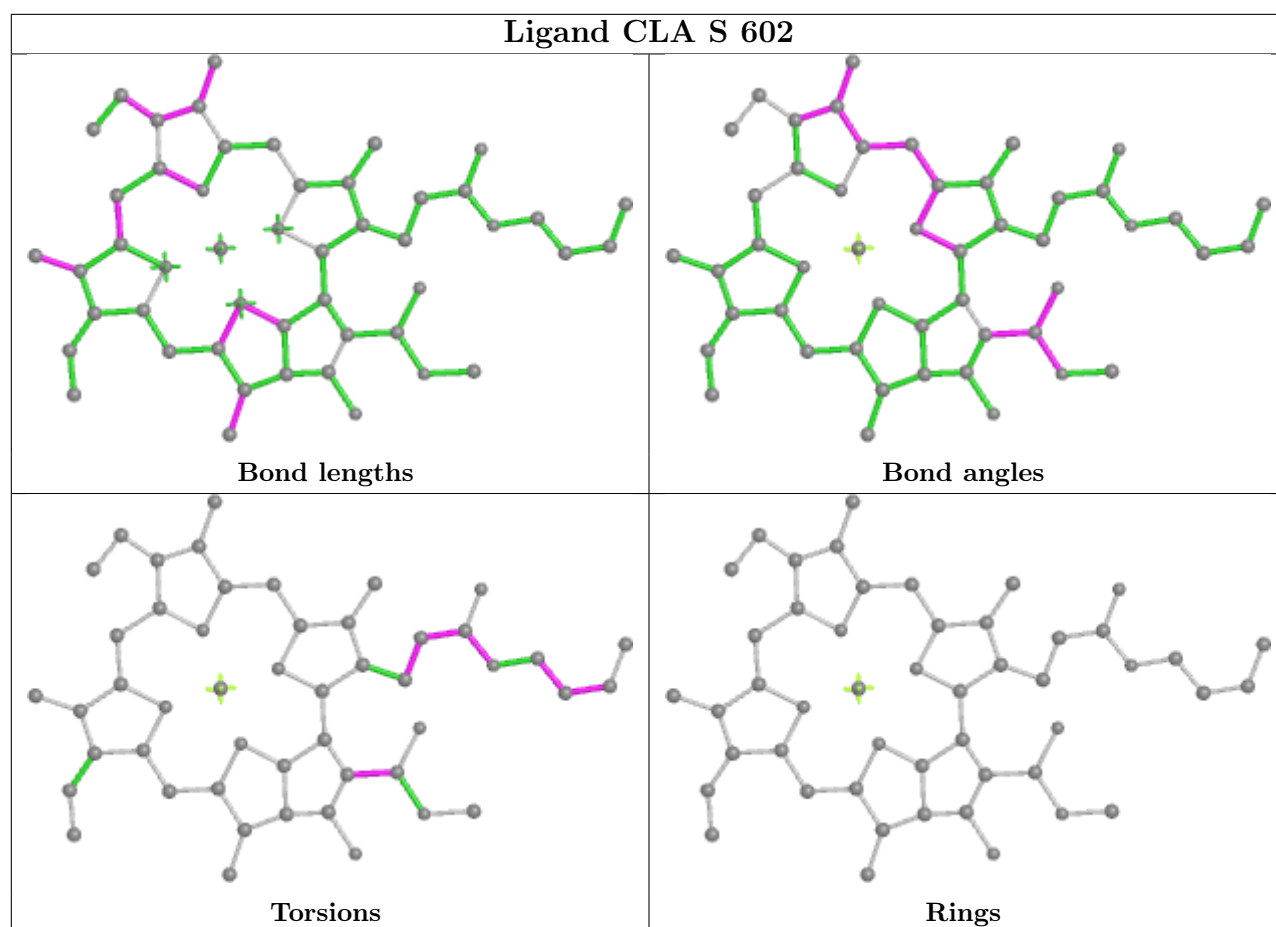
Ligand CLA r 611



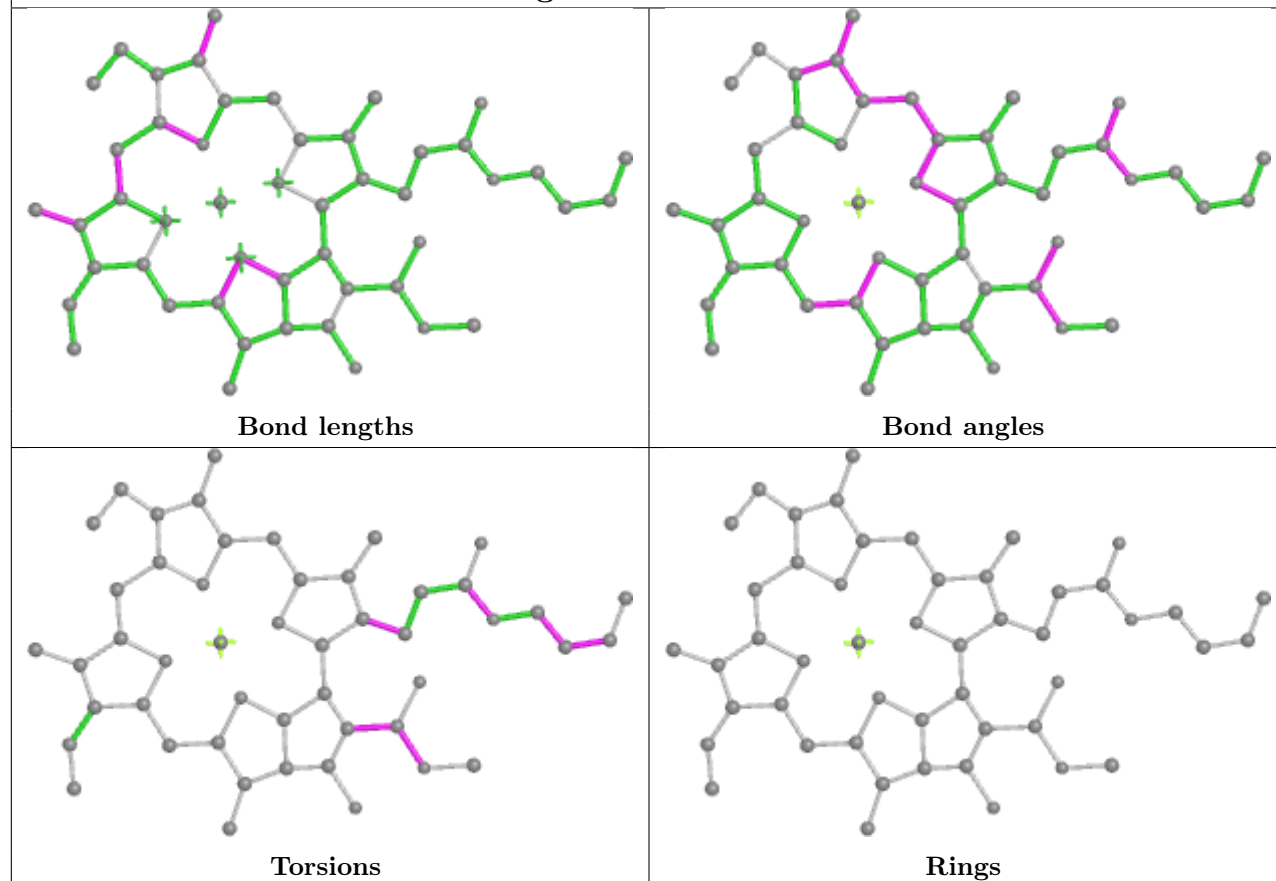




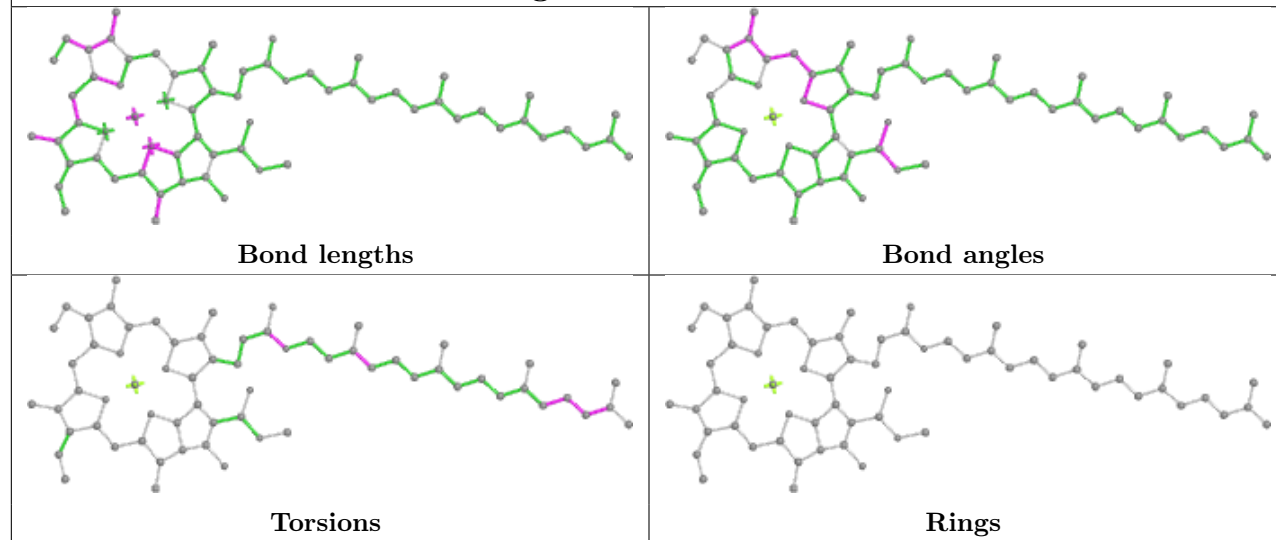




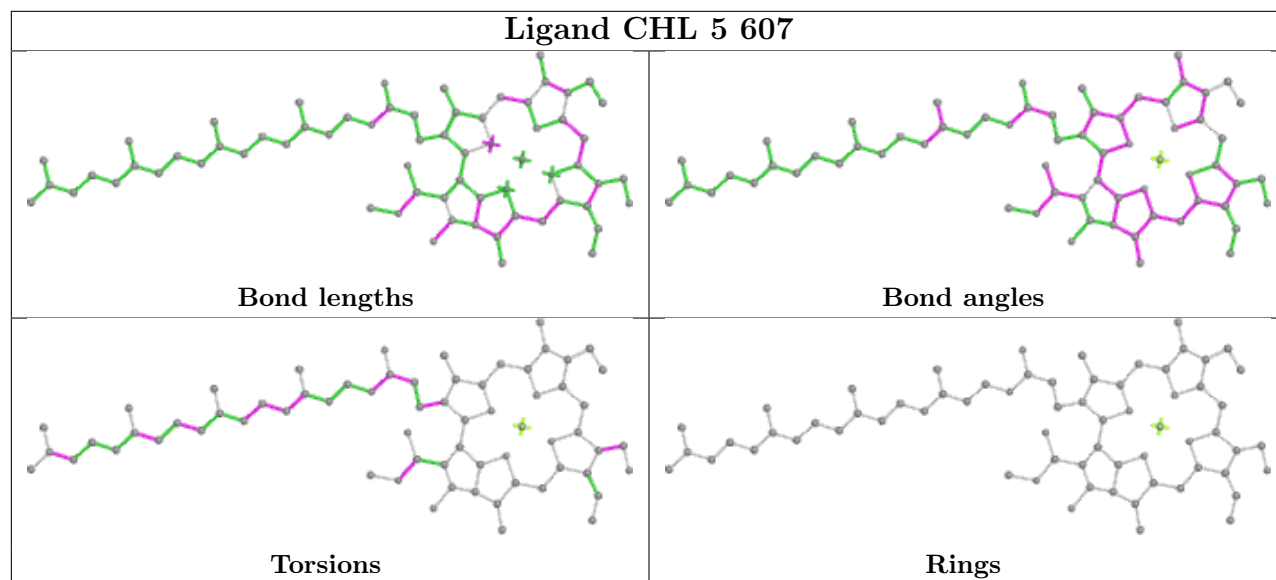
Ligand CLA 2 604



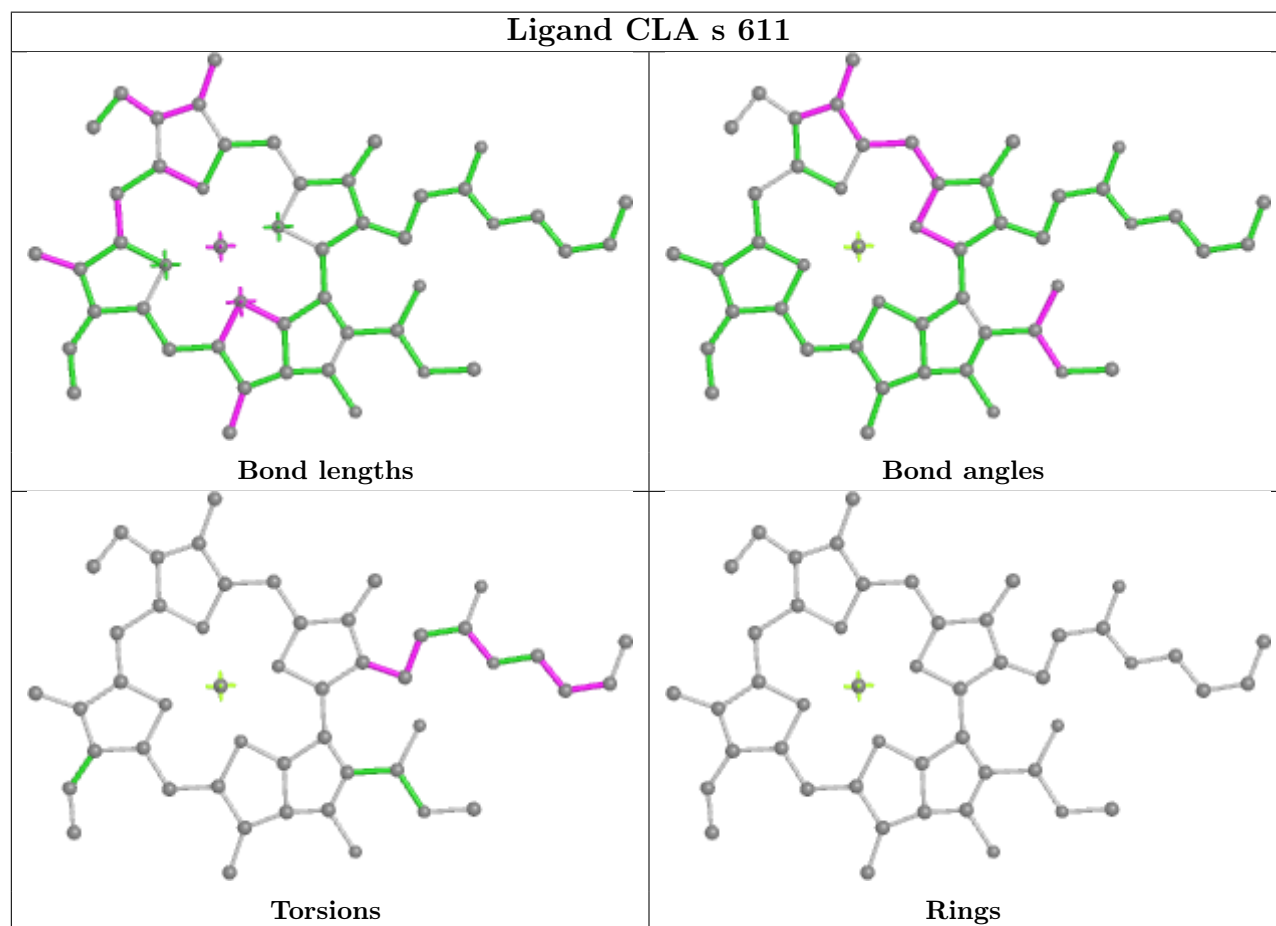
Ligand CLA Y 611



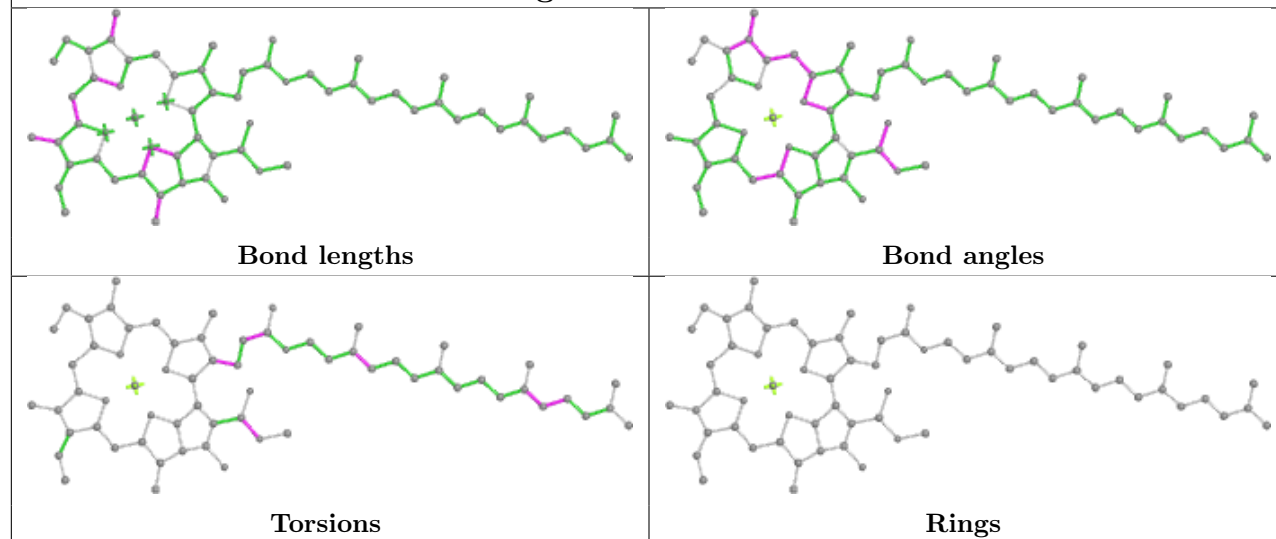
Ligand CHL 5 607



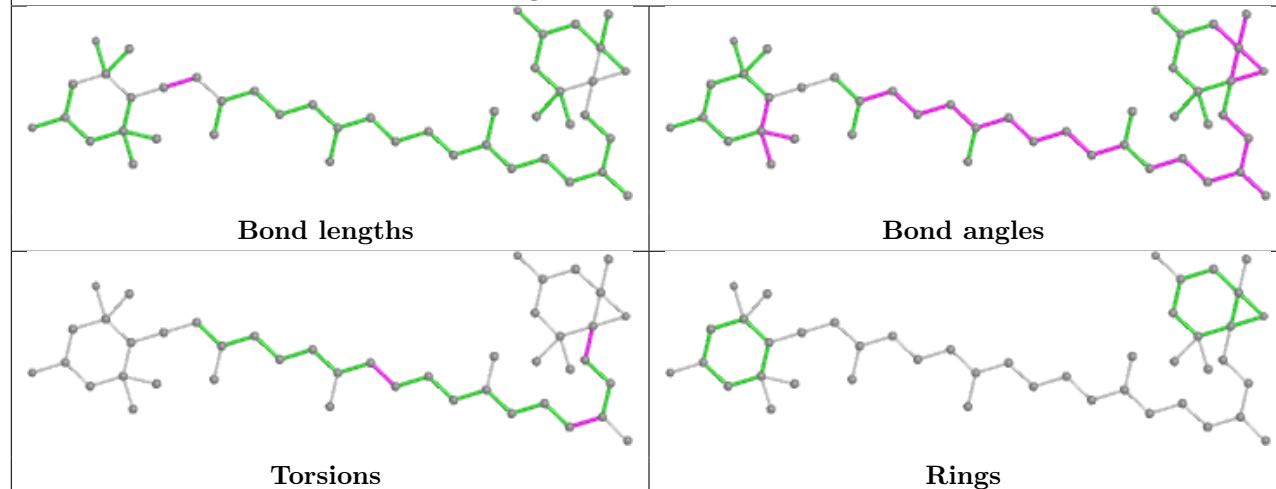
Ligand CLA s 611



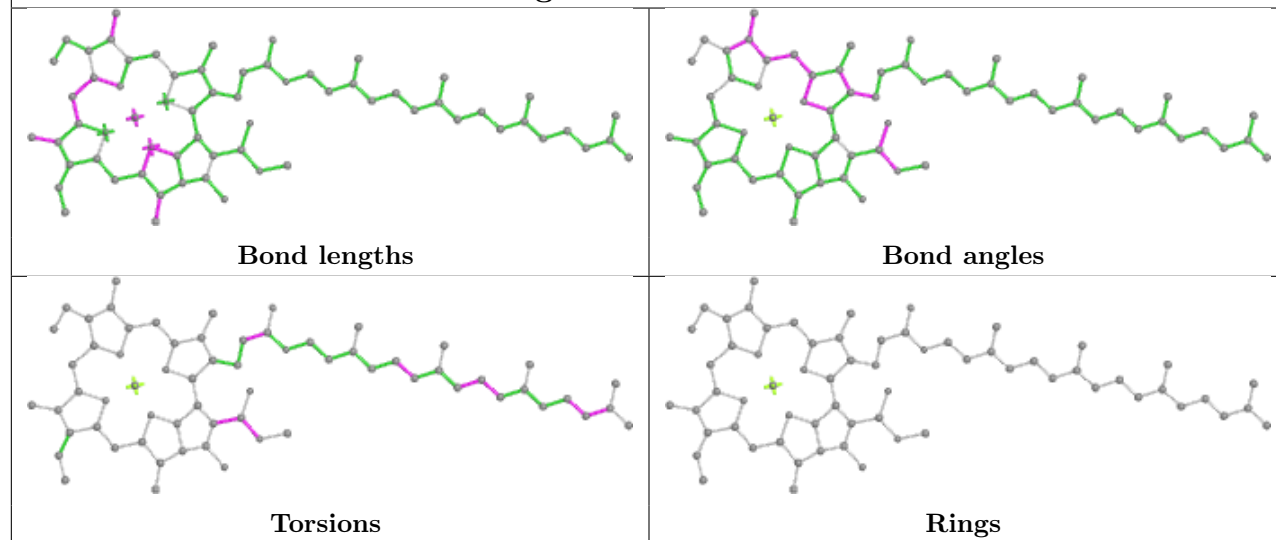
Ligand CLA 8 604

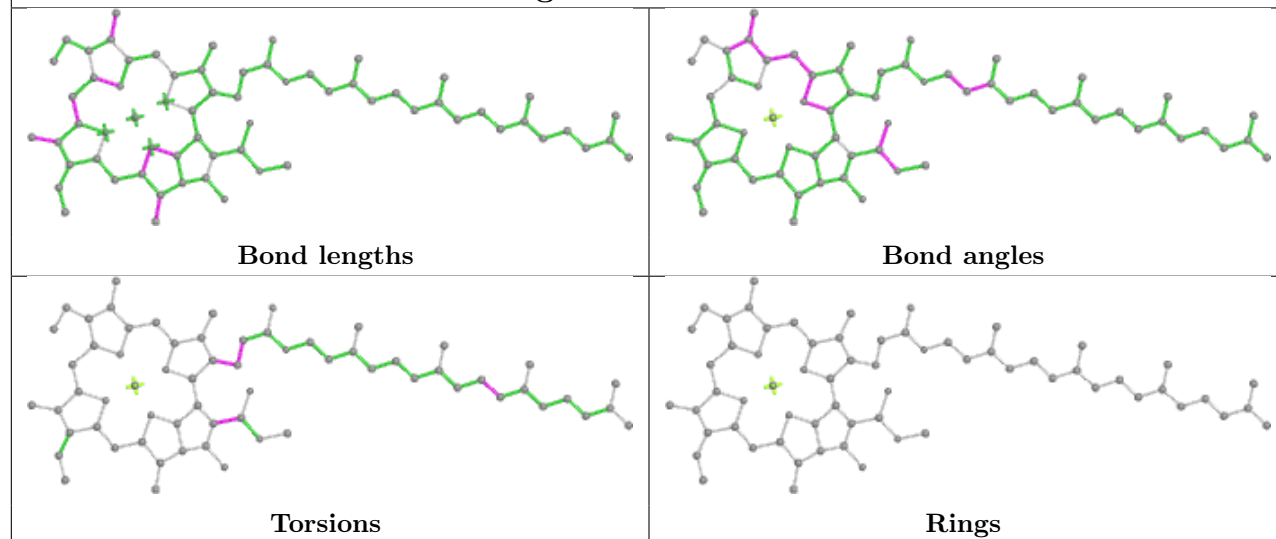
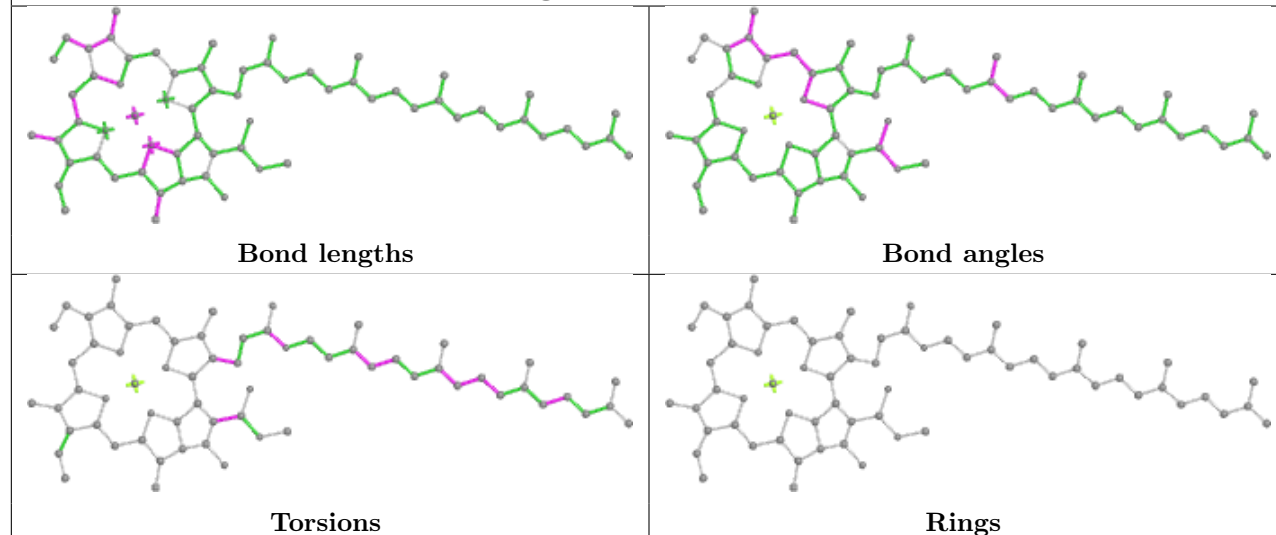
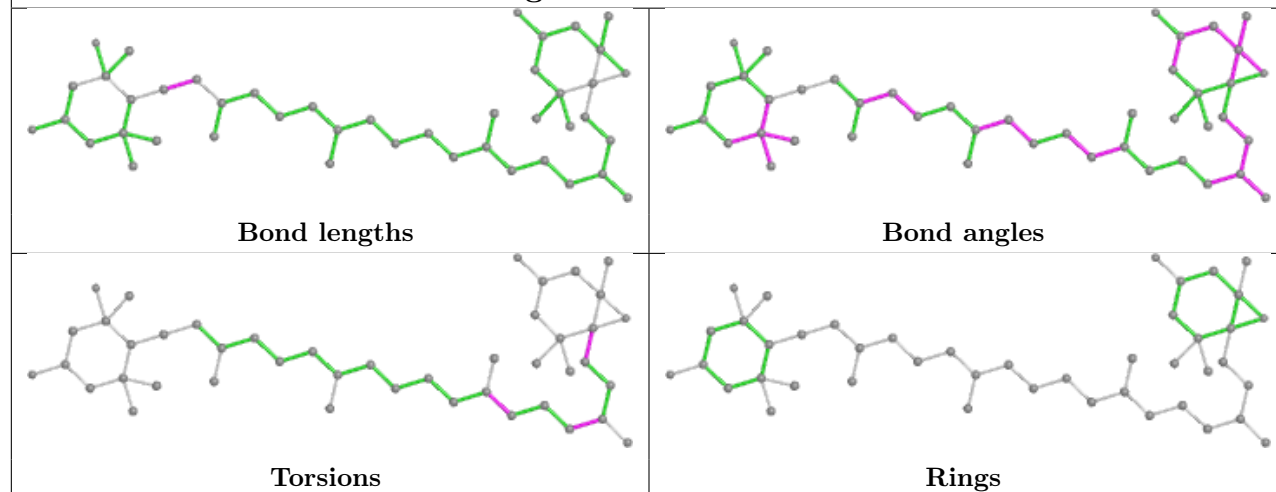


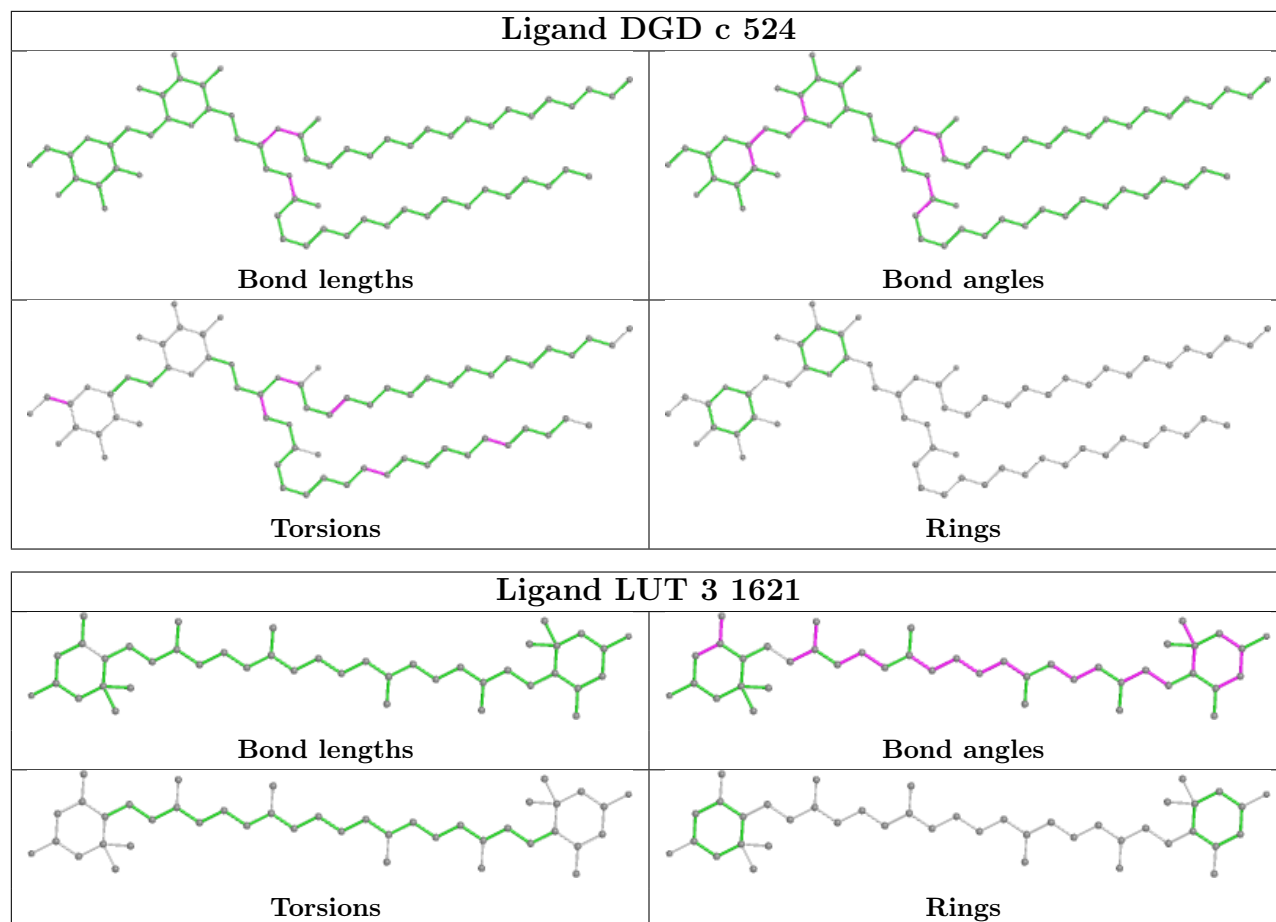
Ligand NEX 5 1623

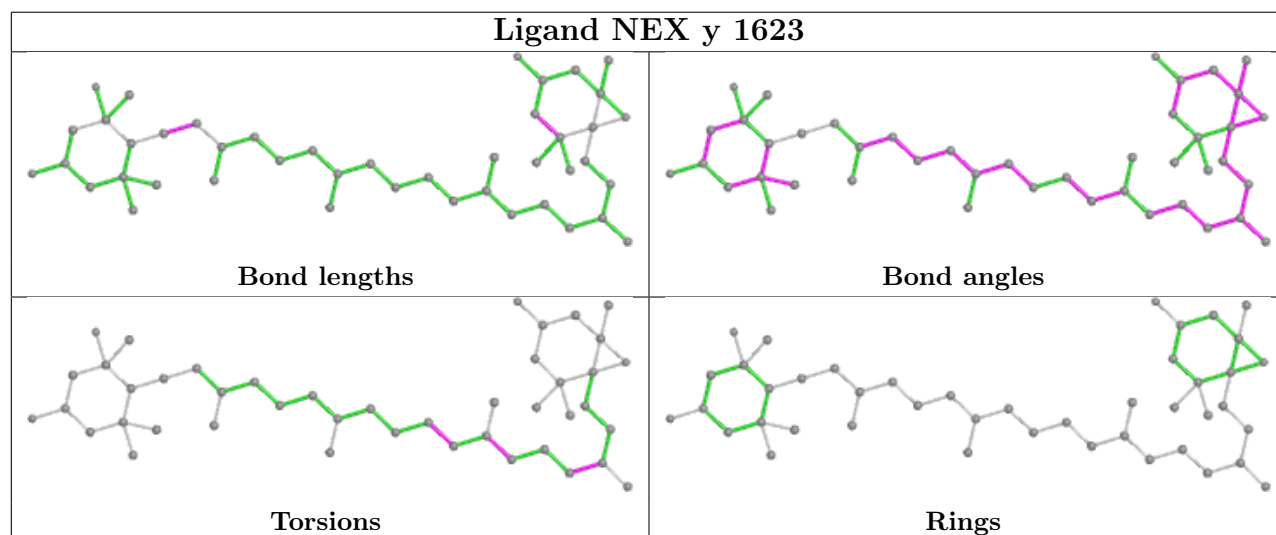
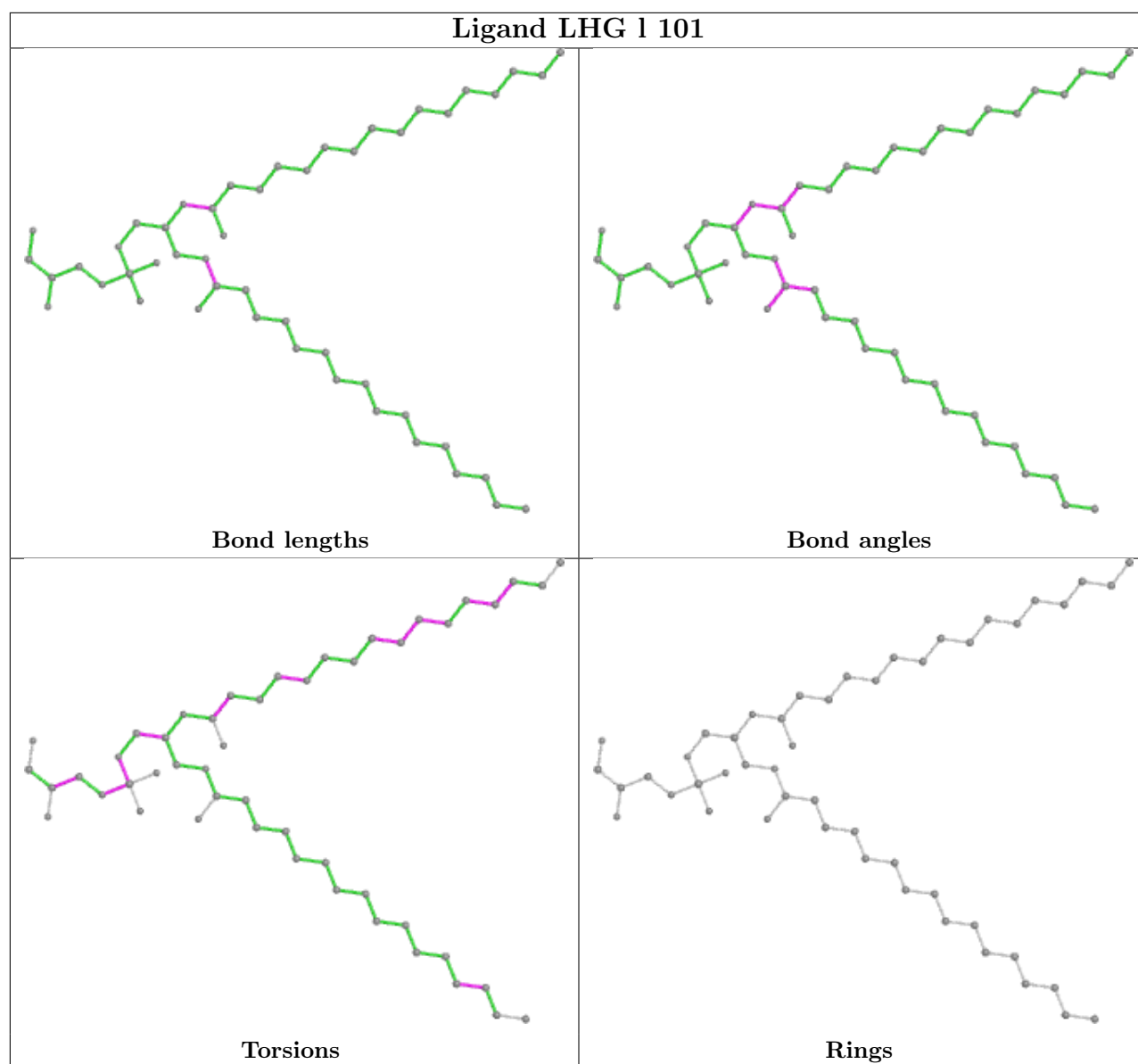


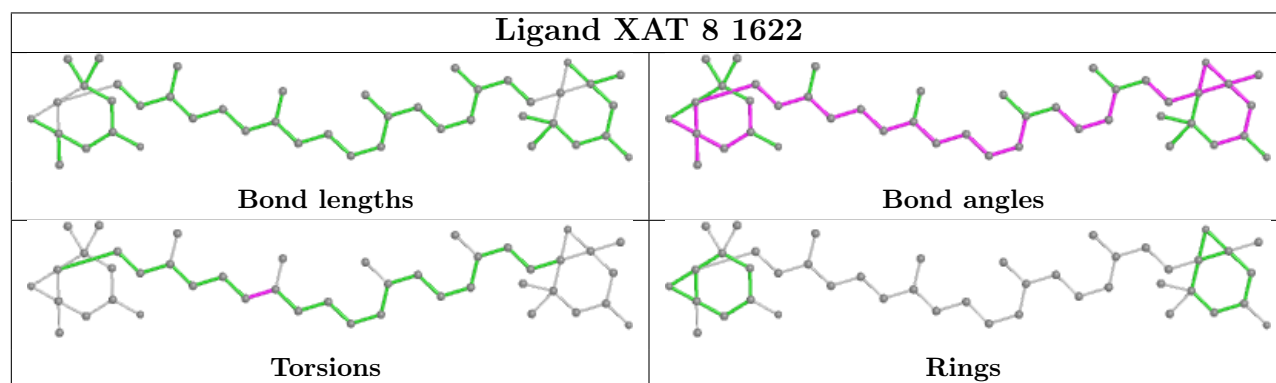
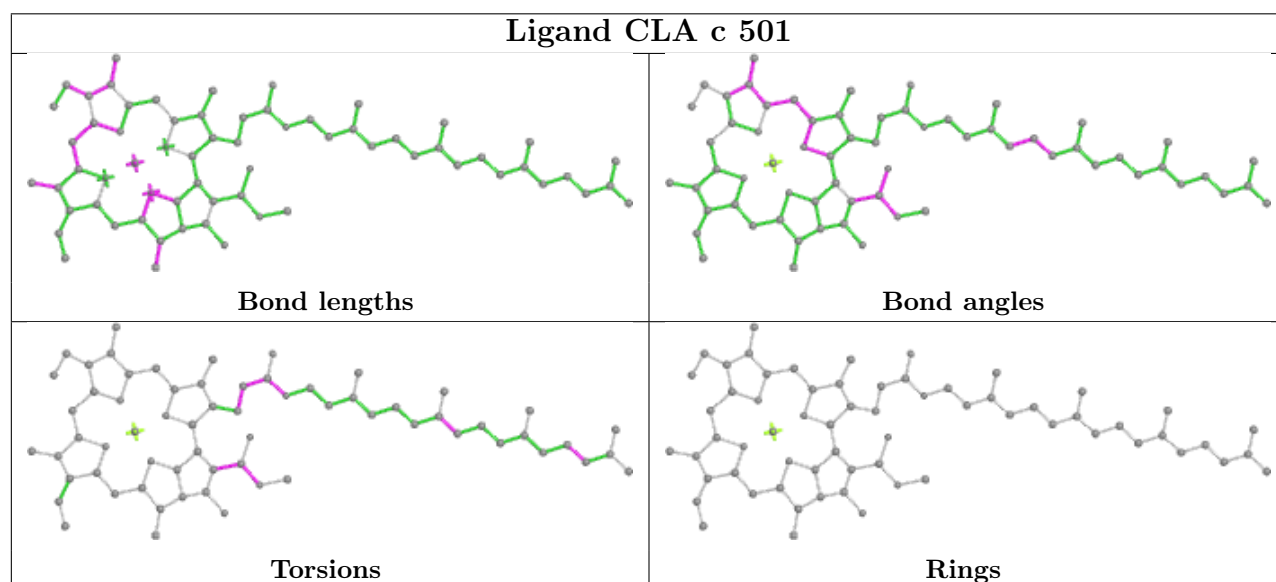
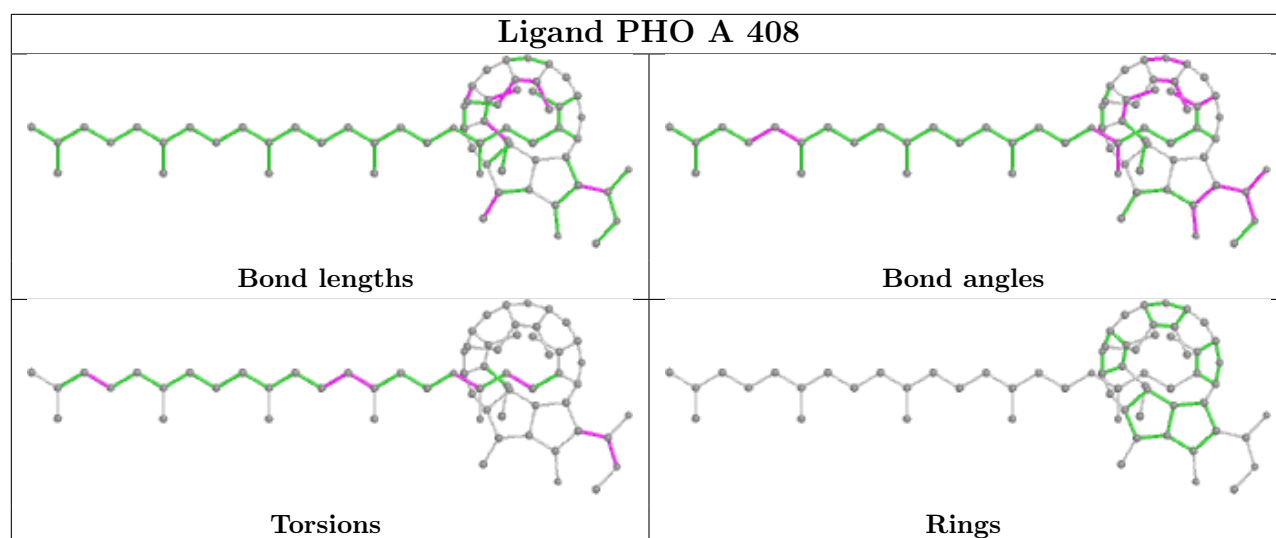
Ligand CLA b 614

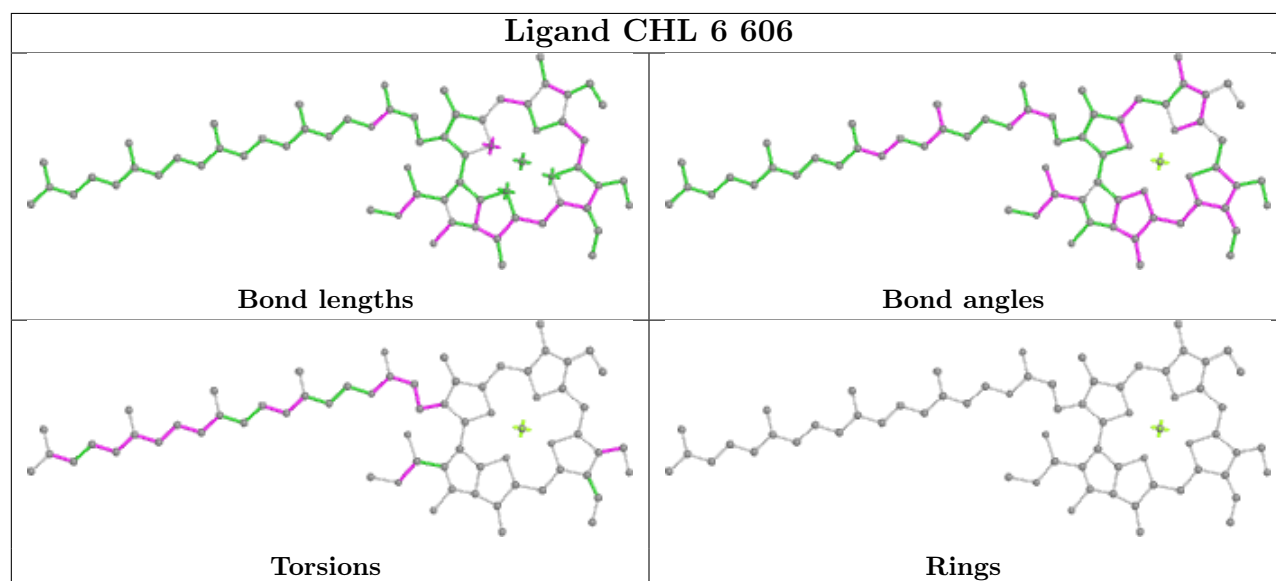
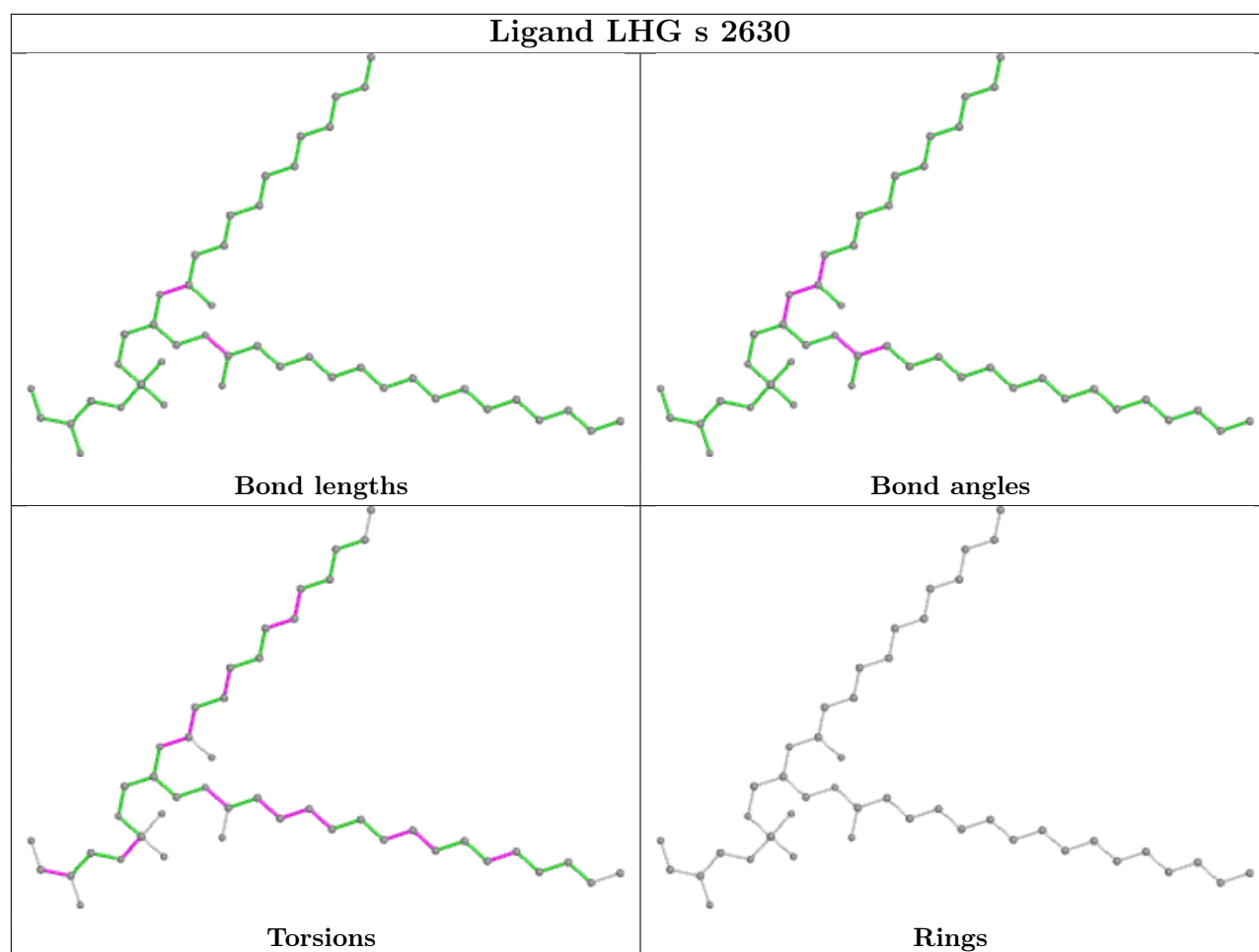


Ligand CLA 2 610**Ligand CLA c 504****Ligand NEX 3 1623**

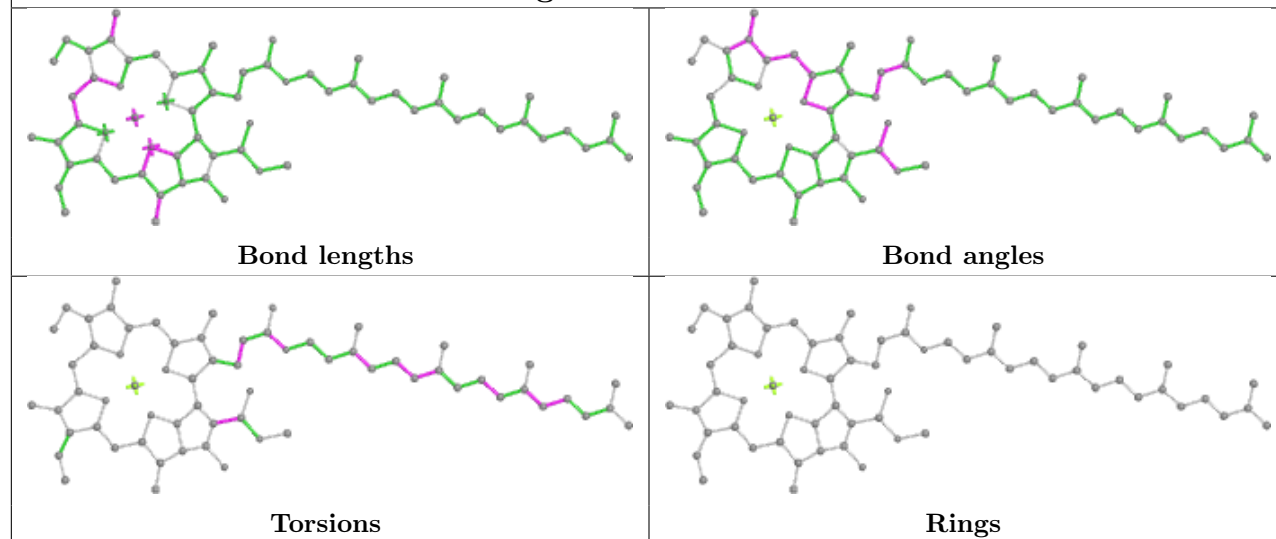




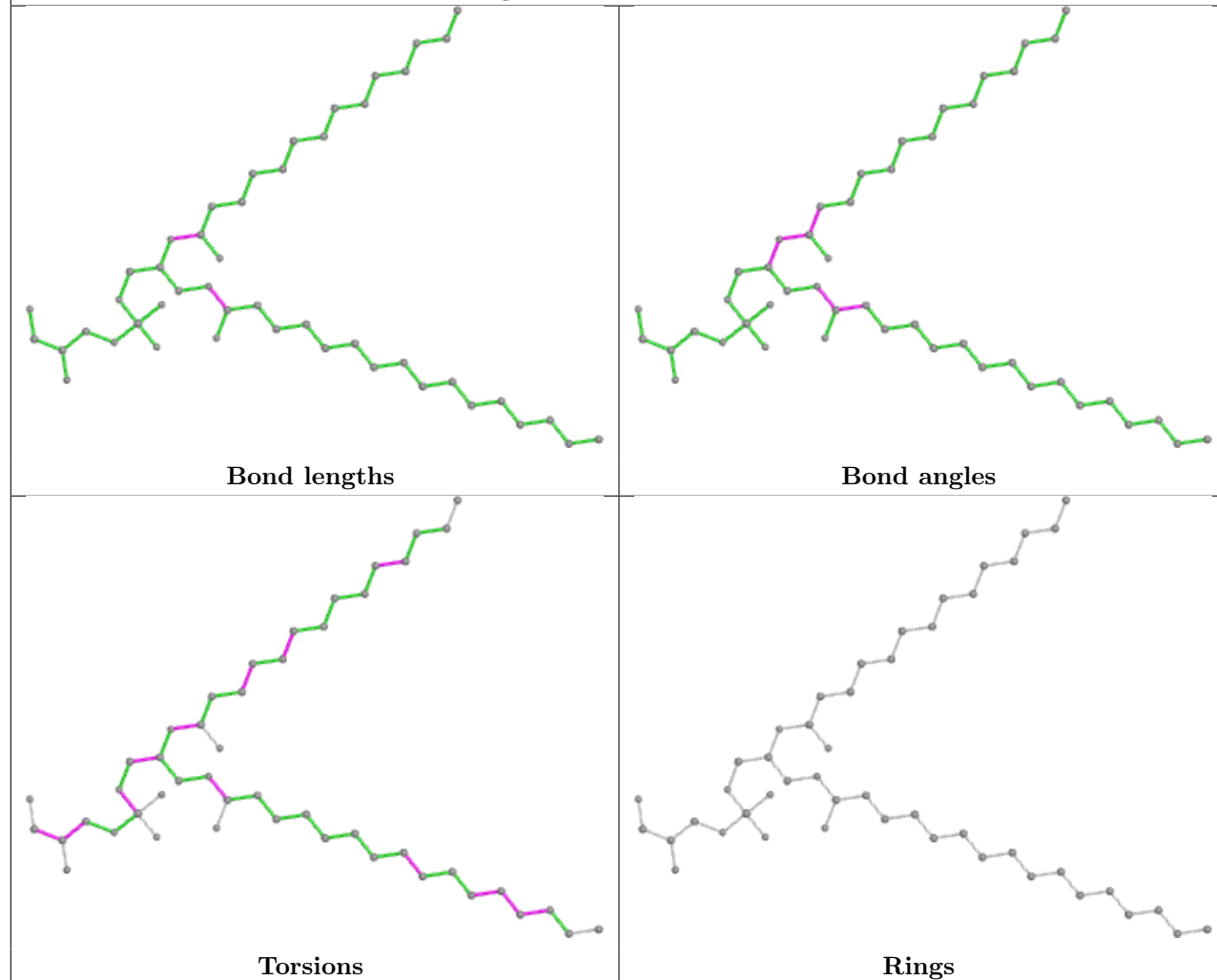


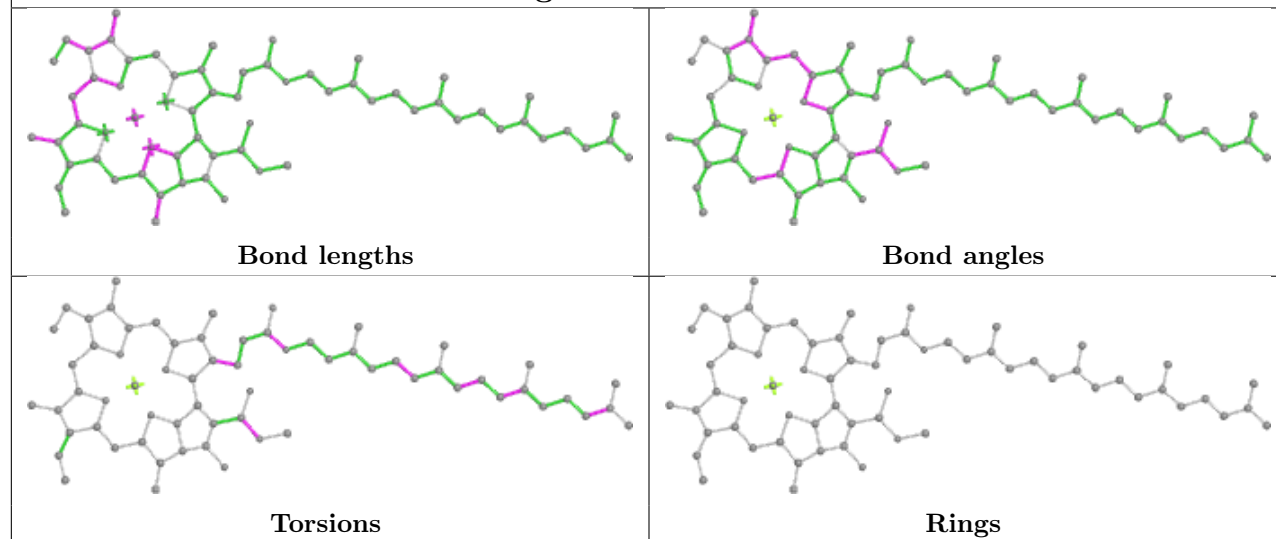
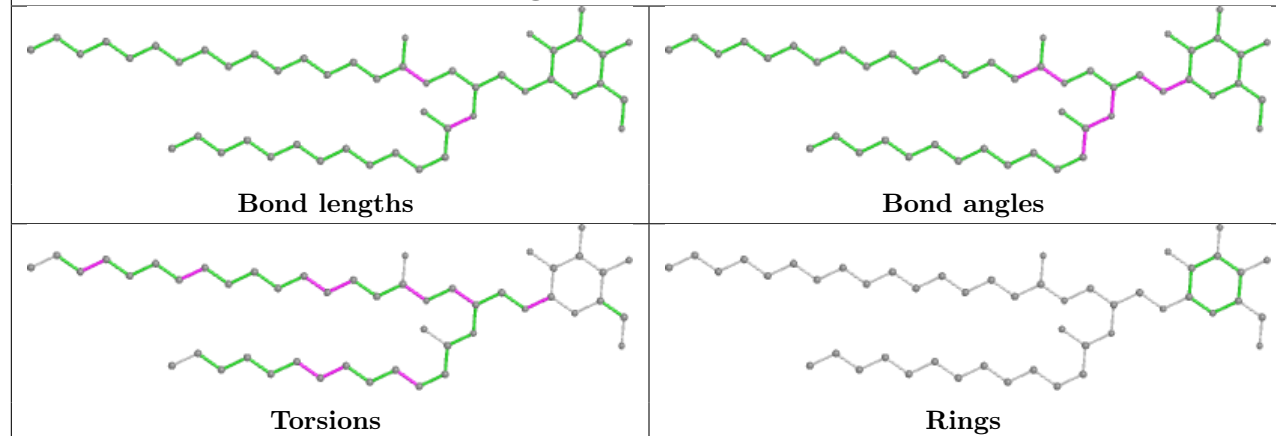


Ligand CLA 1 613

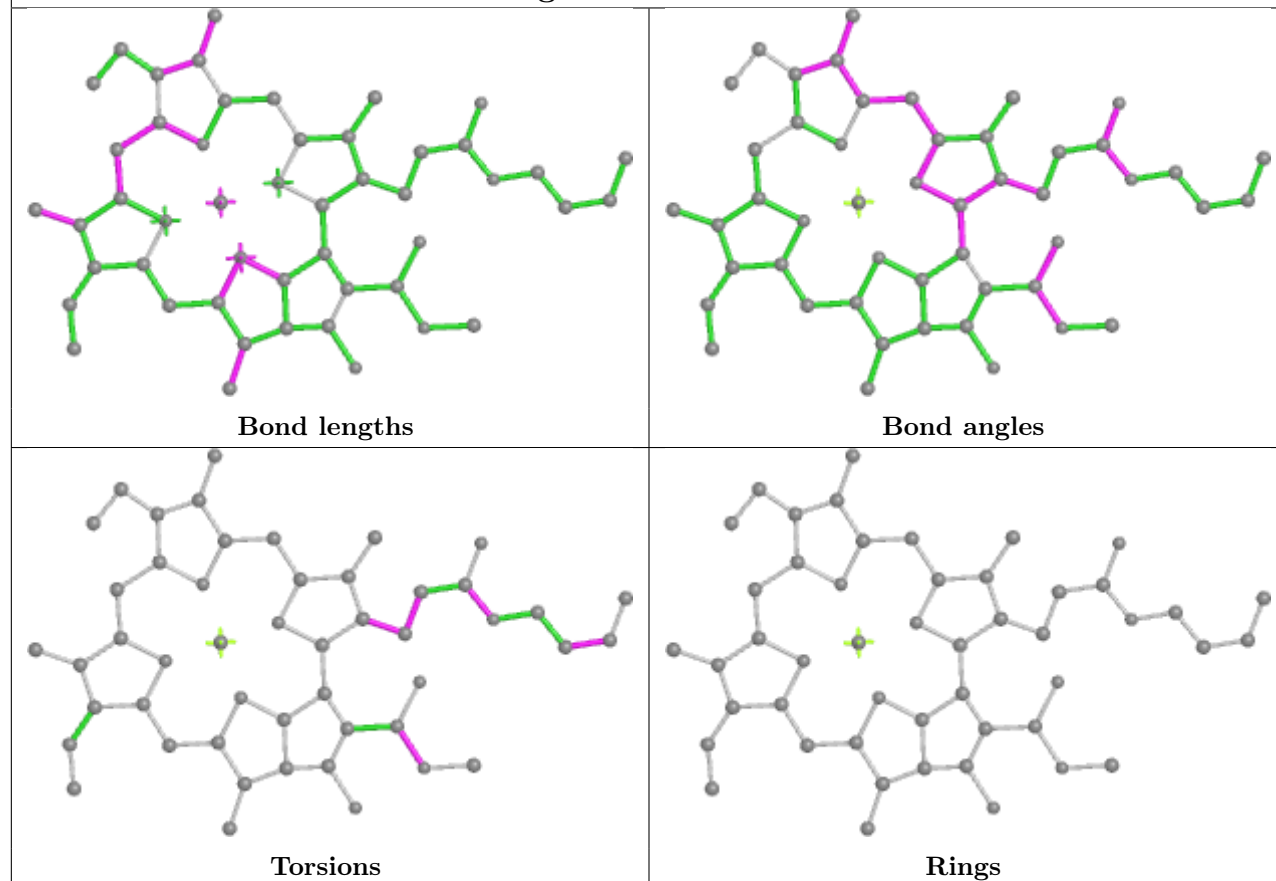


Ligand LHG C 2630

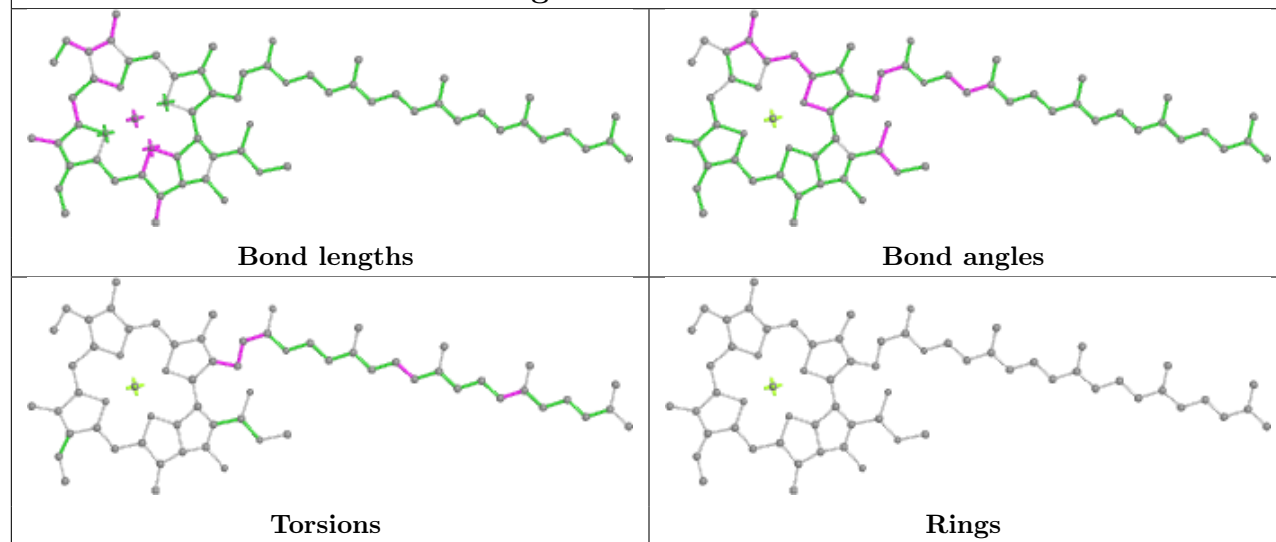


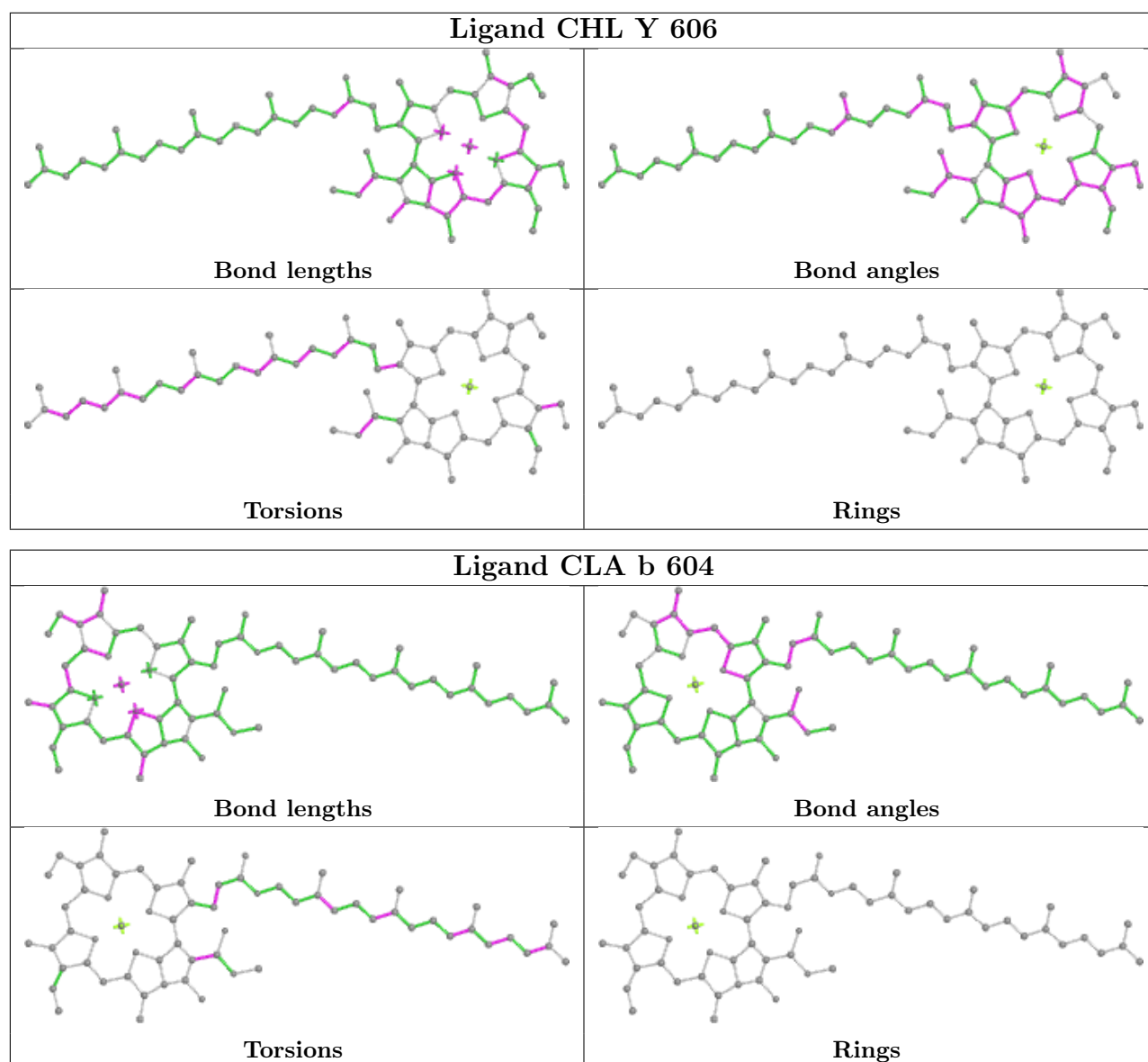
Ligand CLA d 403**Ligand LMG A 413**

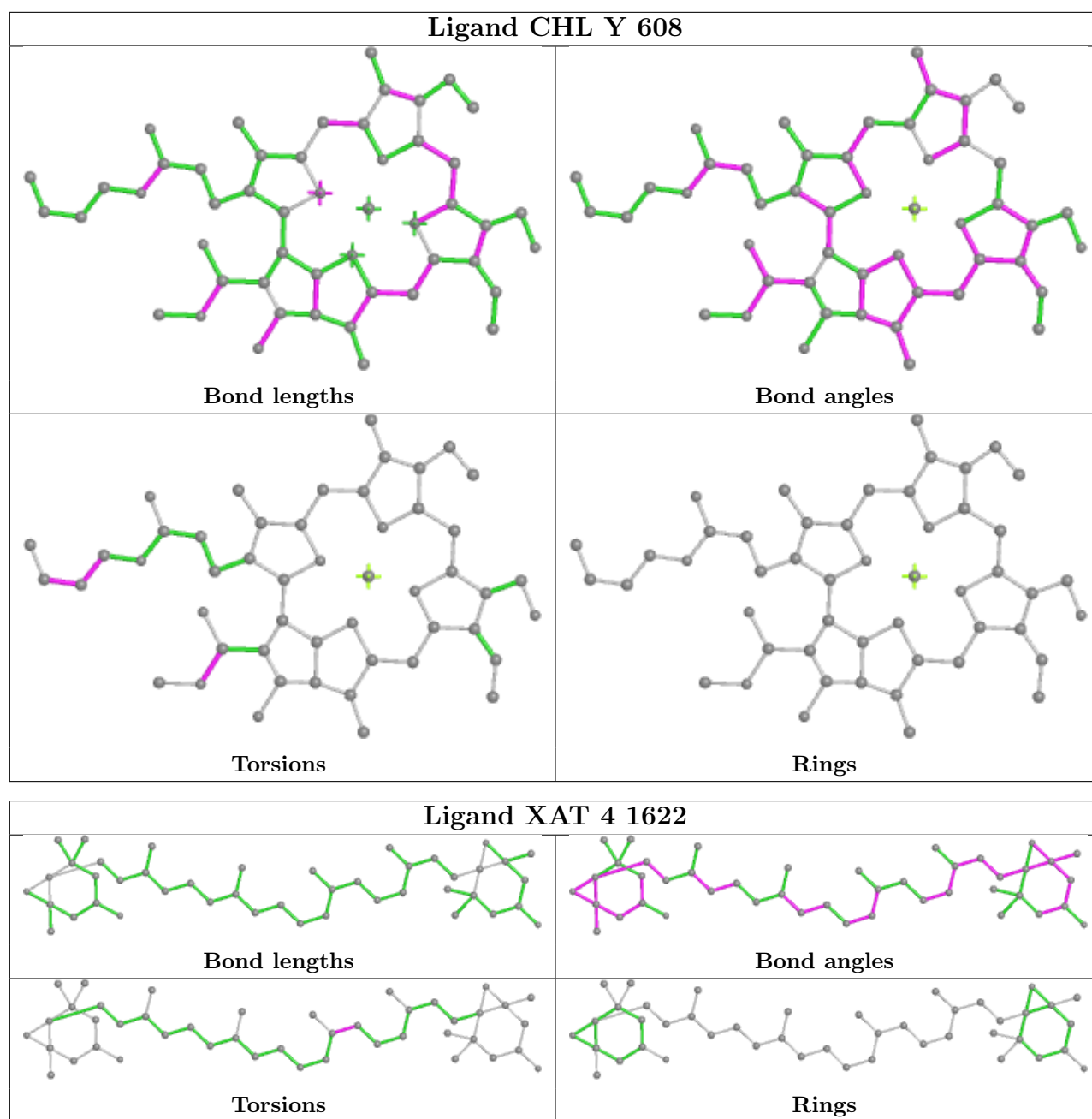
Ligand CLA r 601



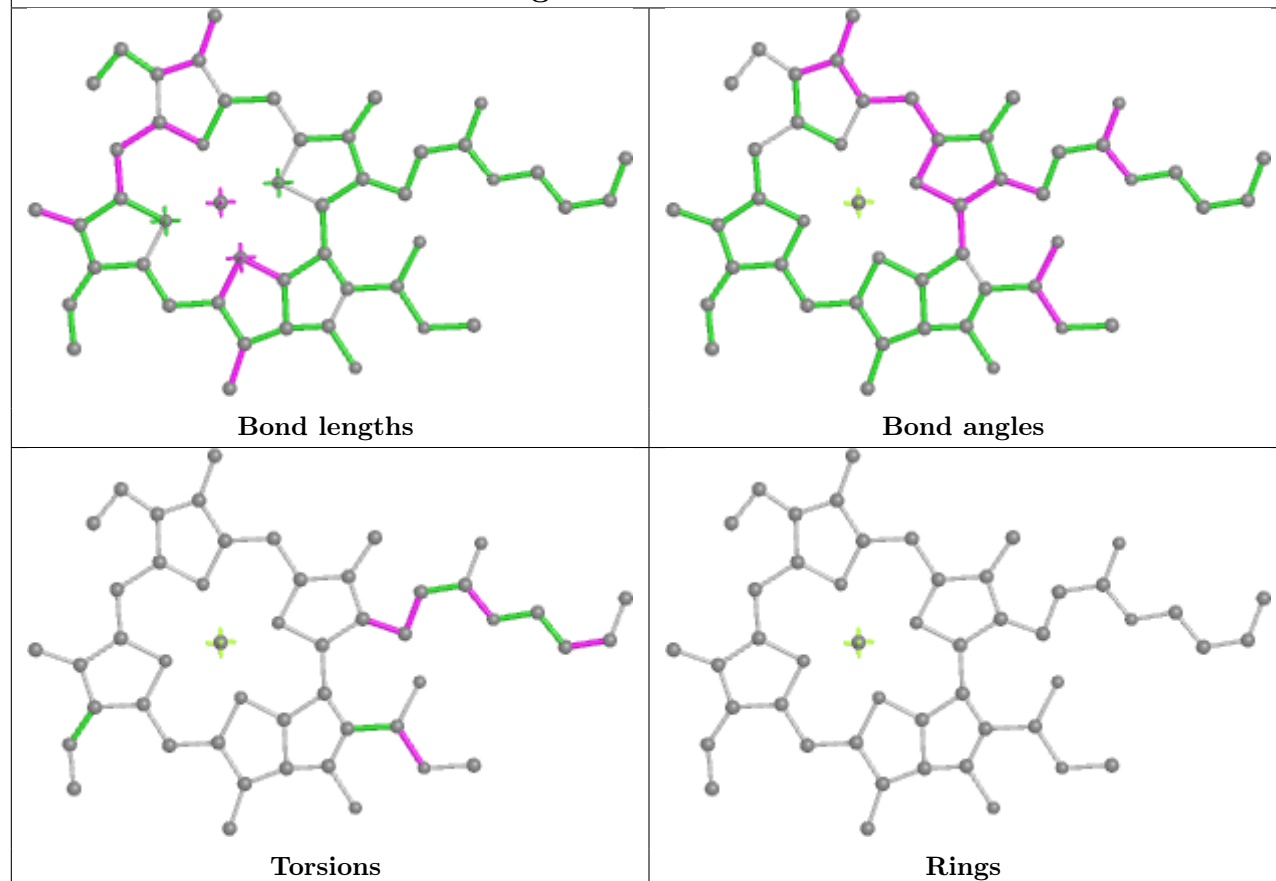
Ligand CLA N 602



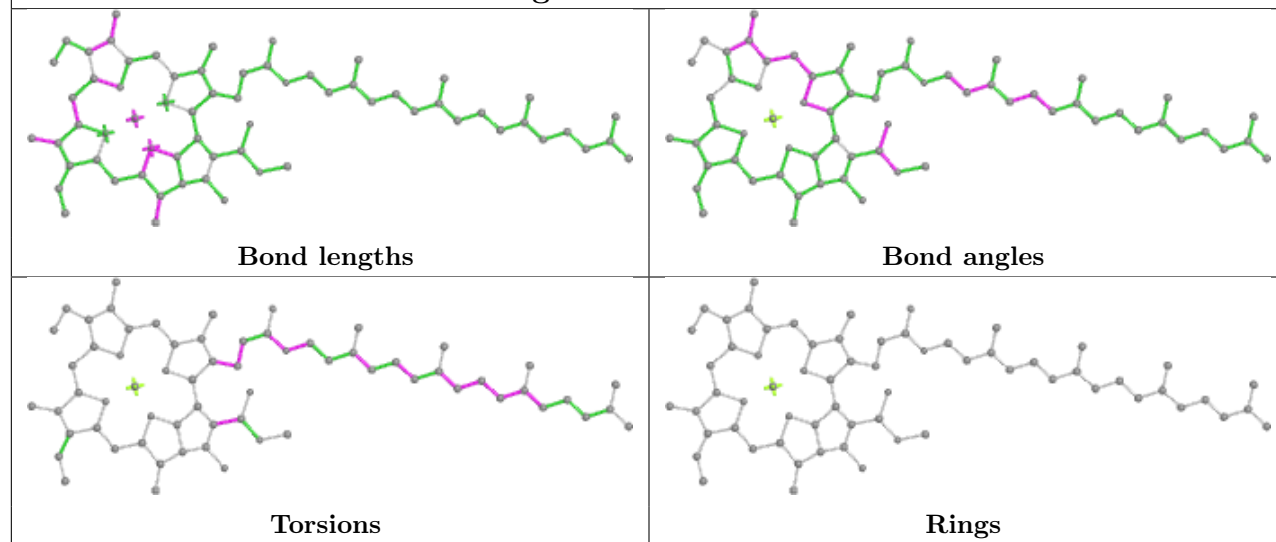




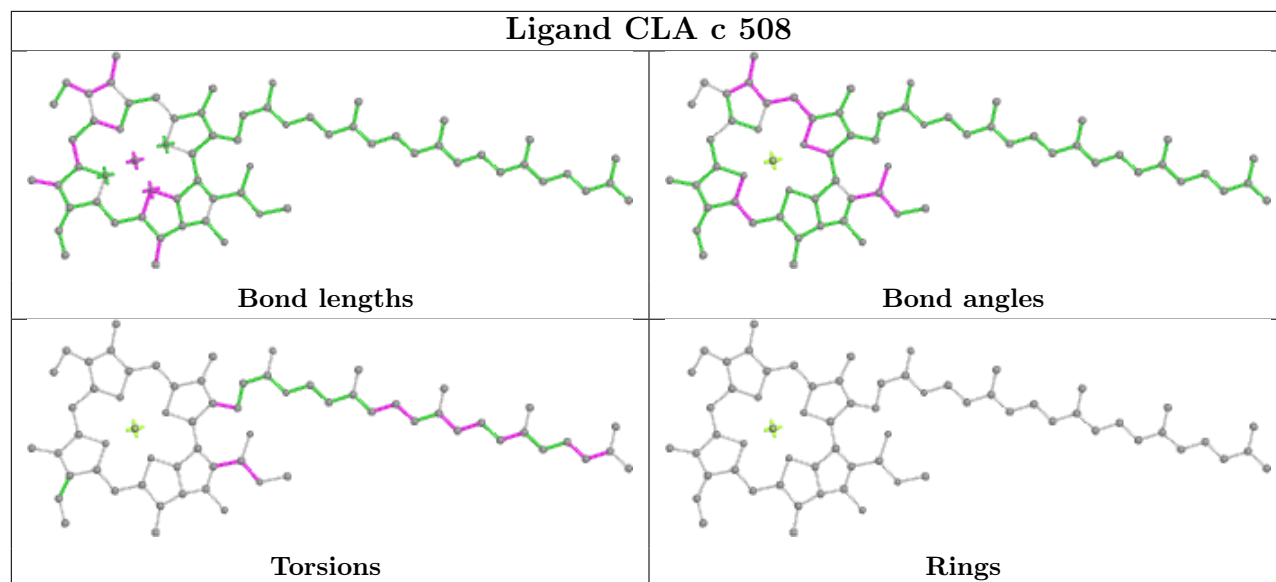
Ligand CLA R 601



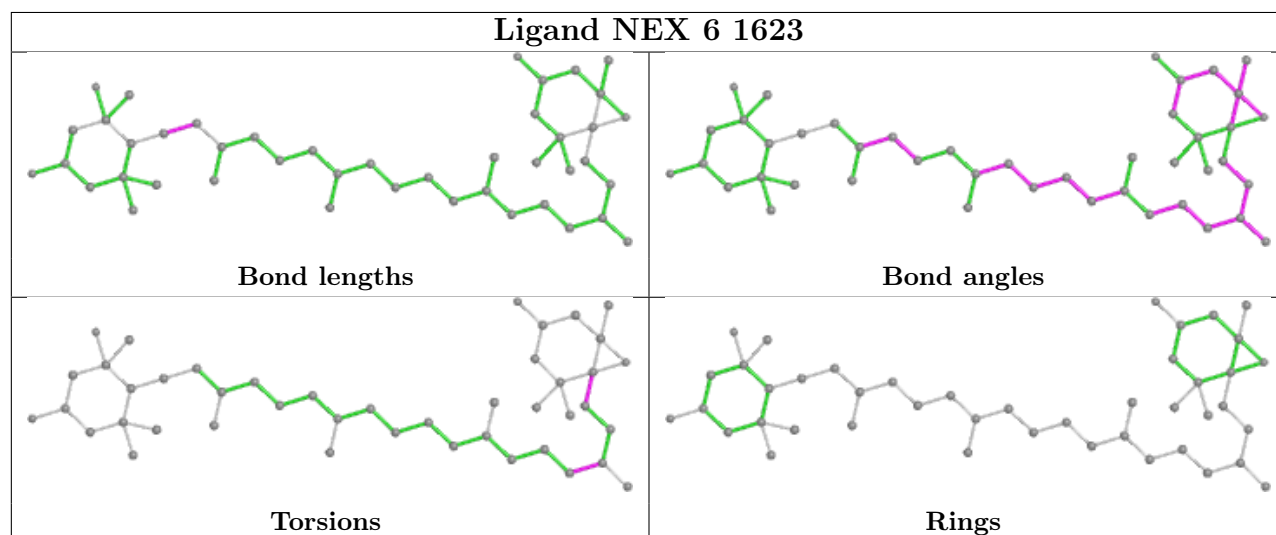
Ligand CLA C 505



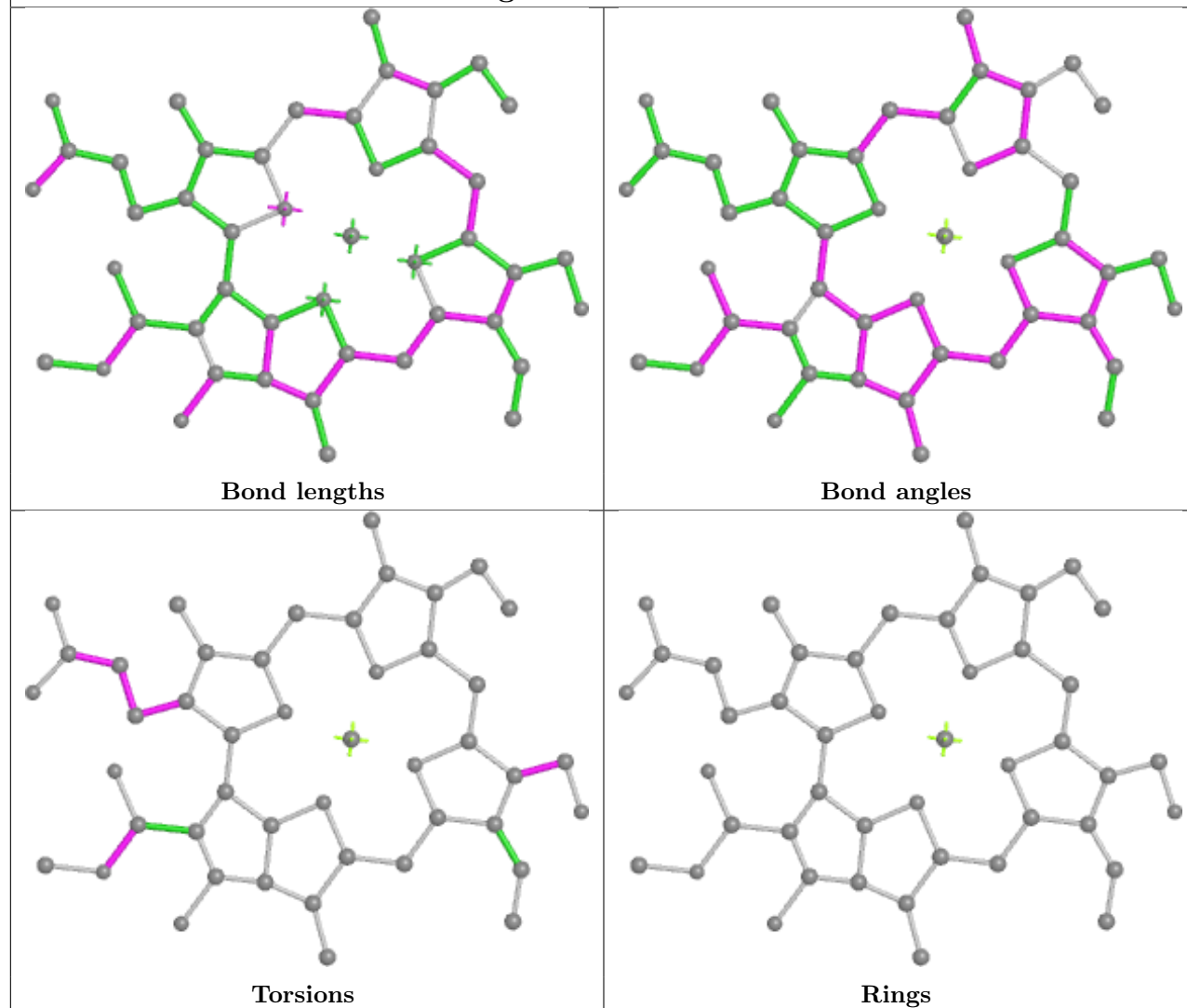
Ligand CLA c 508



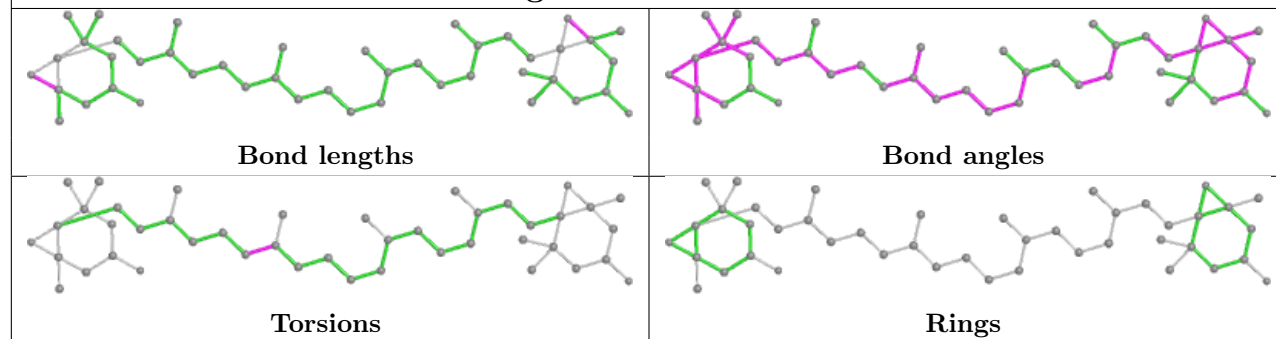
Ligand NEX 6 1623

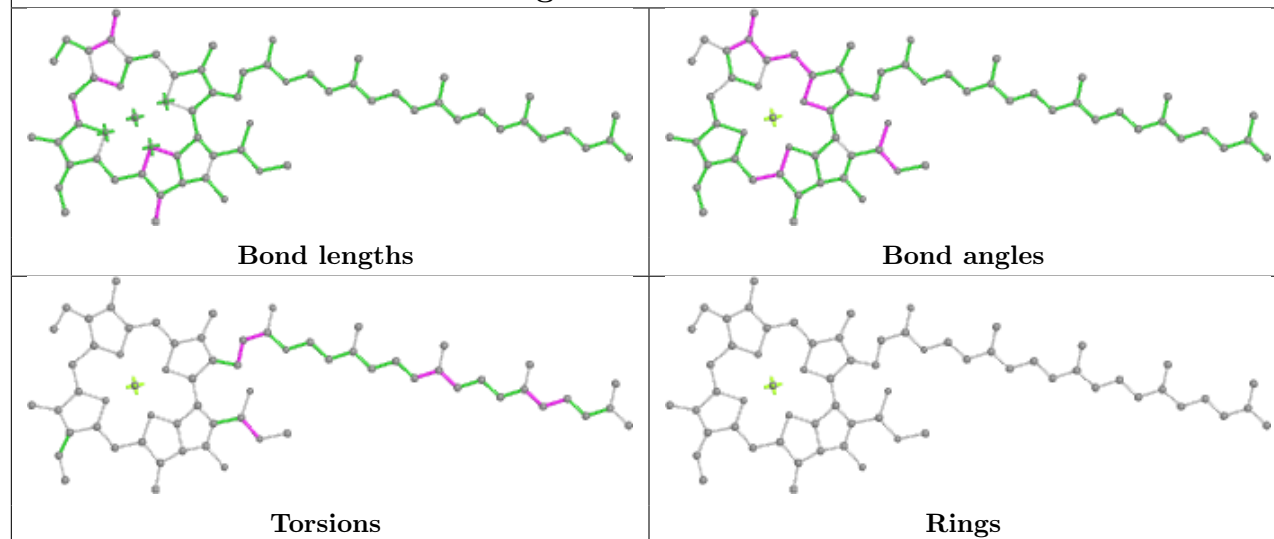
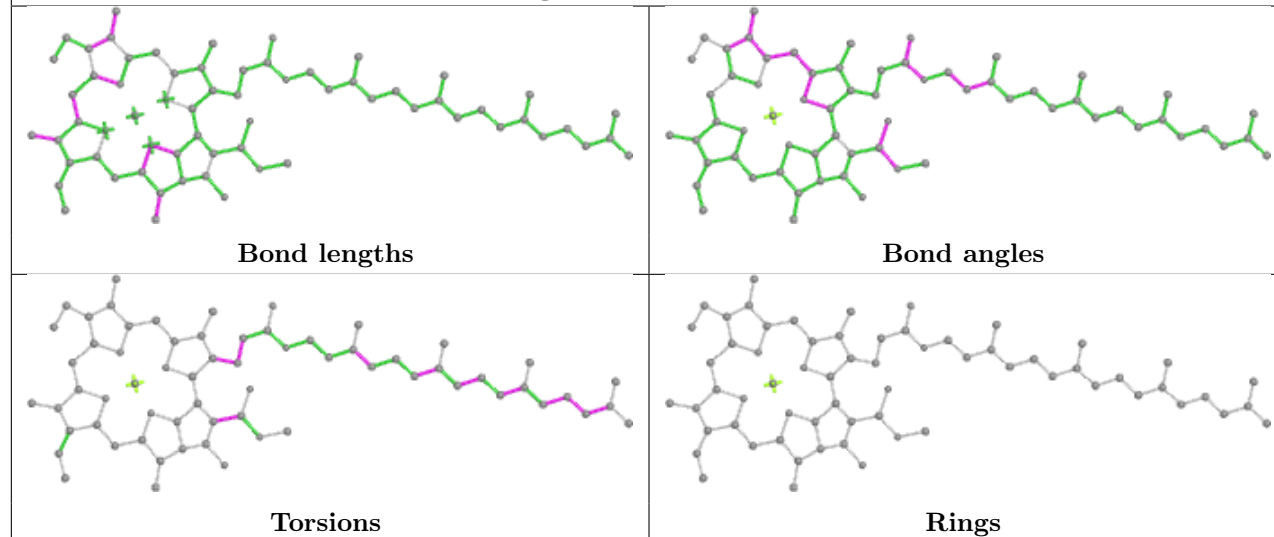


Ligand CHL 8 606

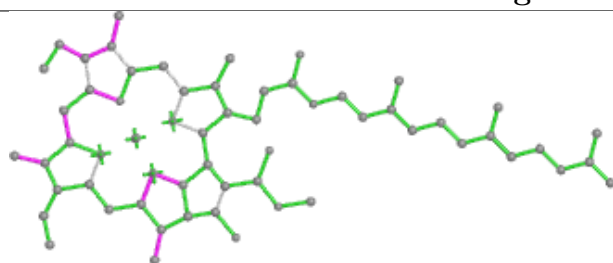


Ligand XAT 1 1622

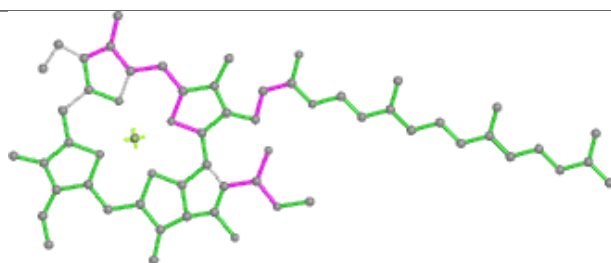


Ligand CLA 5 613**Ligand CLA 1 610**

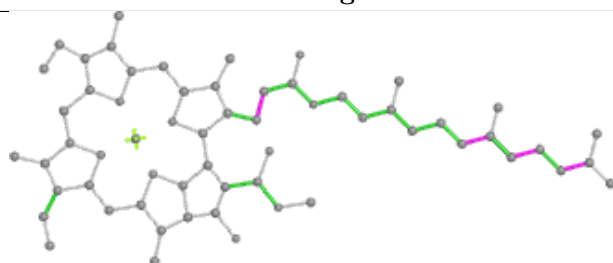
Ligand CLA R 602



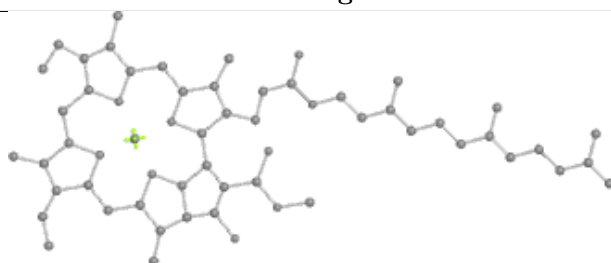
Bond lengths



Bond angles

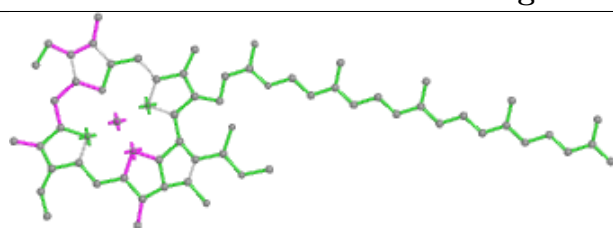


Torsions

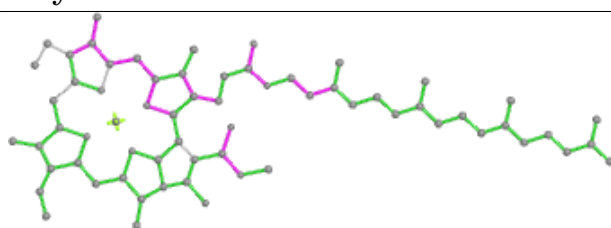


Rings

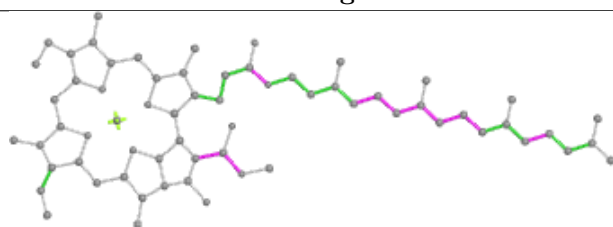
Ligand CLA y 612



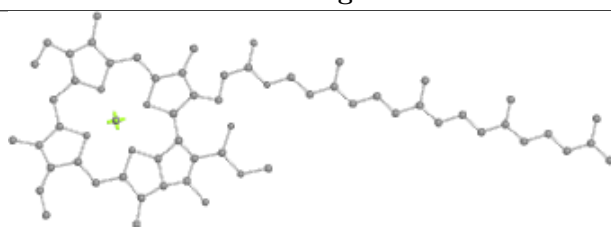
Bond lengths



Bond angles

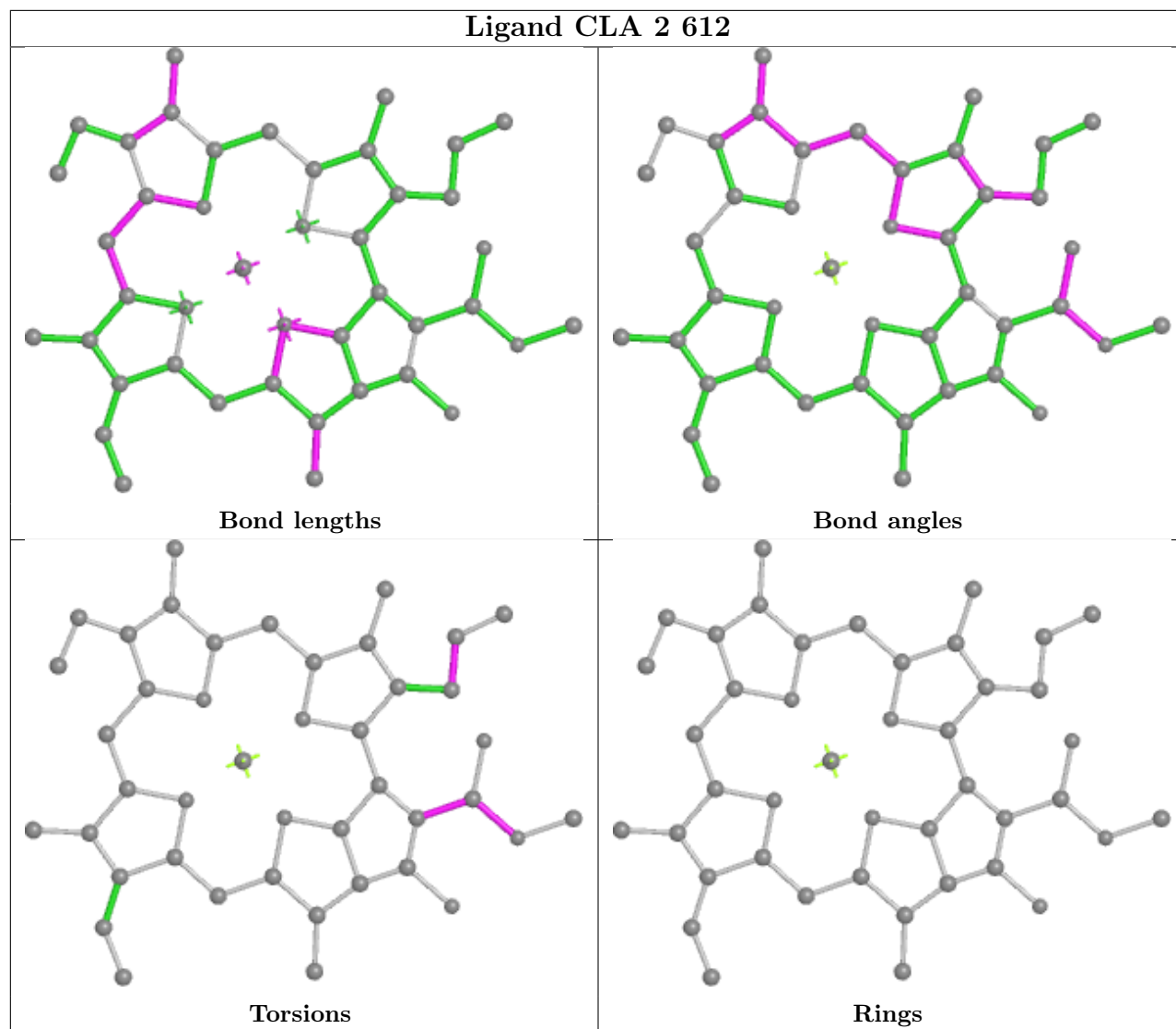


Torsions

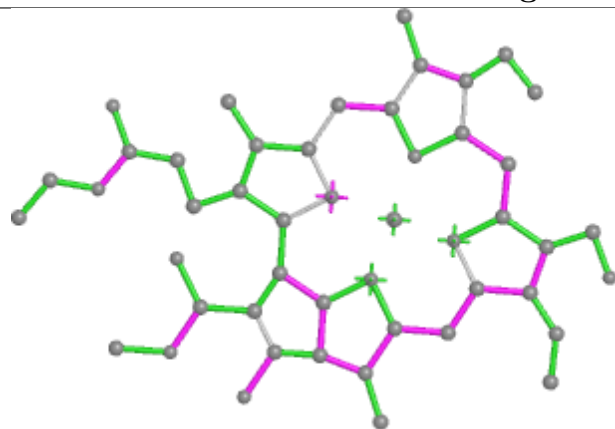


Rings

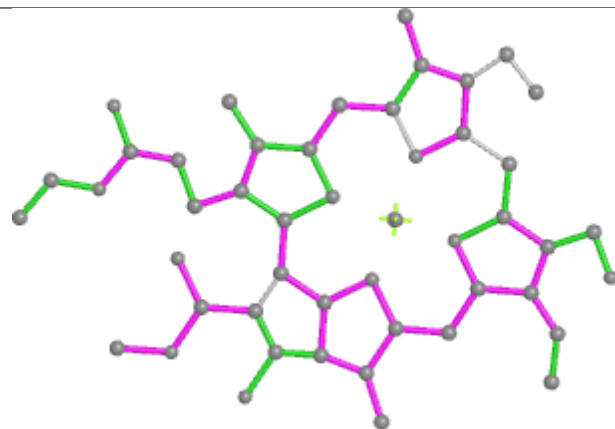
Ligand CLA 2 612



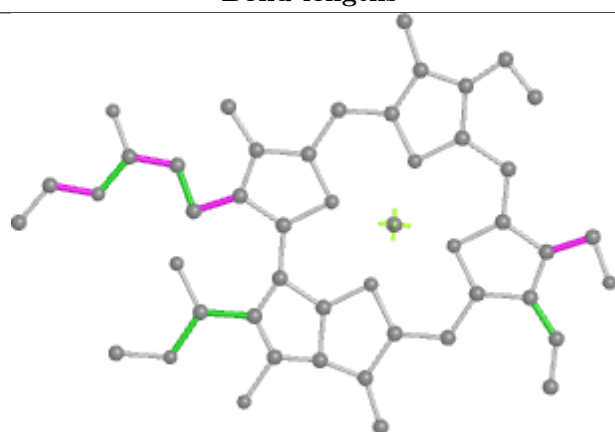
Ligand CHL 9 605



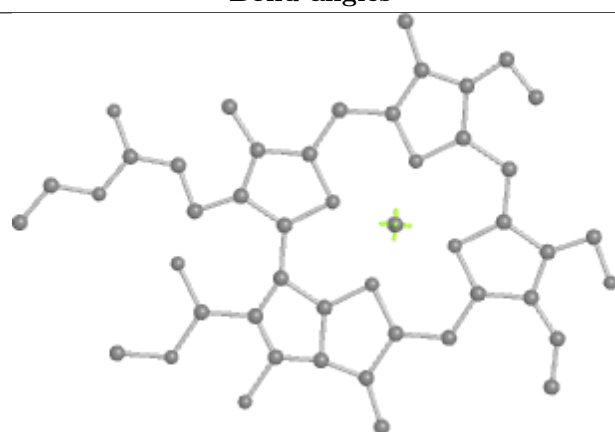
Bond lengths



Bond angles

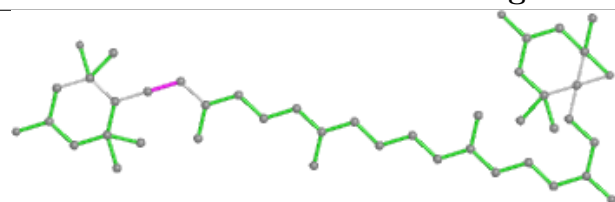


Torsions

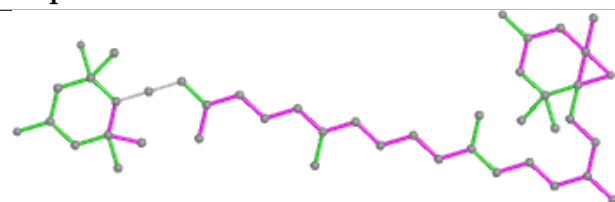


Rings

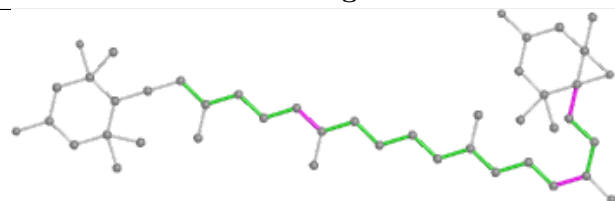
Ligand NEX p 1623



Bond lengths



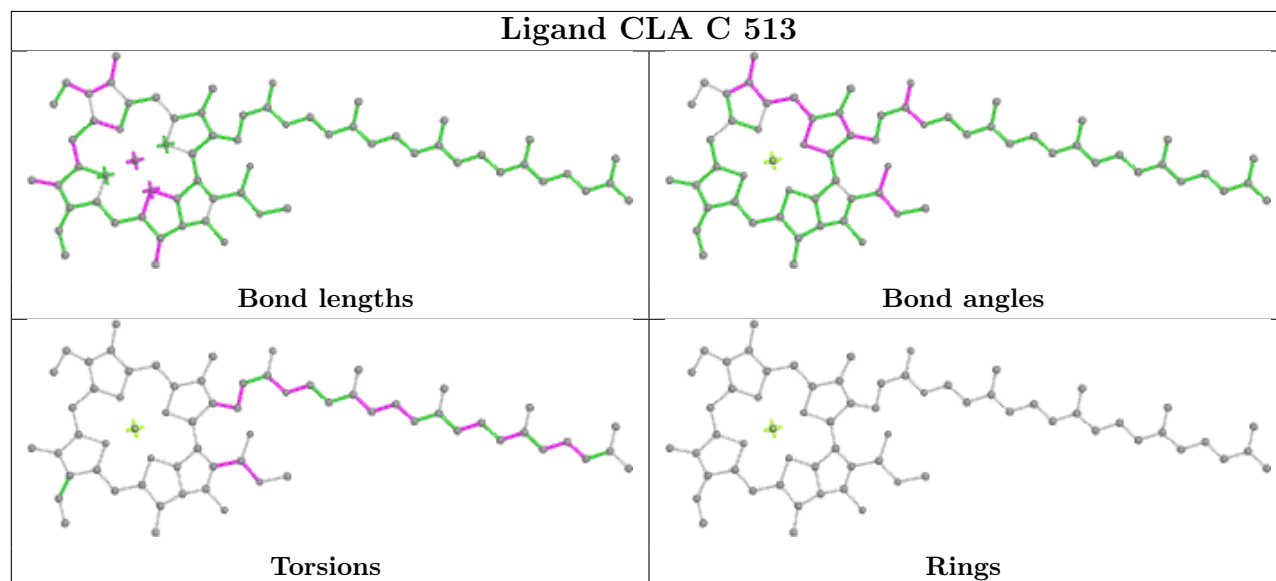
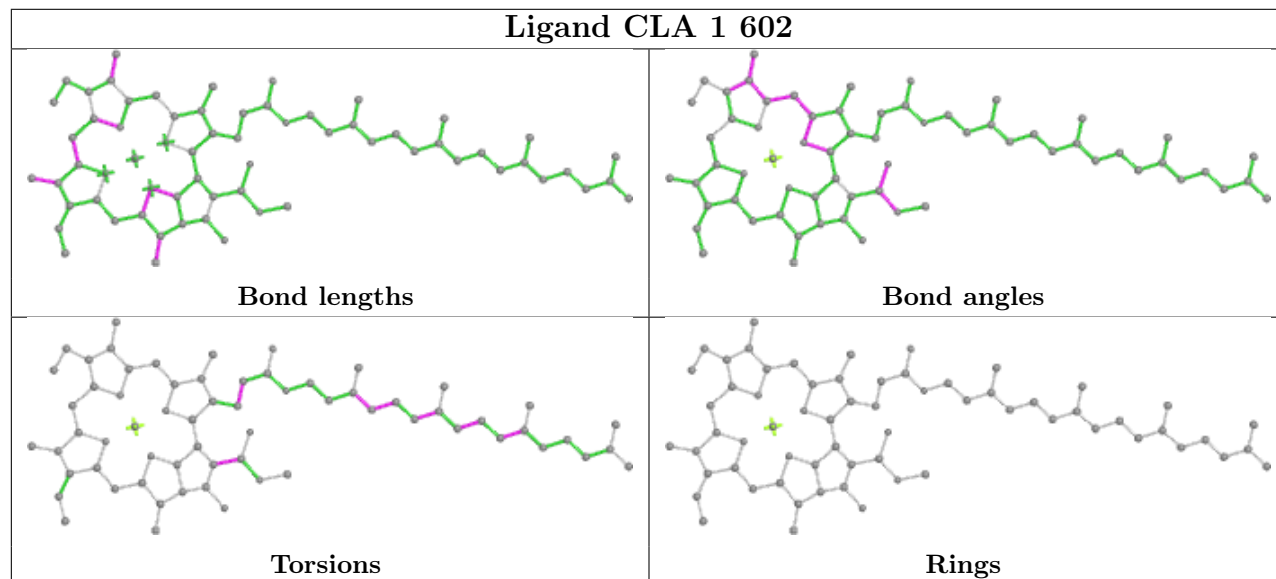
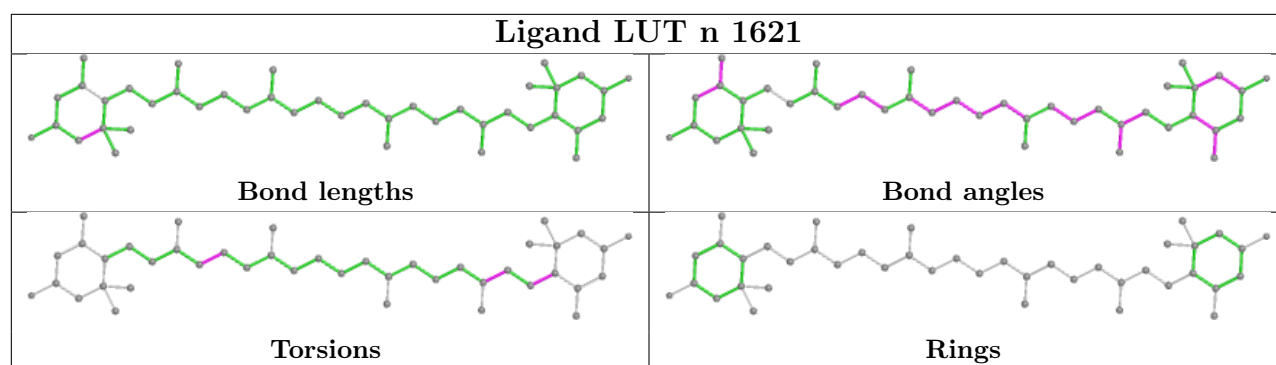
Bond angles



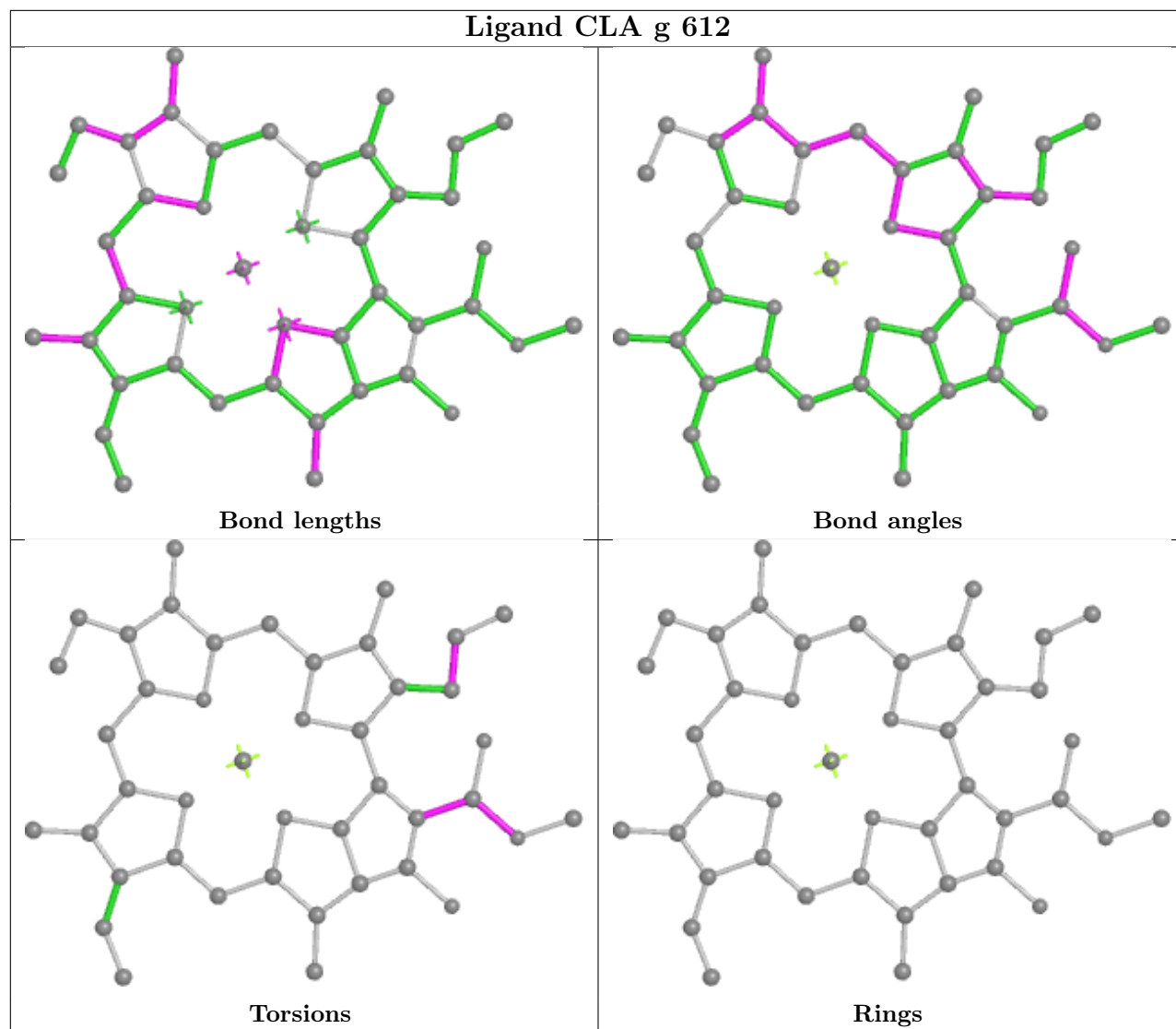
Torsions



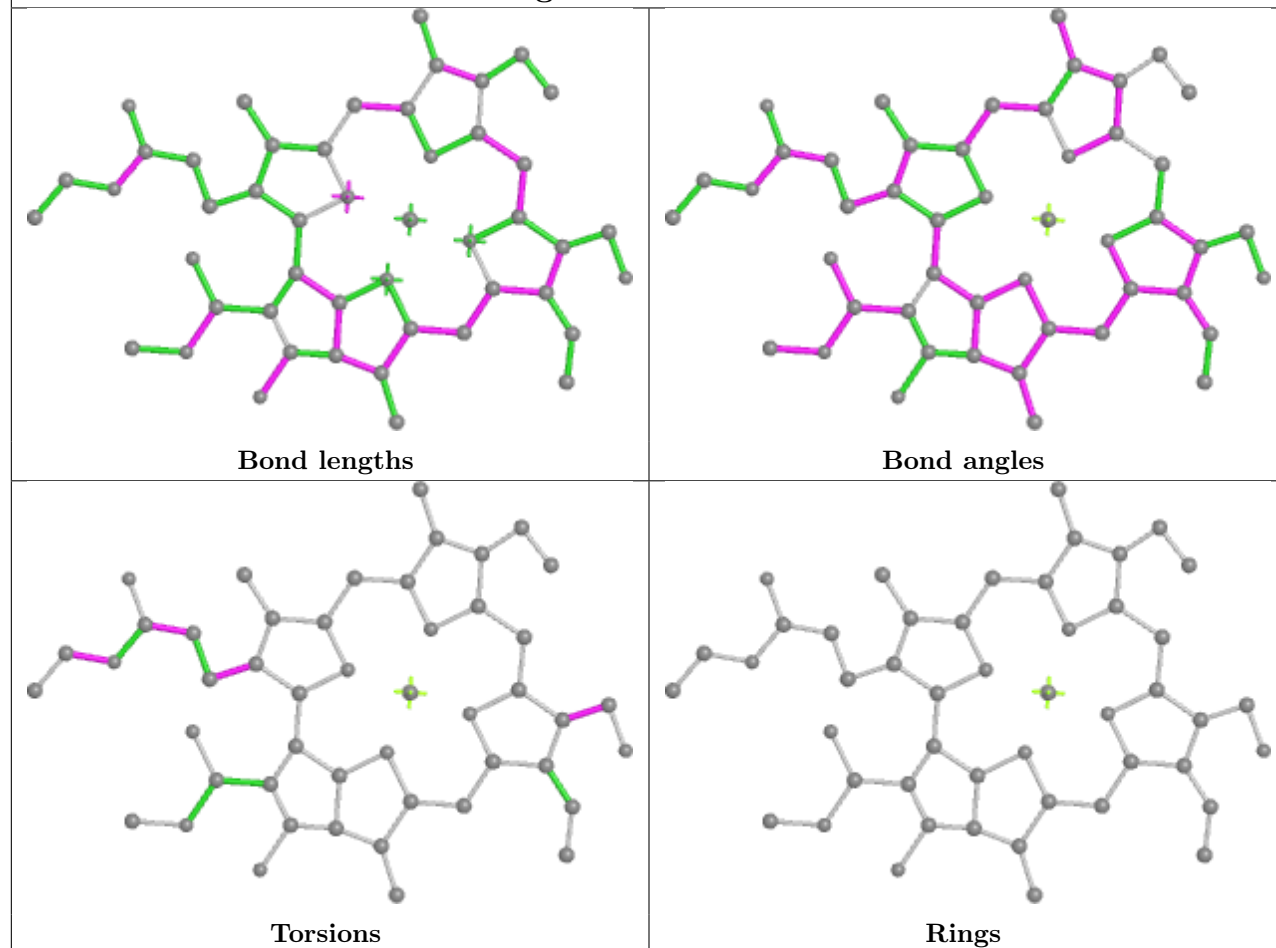
Rings



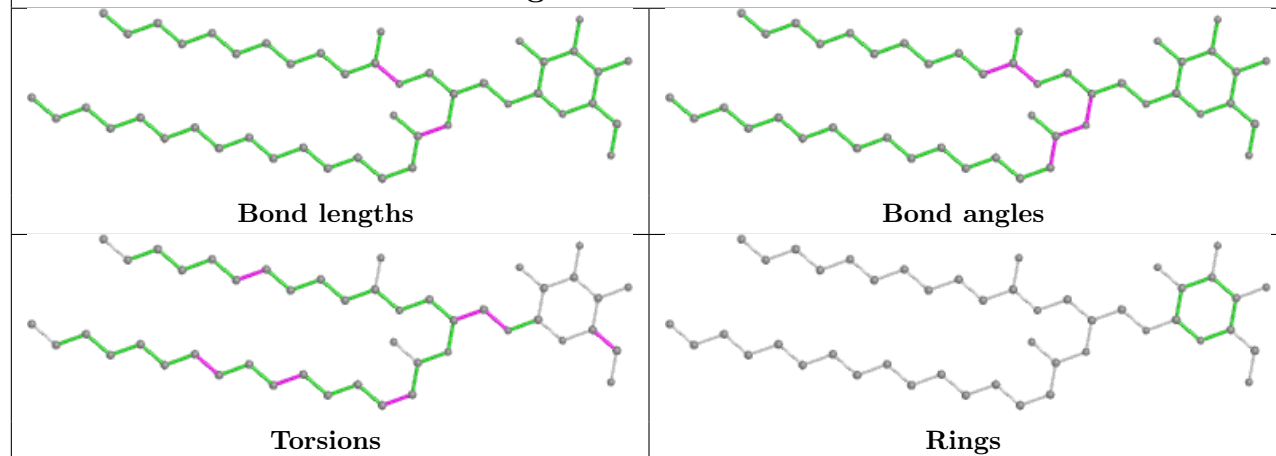
Ligand CLA g 612

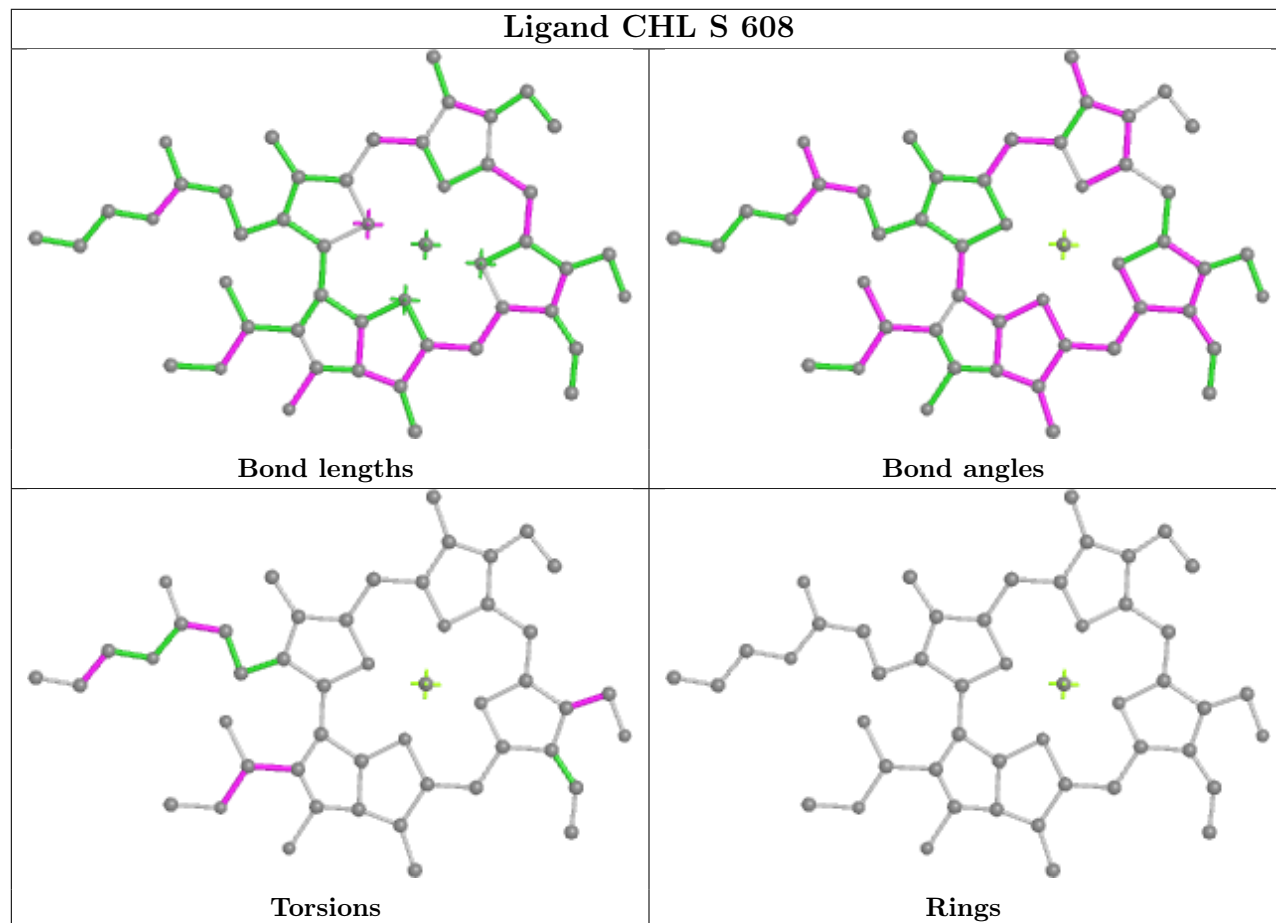
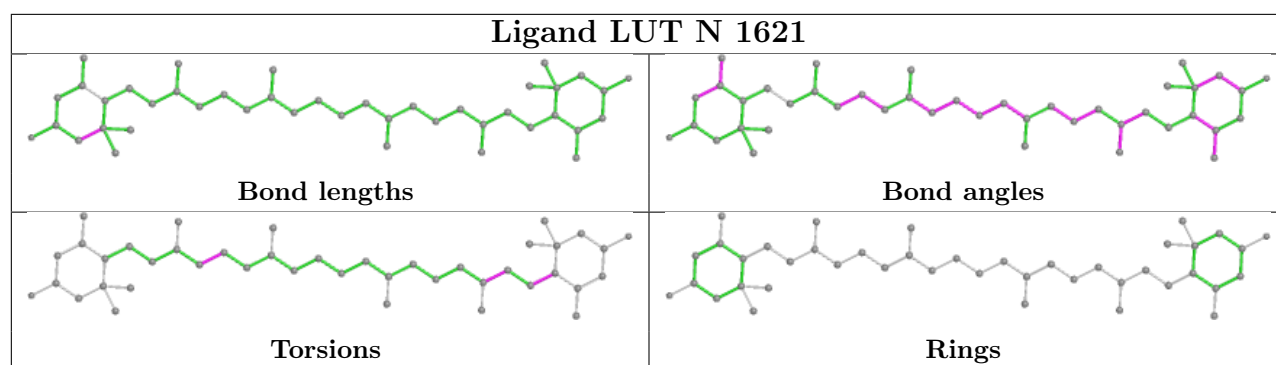


Ligand CHL 2 605

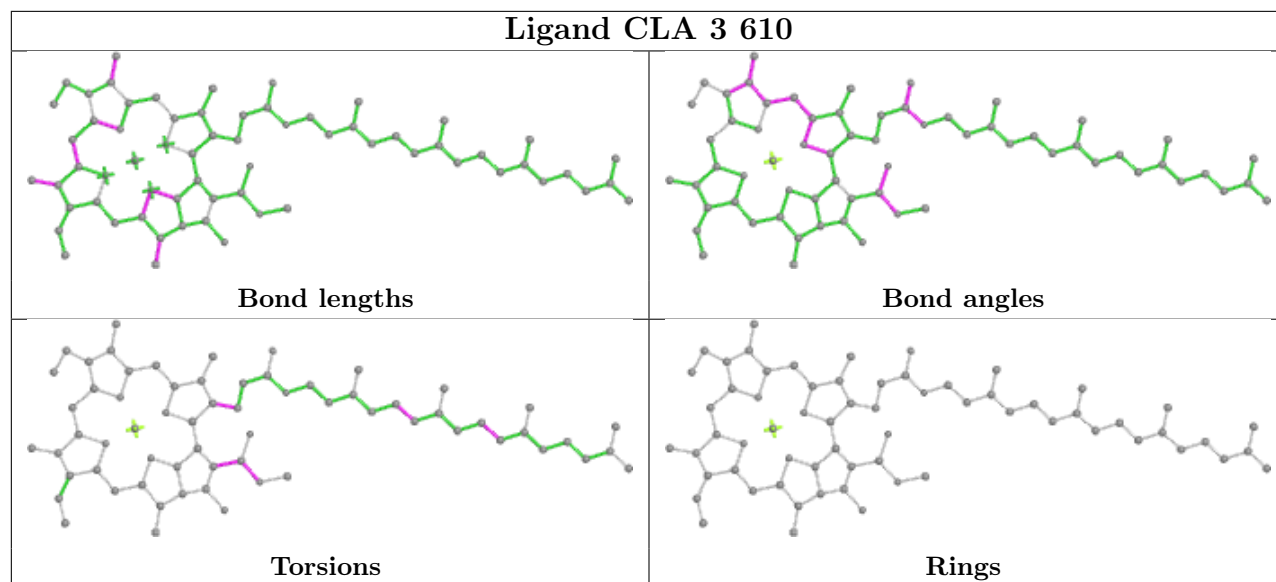


Ligand LMG D 411

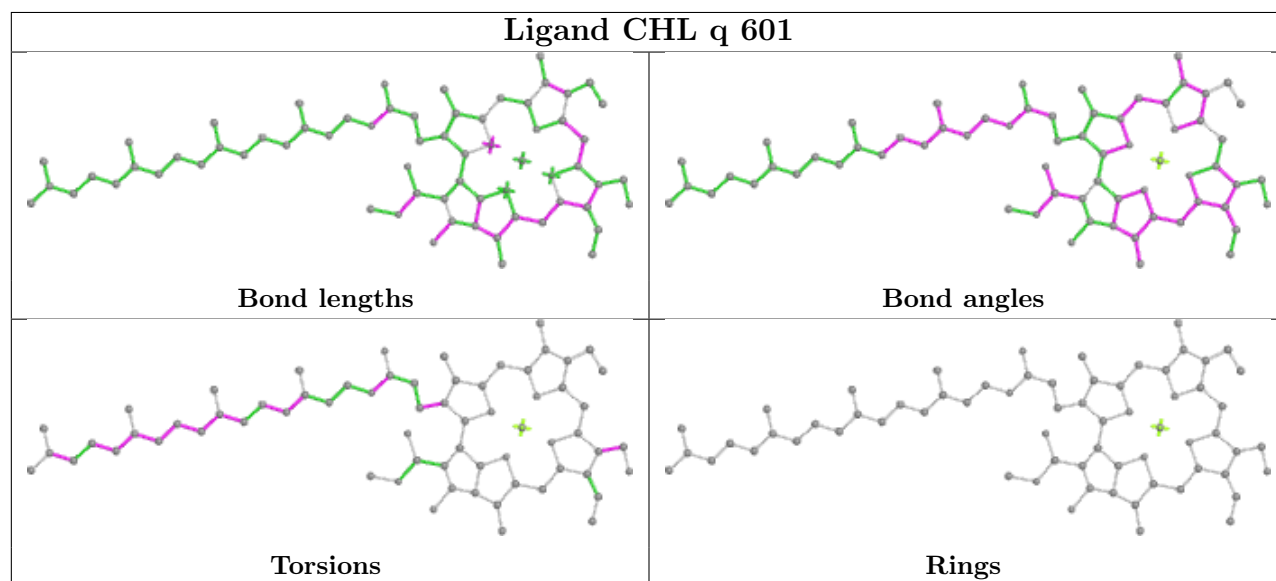




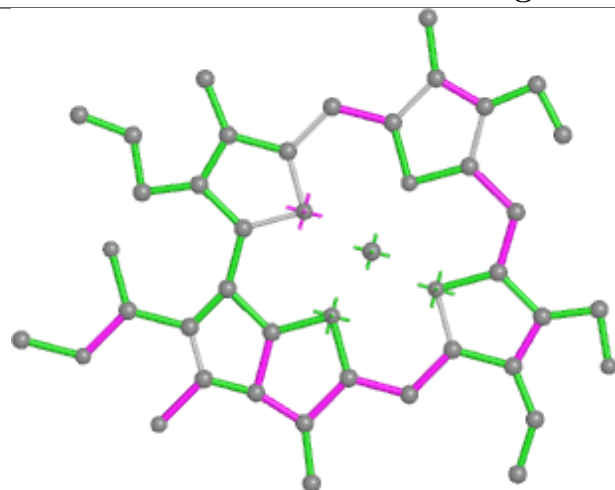
Ligand CLA 3 610



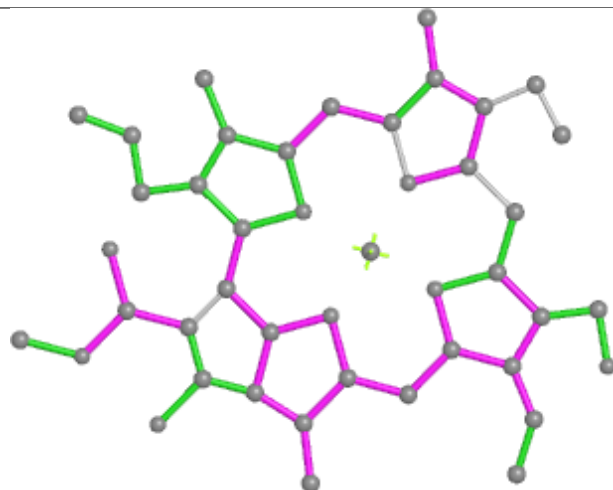
Ligand CHL q 601



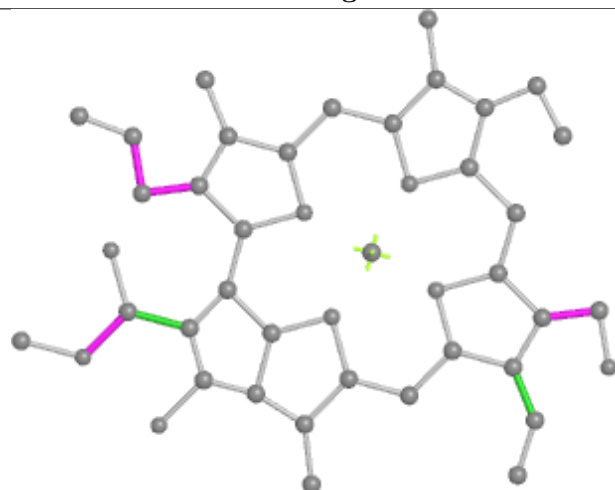
Ligand CHL G 608



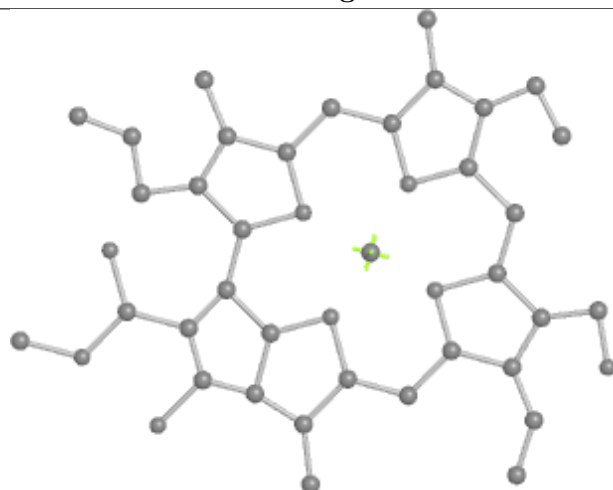
Bond lengths



Bond angles

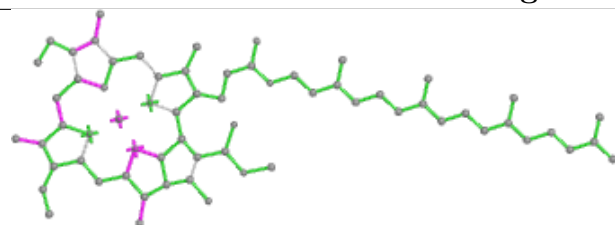


Torsions

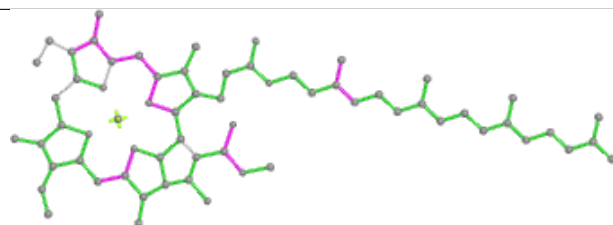


Rings

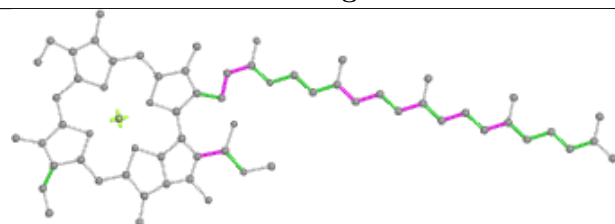
Ligand CLA 7 602



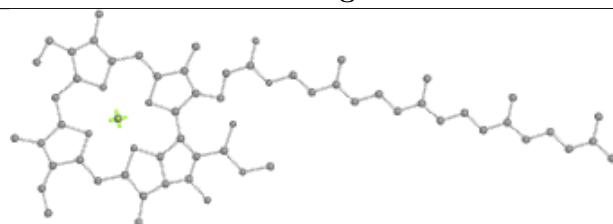
Bond lengths



Bond angles

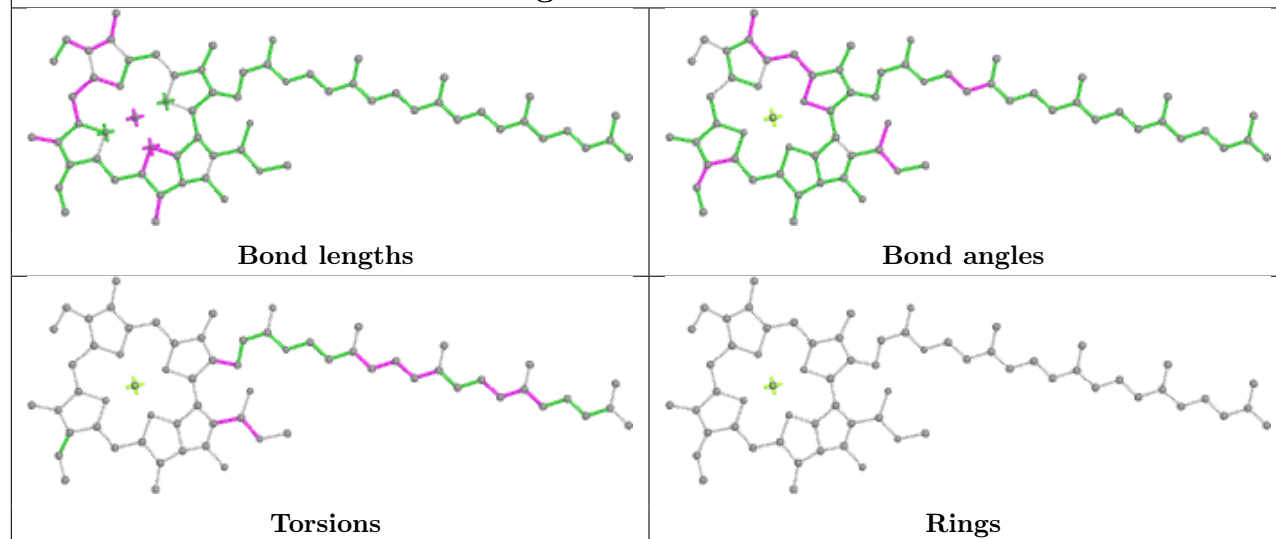


Torsions

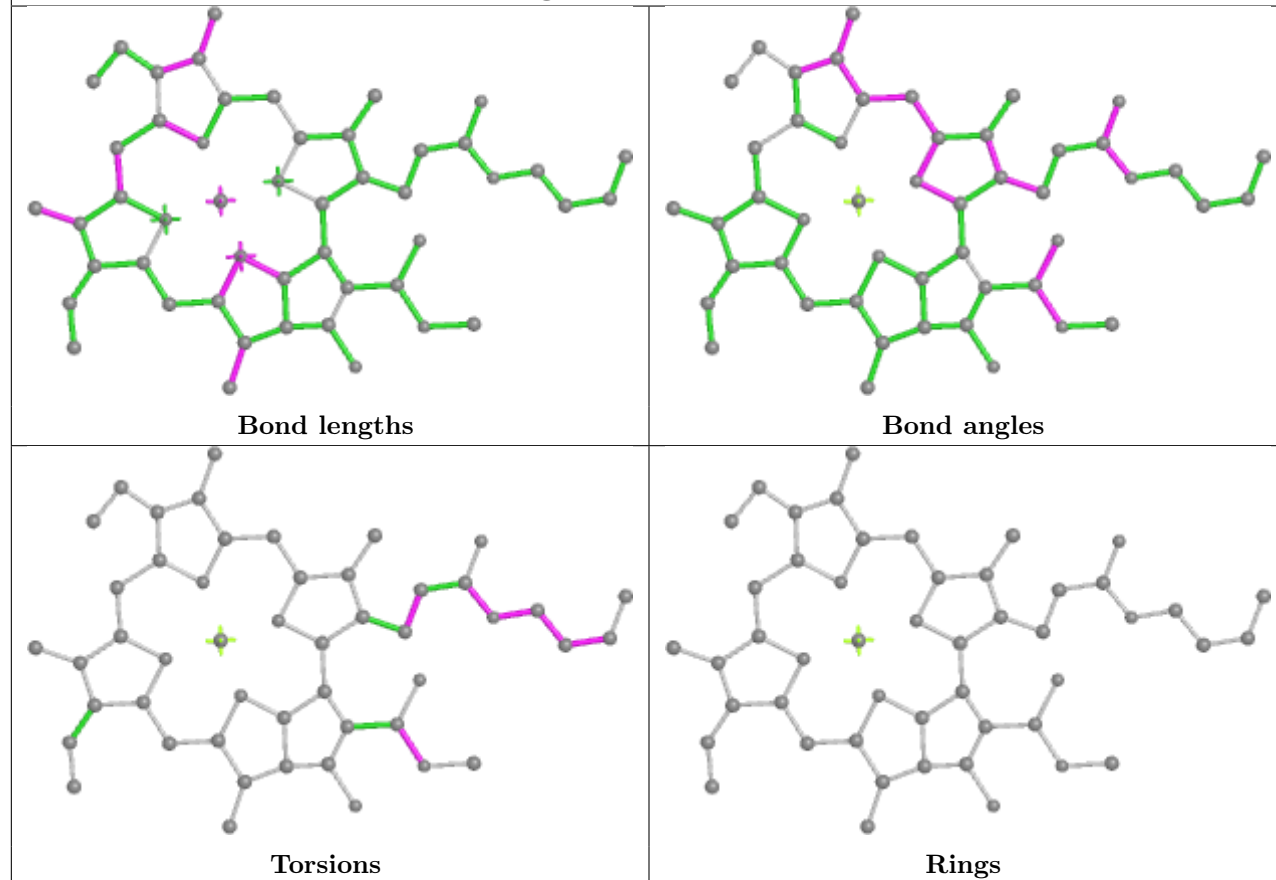


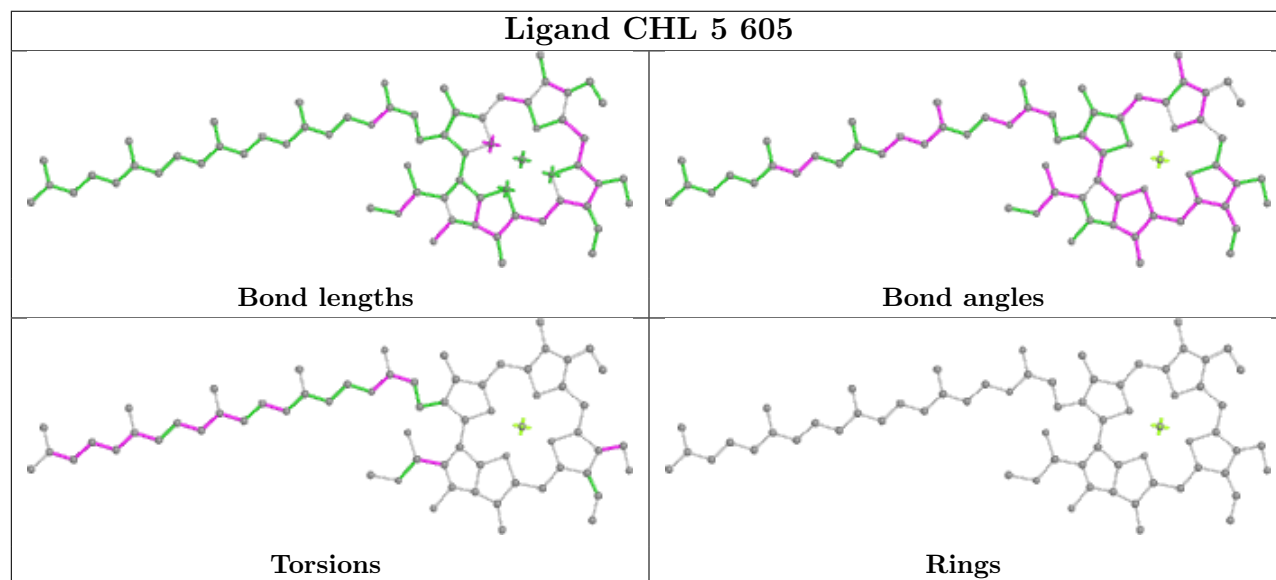
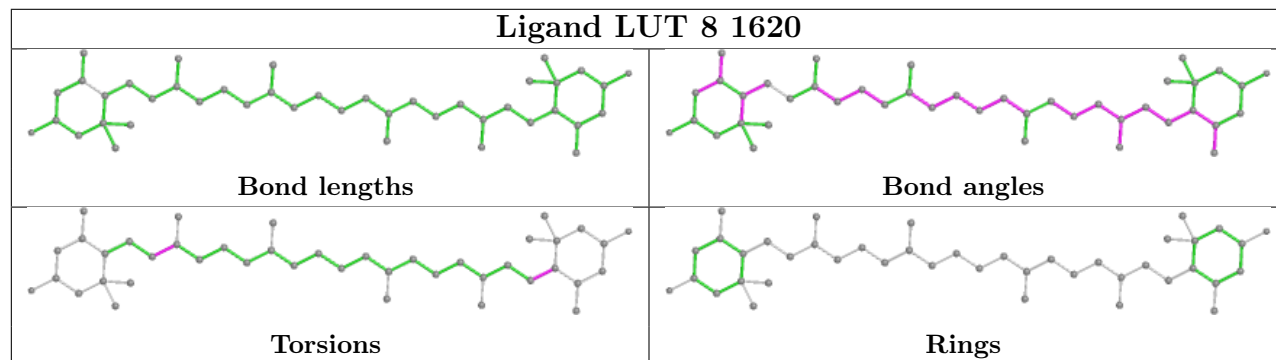
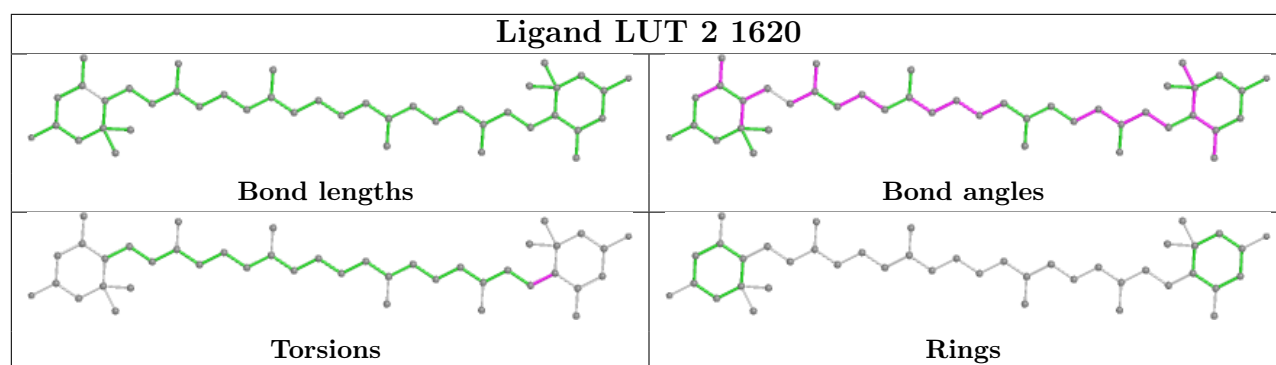
Rings

Ligand CLA 1 604

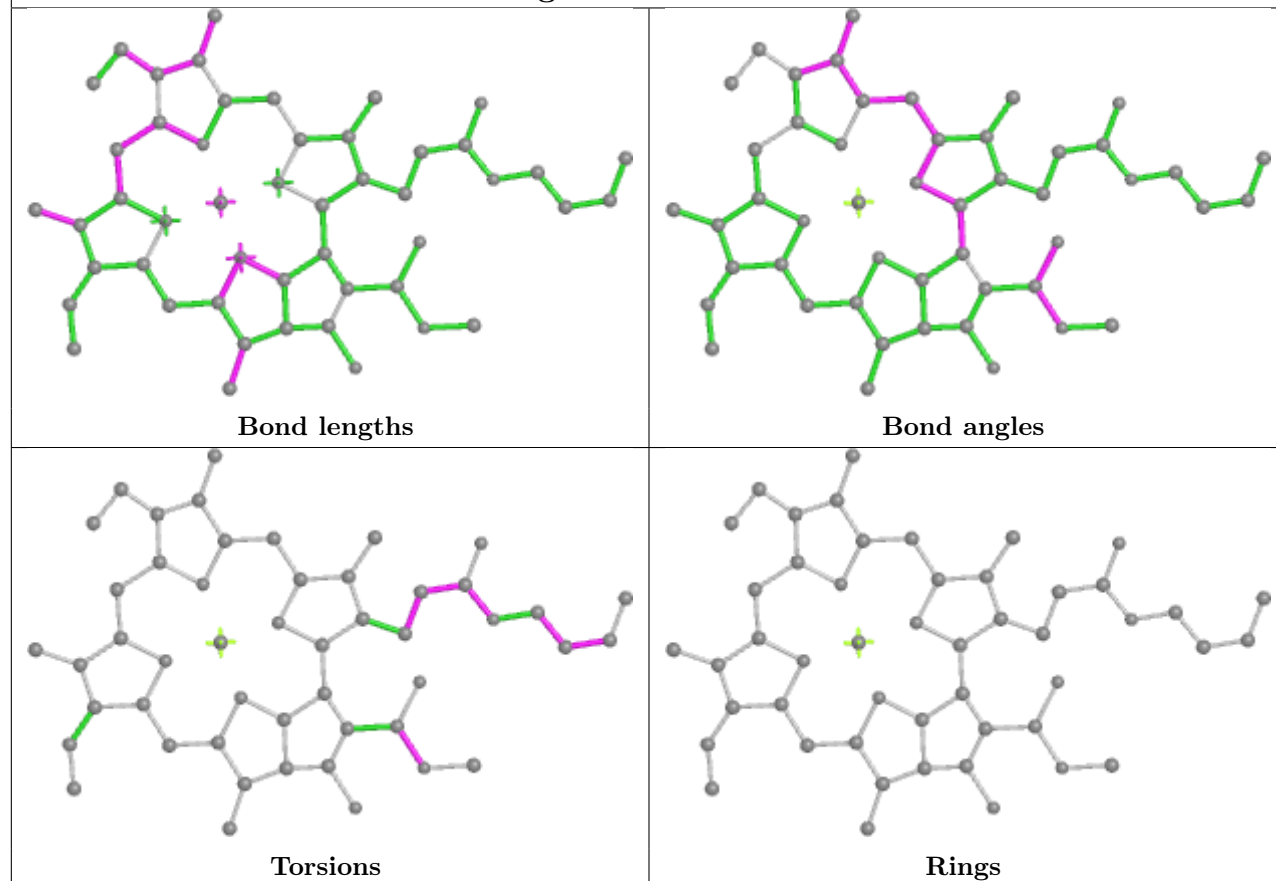


Ligand CLA r 612

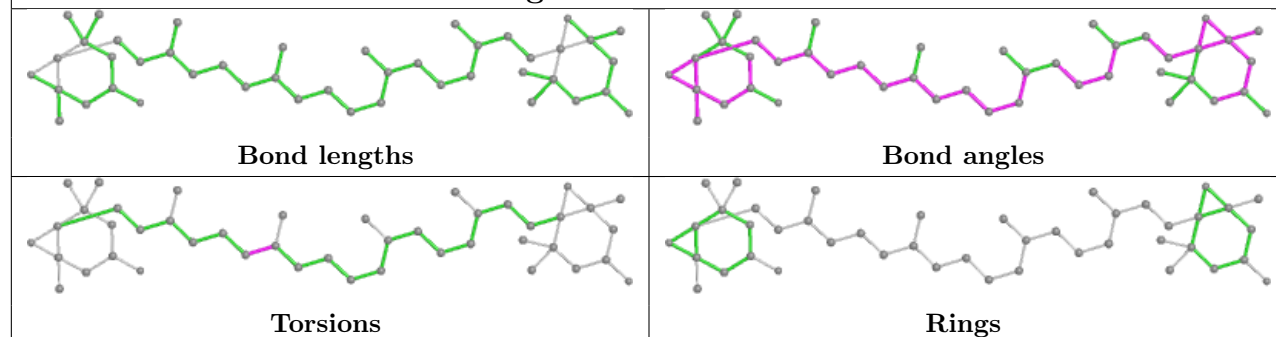


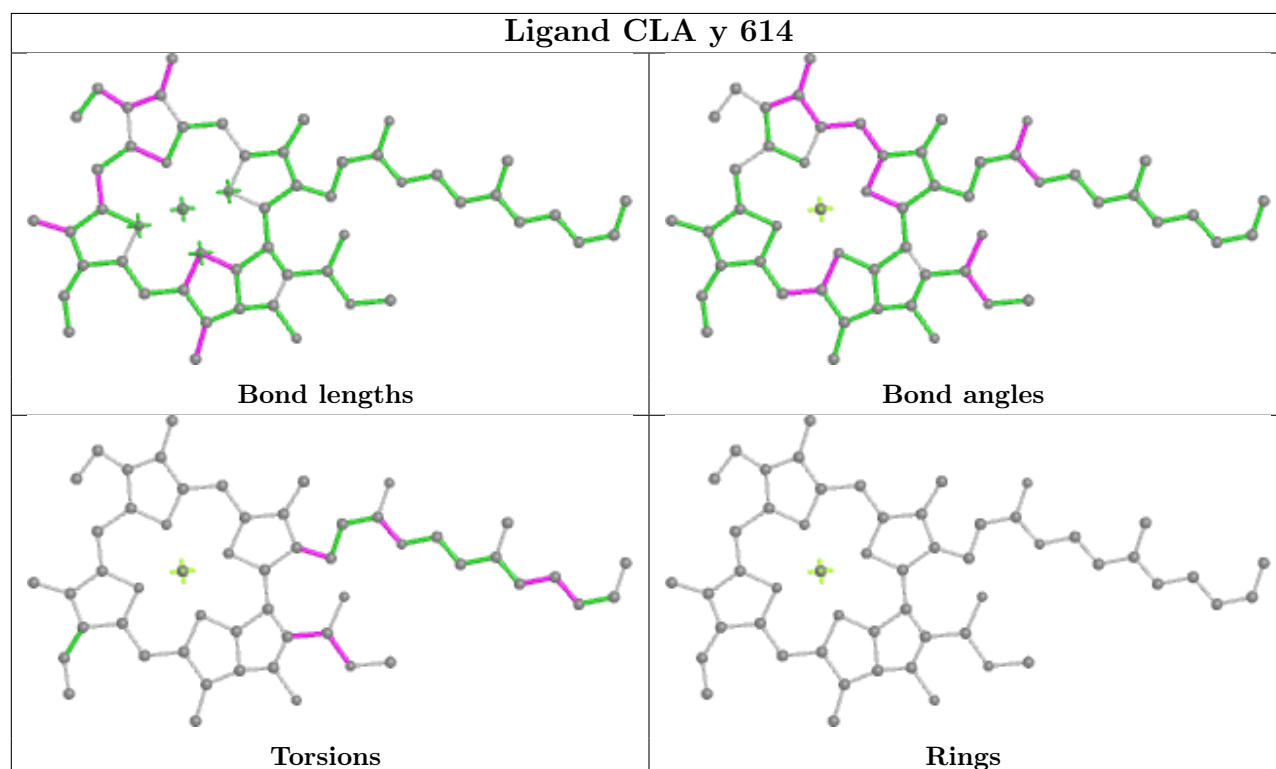
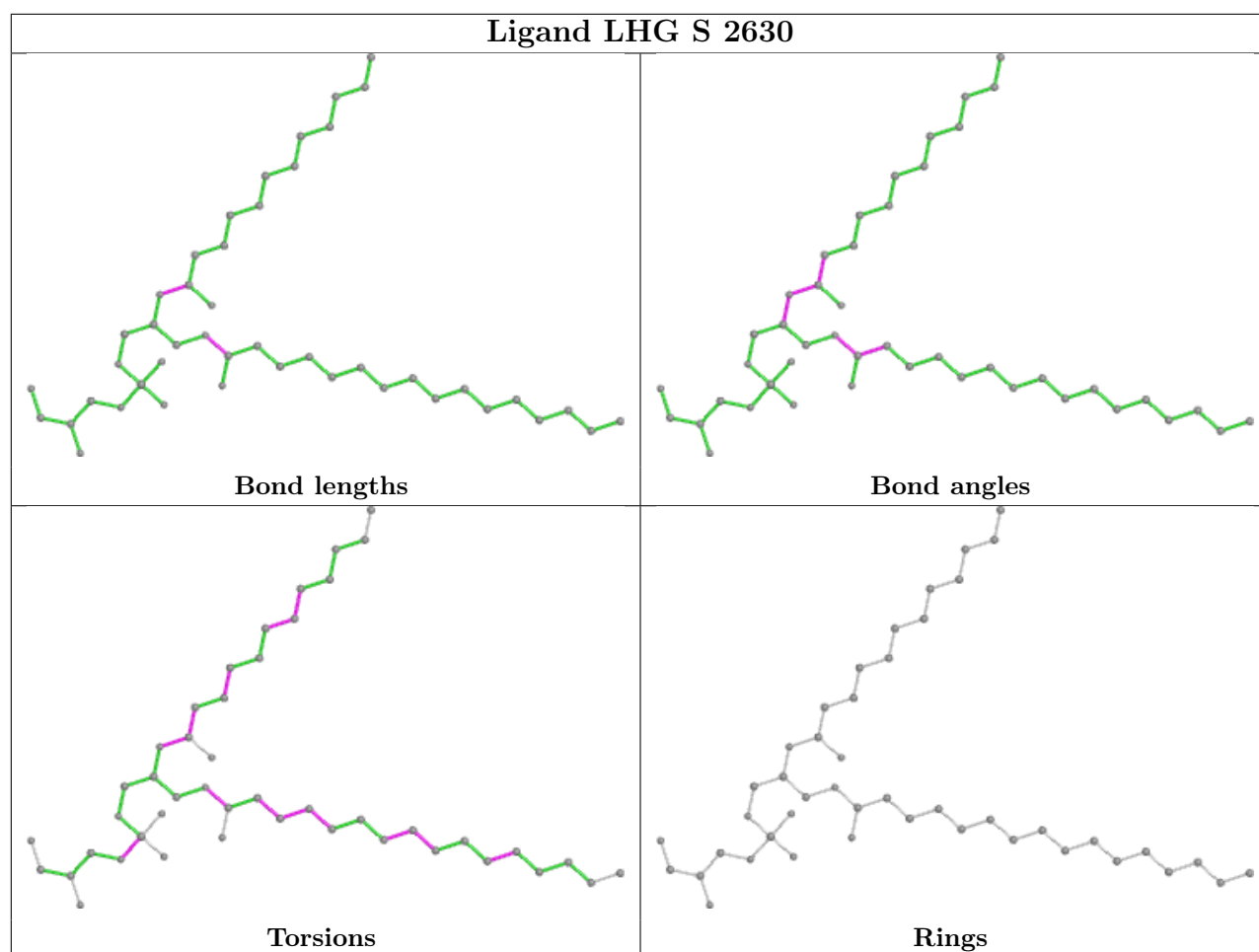


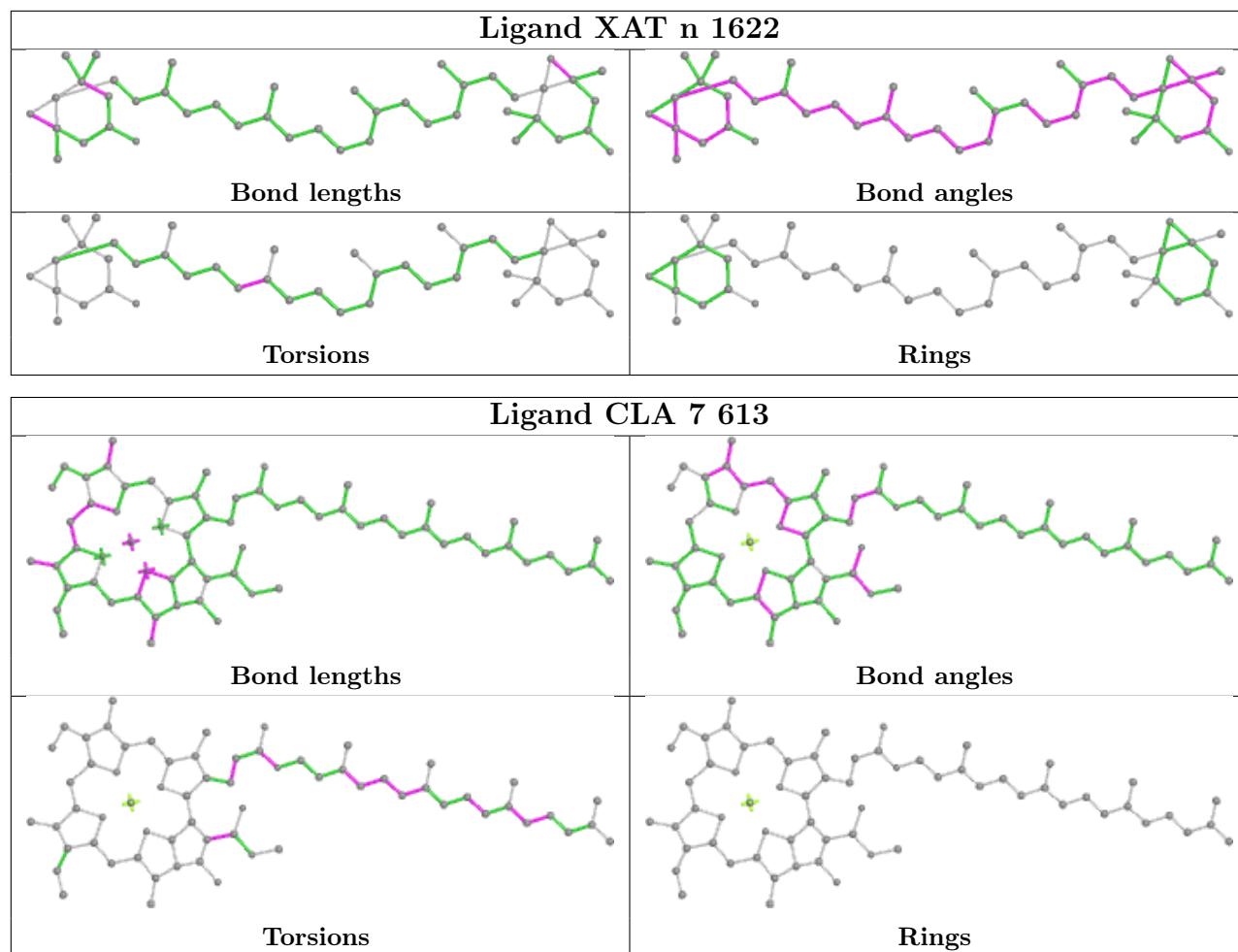
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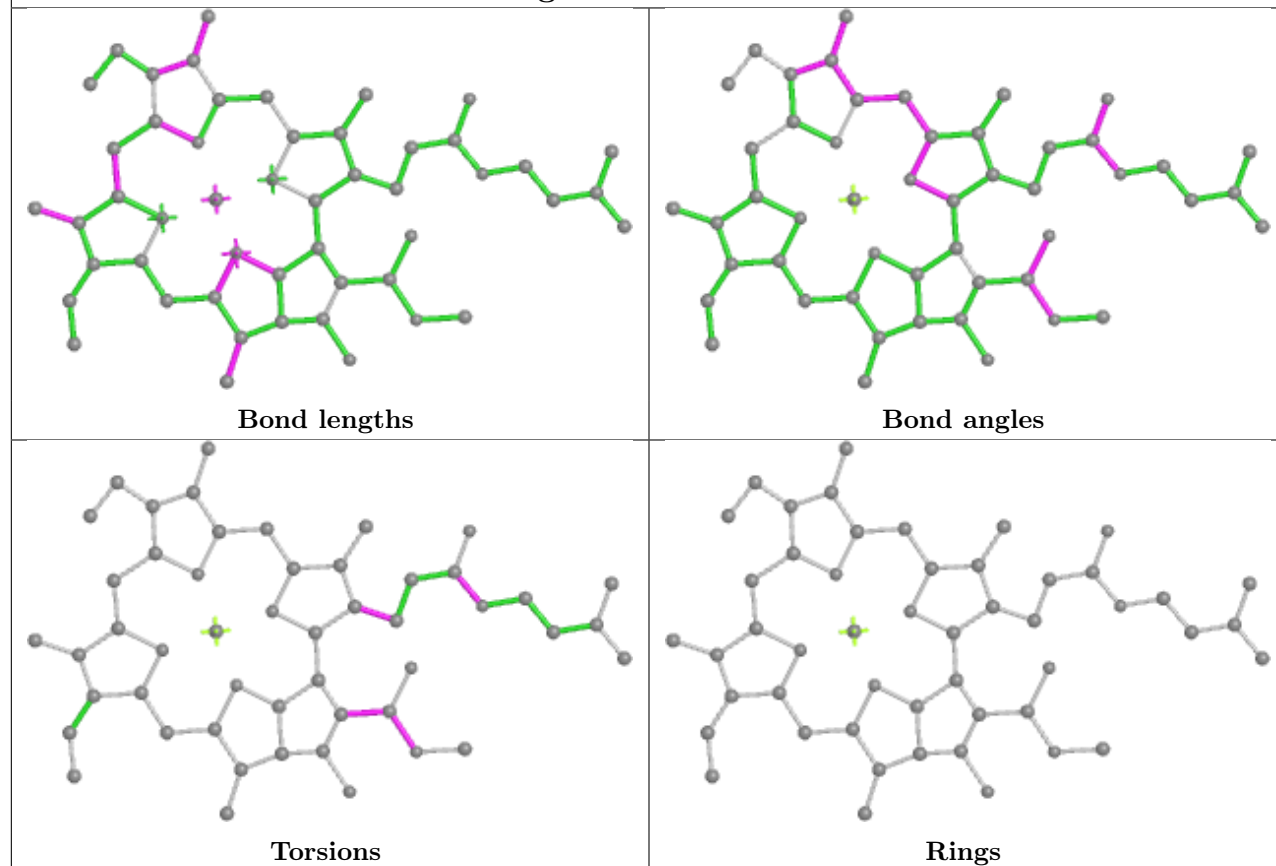
Ligand XAT 3 1622



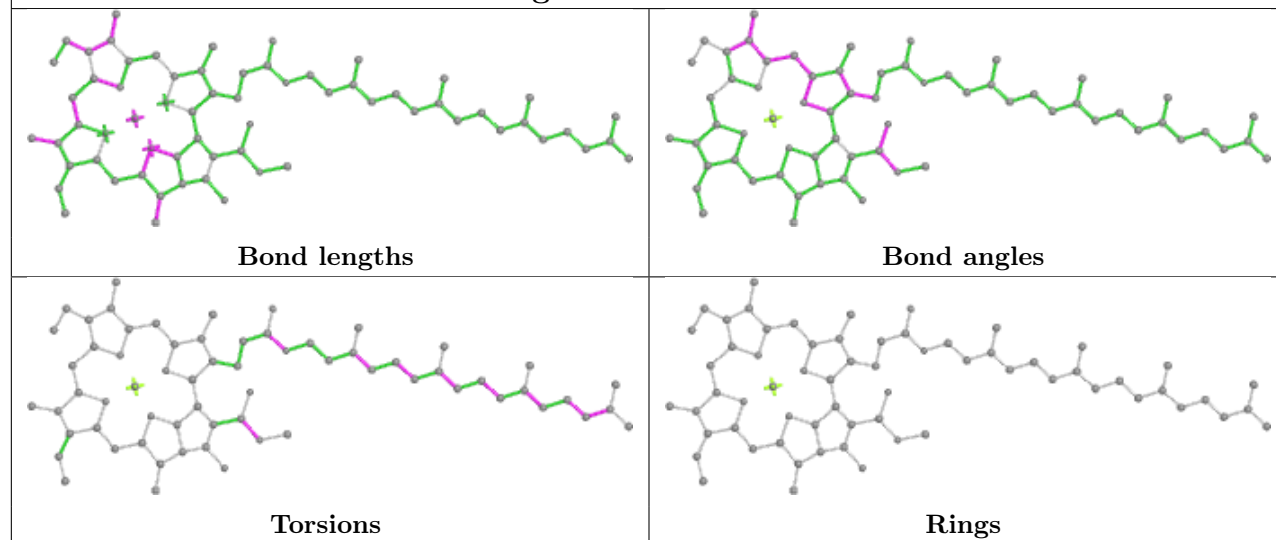


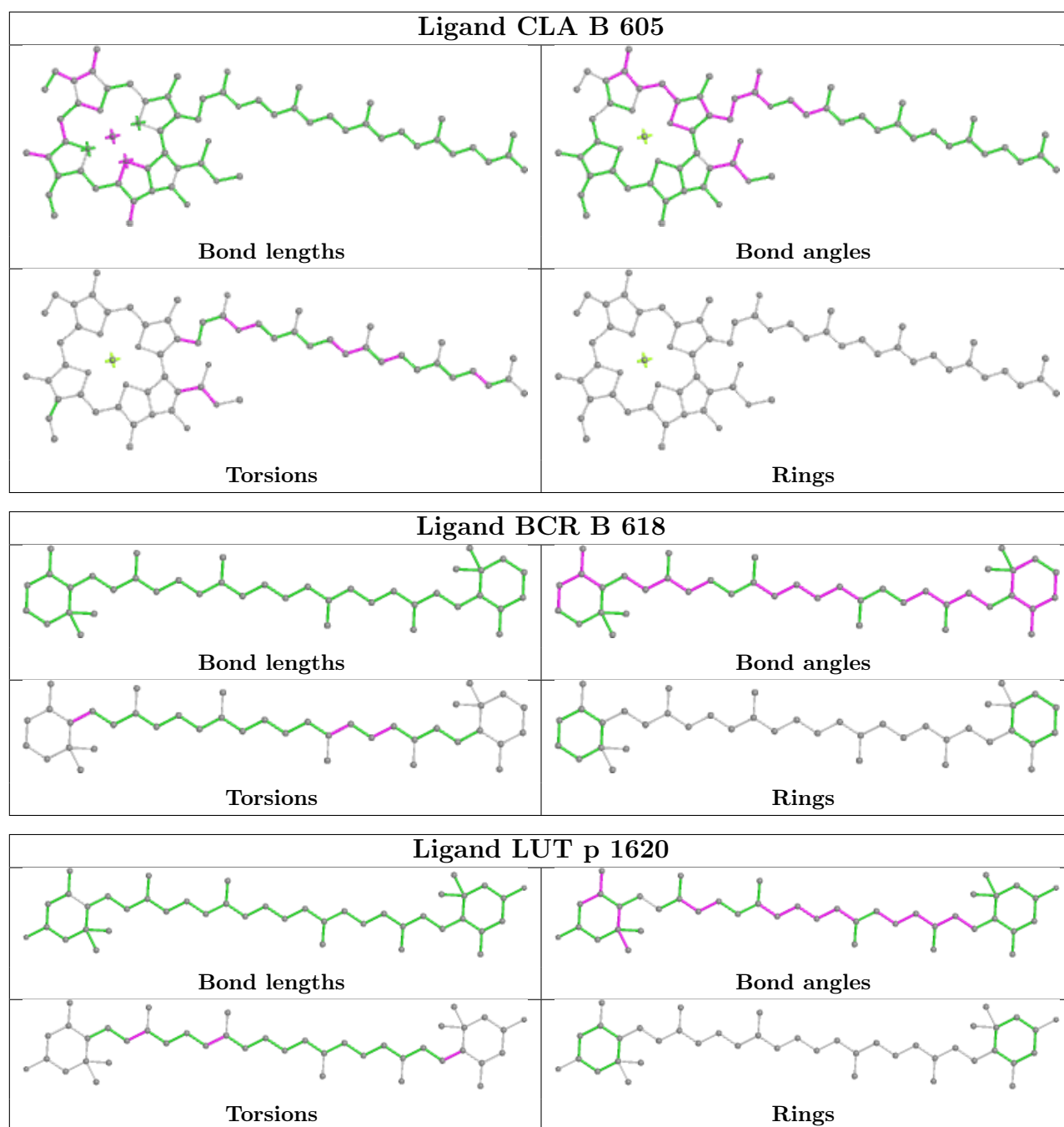


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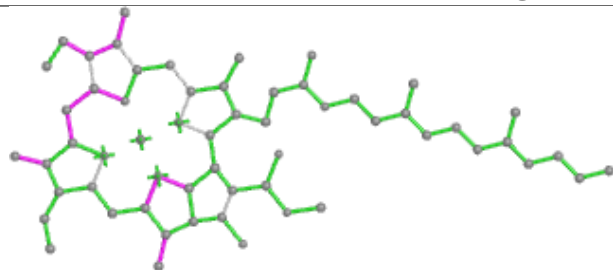


Ligand CLA C 512

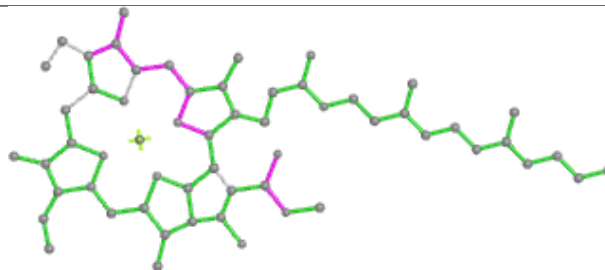




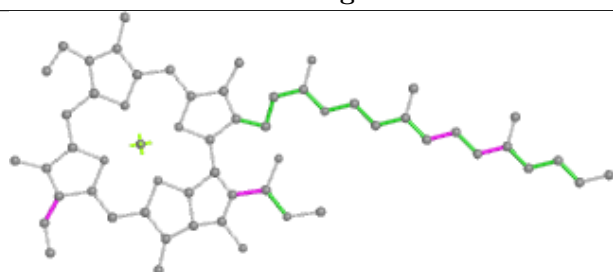
Ligand CLA R 609



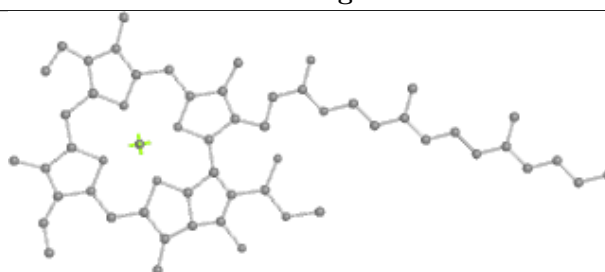
Bond lengths



Bond angles

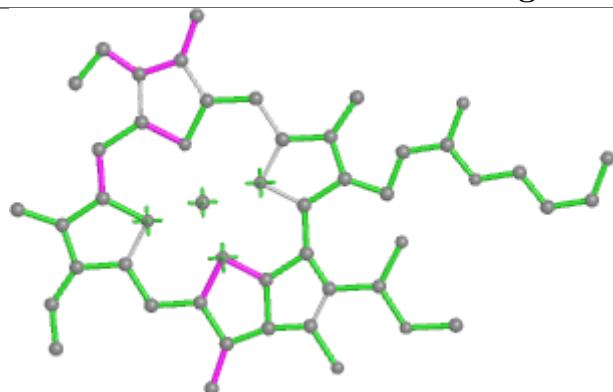


Torsions

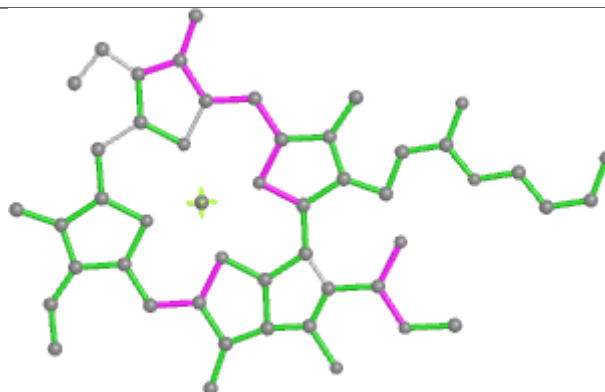


Rings

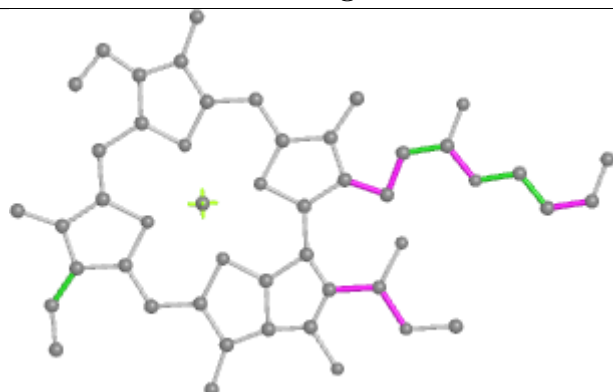
Ligand CLA 9 614



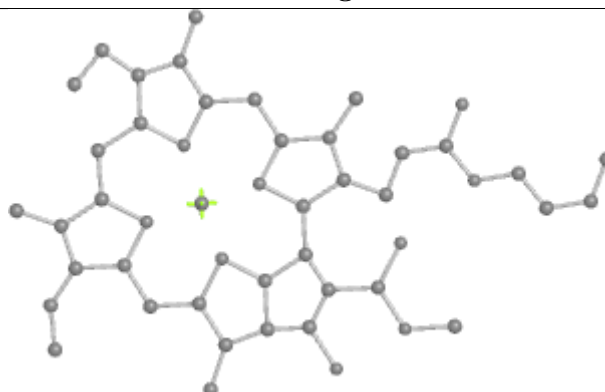
Bond lengths



Bond angles

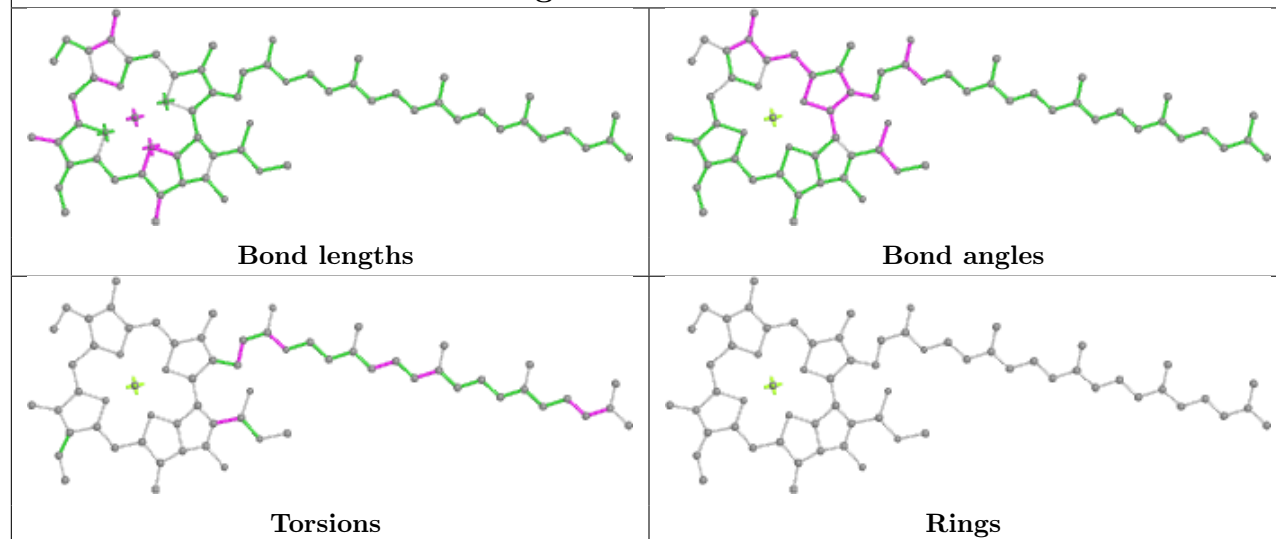


Torsions

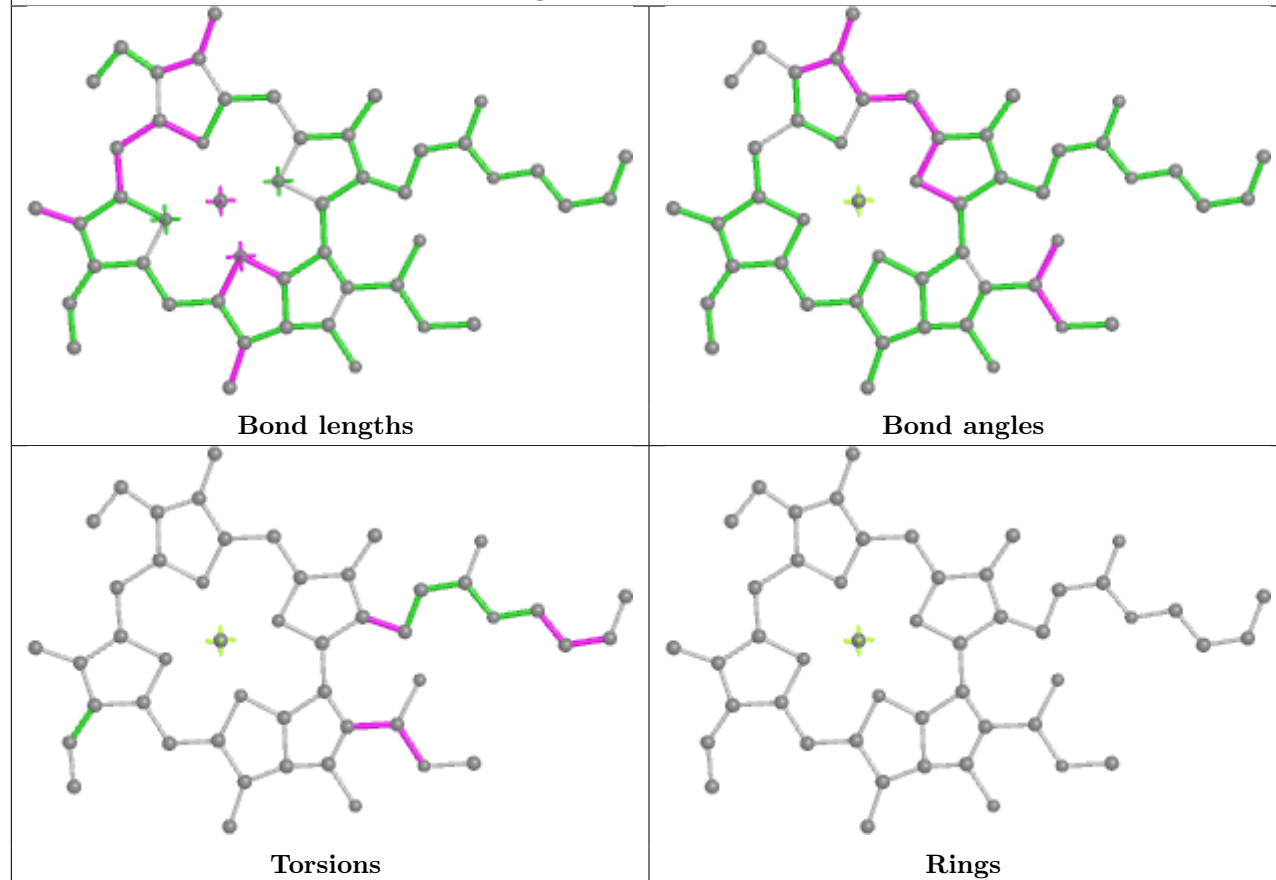


Rings

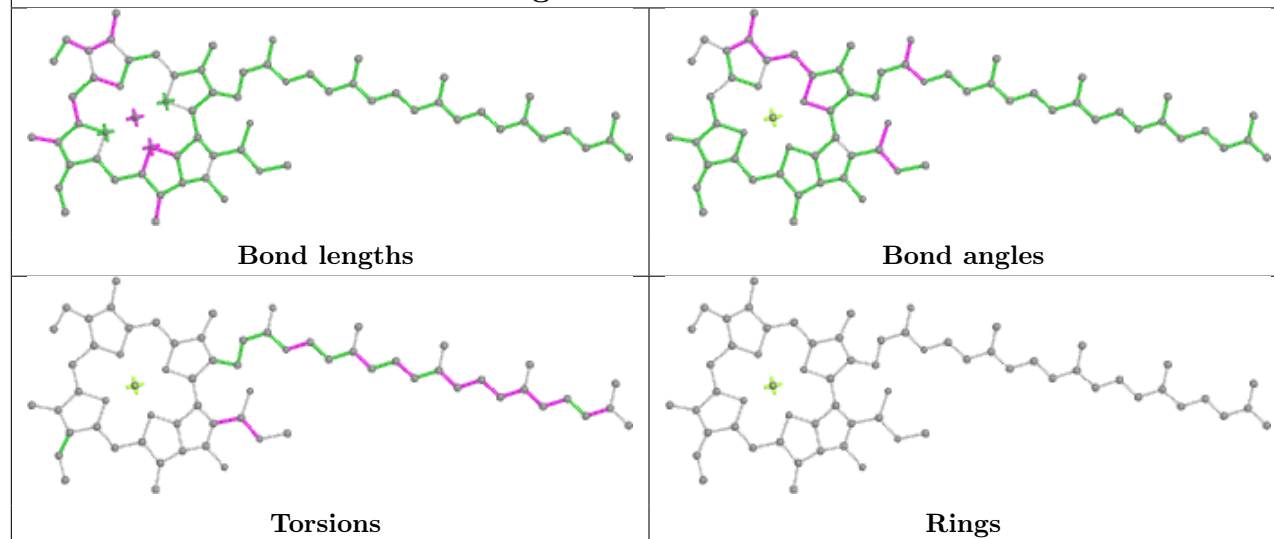
Ligand CLA b 617



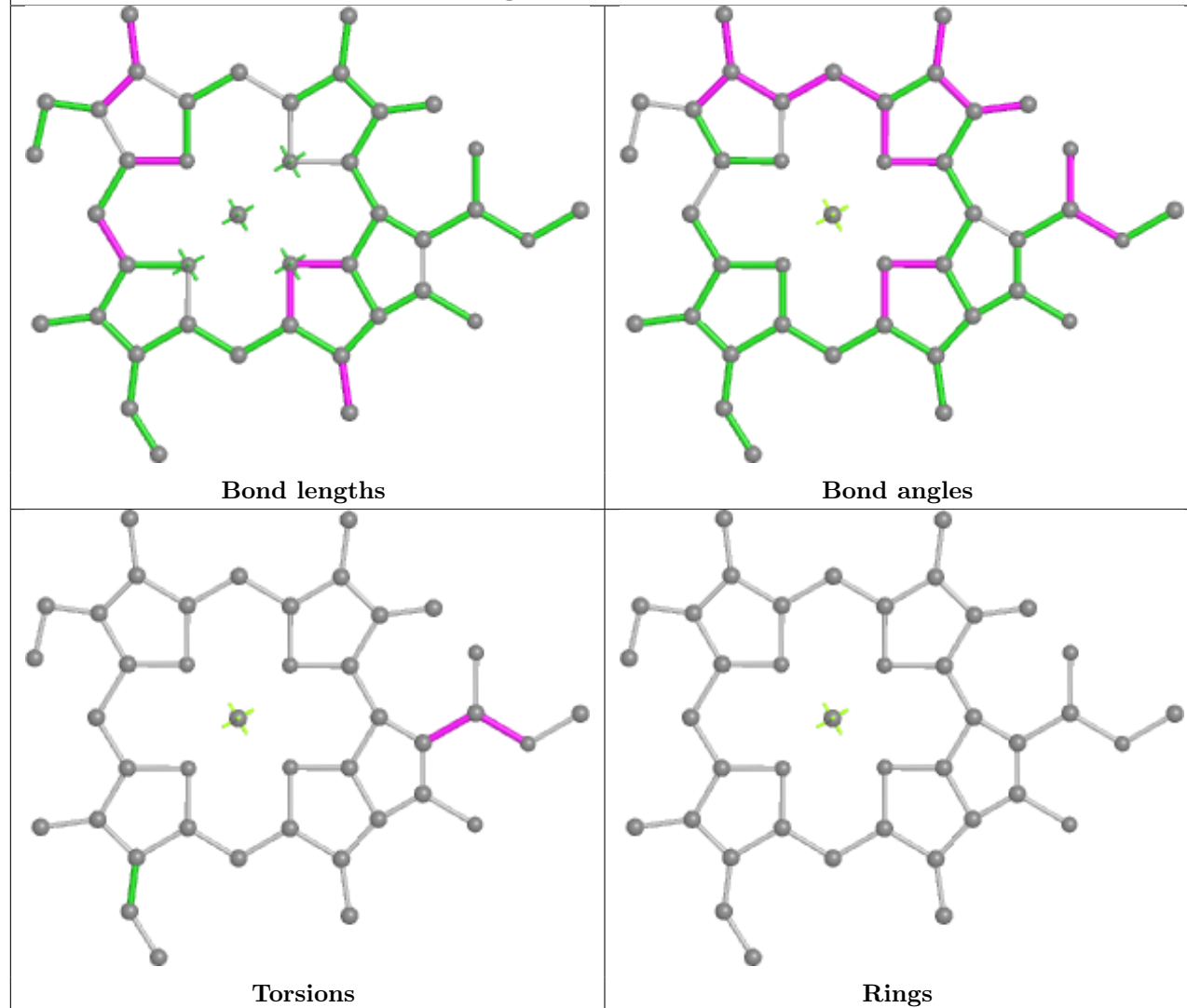
Ligand CLA N 611



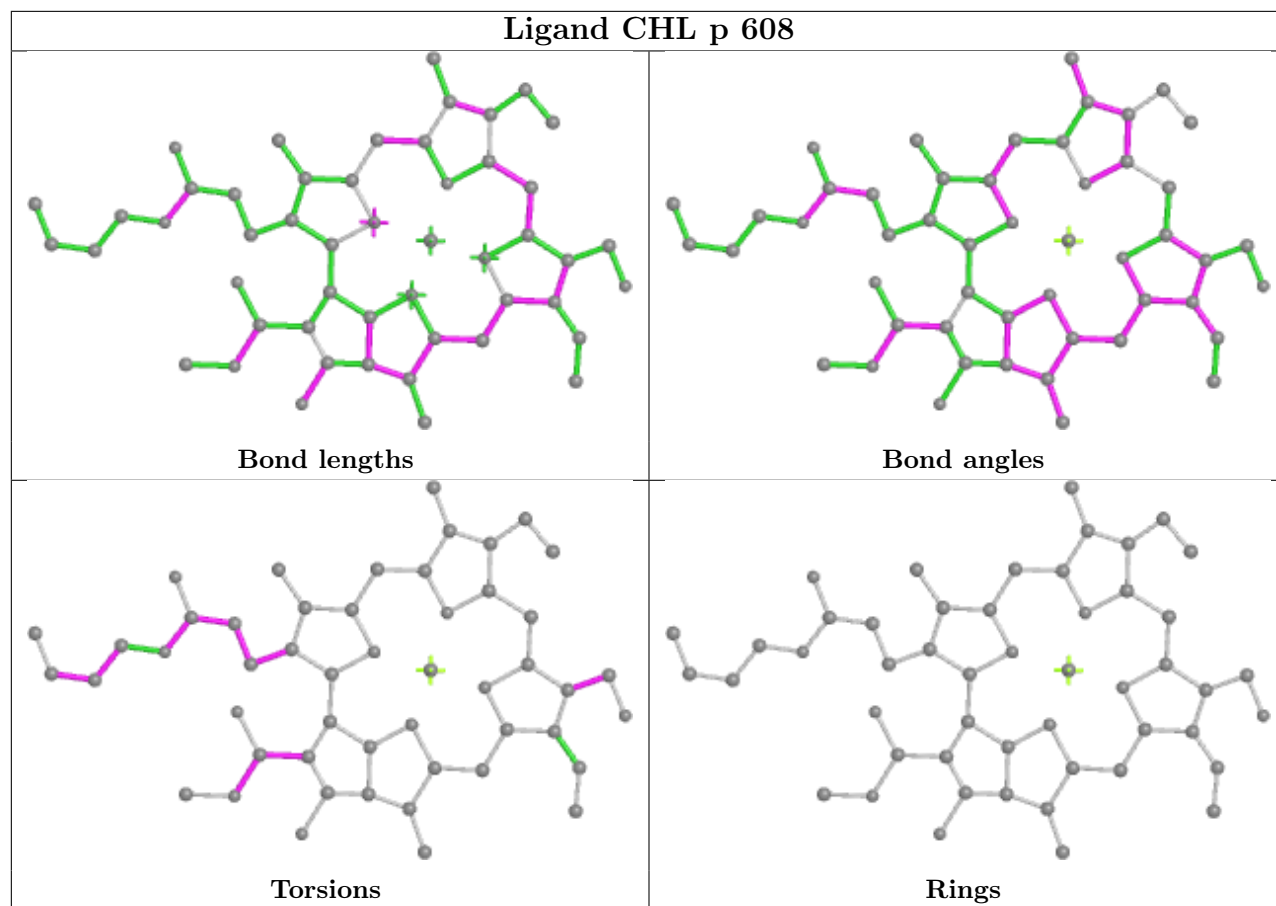
Ligand CLA C 506



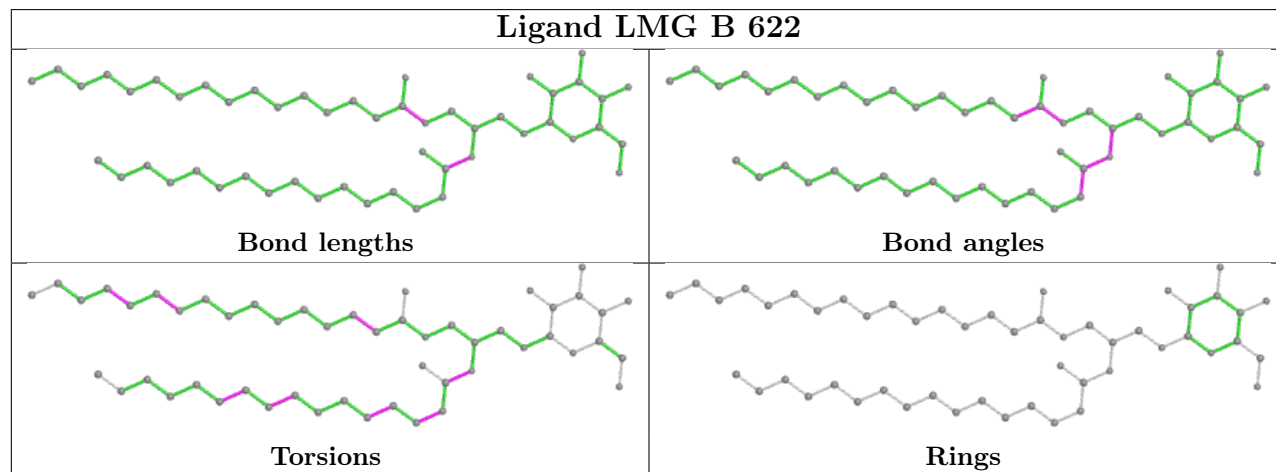
Ligand CLA s 609

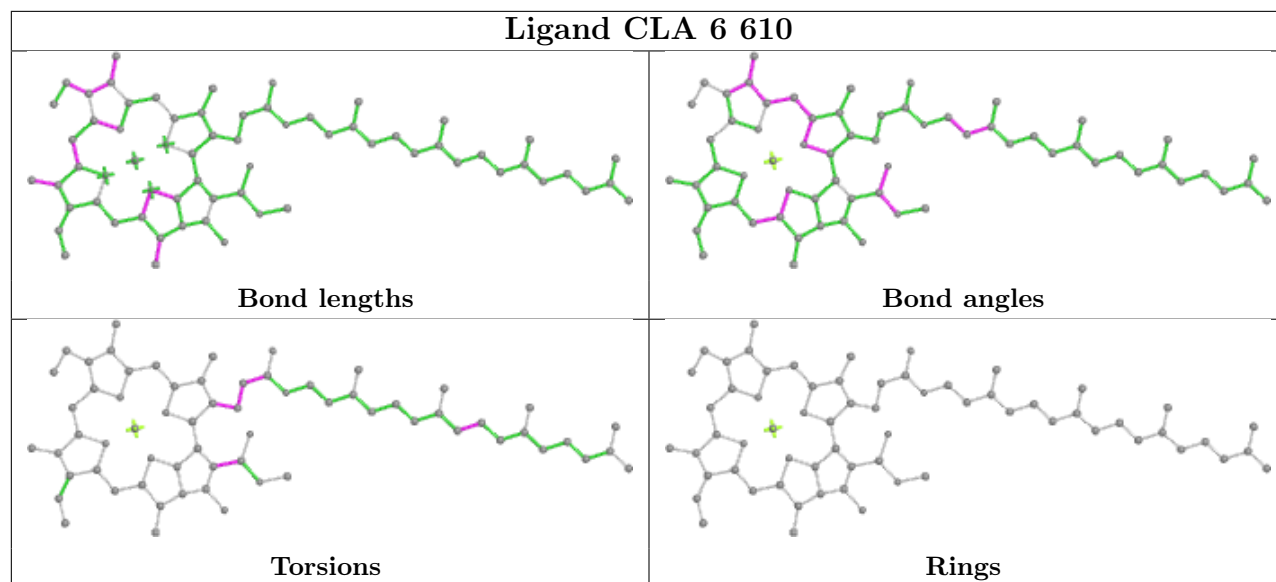
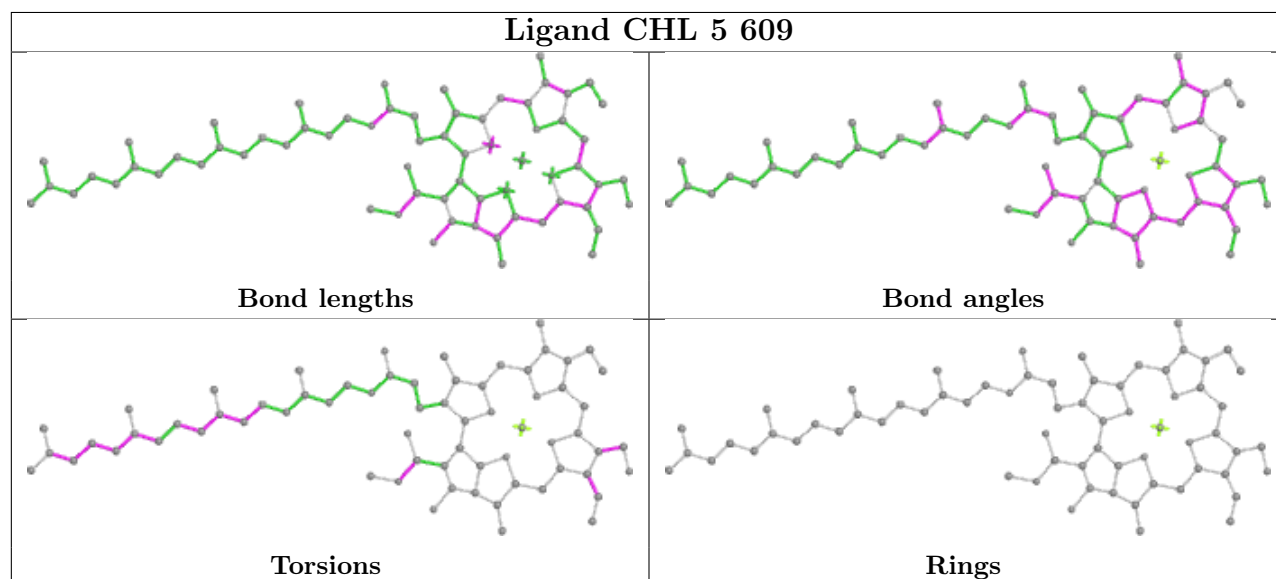


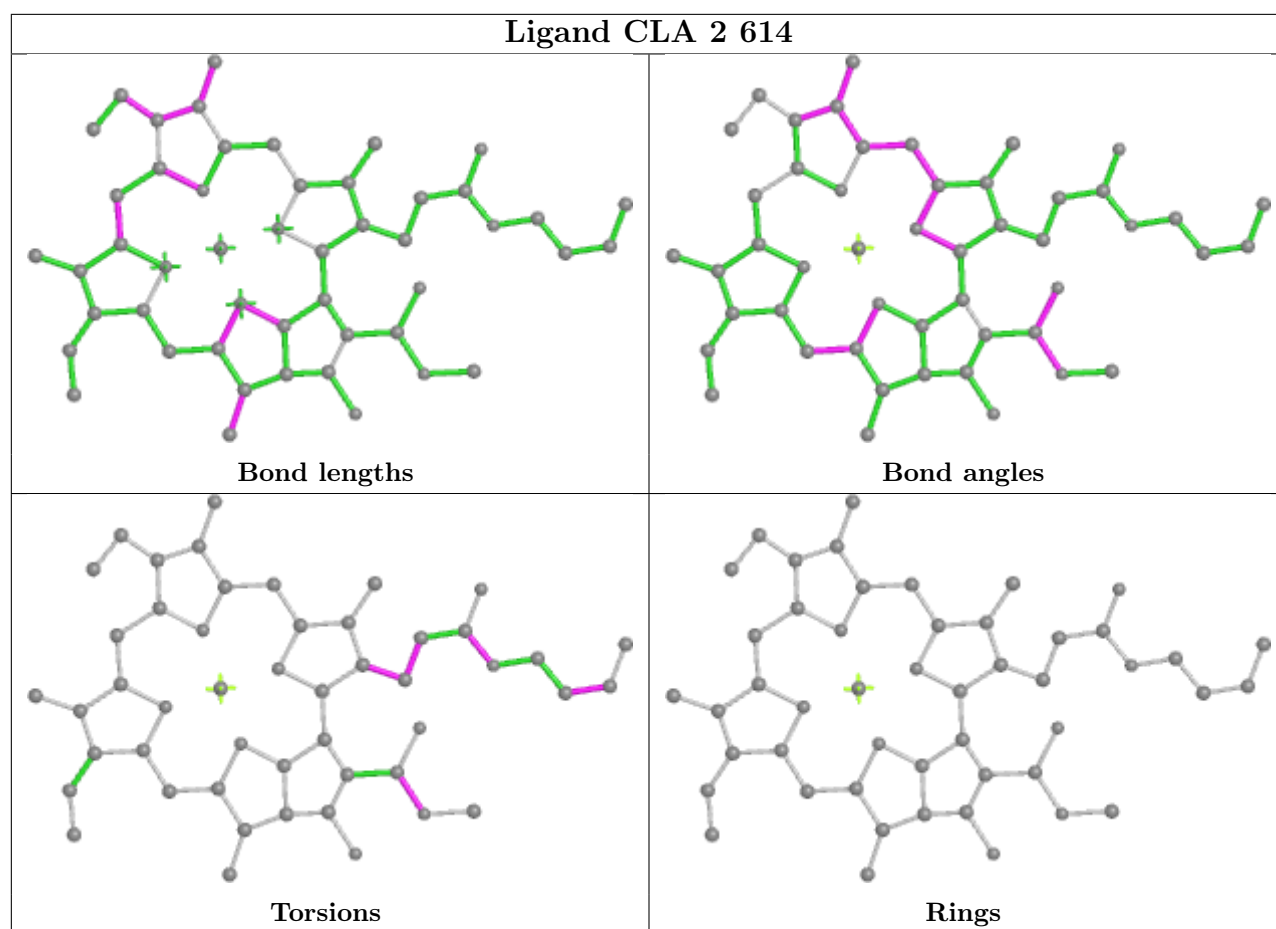
Ligand CHL p 608

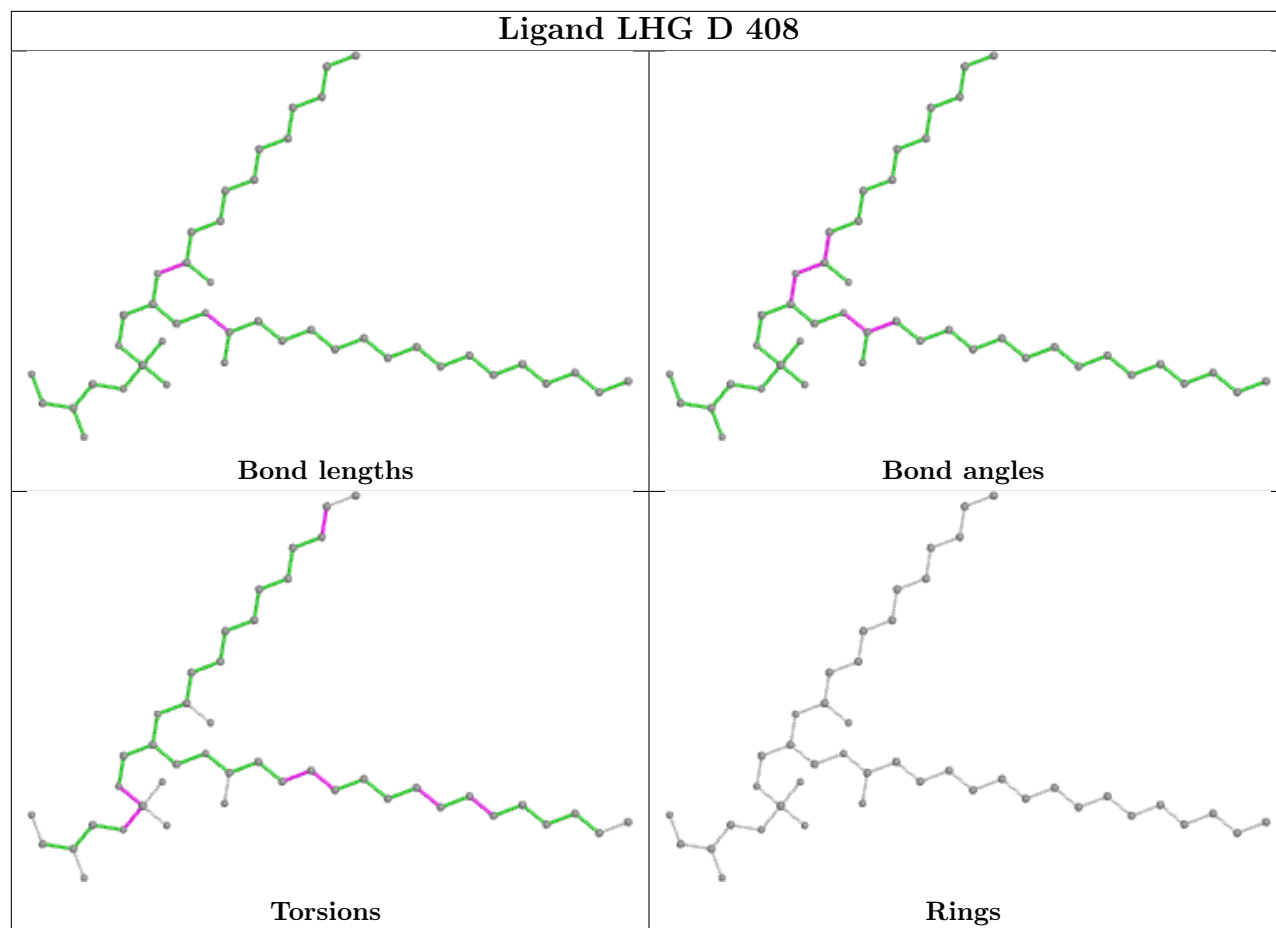


Ligand LMG B 622

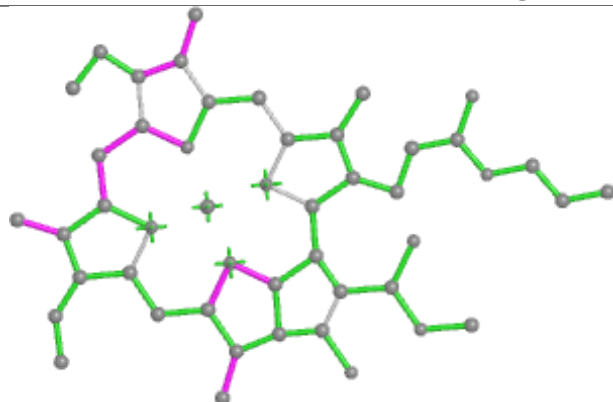


Ligand CLA 6 610**Ligand CHL 5 609**

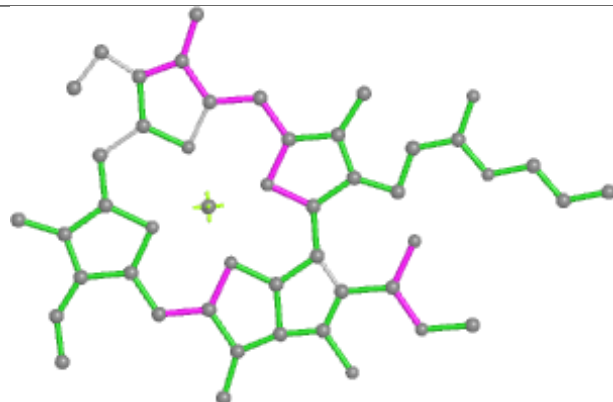




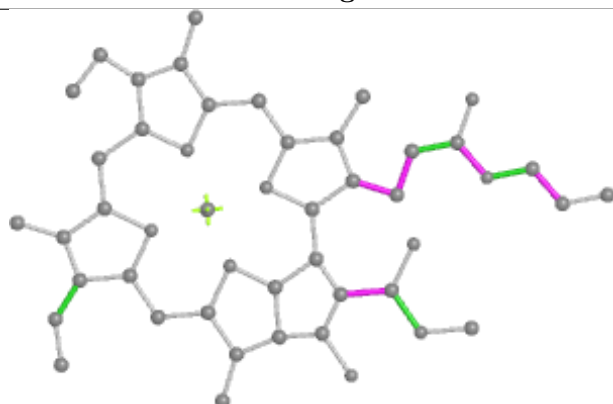
Ligand CLA R 604



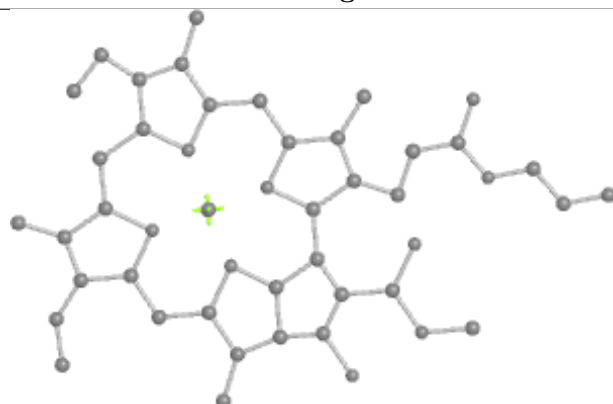
Bond lengths



Bond angles

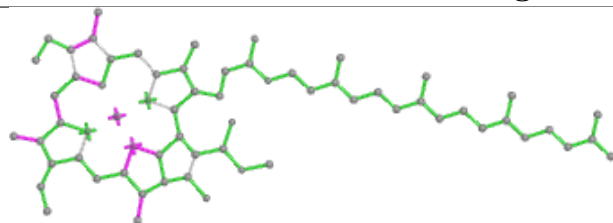


Torsions

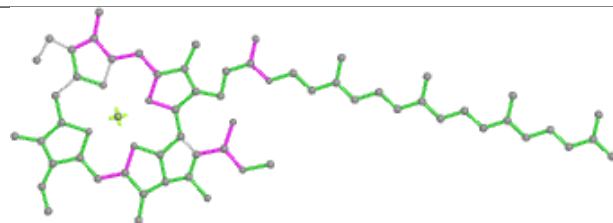


Rings

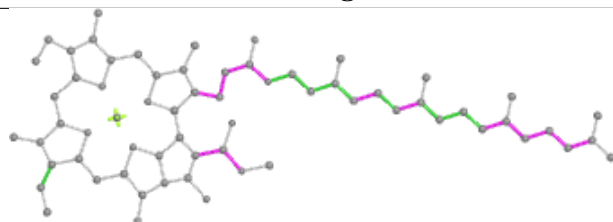
Ligand CLA R 616



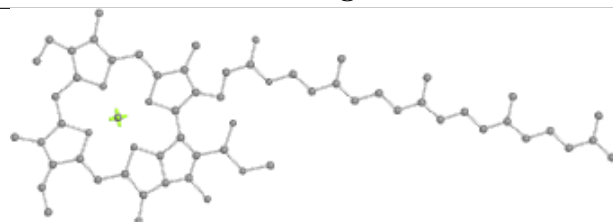
Bond lengths



Bond angles

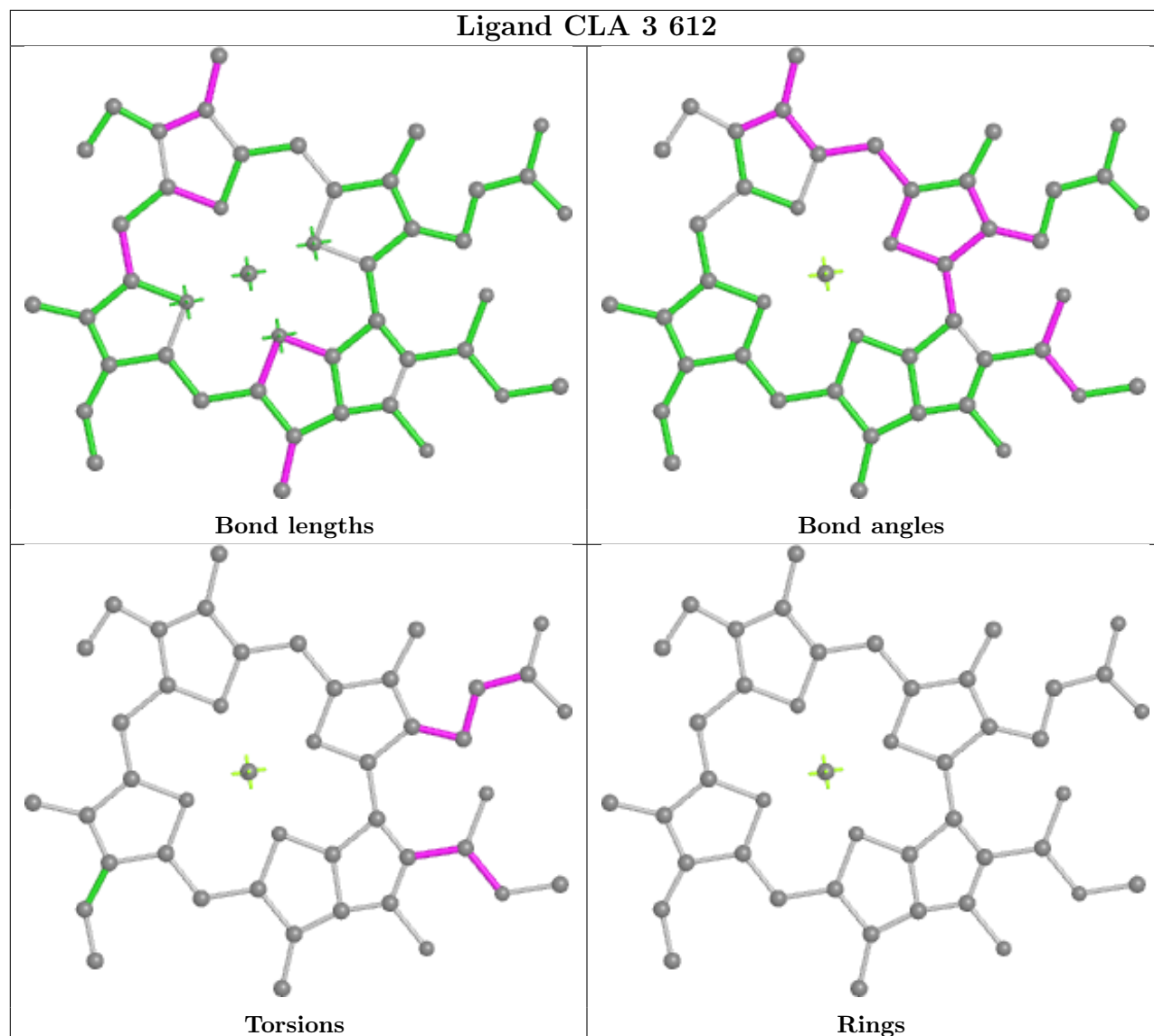


Torsions

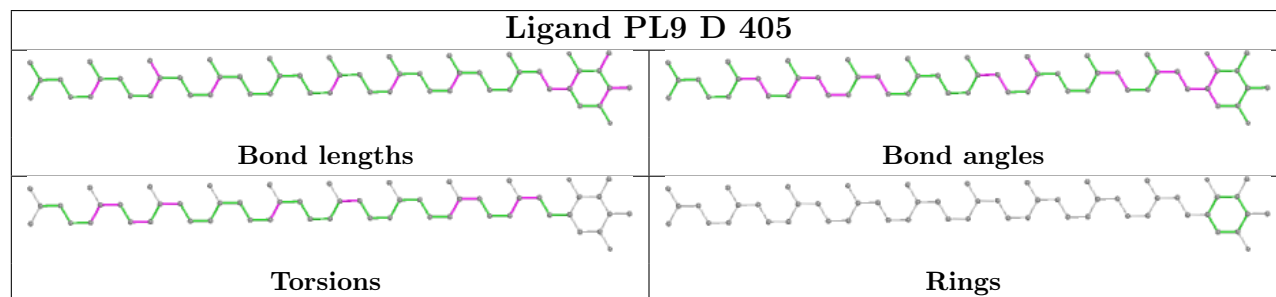


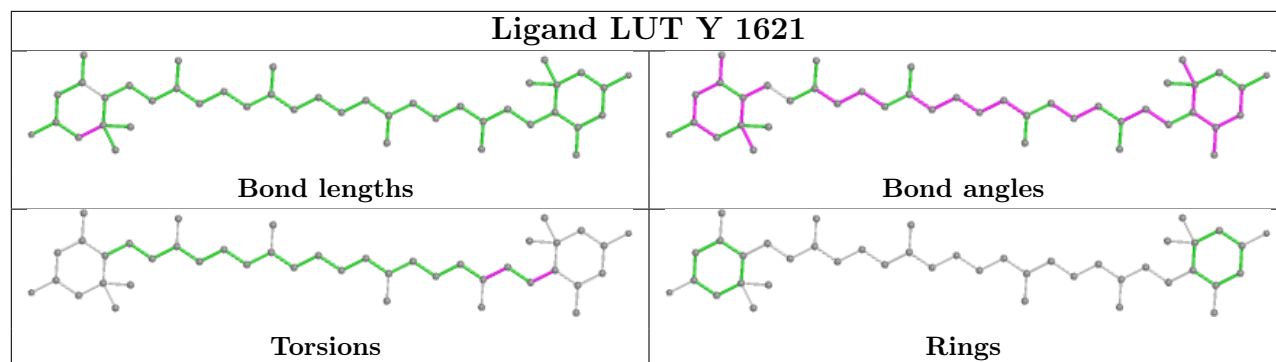
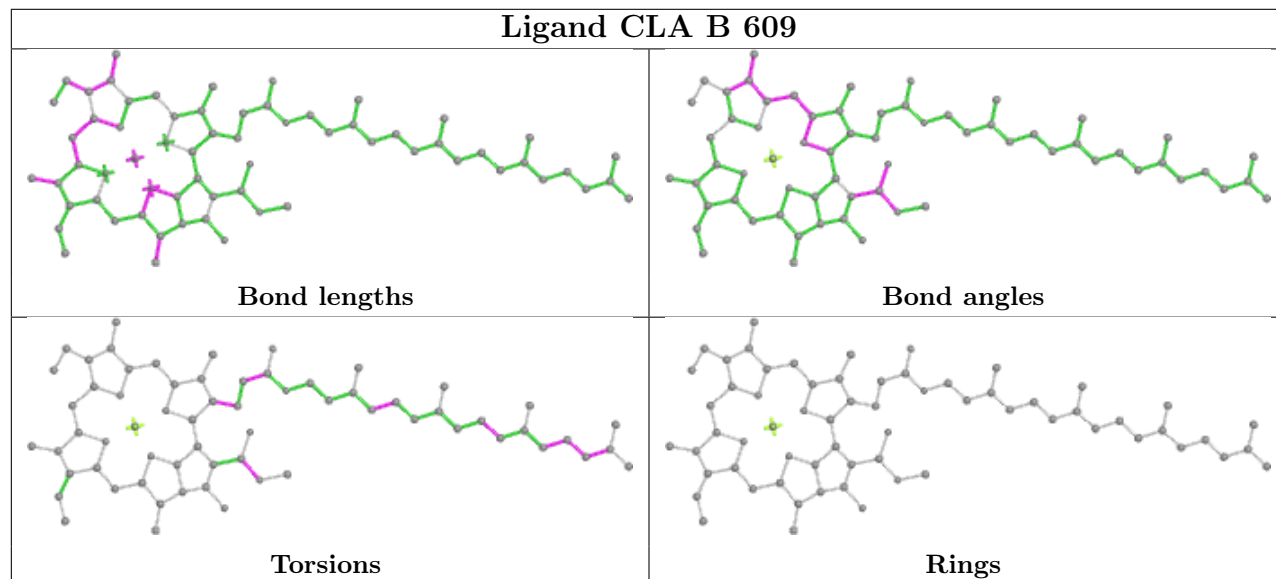
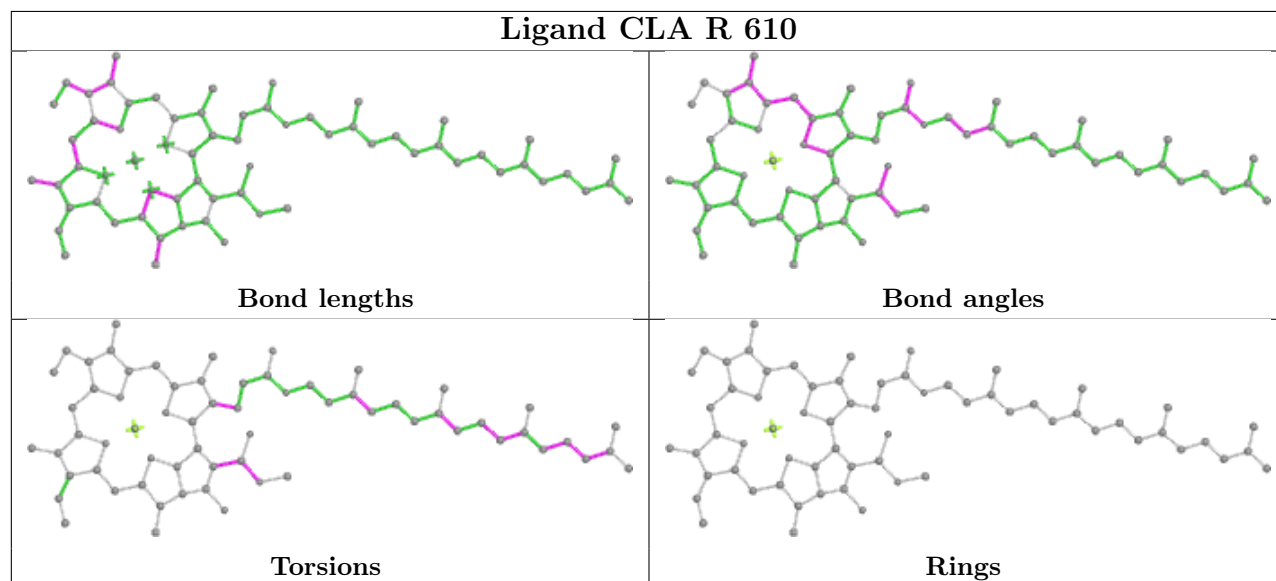
Rings

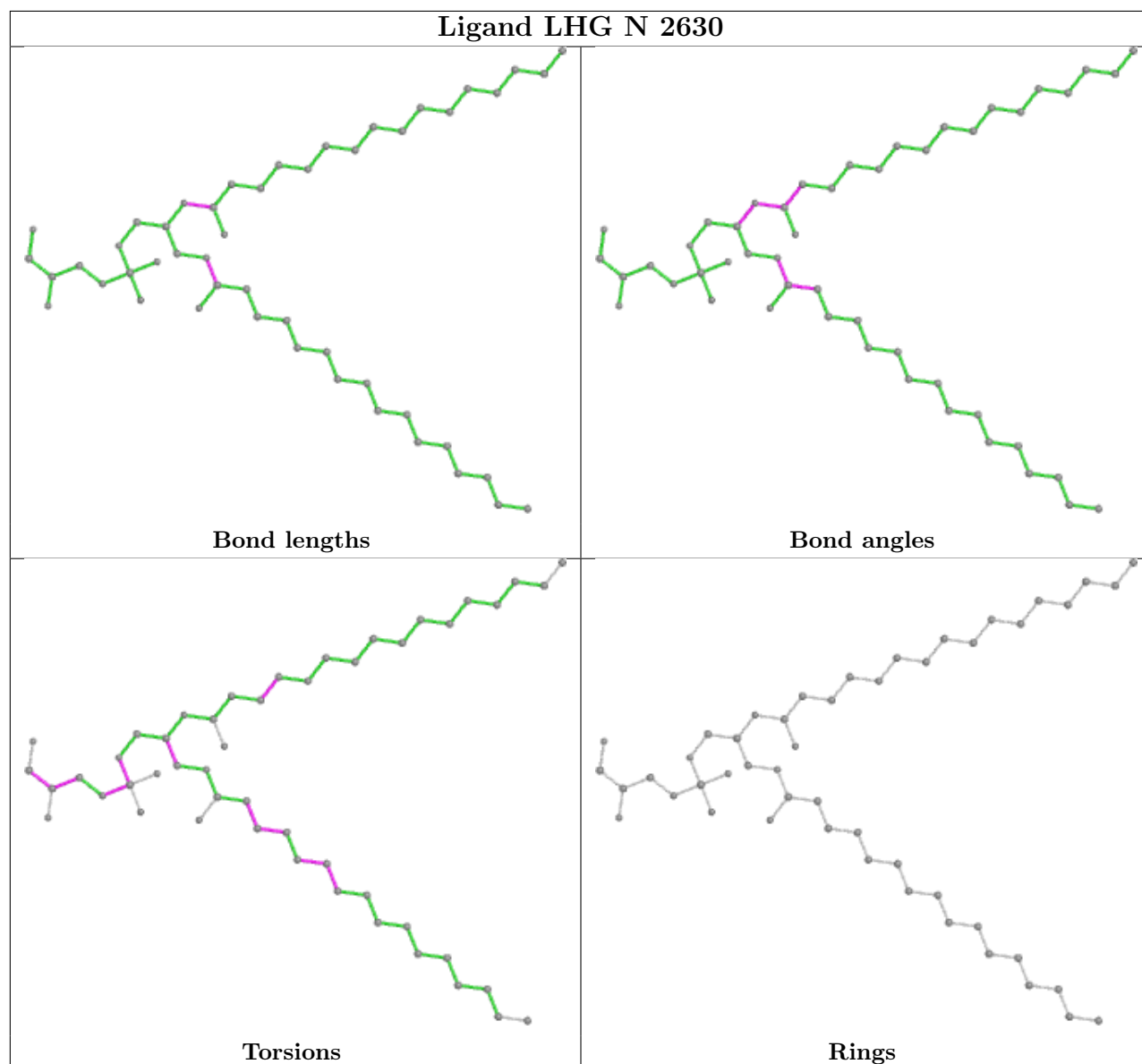
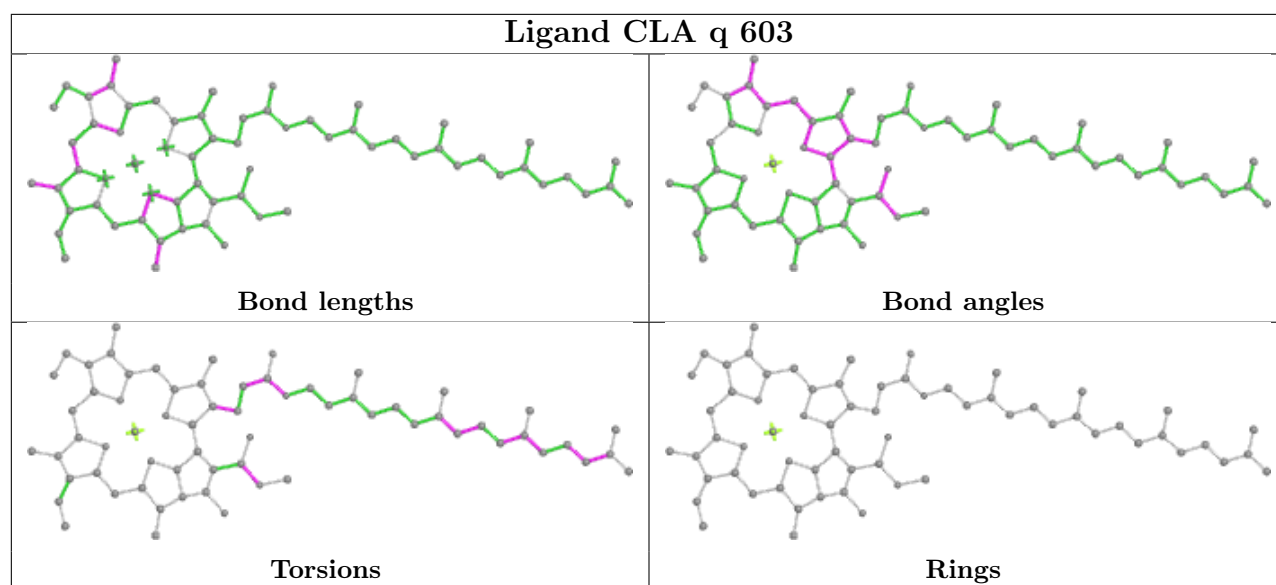
Ligand CLA 3 612



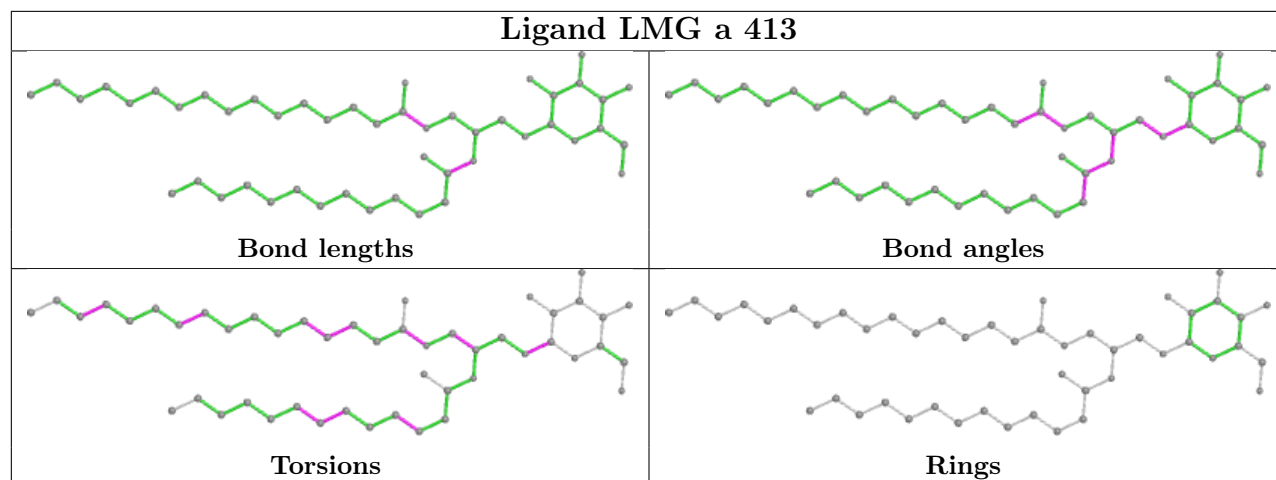
Ligand PL9 D 405



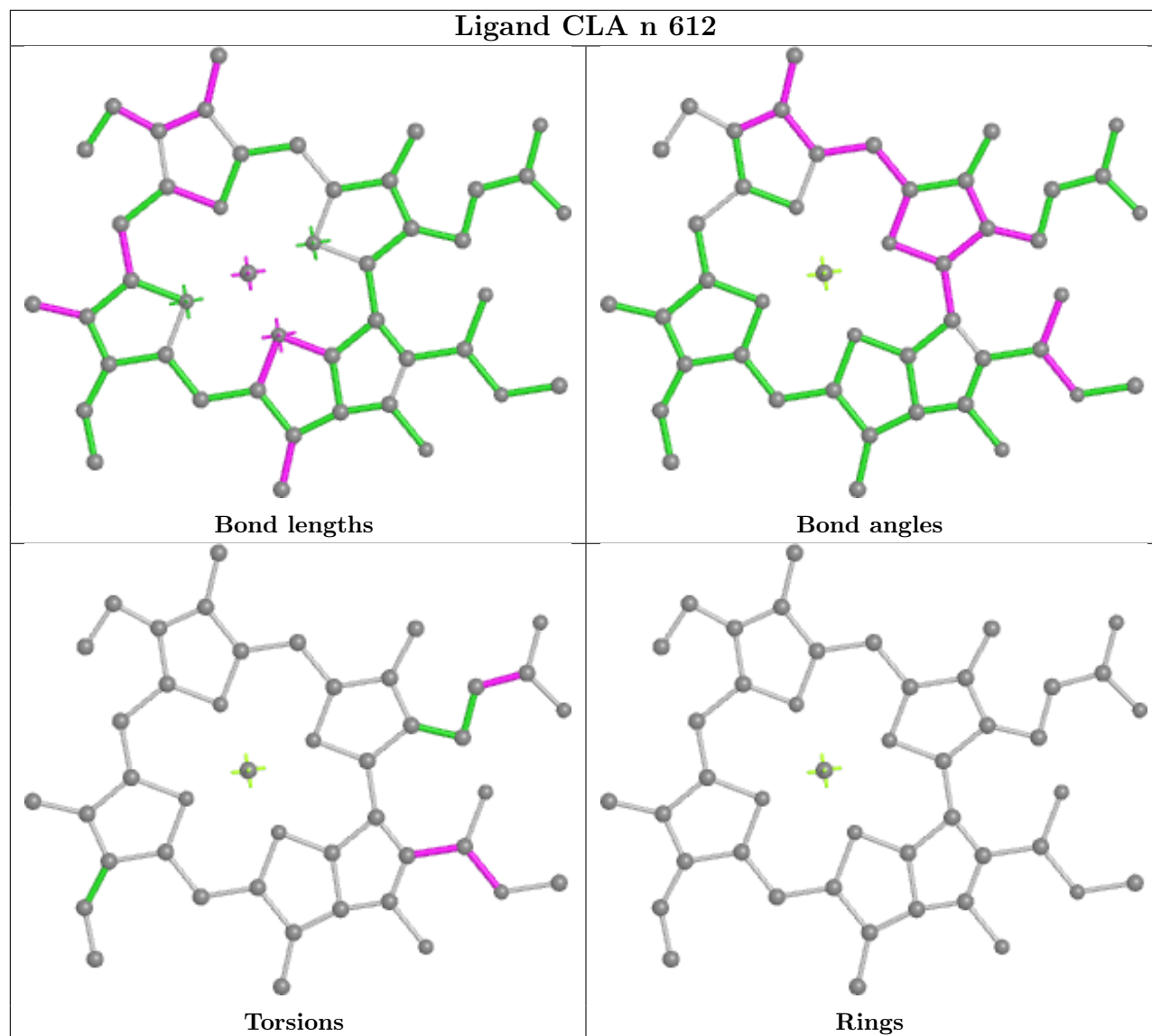
Ligand LUT Y 1621**Ligand CLA B 609****Ligand CLA R 610**

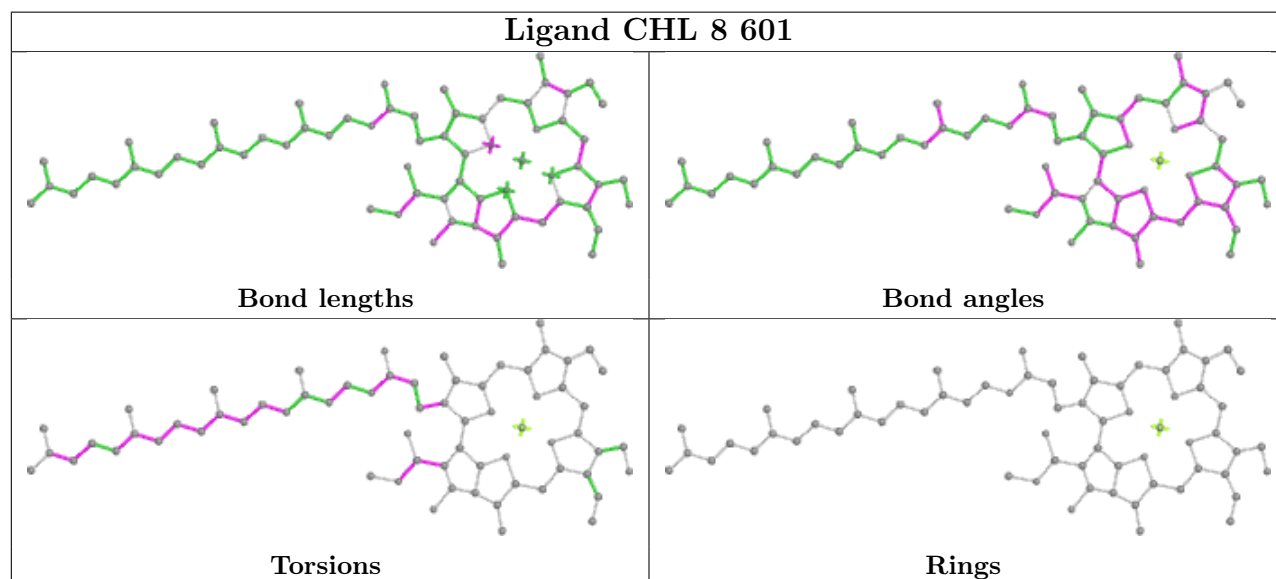
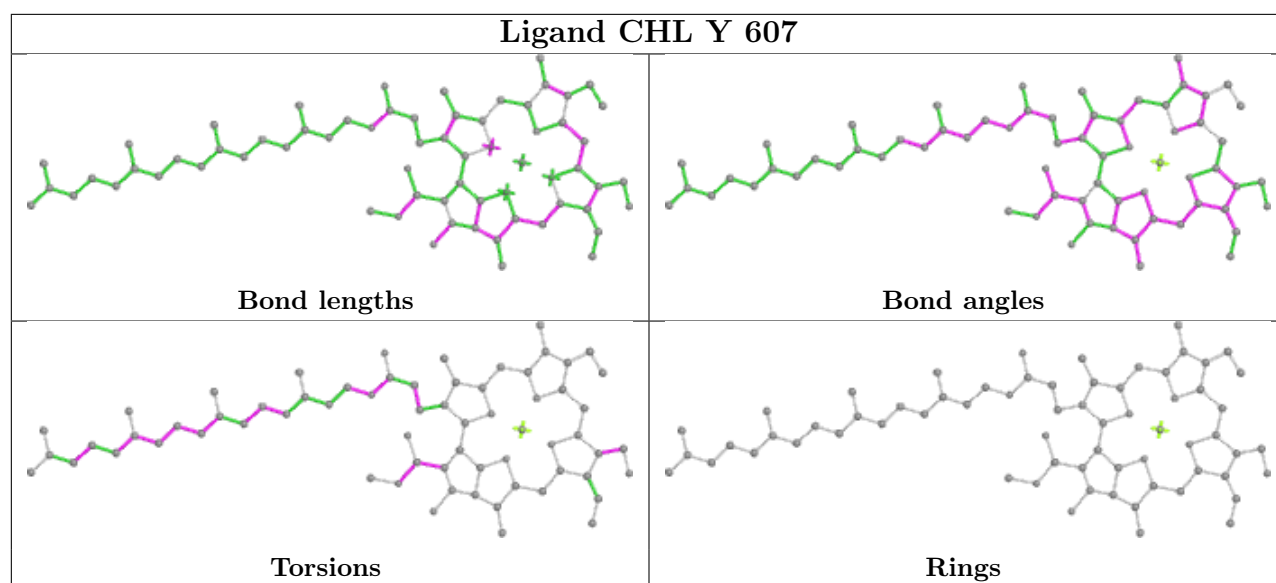


Ligand LMG a 413

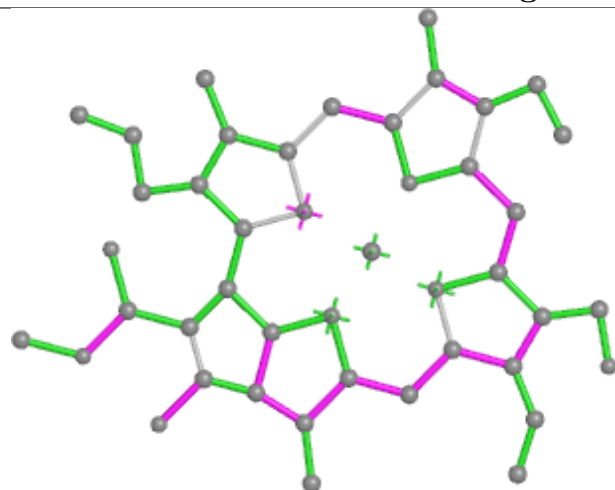


Ligand CLA n 612

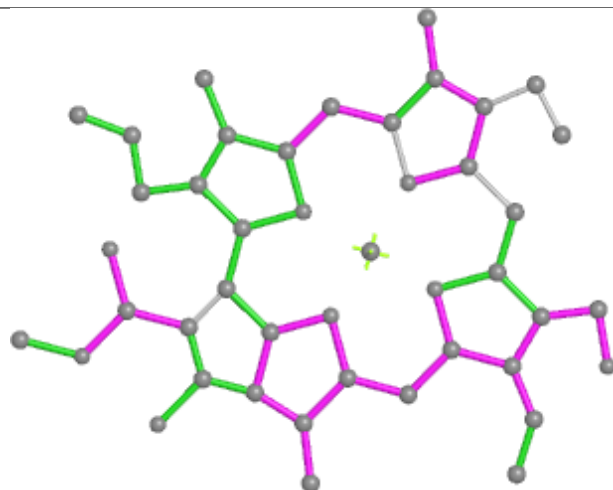




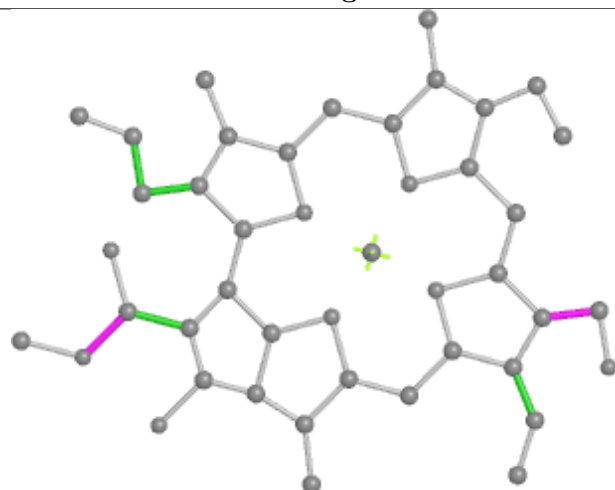
Ligand CHL 4 608



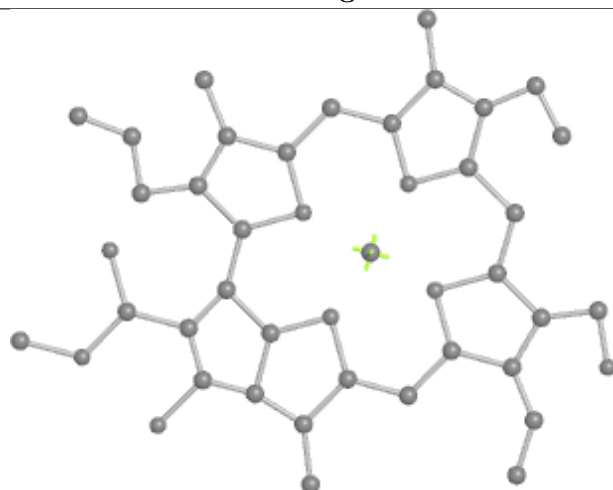
Bond lengths



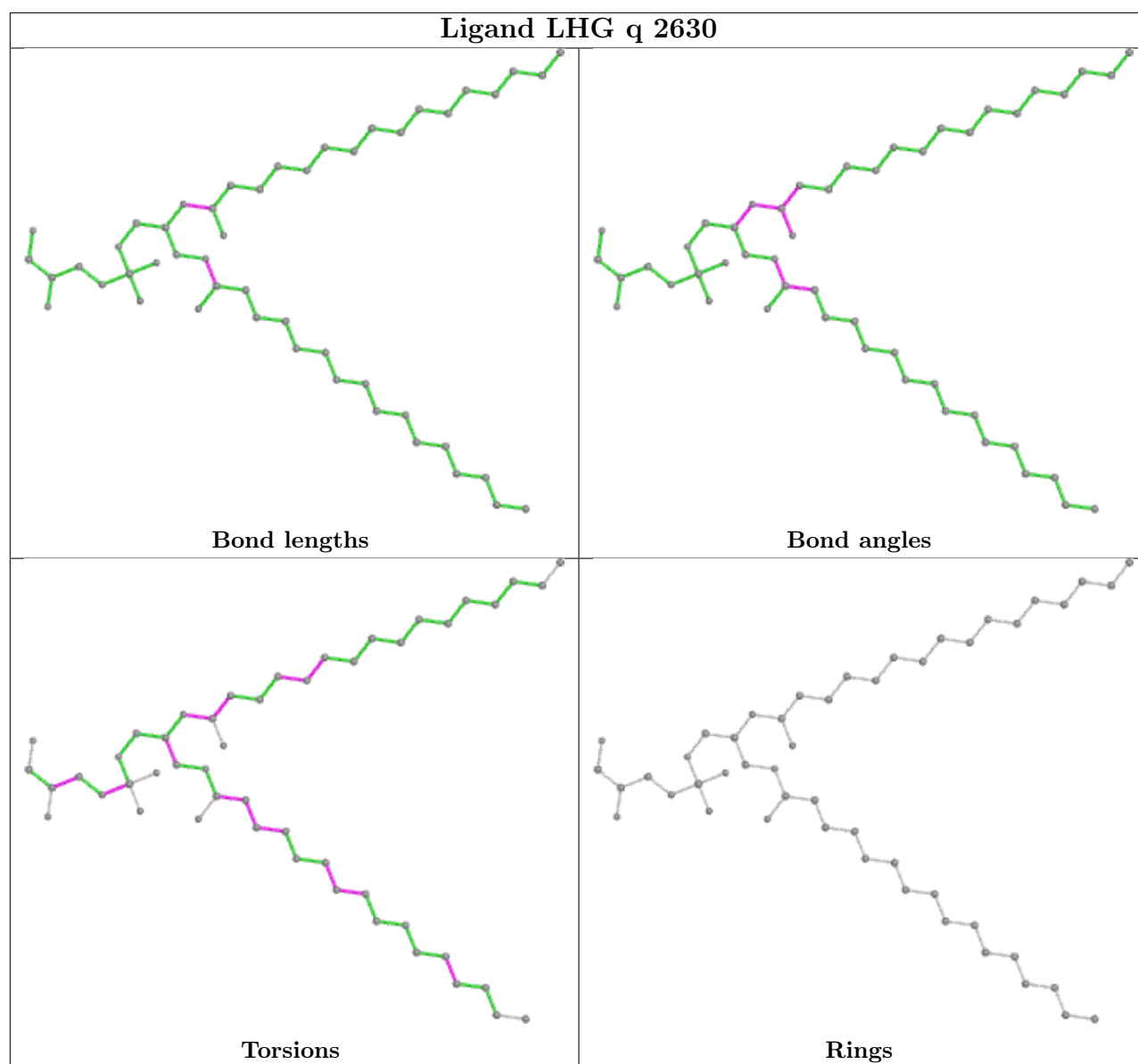
Bond angles

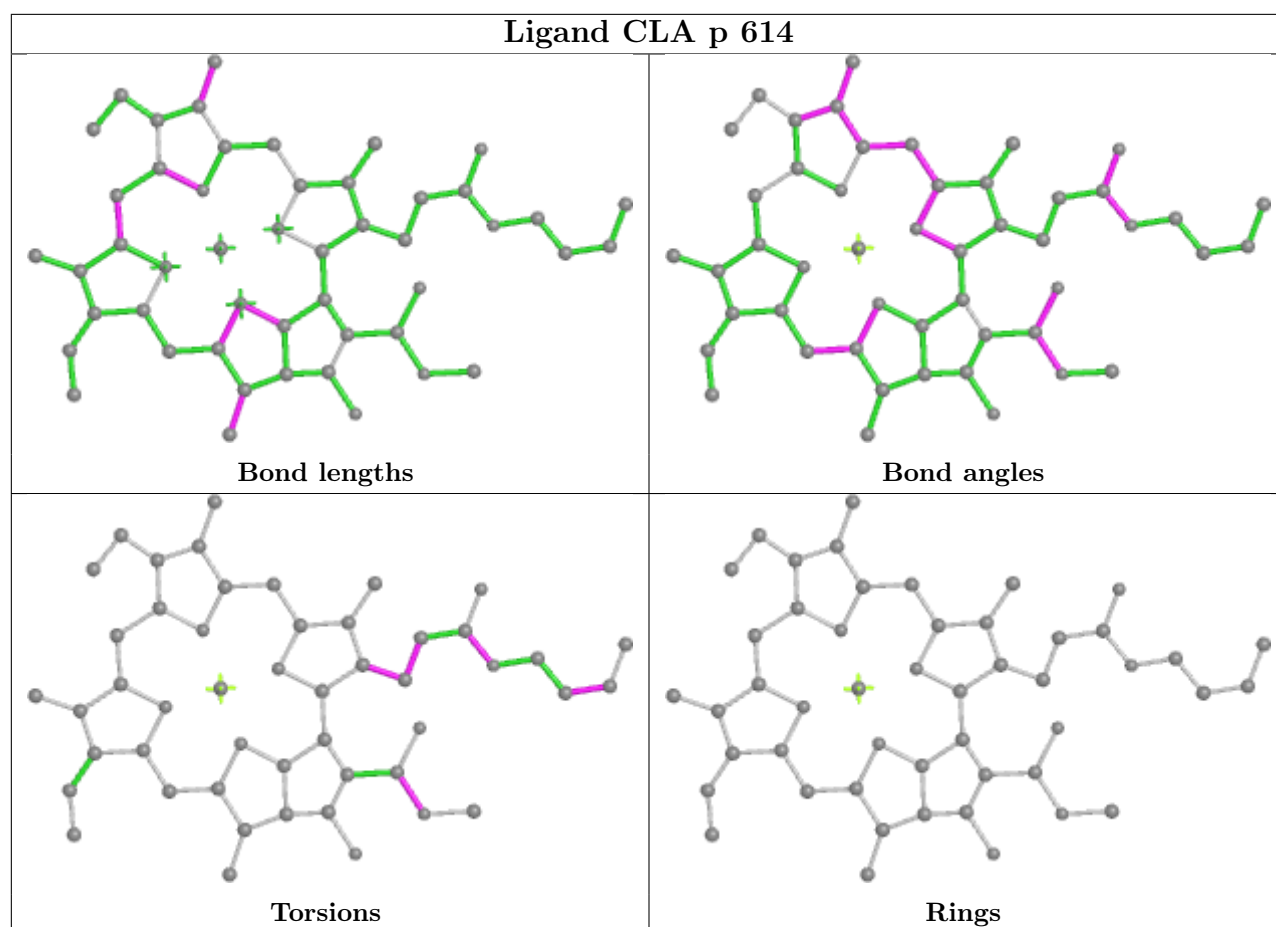


Torsions

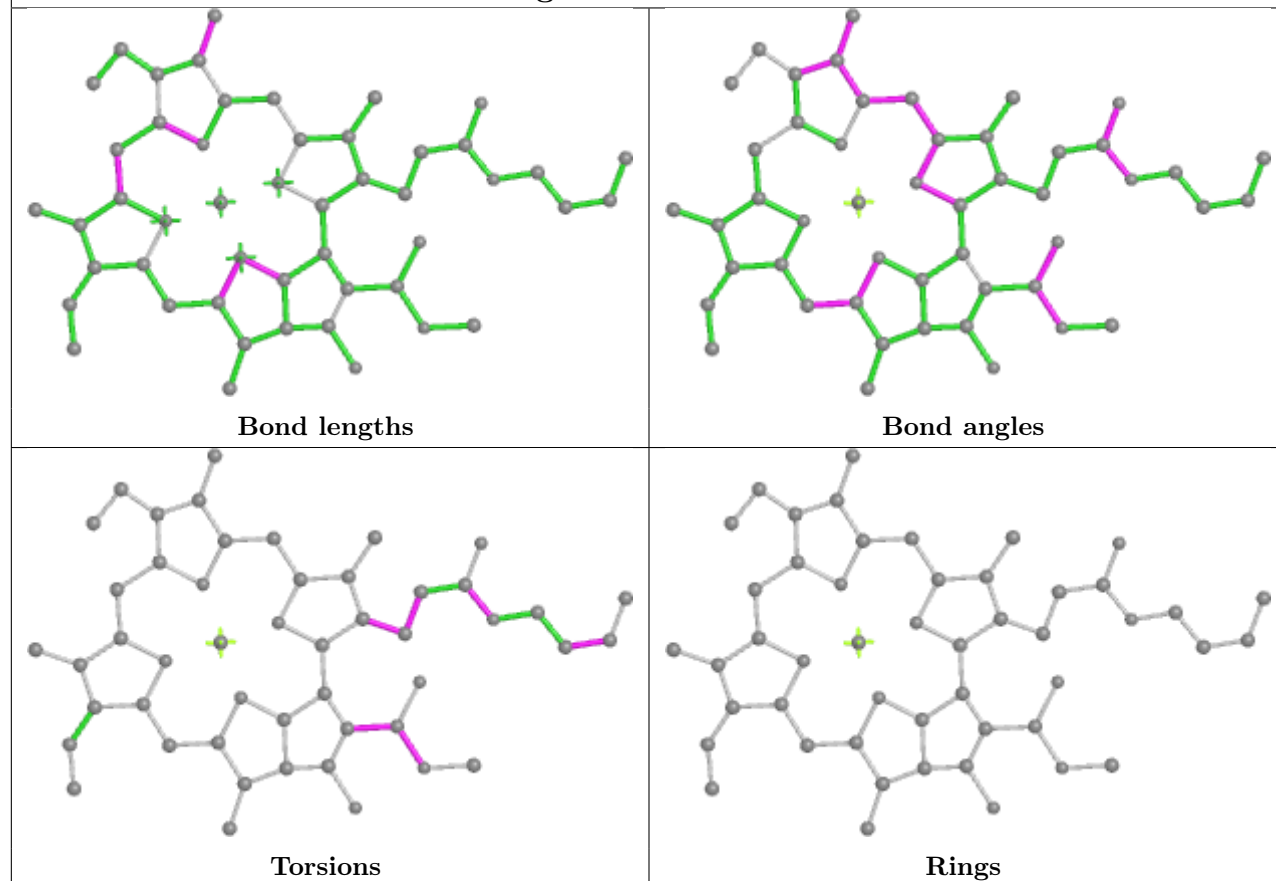


Rings

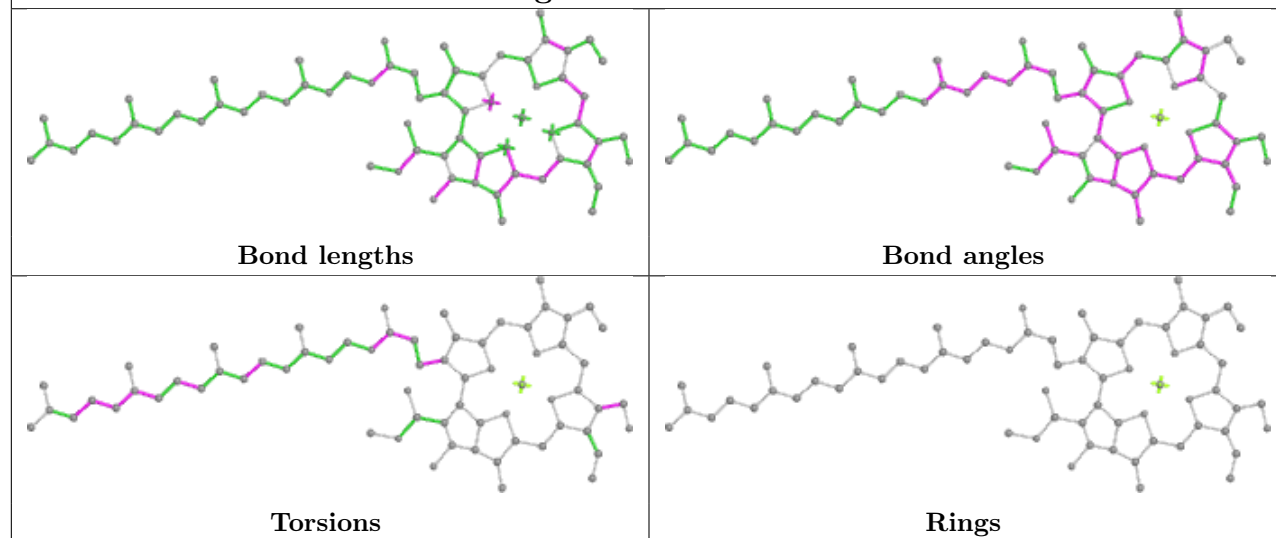




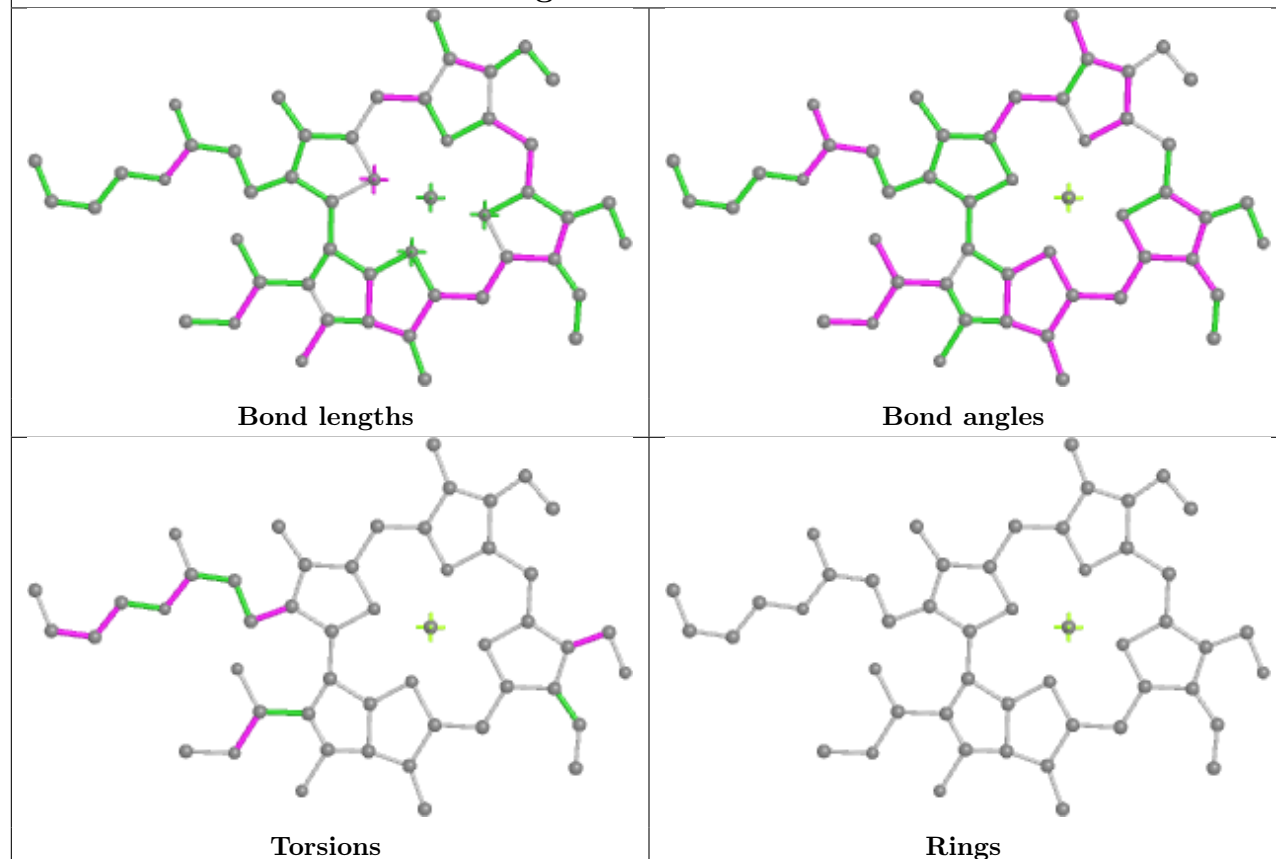
Ligand CLA 8 614



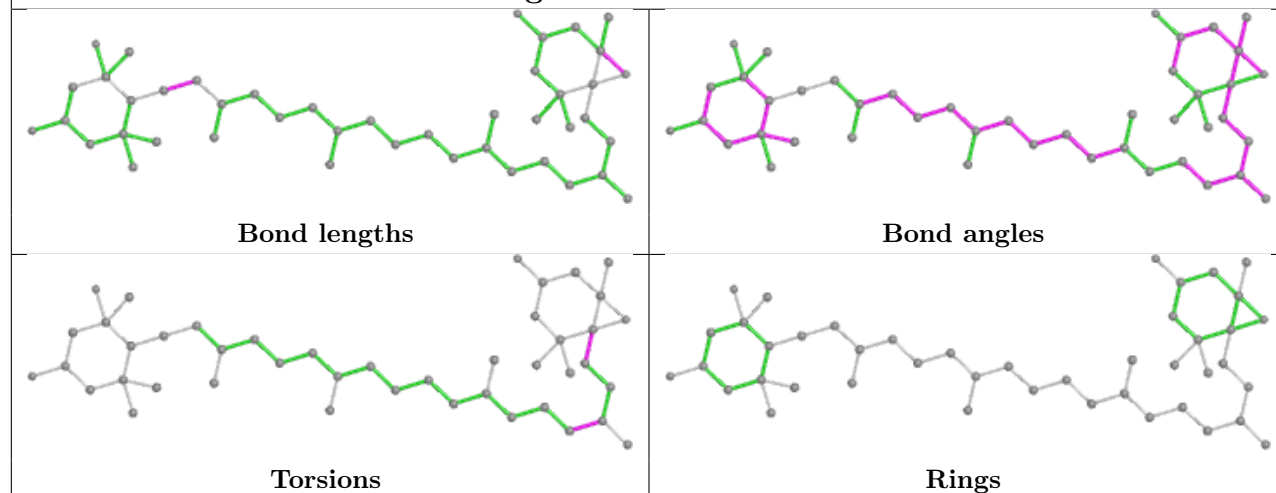
Ligand CHL n 607

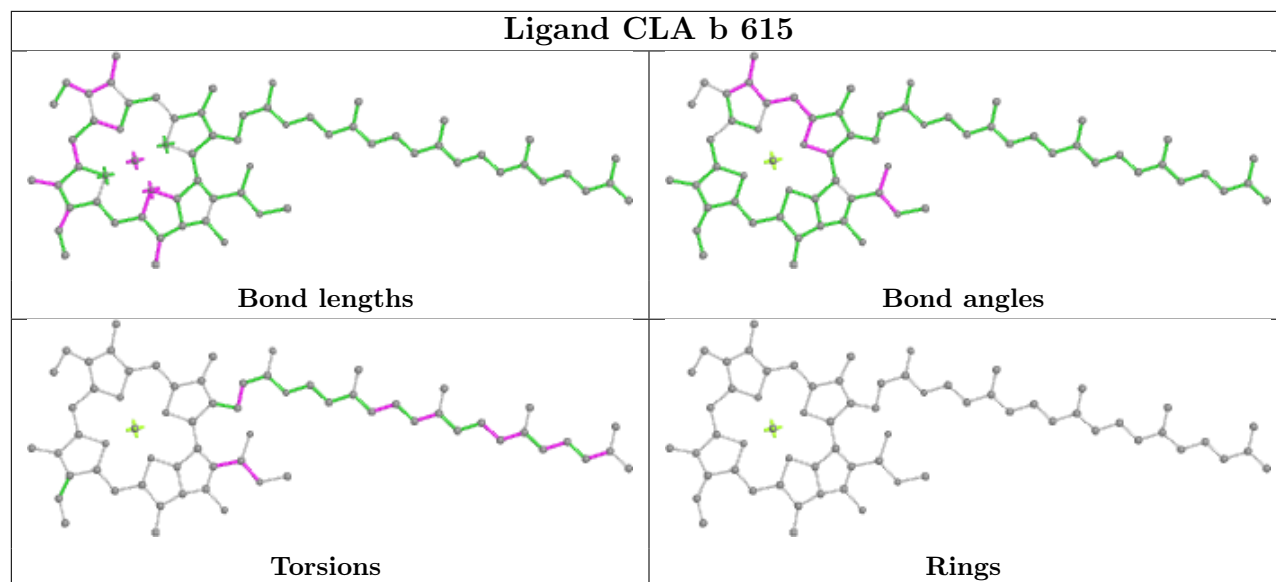
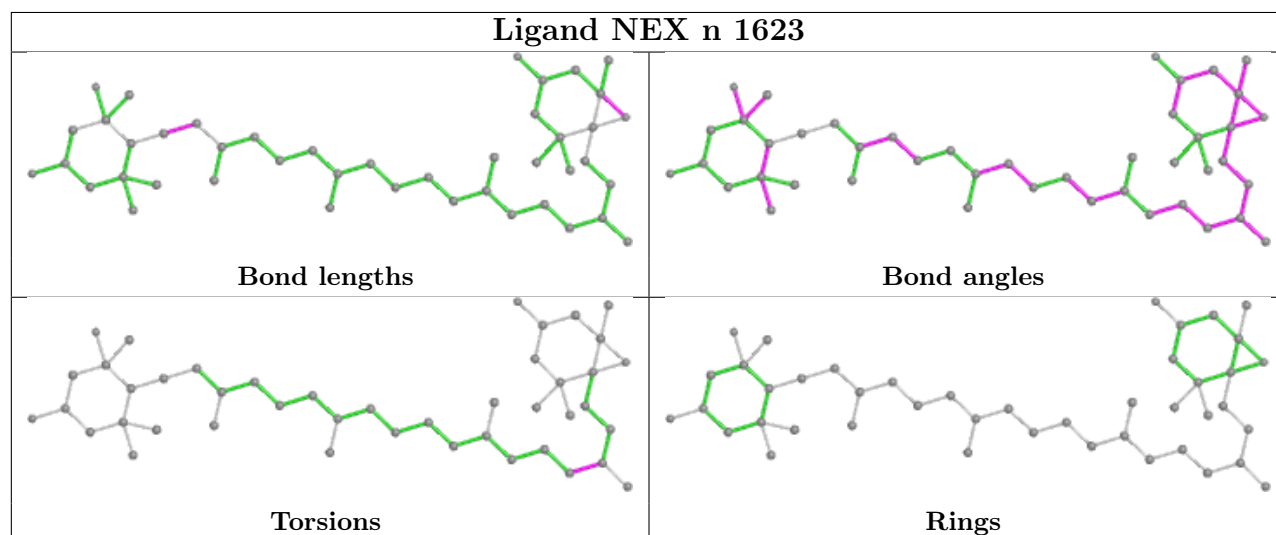


Ligand CHL 9 606

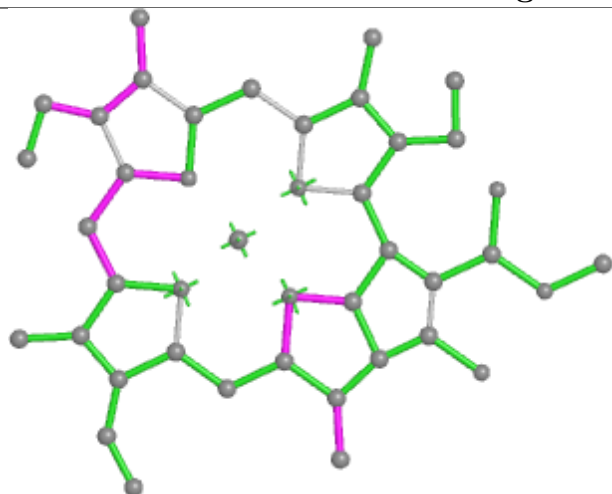


Ligand NEX 4 1623

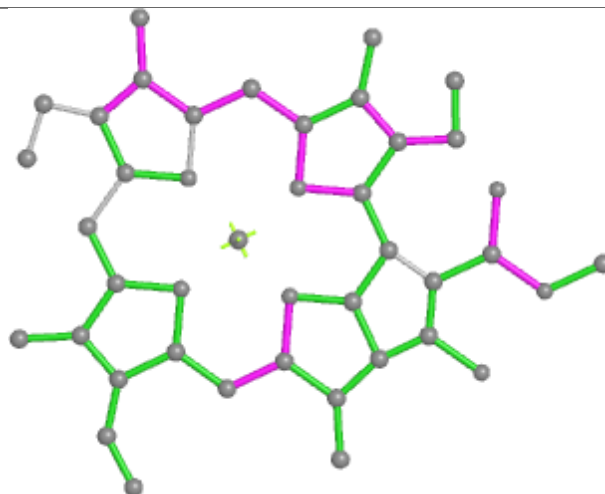


Ligand CLA b 615**Ligand NEX n 1623**

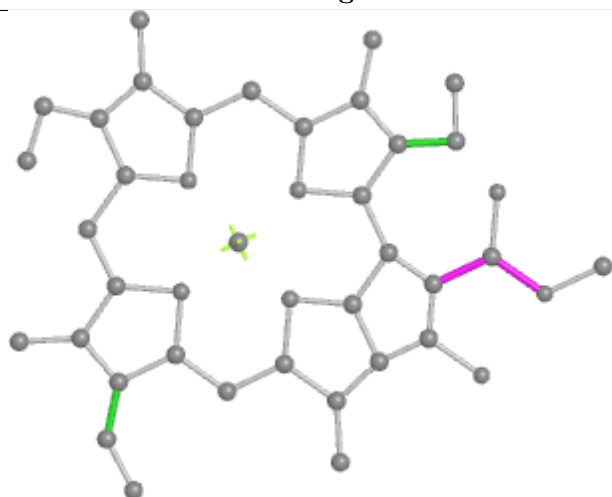
Ligand CLA S 603



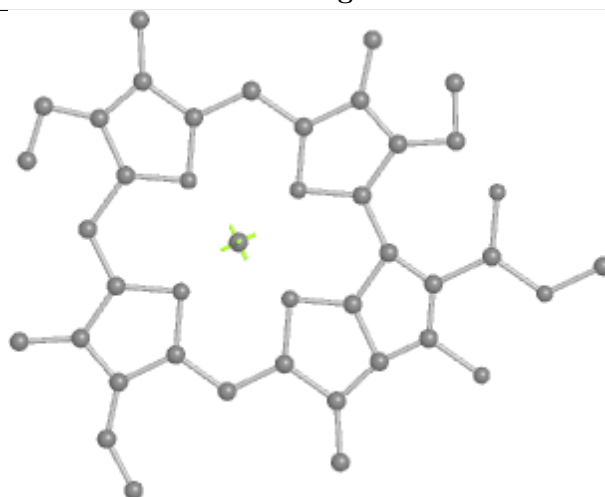
Bond lengths



Bond angles

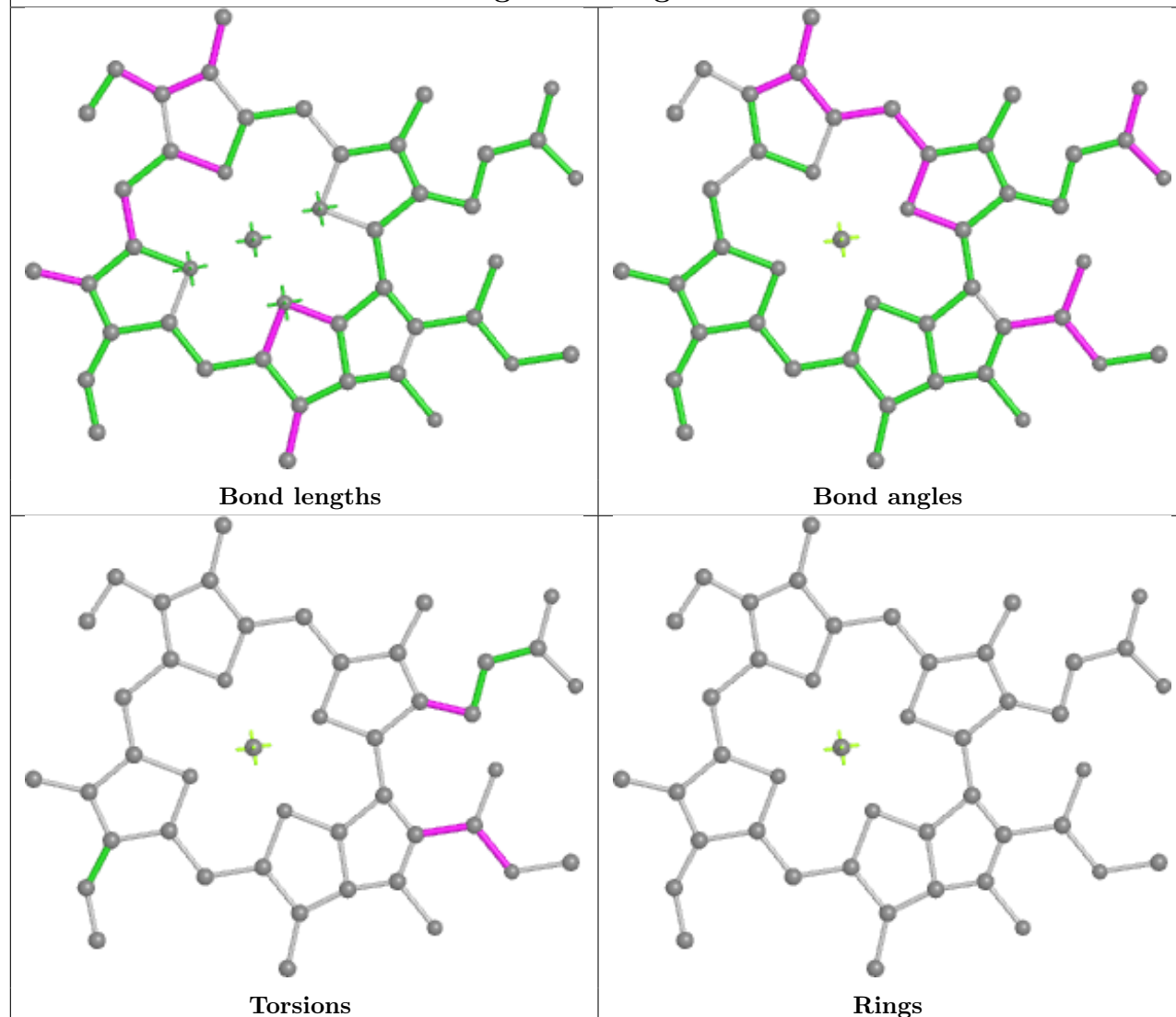


Torsions

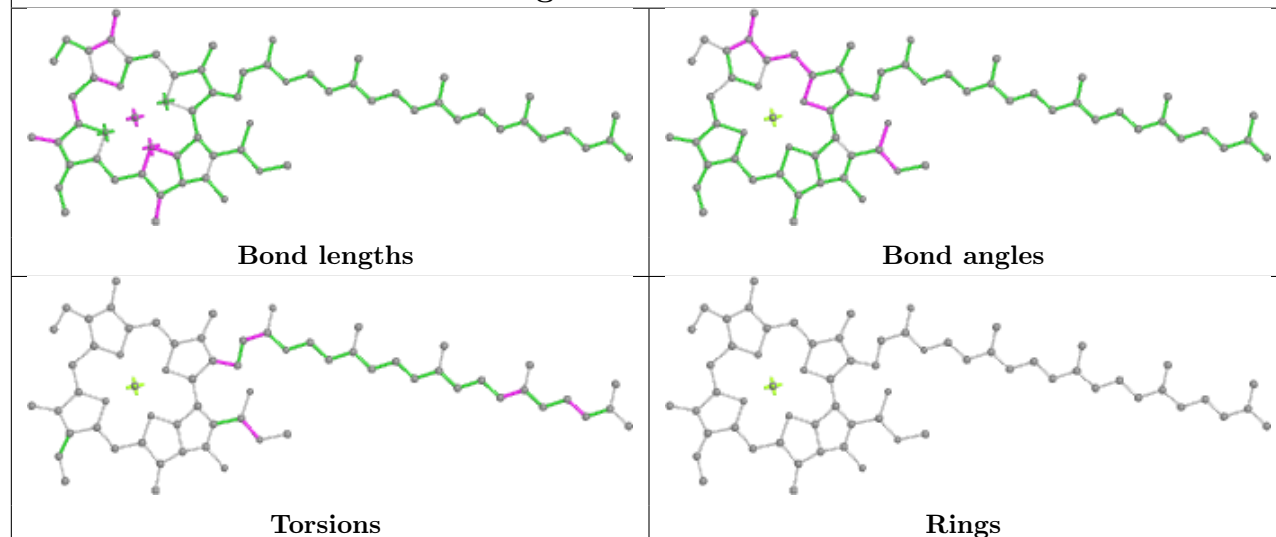


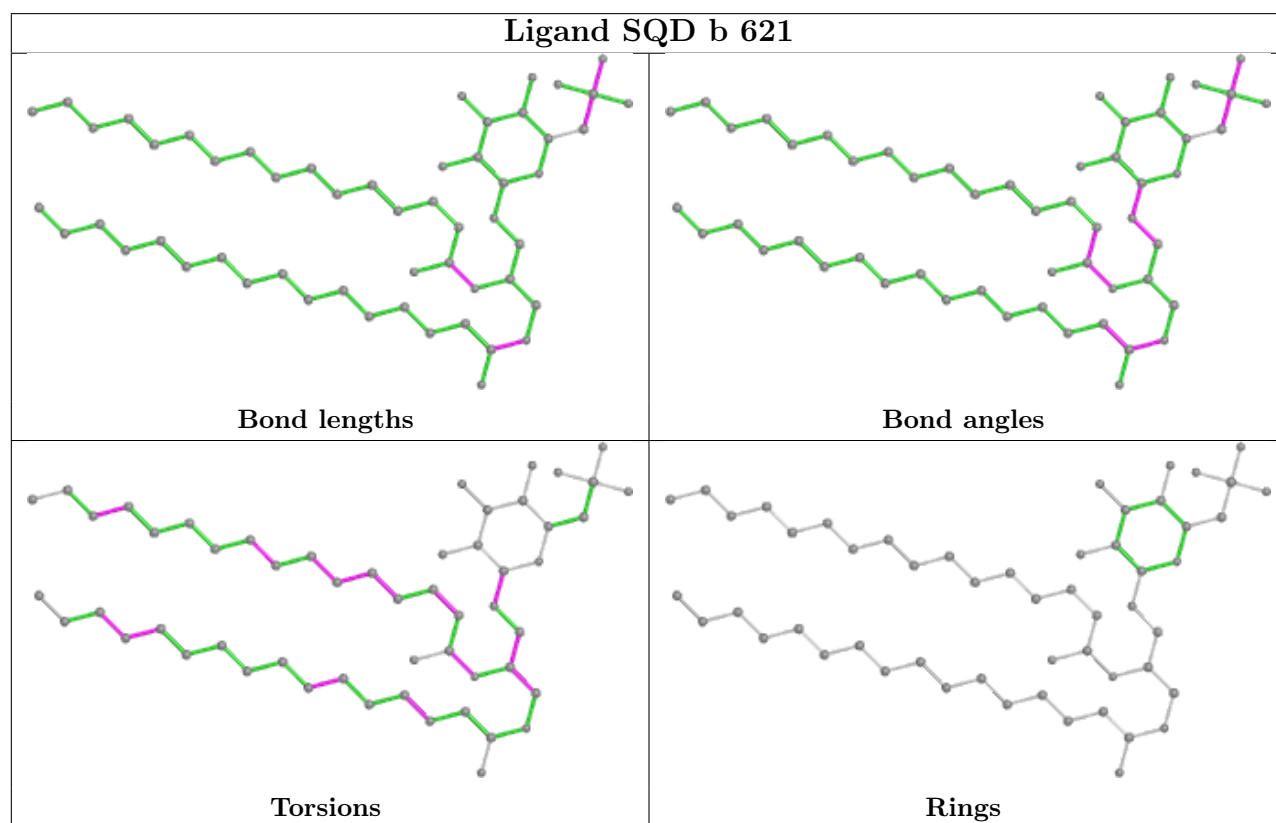
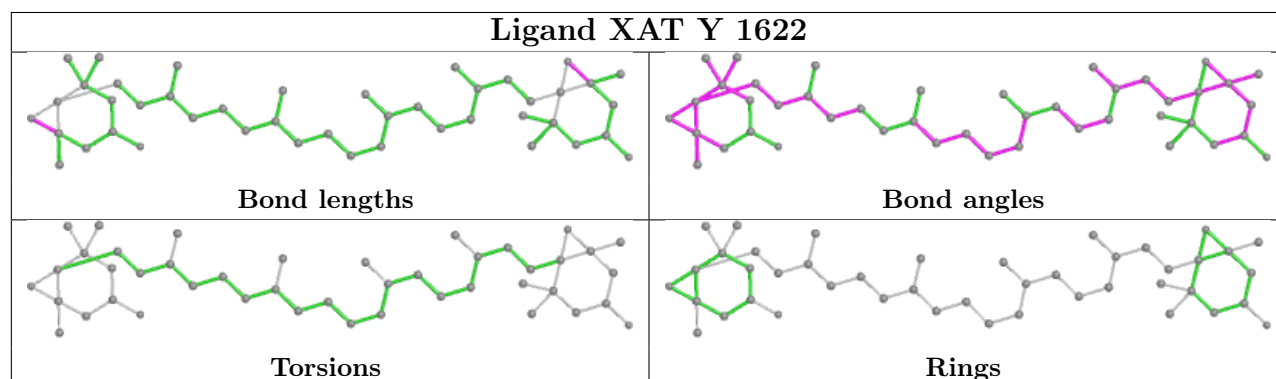
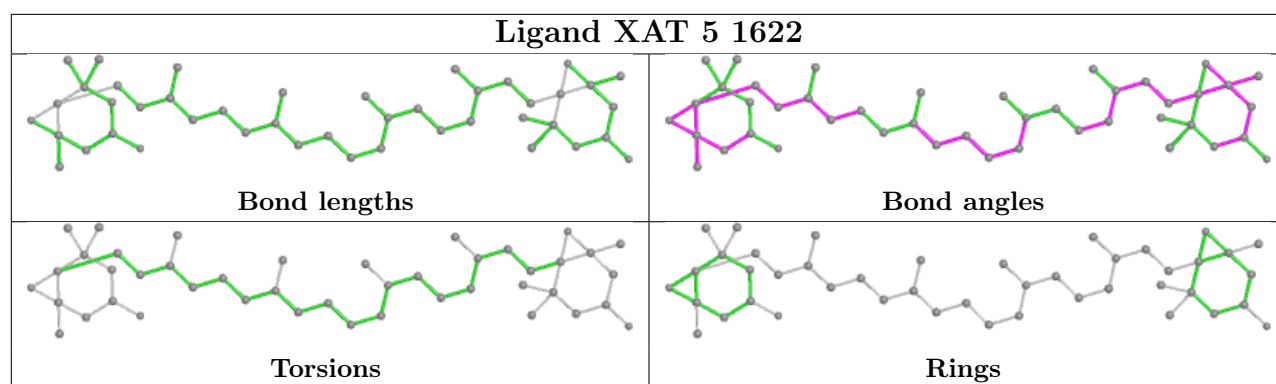
Rings

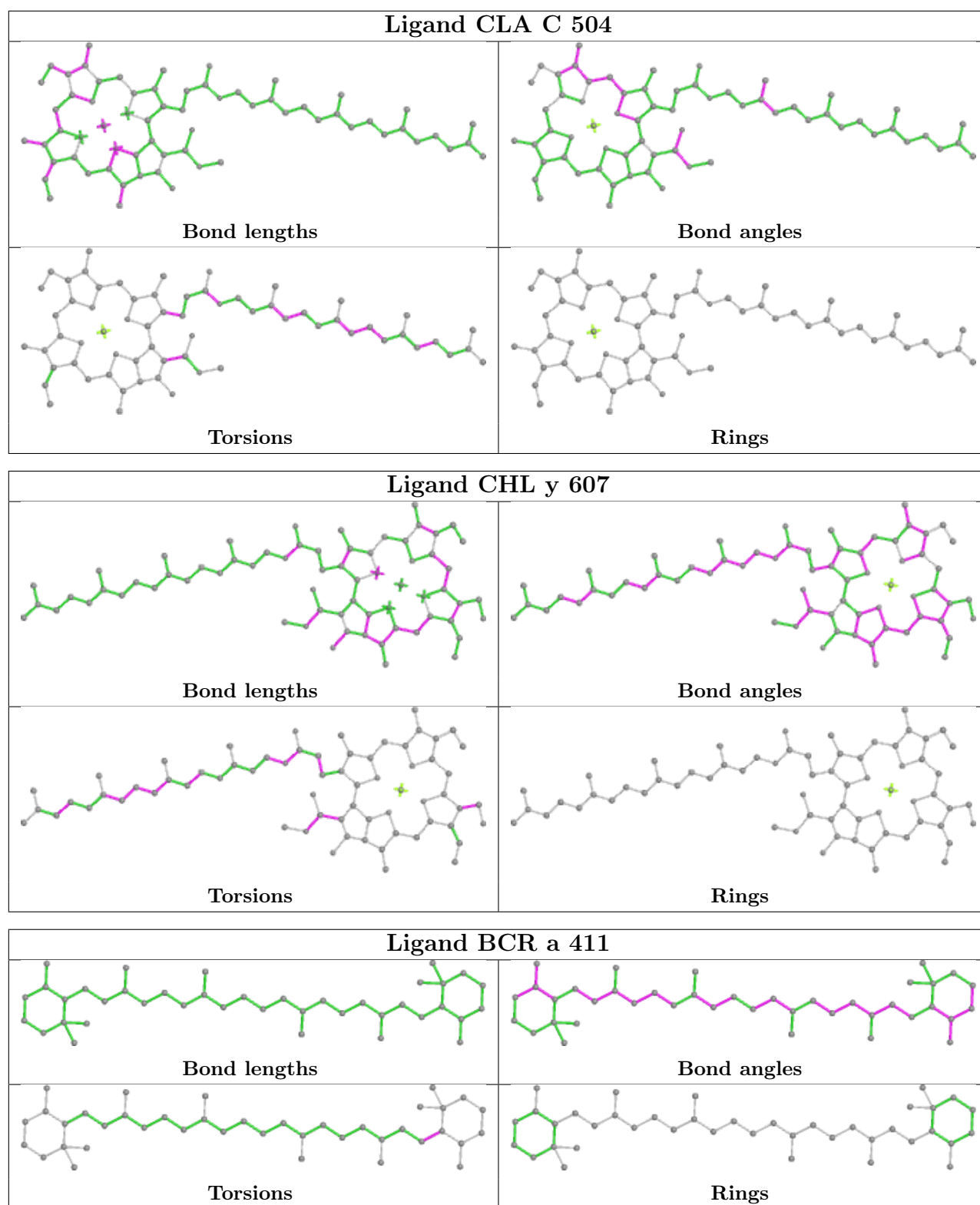
Ligand CLA g 611

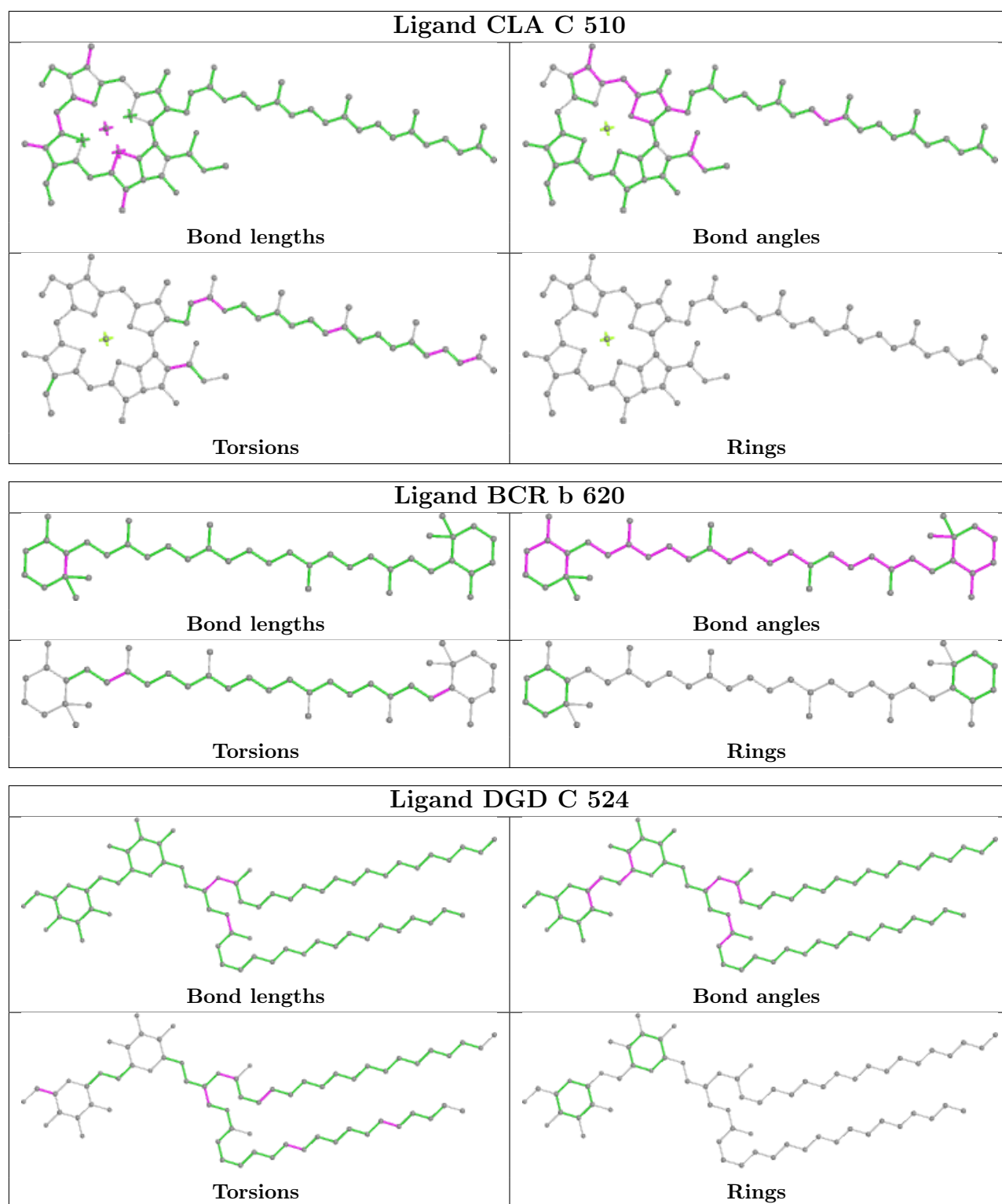


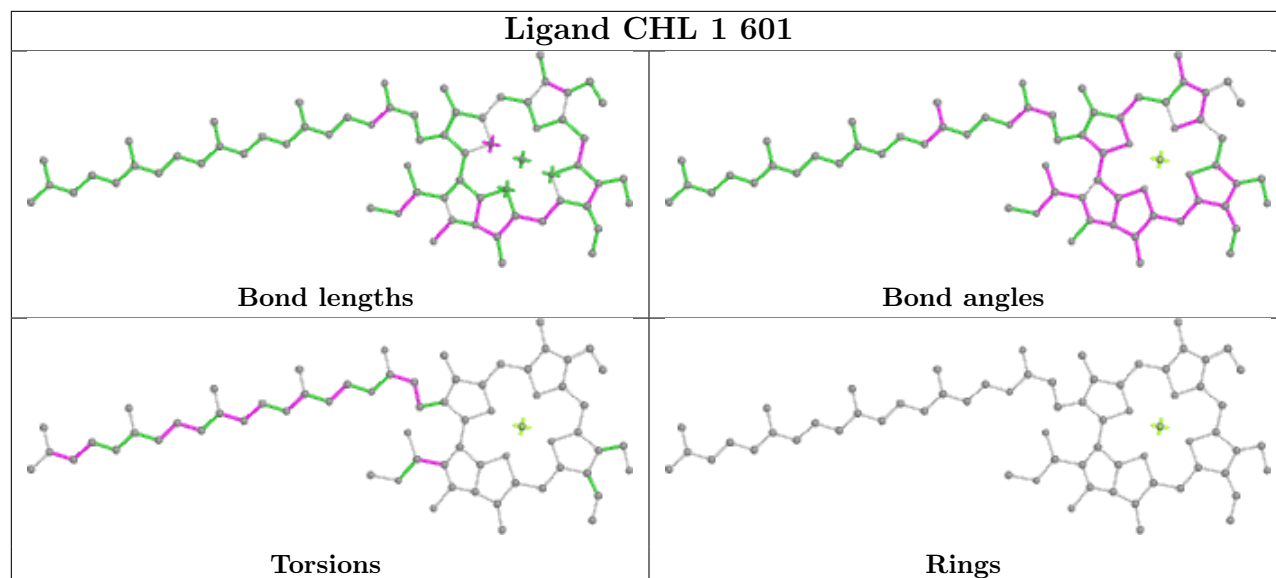
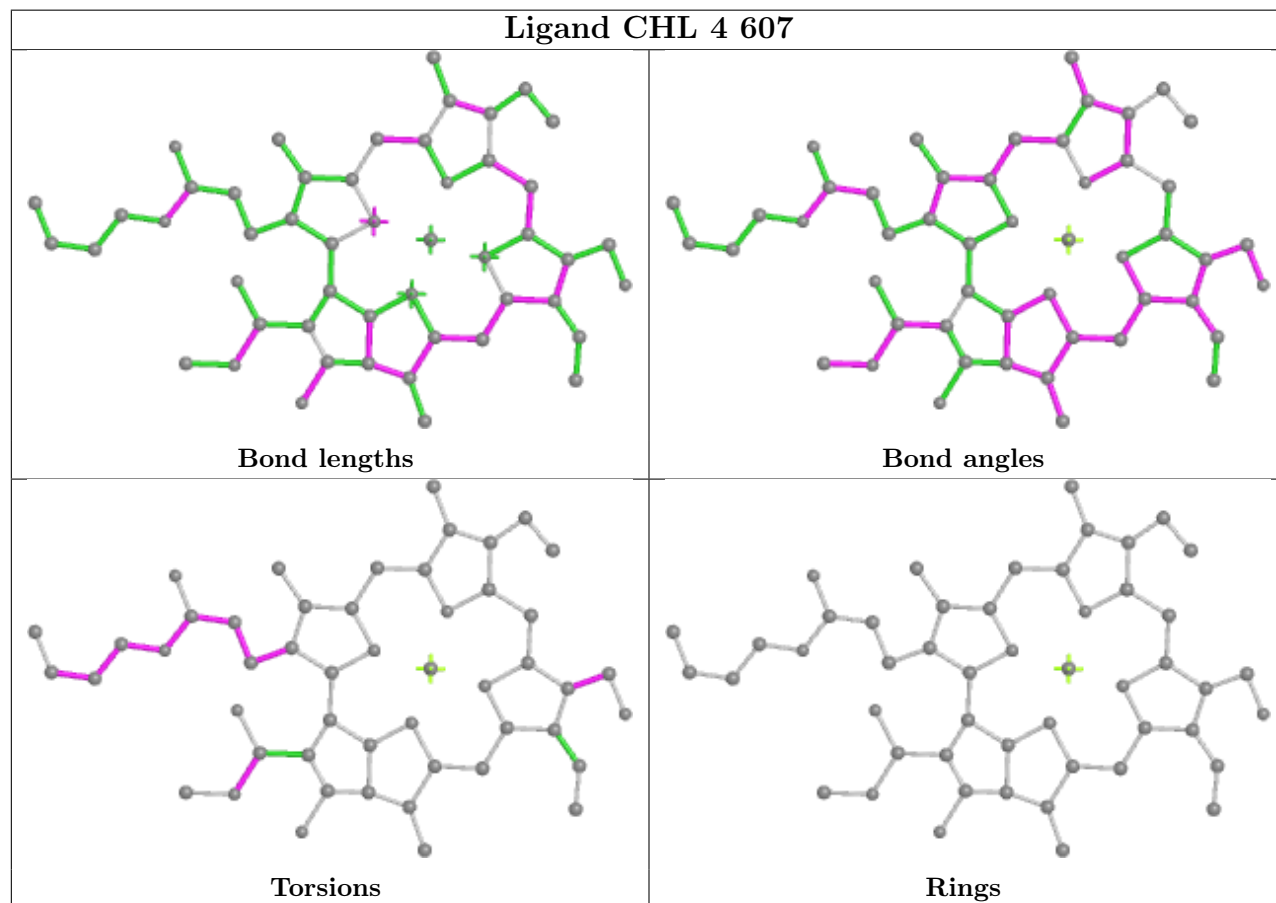
Ligand CLA 7 611



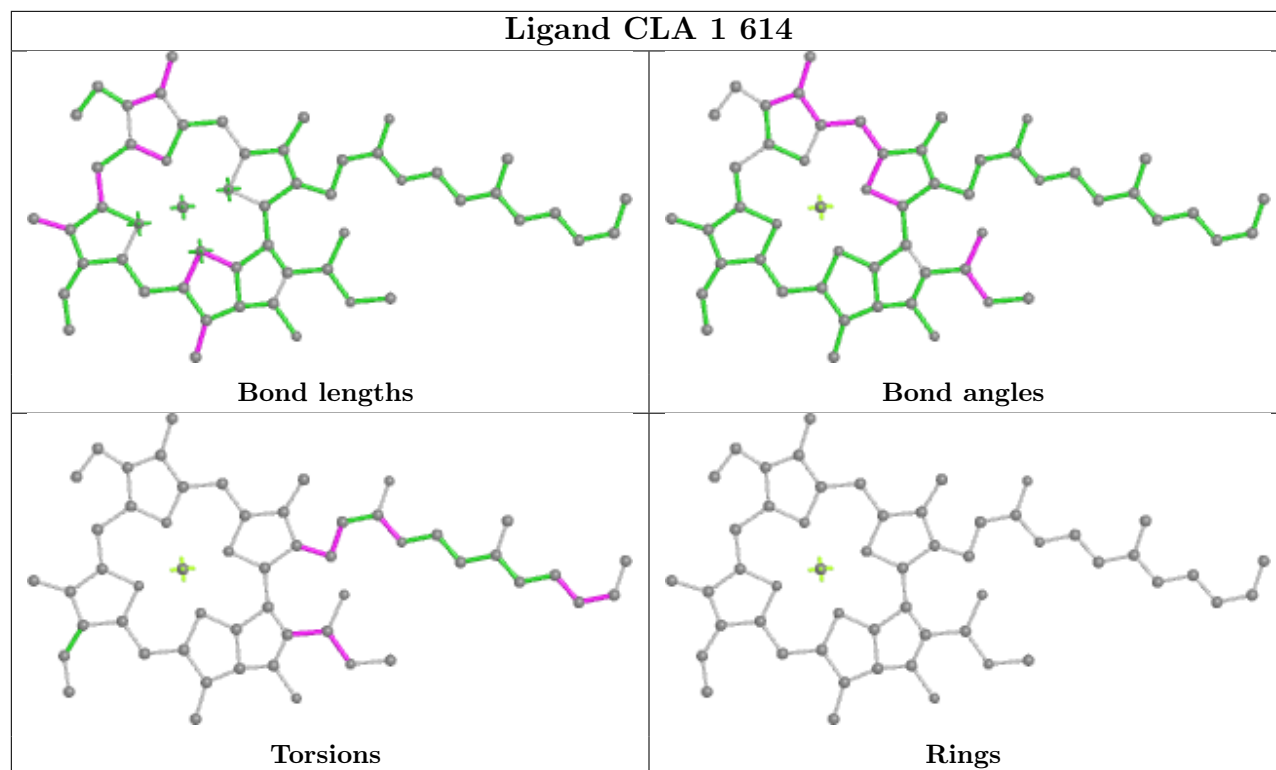




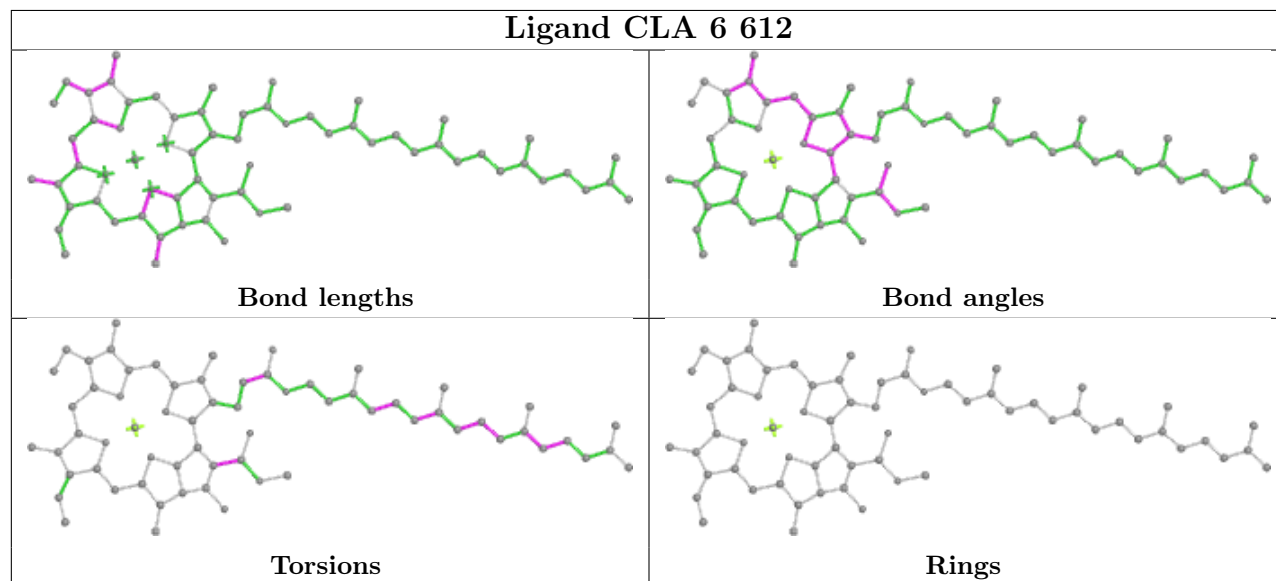


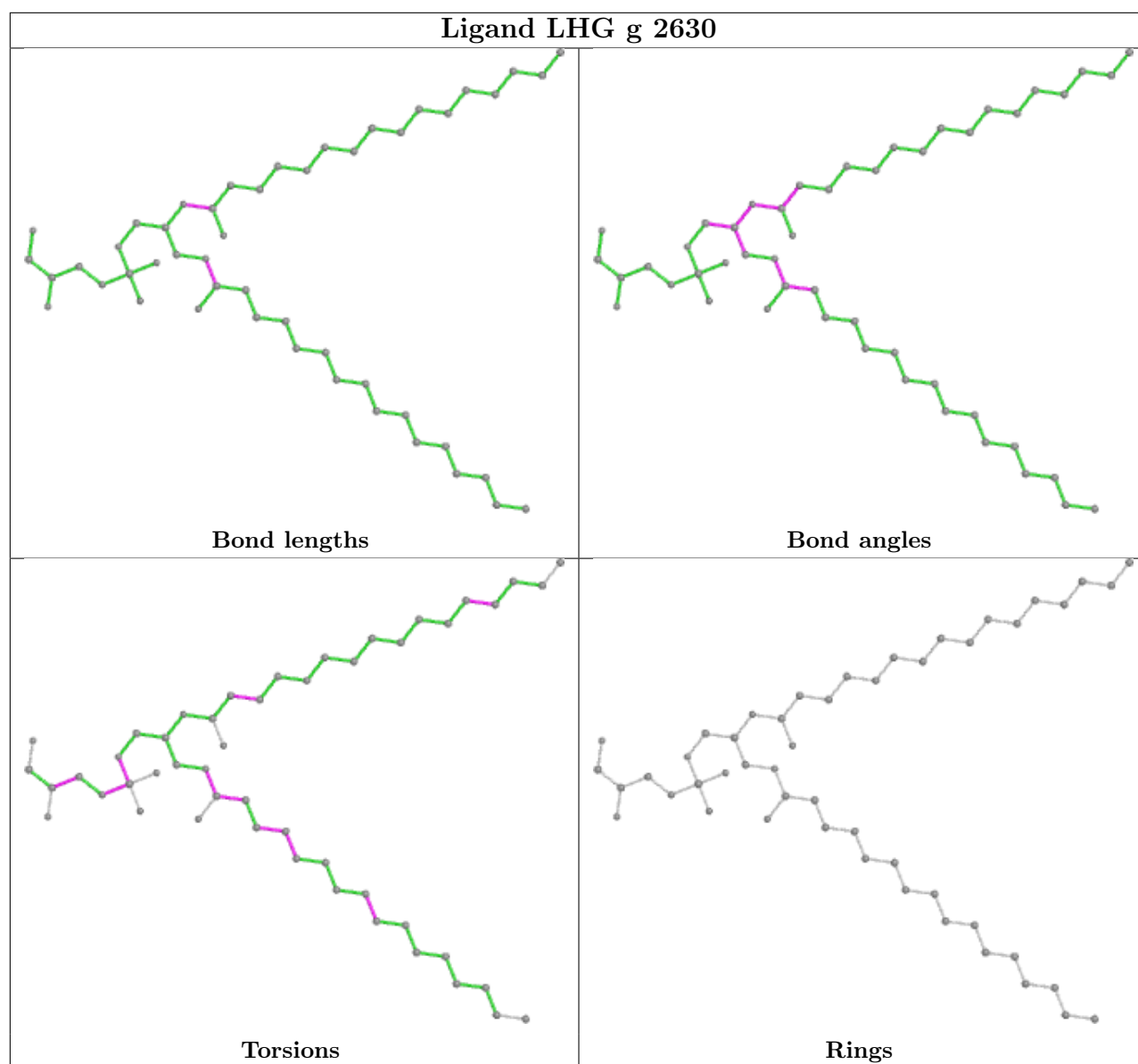
Ligand CHL 1 601**Ligand CHL 4 607**

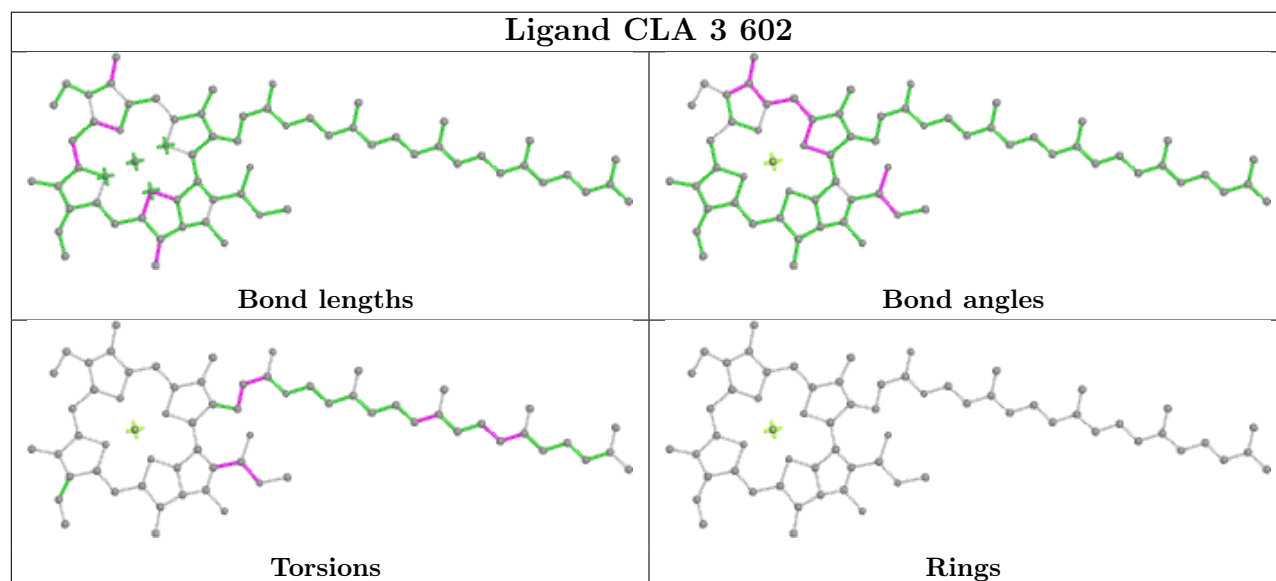
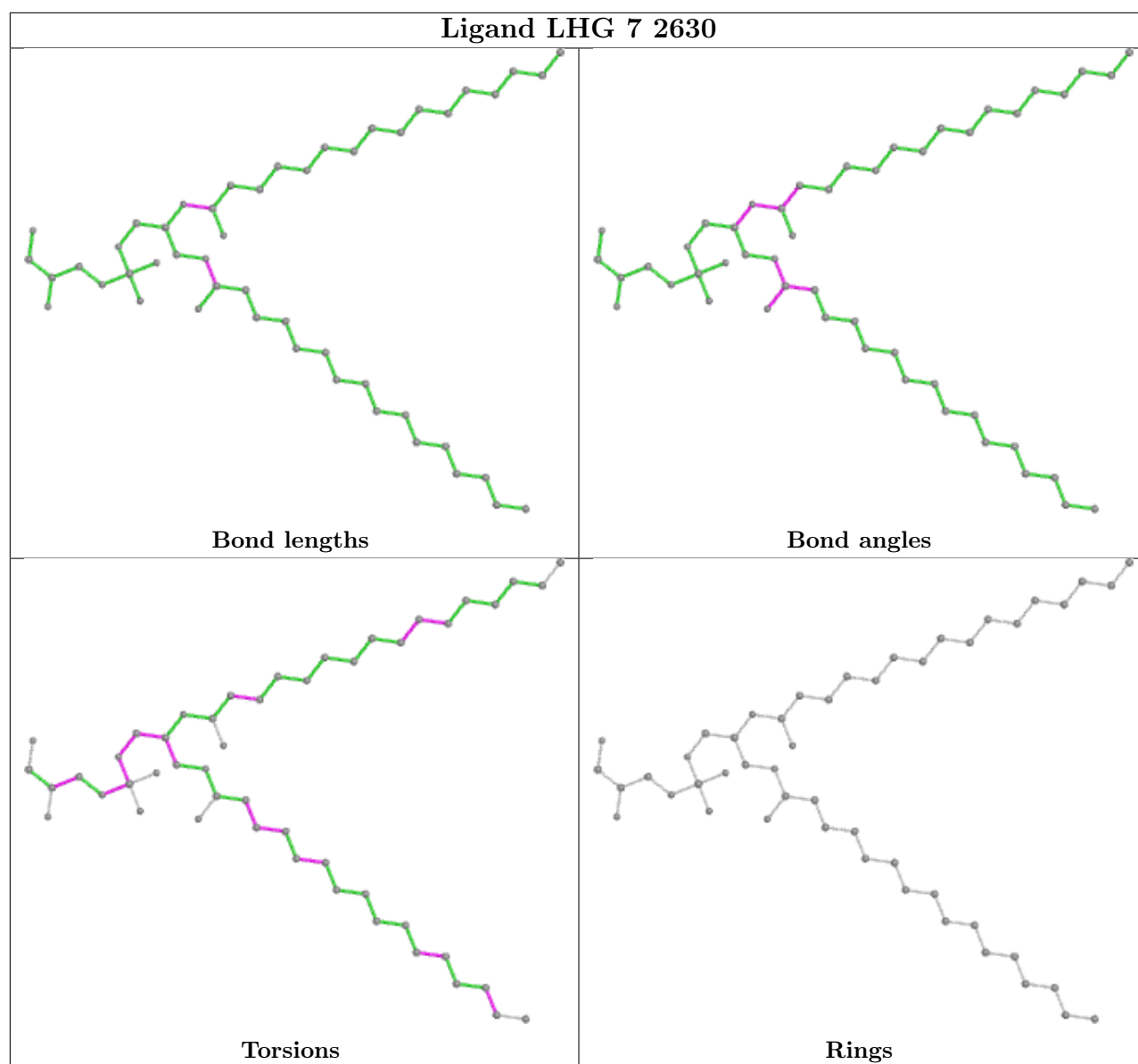
Ligand CLA 1 614



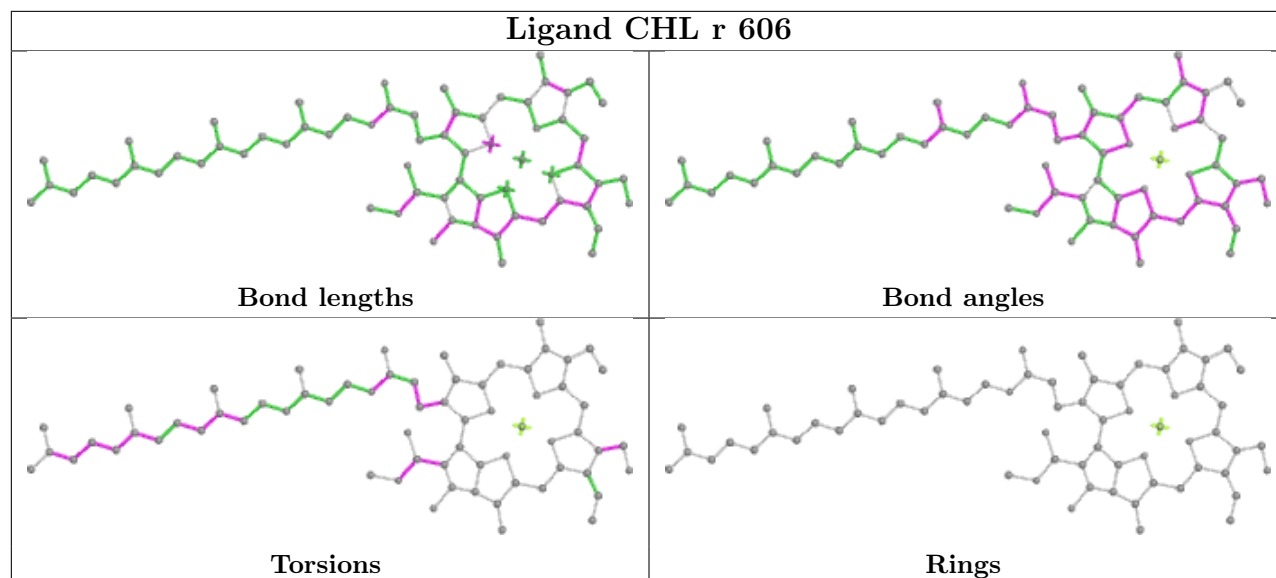
Ligand CLA 6 612



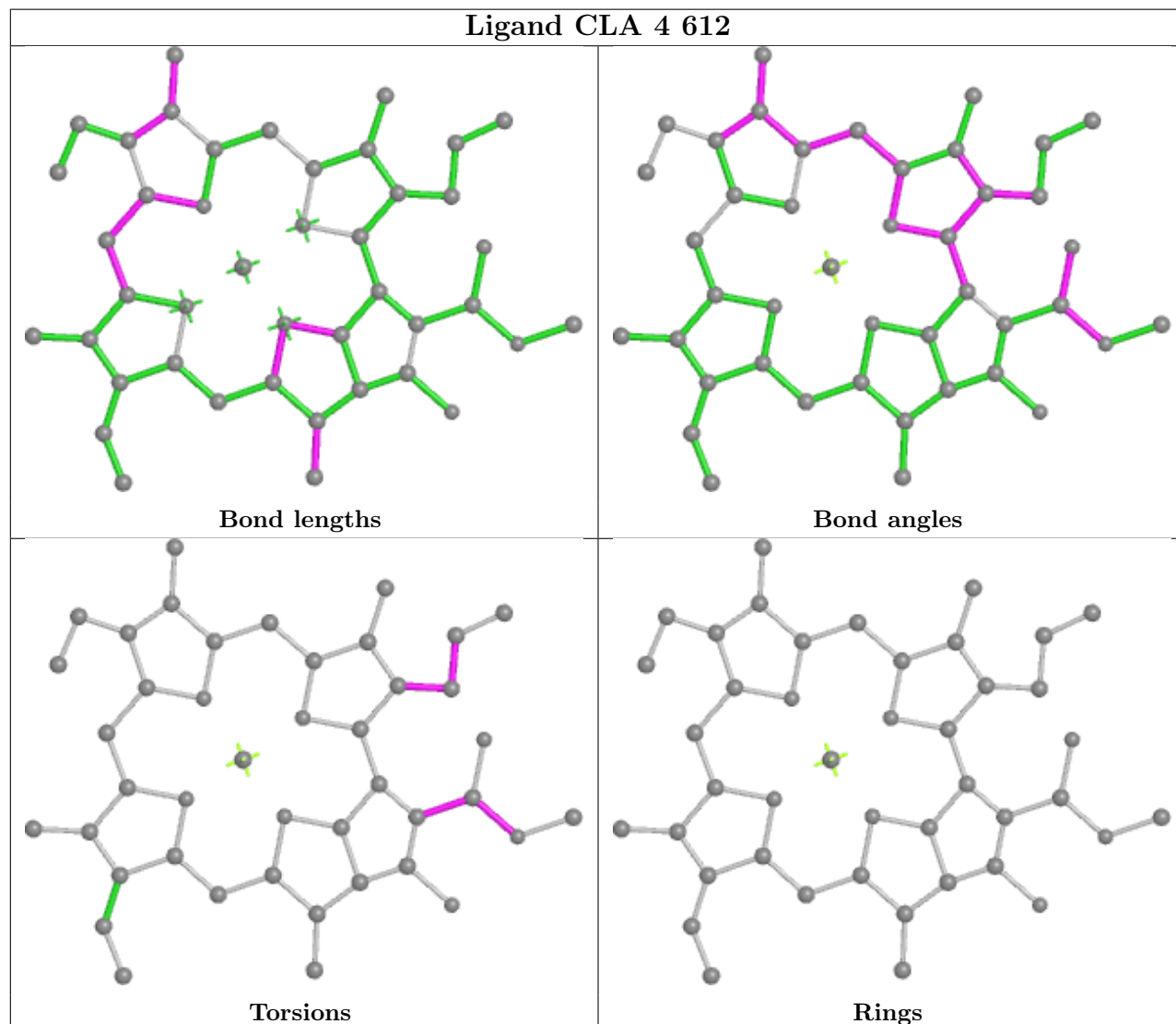




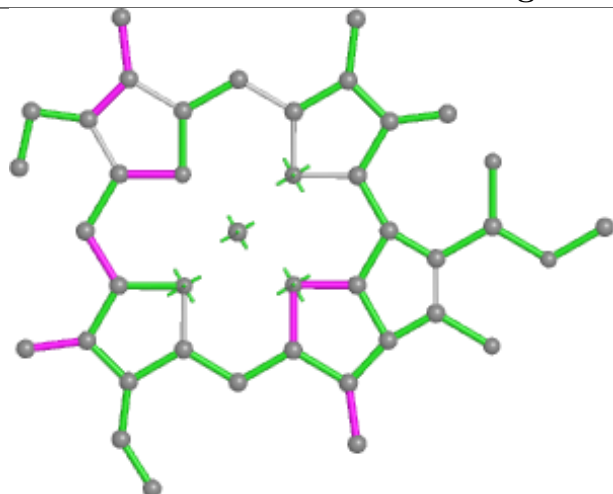
Ligand CHL r 606



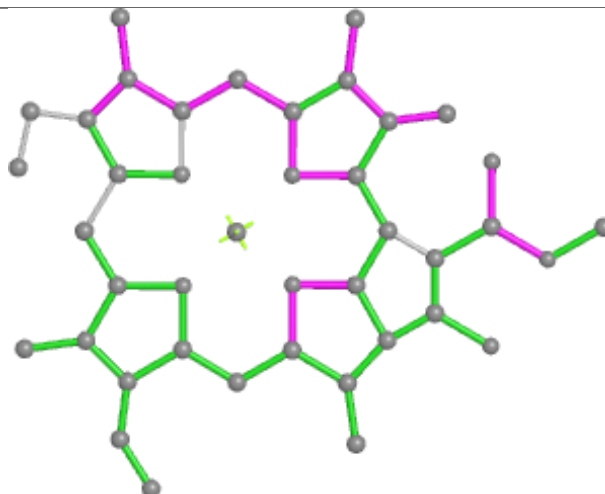
Ligand CLA 4 612



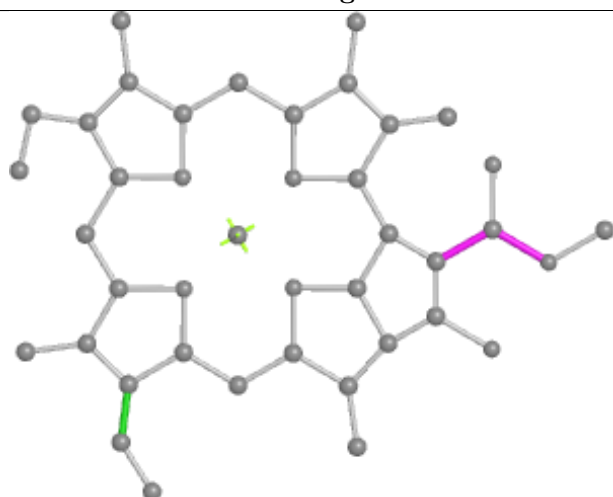
Ligand CLA S 609



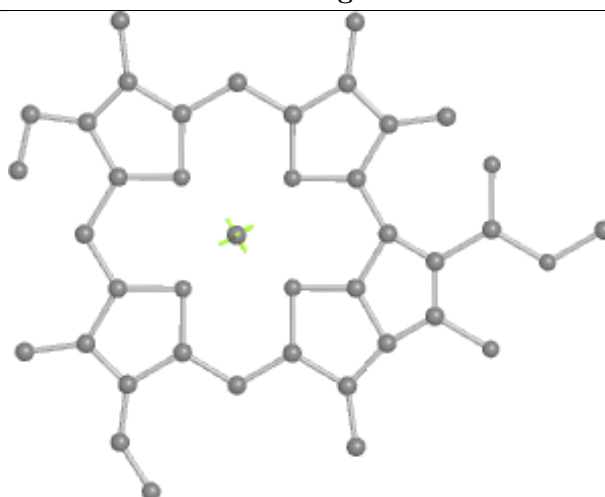
Bond lengths



Bond angles

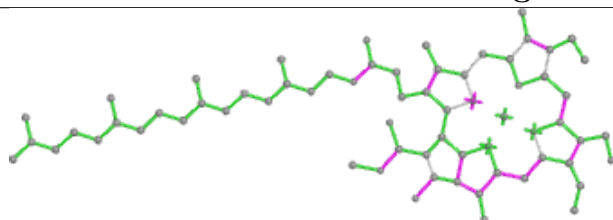


Torsions

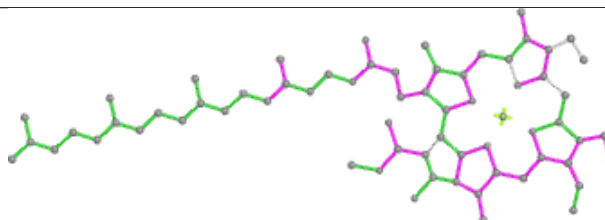


Rings

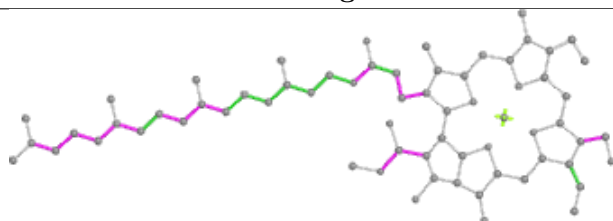
Ligand CHL R 606



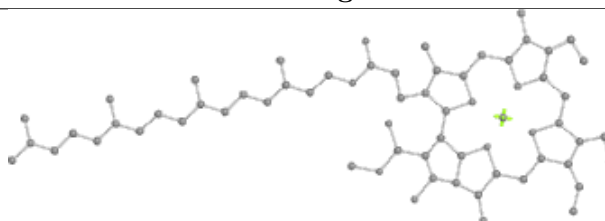
Bond lengths



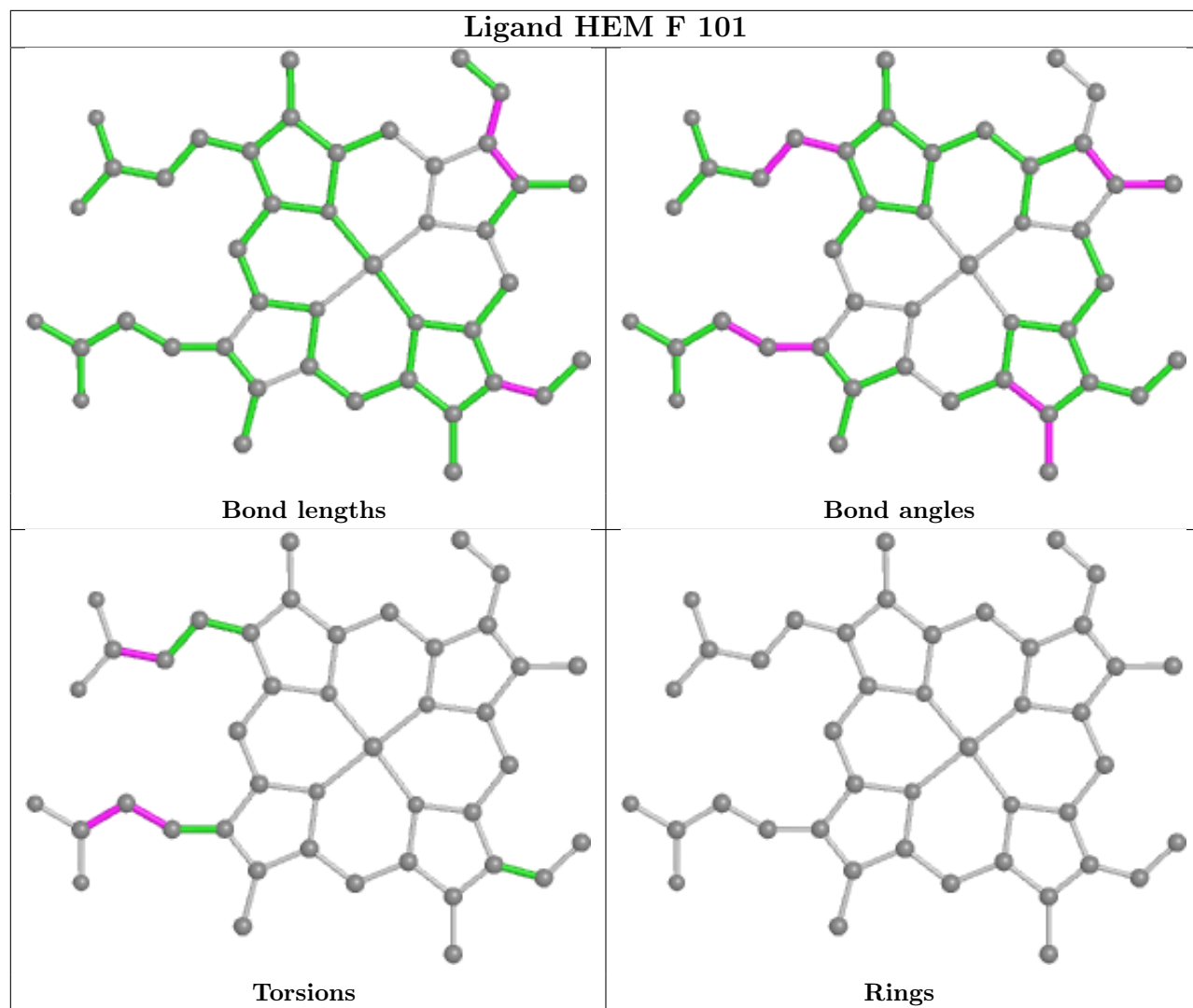
Bond angles



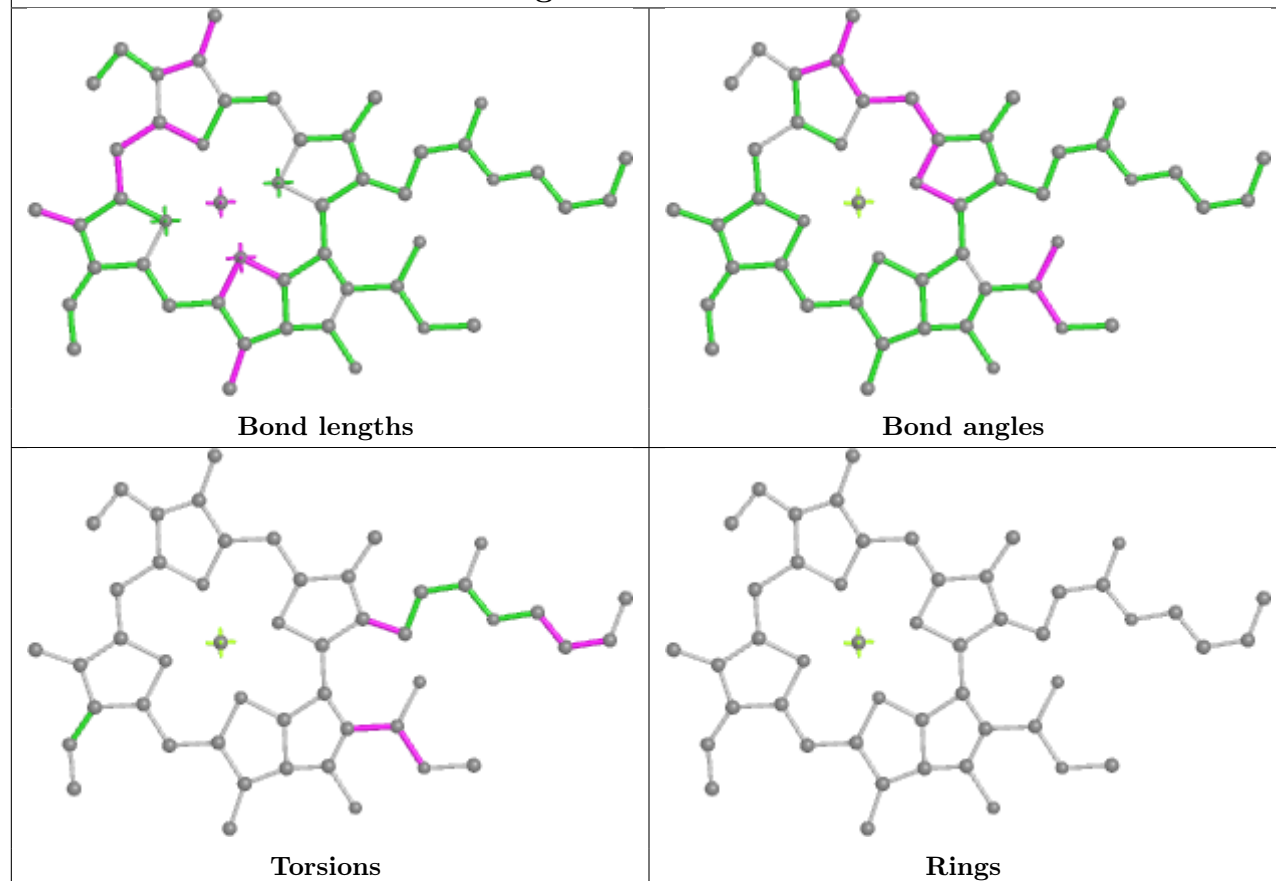
Torsions



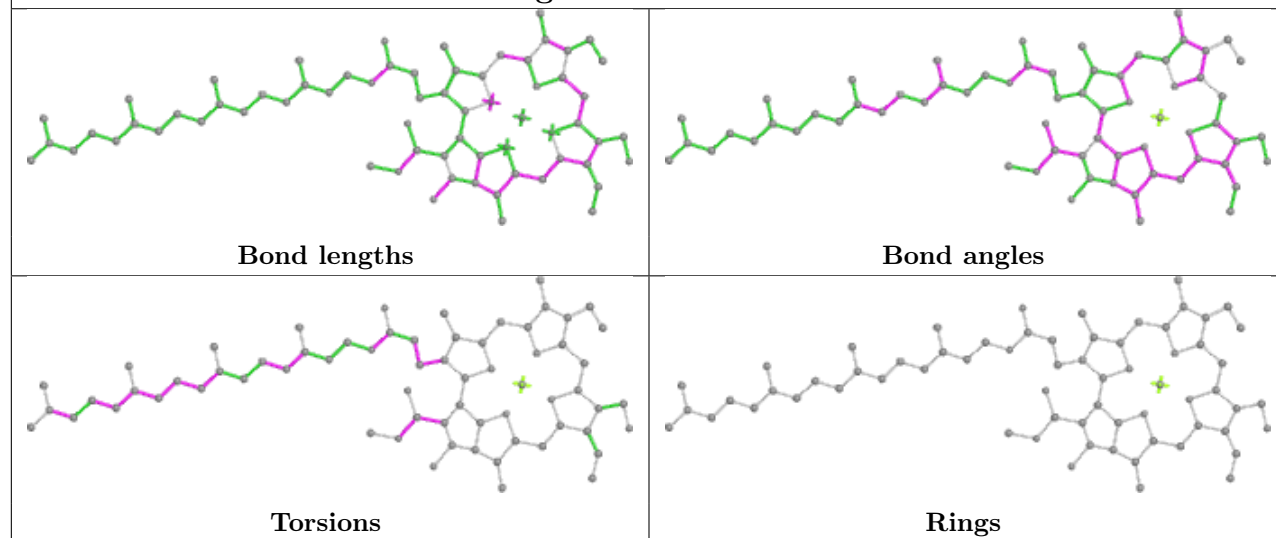
Rings

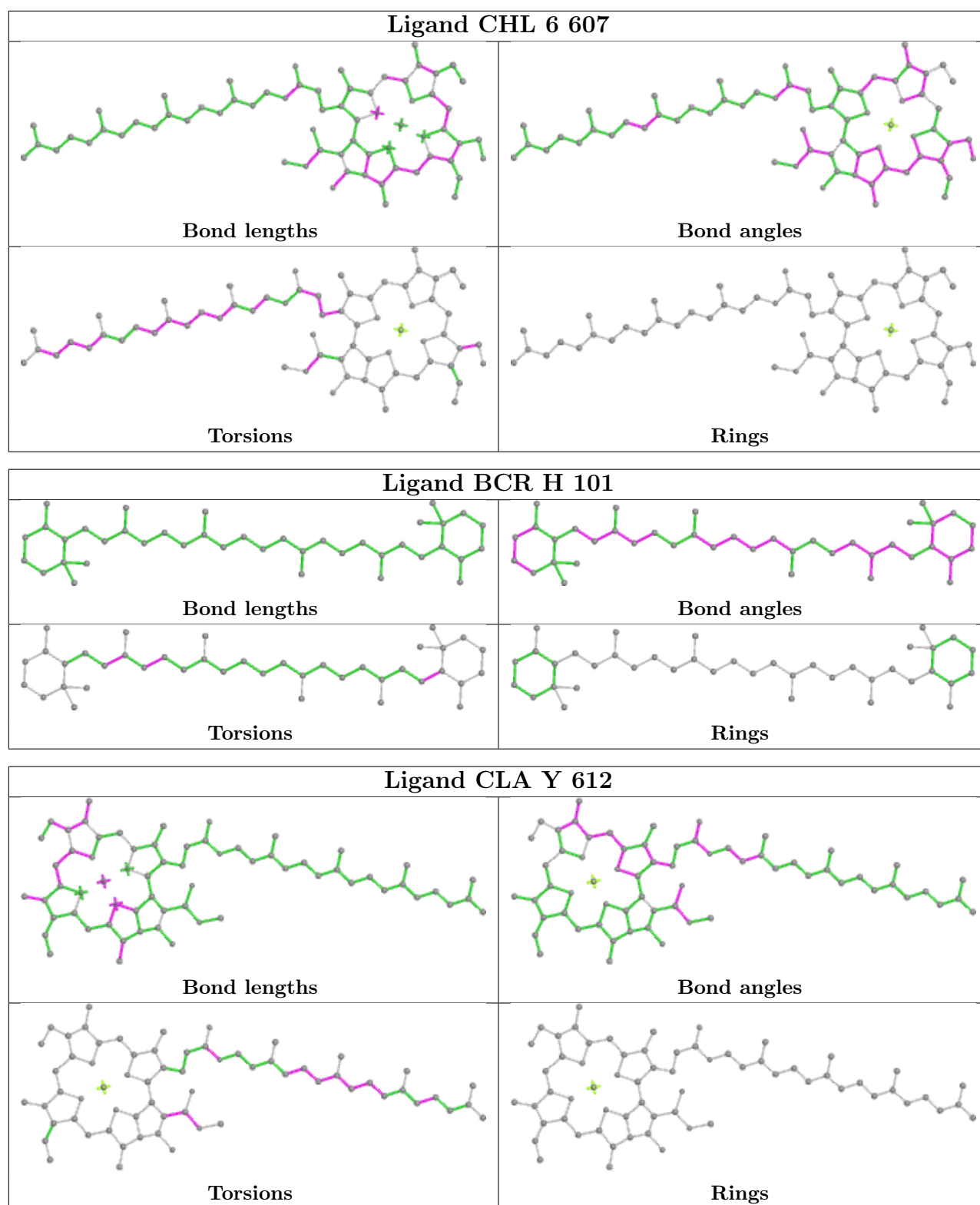


Ligand CLA n 611

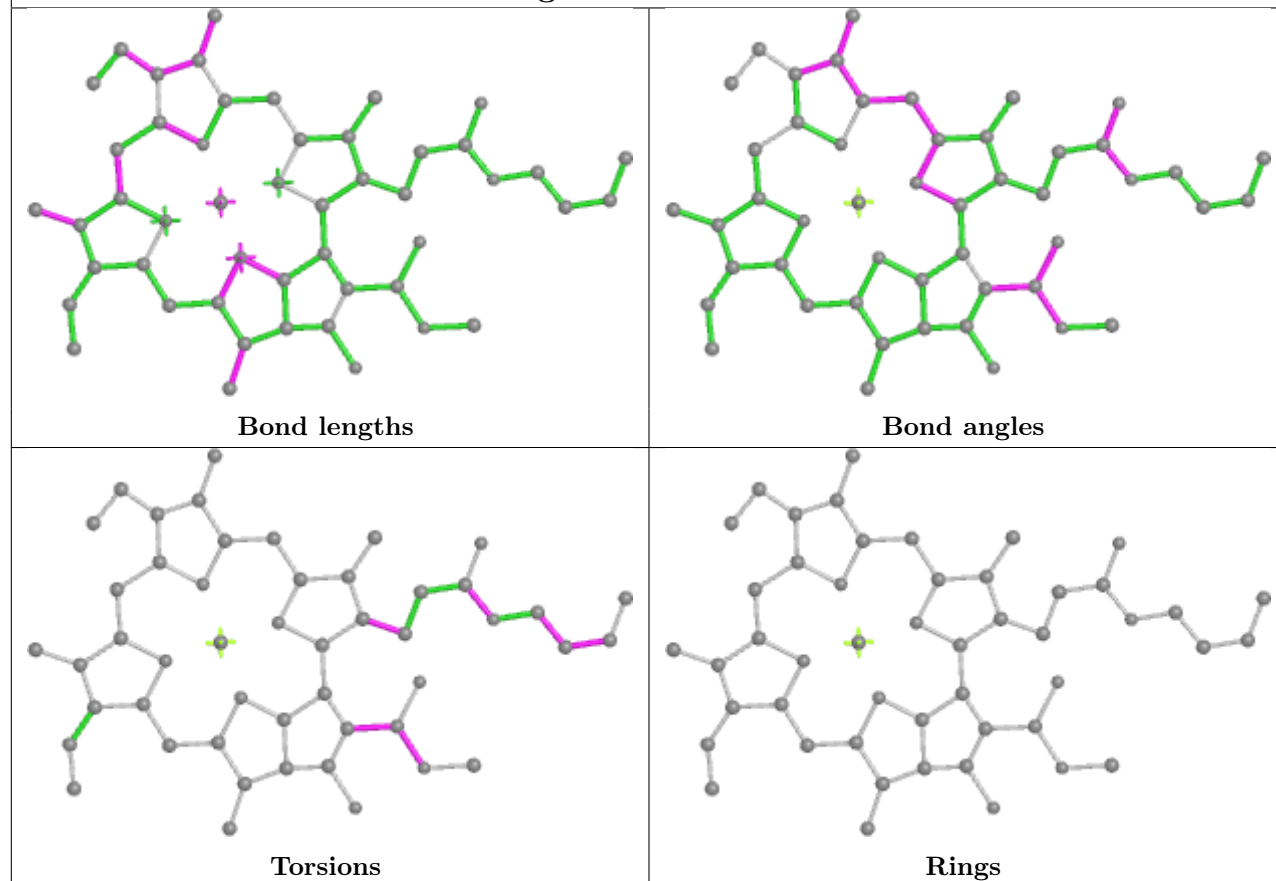


Ligand CHL 0 606

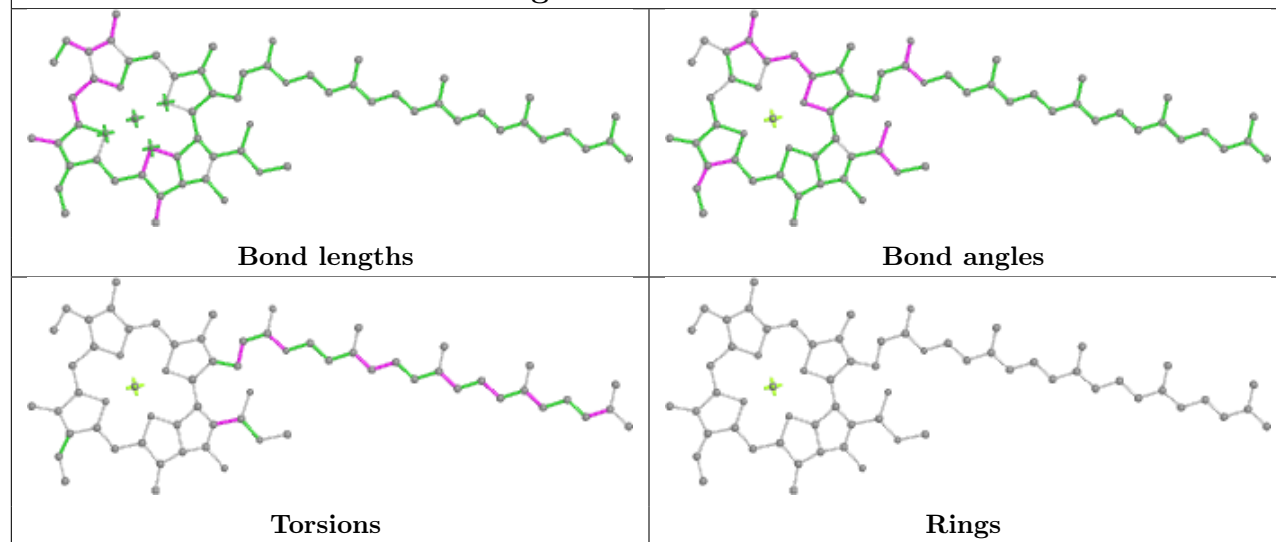




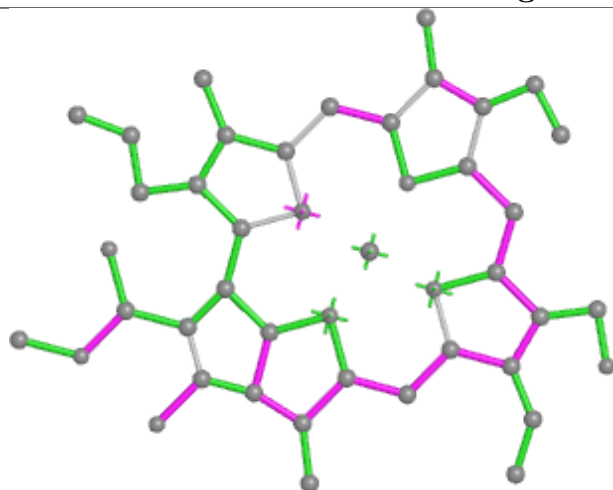
Ligand CLA s 610



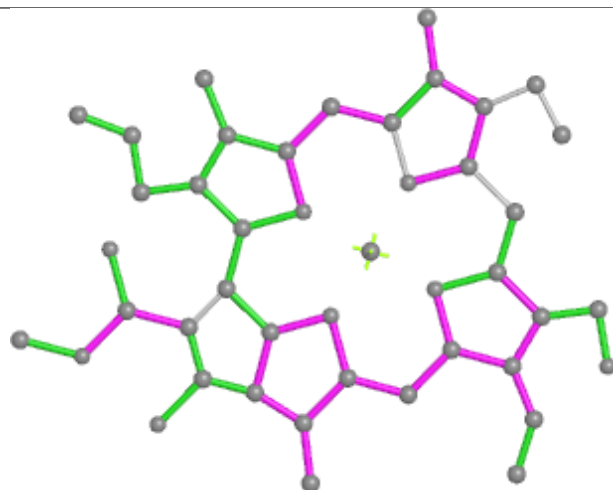
Ligand CLA N 613



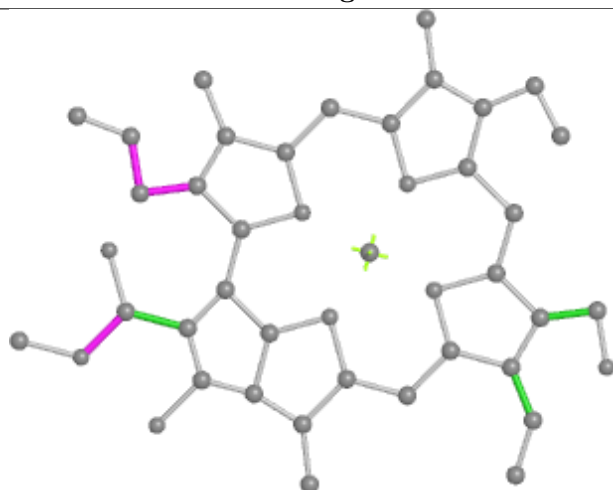
Ligand CHL 9 608



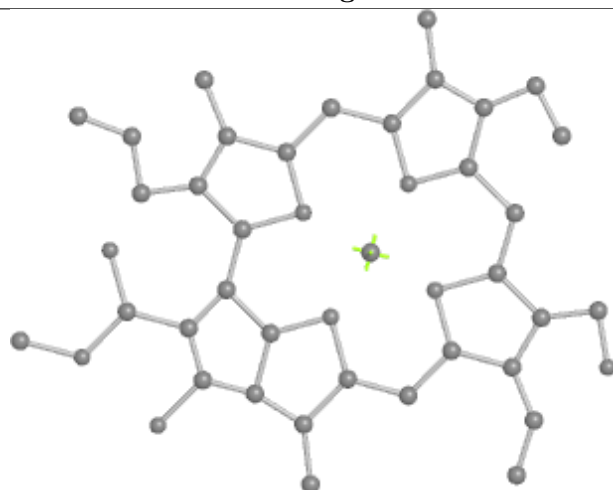
Bond lengths



Bond angles

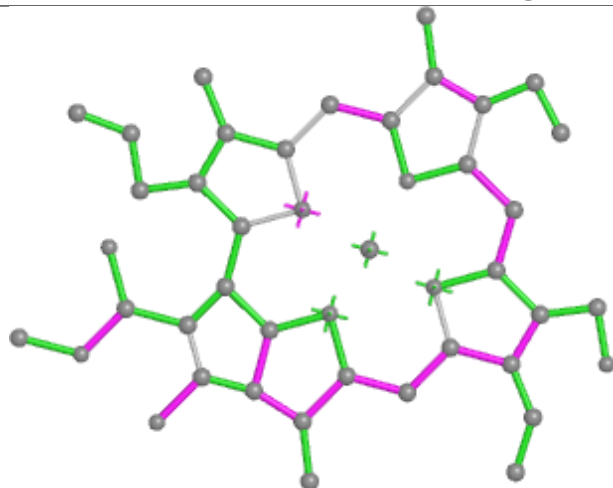


Torsions

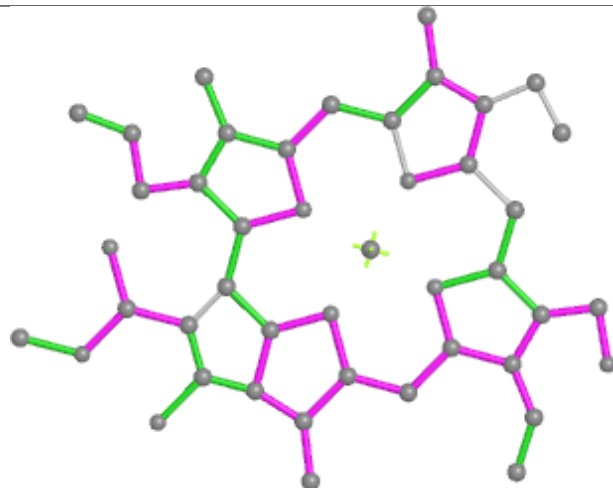


Rings

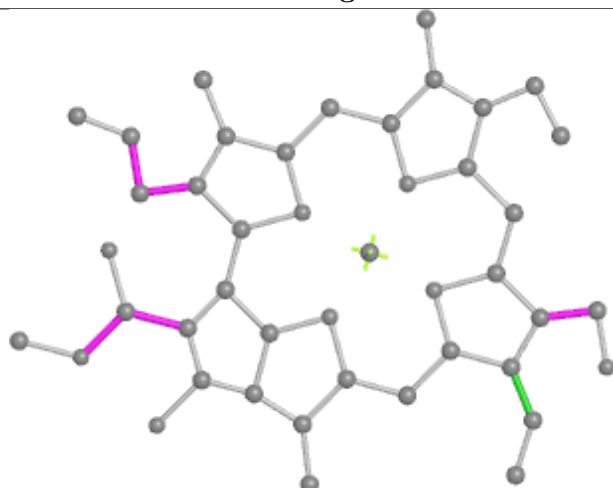
Ligand CHL s 606



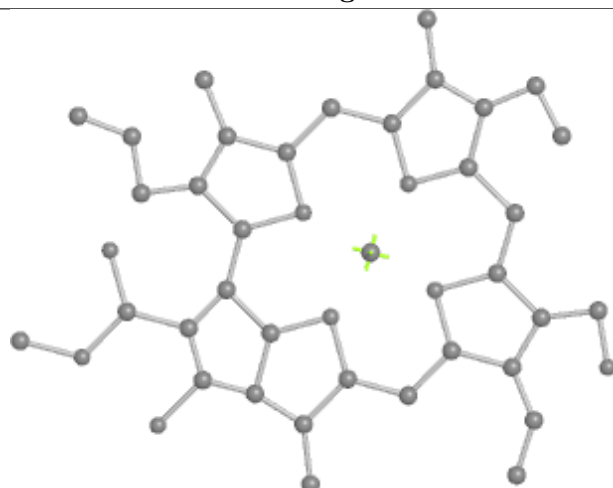
Bond lengths



Bond angles

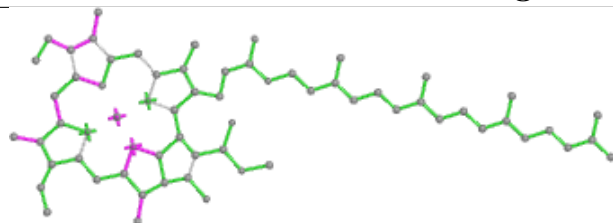


Torsions

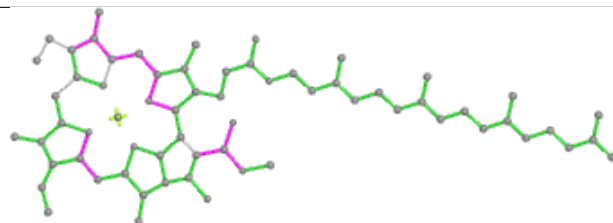


Rings

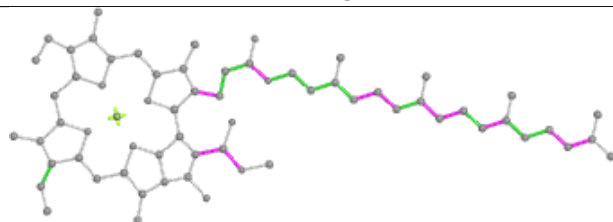
Ligand CLA C 508



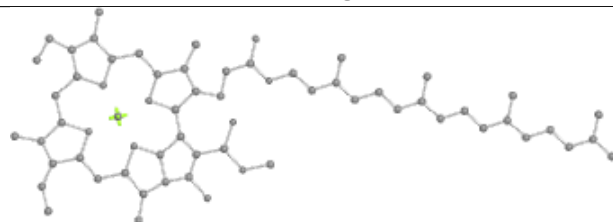
Bond lengths



Bond angles

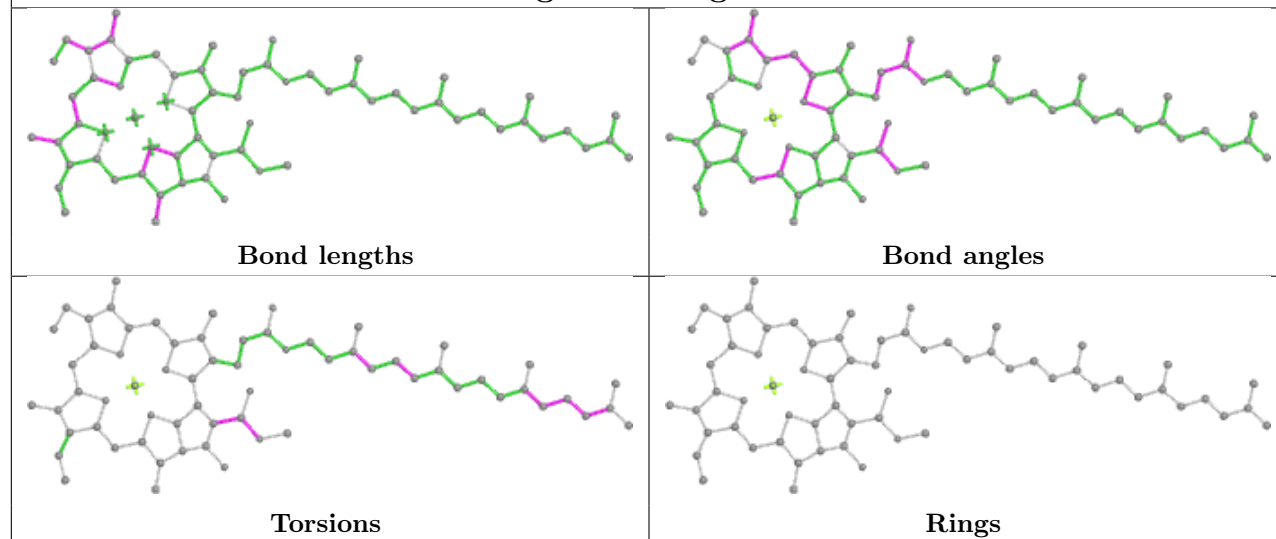


Torsions

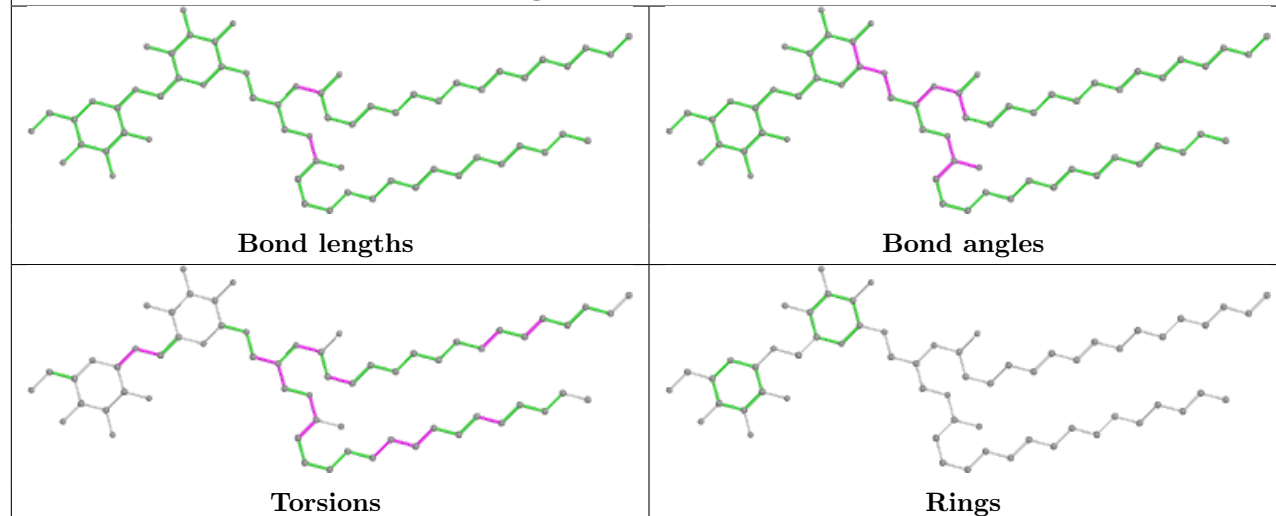


Rings

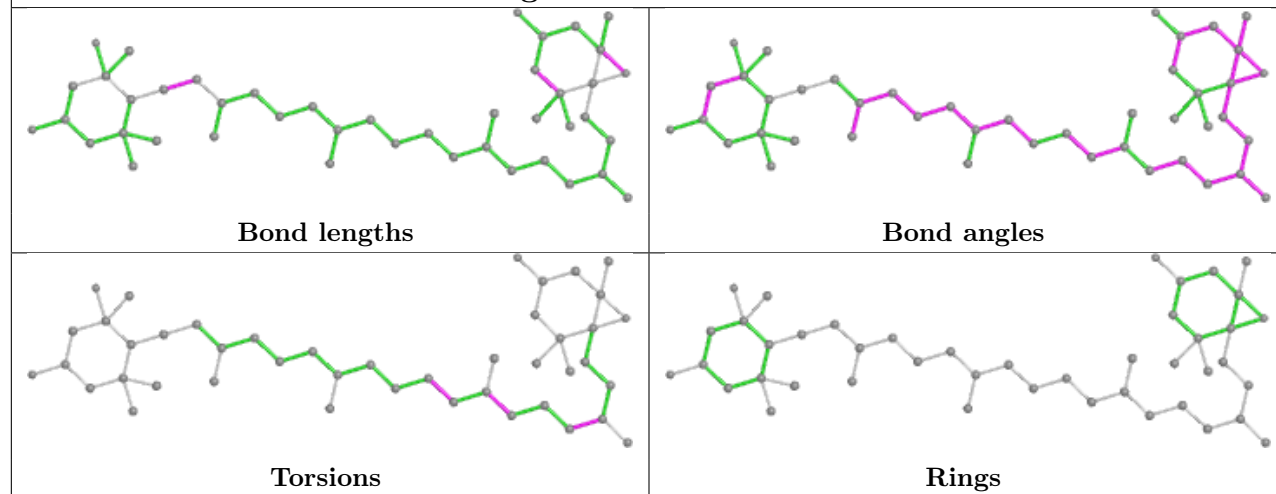
Ligand CLA g 610



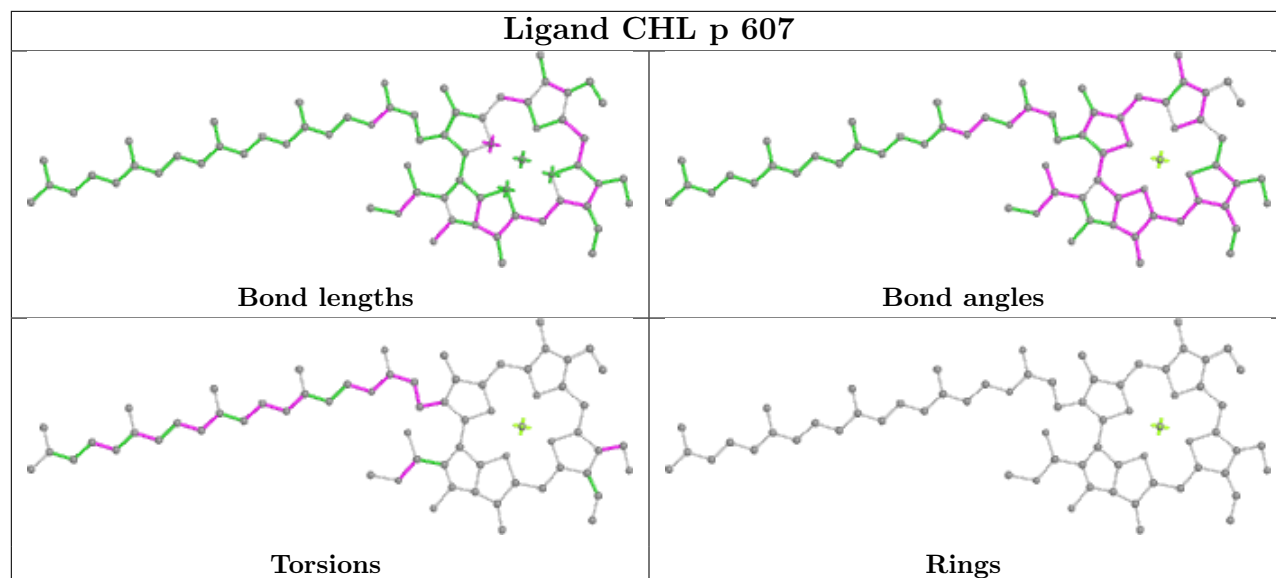
Ligand DGD C 519



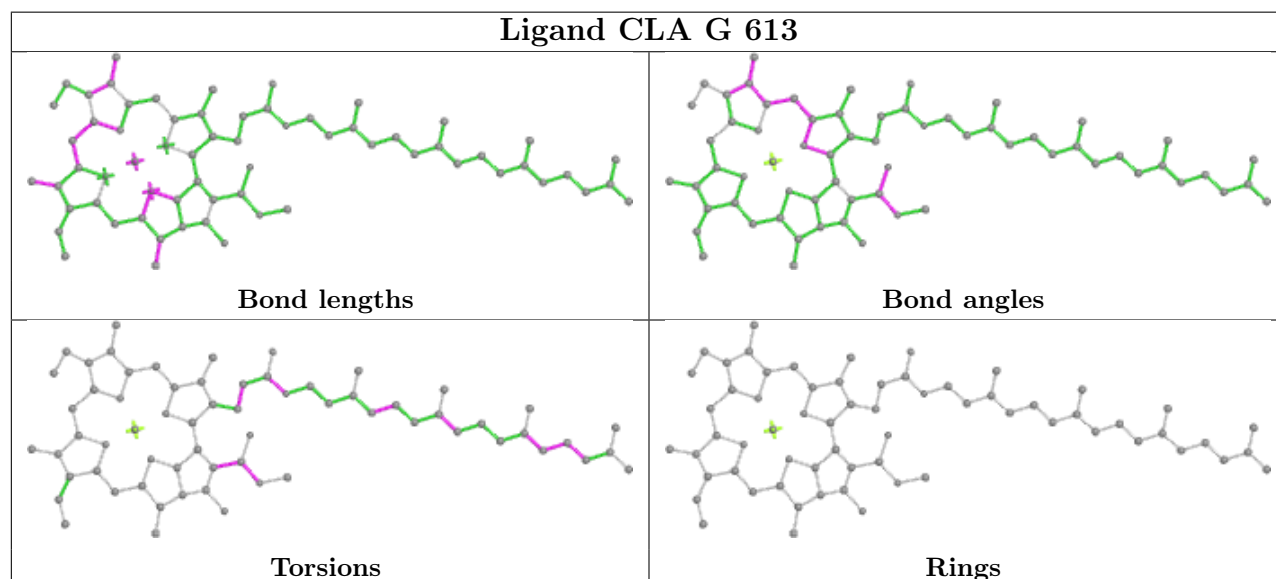
Ligand NEX Y 1623



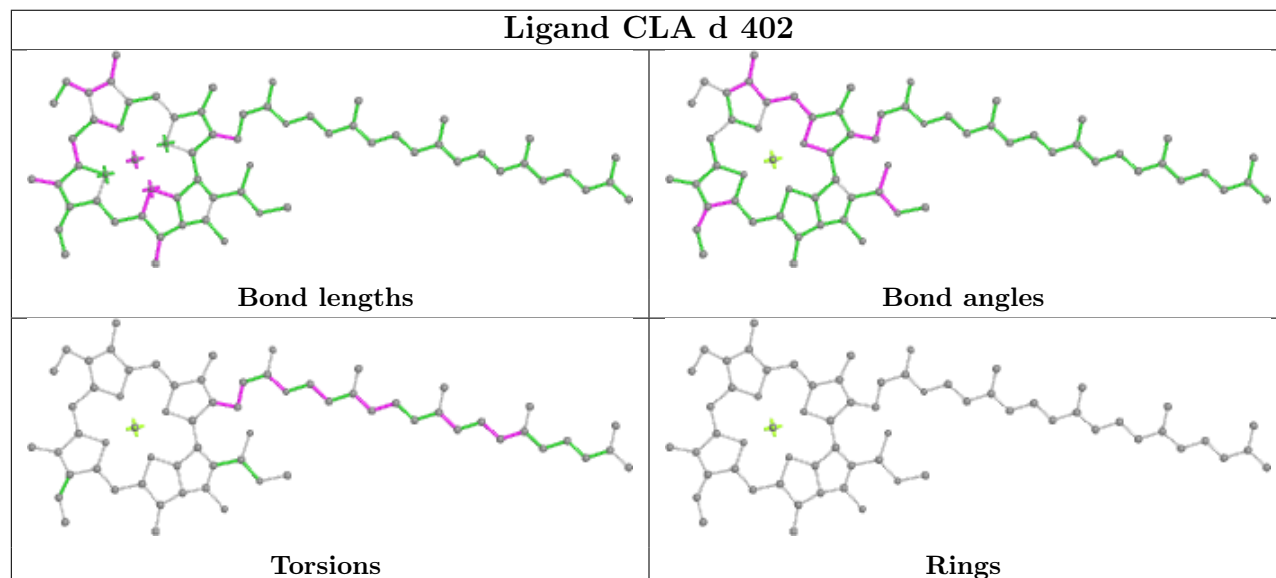
Ligand CHL p 607

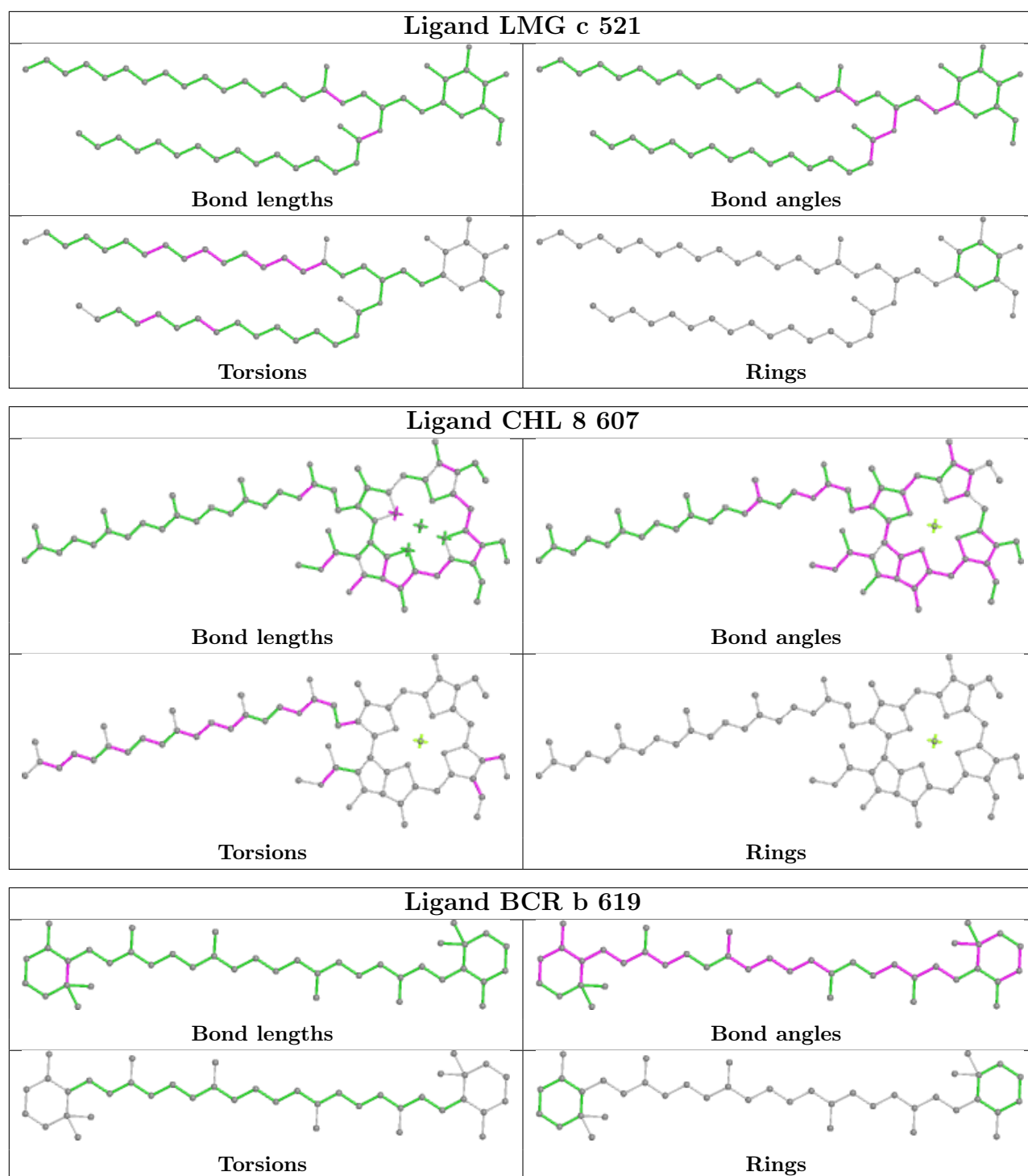


Ligand CLA G 613

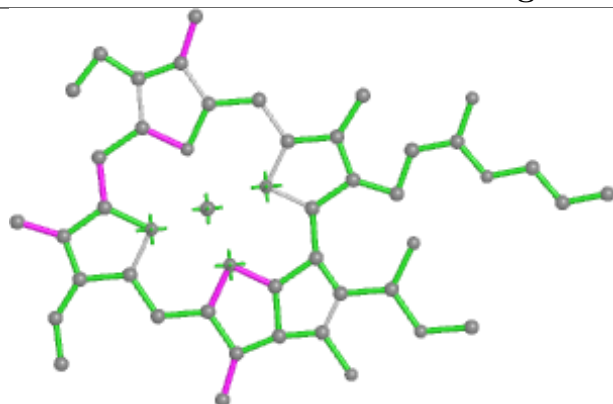


Ligand CLA d 402

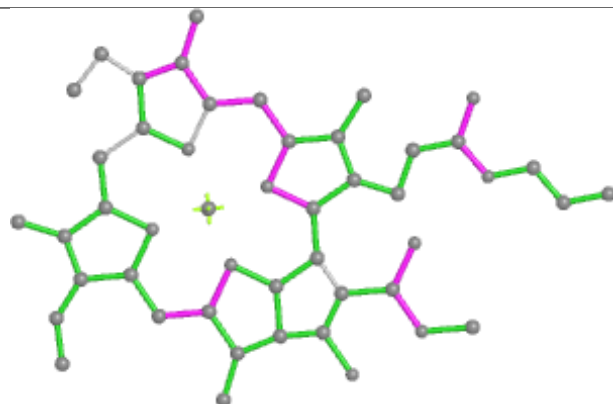




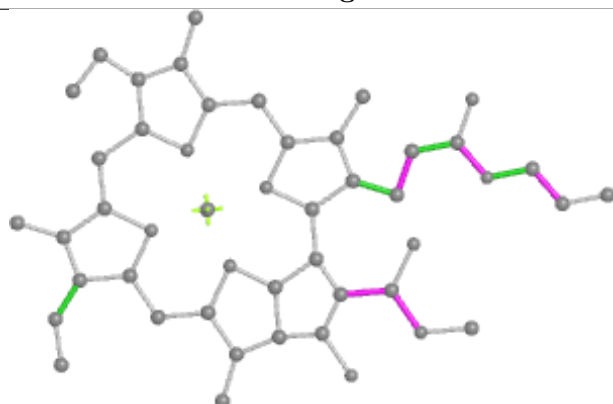
Ligand CLA S 614



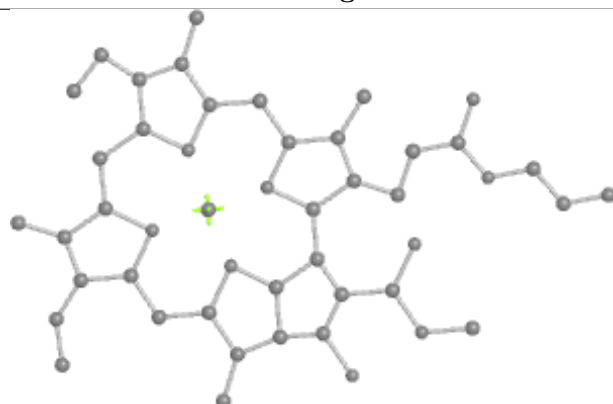
Bond lengths



Bond angles

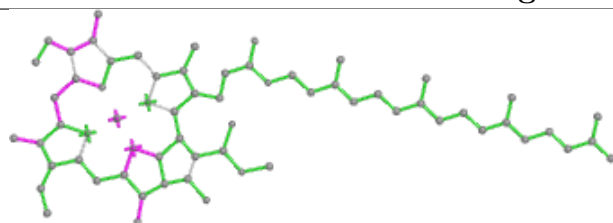


Torsions

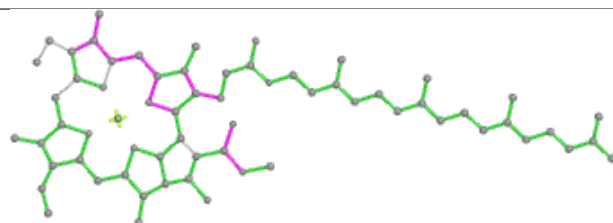


Rings

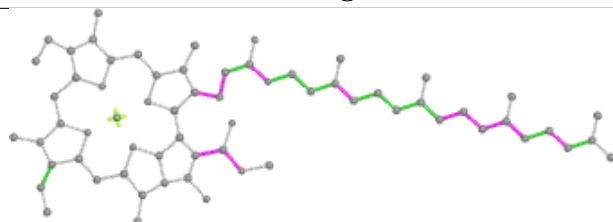
Ligand CLA 1 603



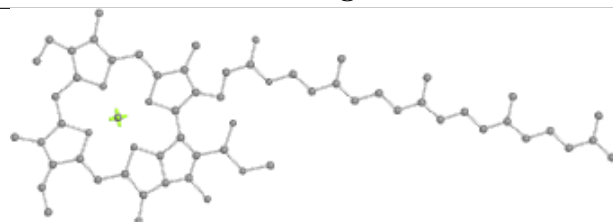
Bond lengths



Bond angles

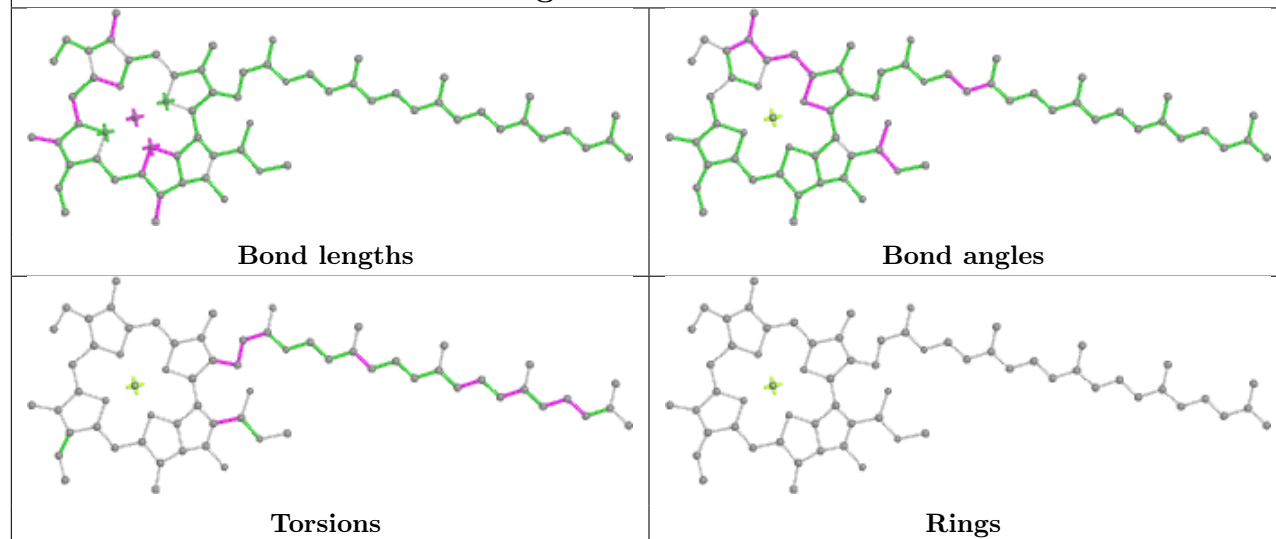


Torsions

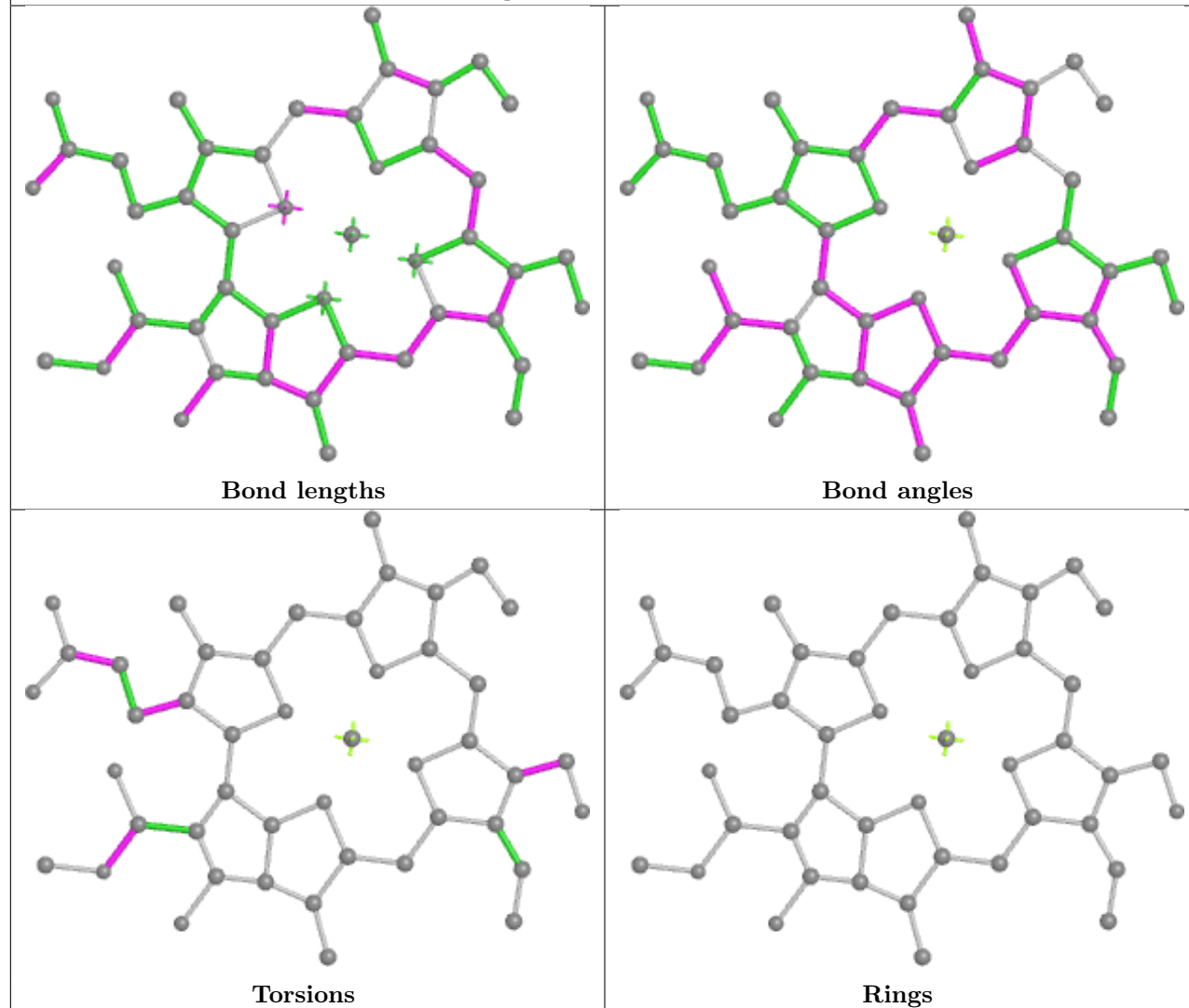


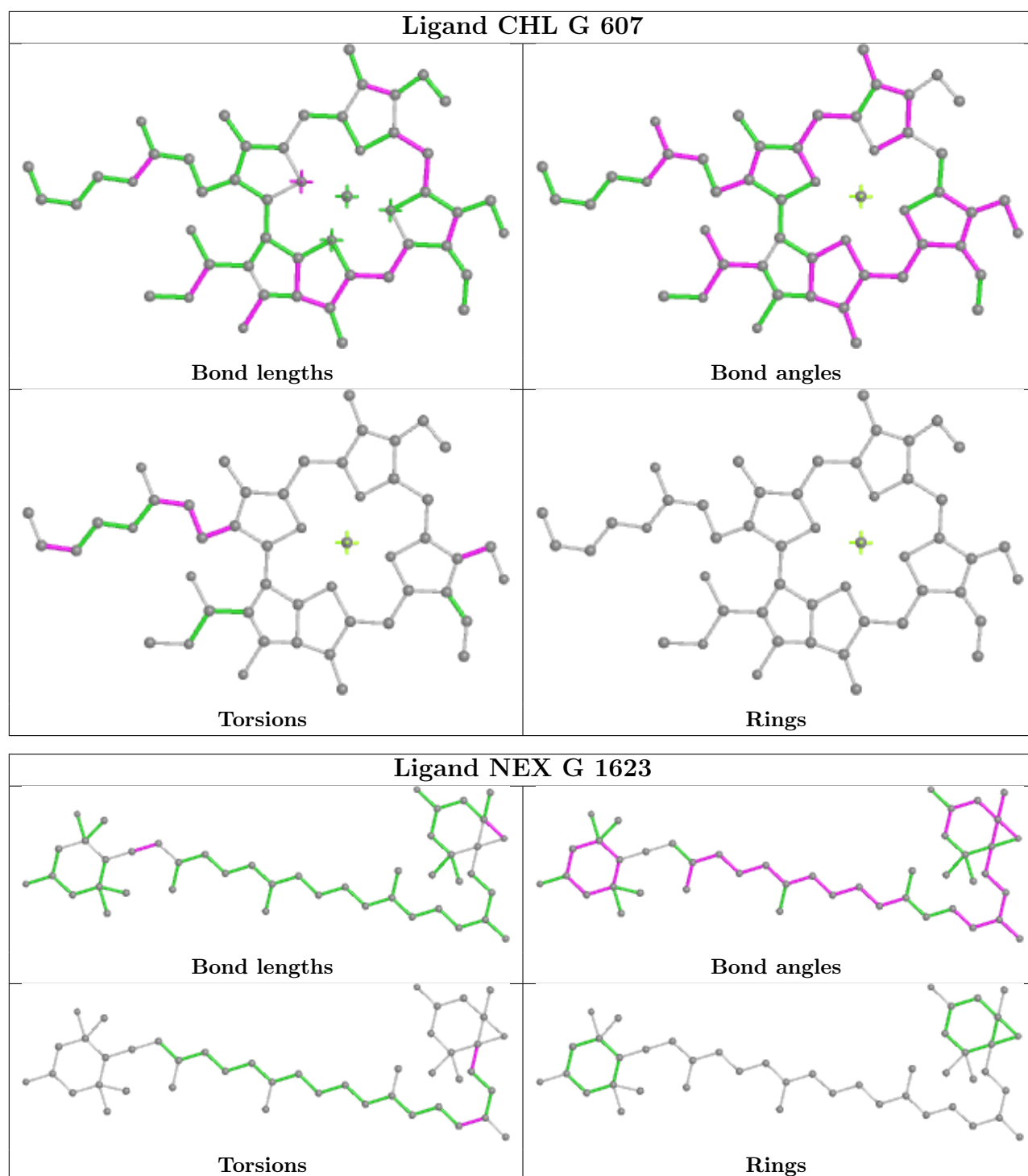
Rings

Ligand CLA 2 602

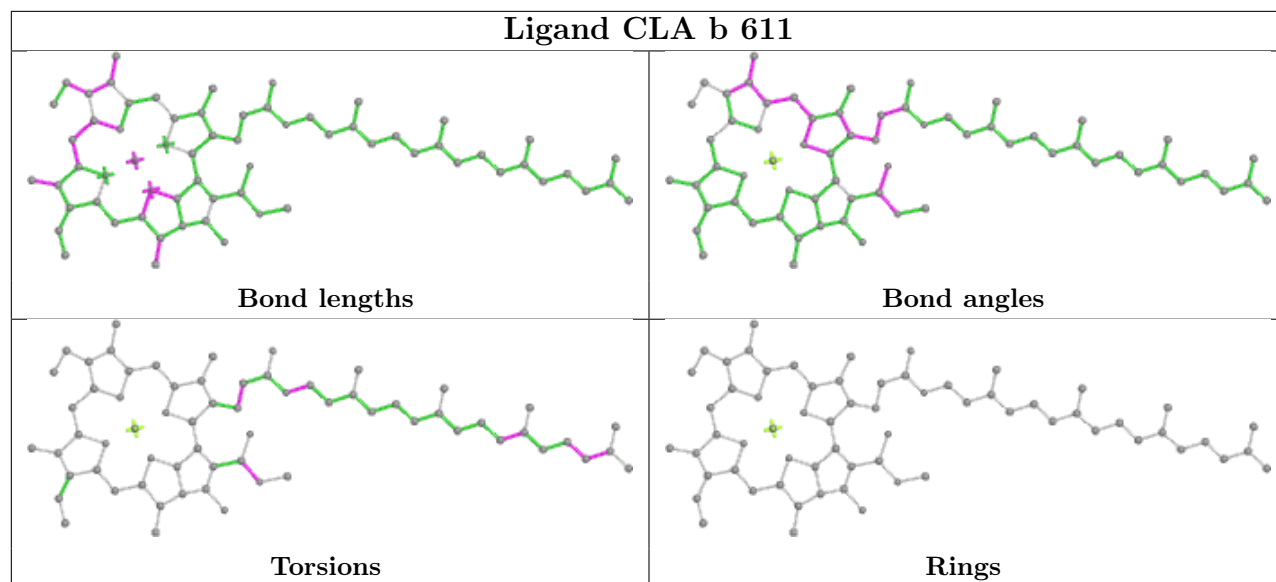


Ligand CHL 3 606

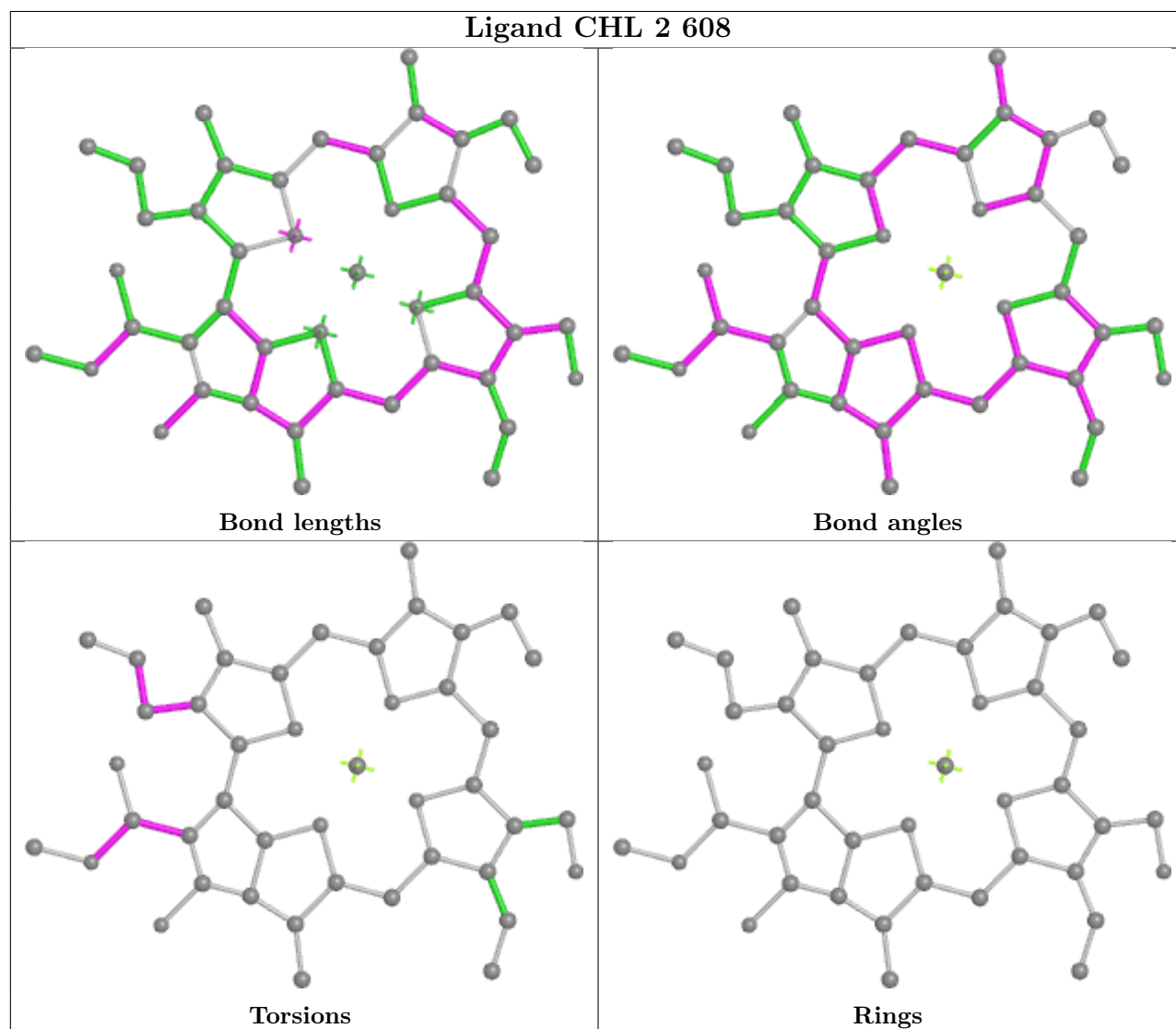




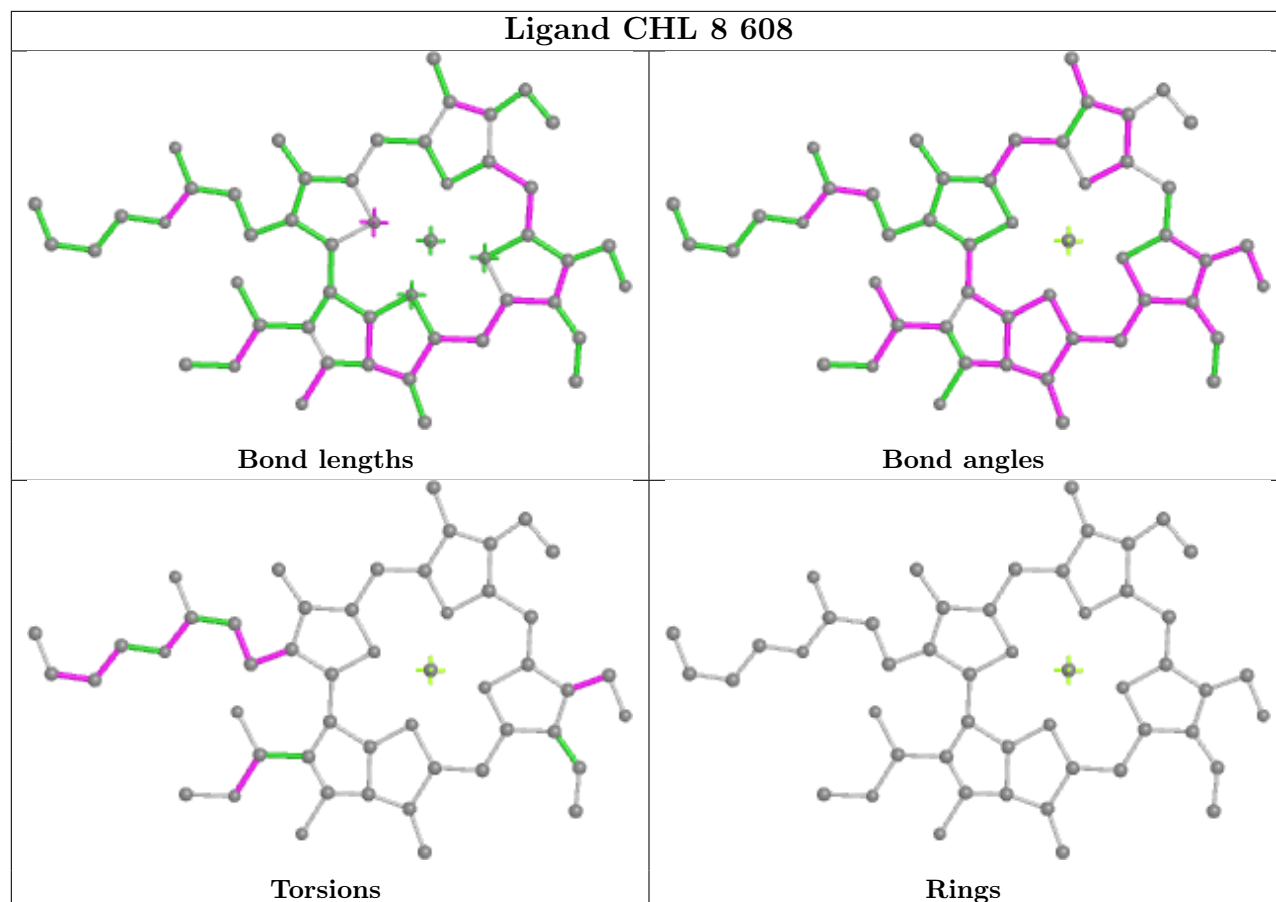
Ligand CLA b 611



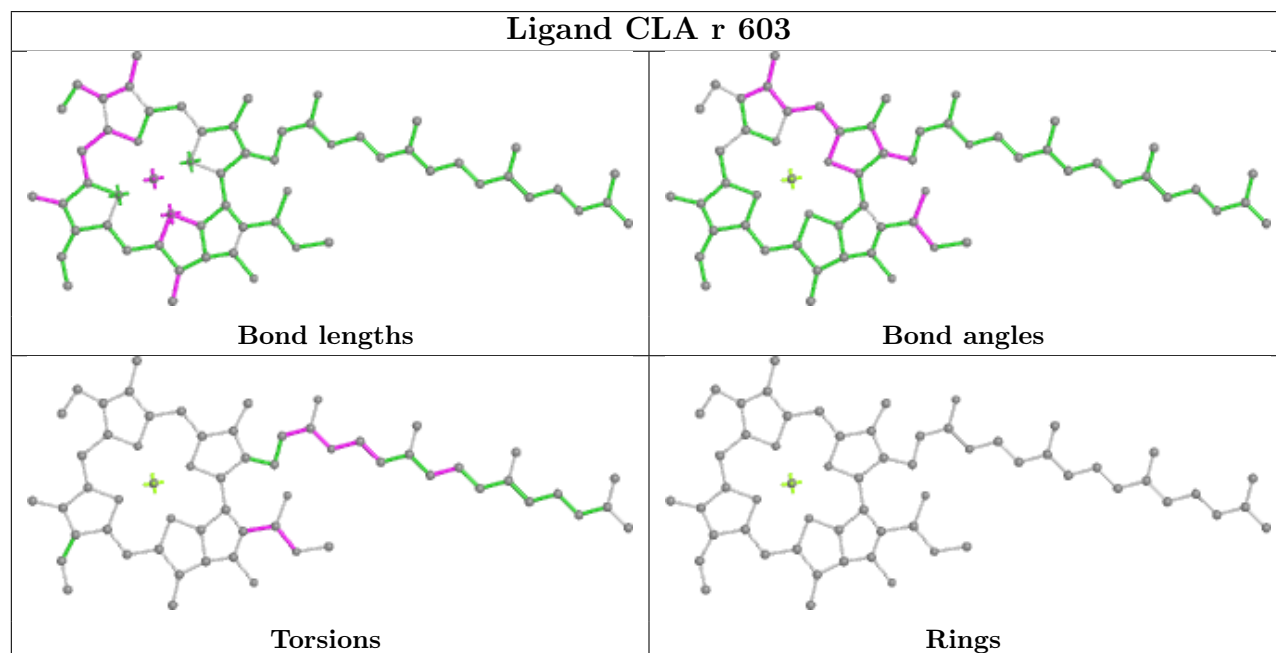
Ligand CHL 2 608

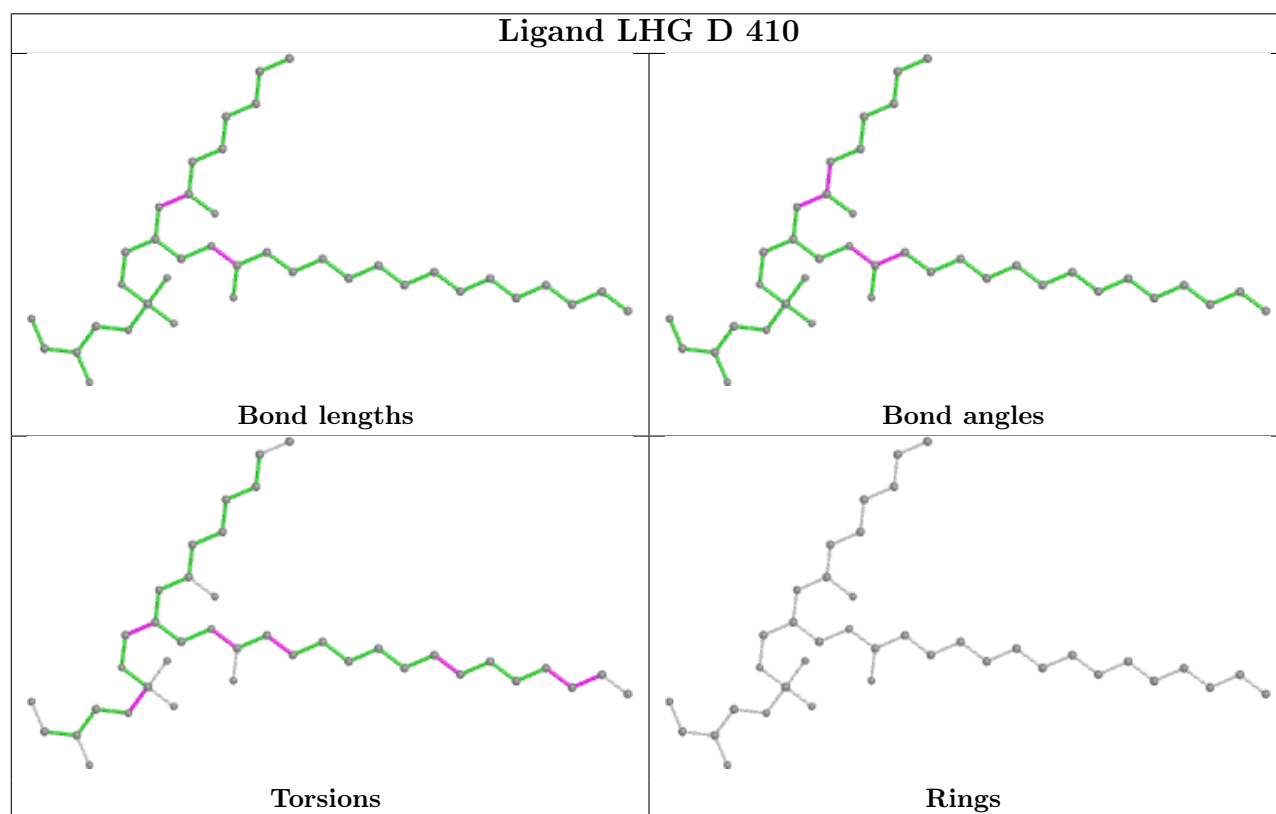
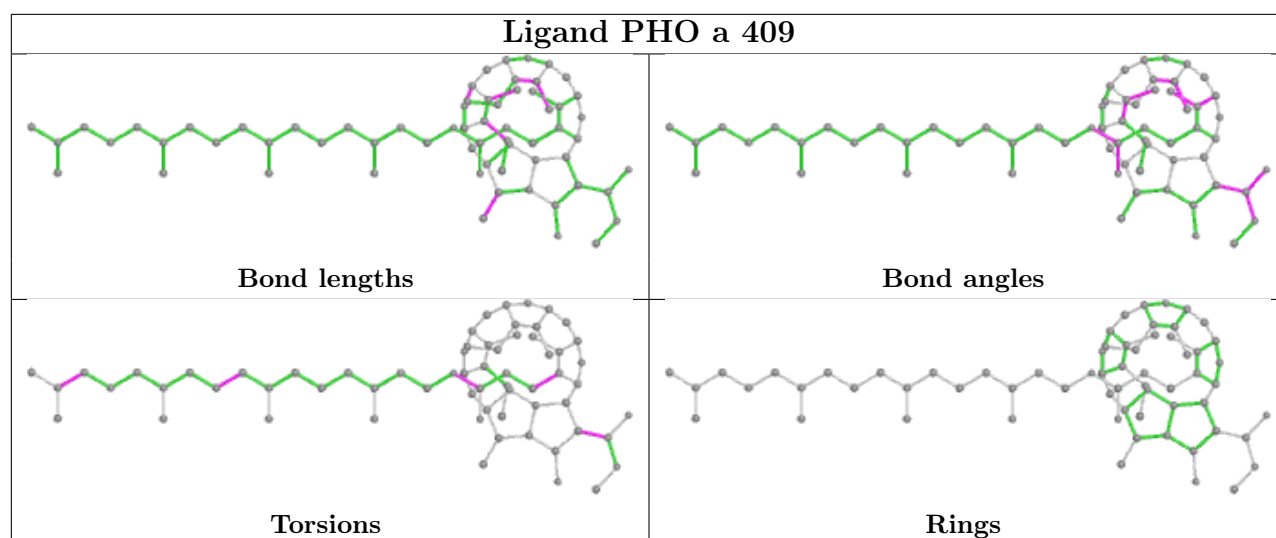


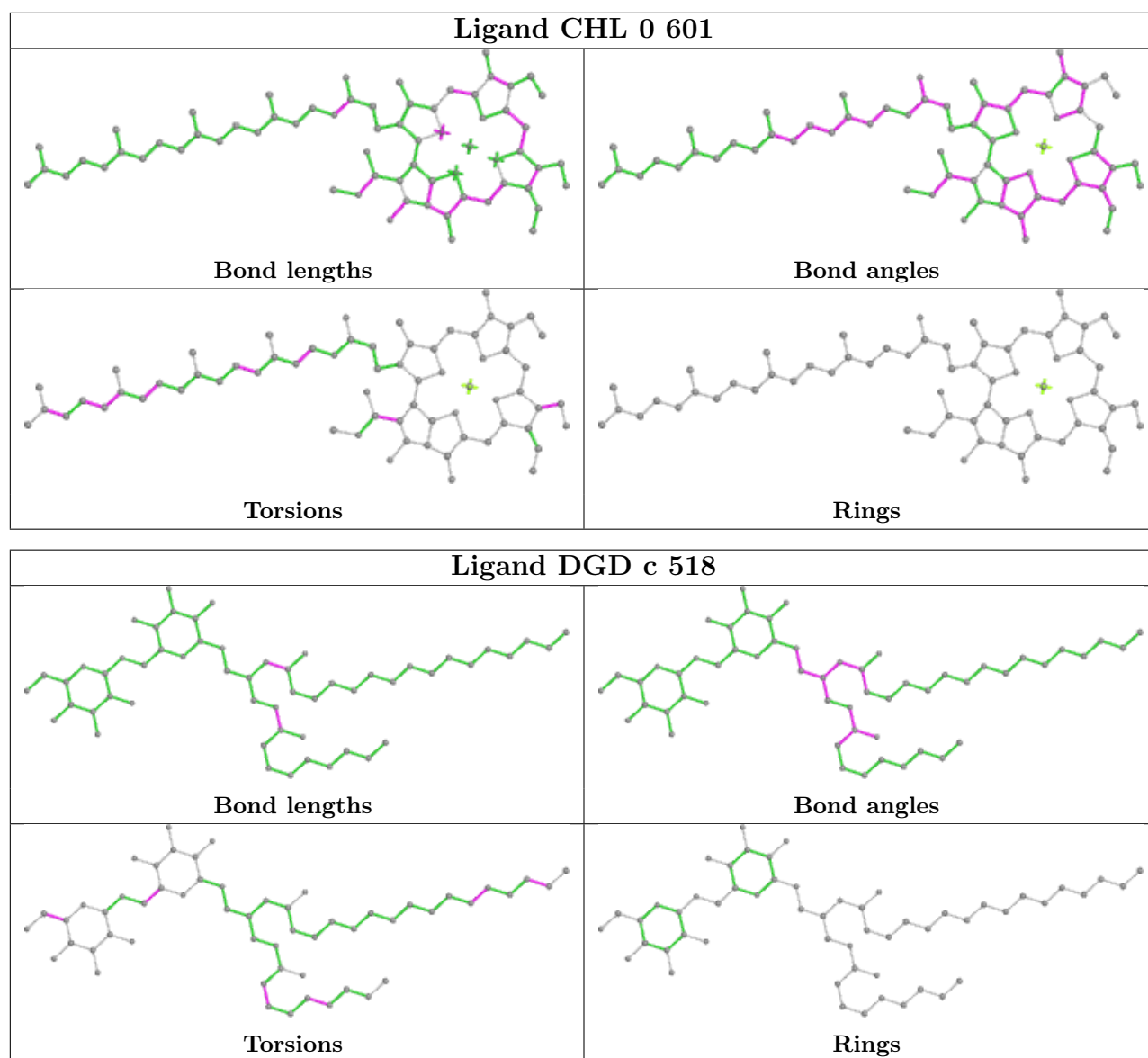
Ligand CHL 8 608



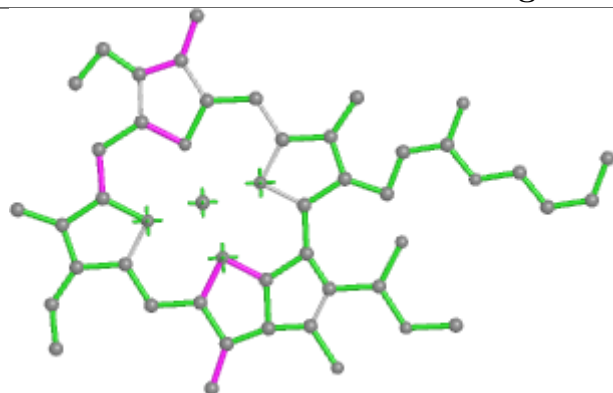
Ligand CLA r 603



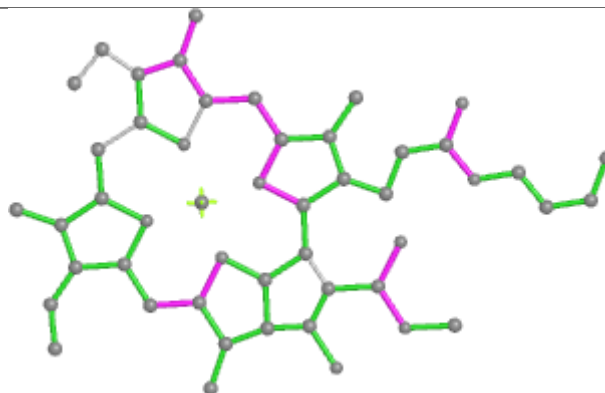




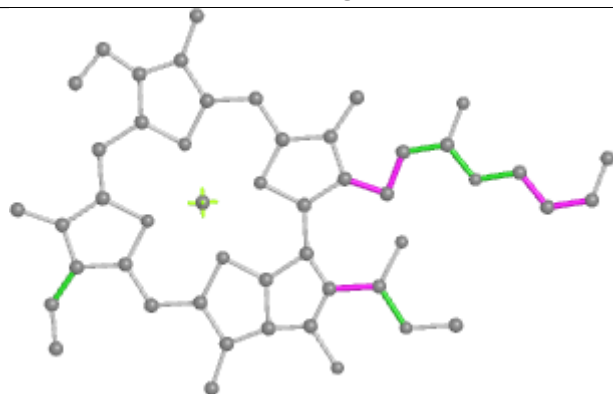
Ligand CLA 8 611



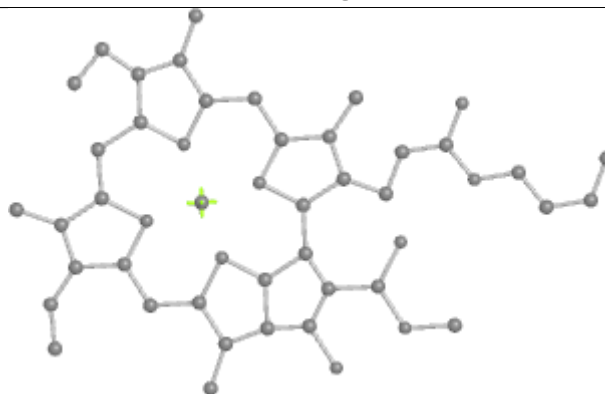
Bond lengths



Bond angles

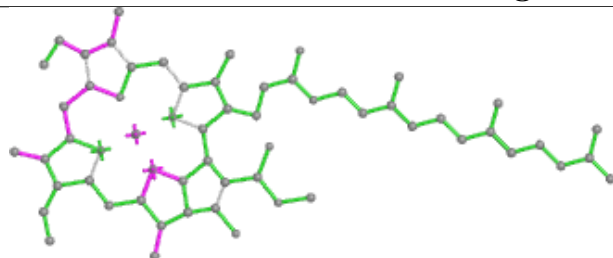


Torsions

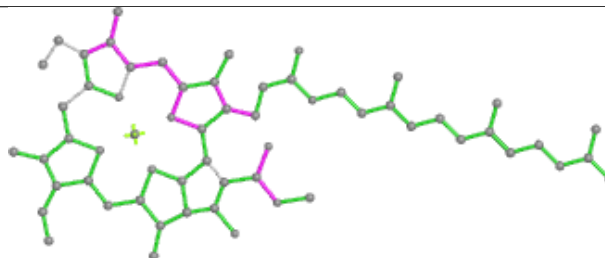


Rings

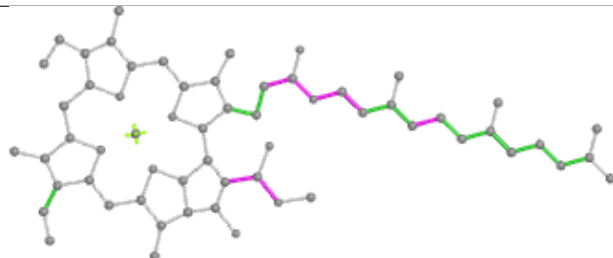
Ligand CLA R 603



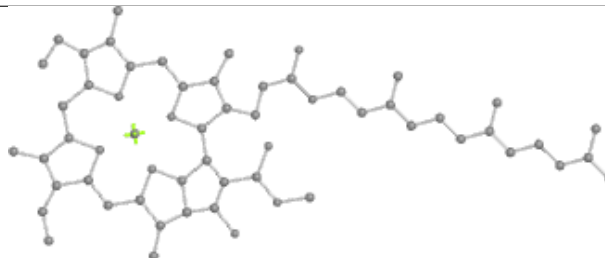
Bond lengths



Bond angles

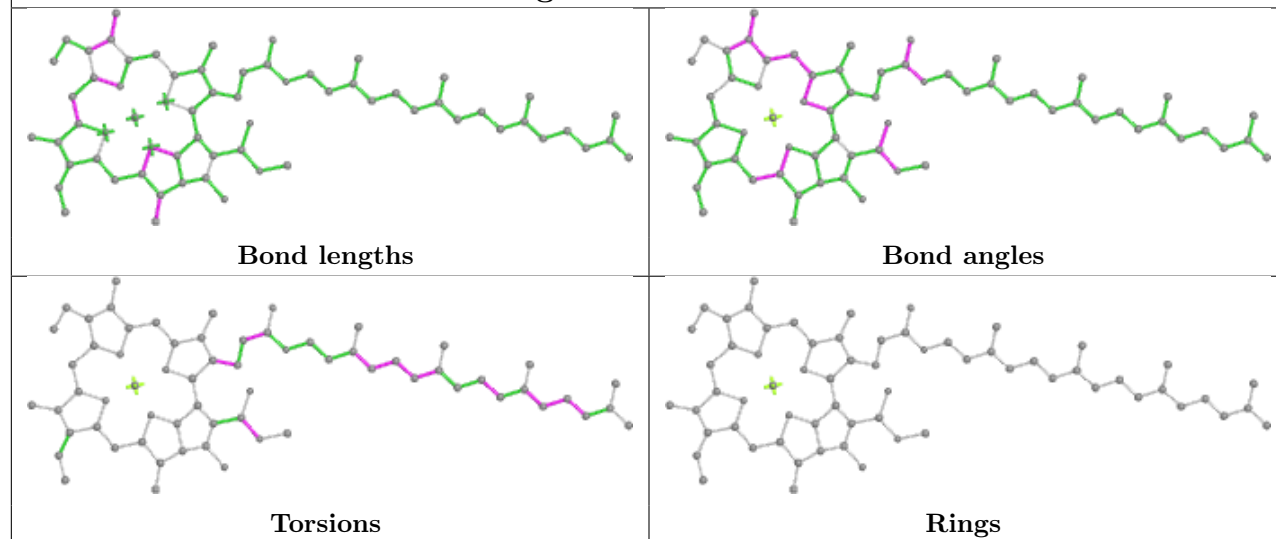


Torsions

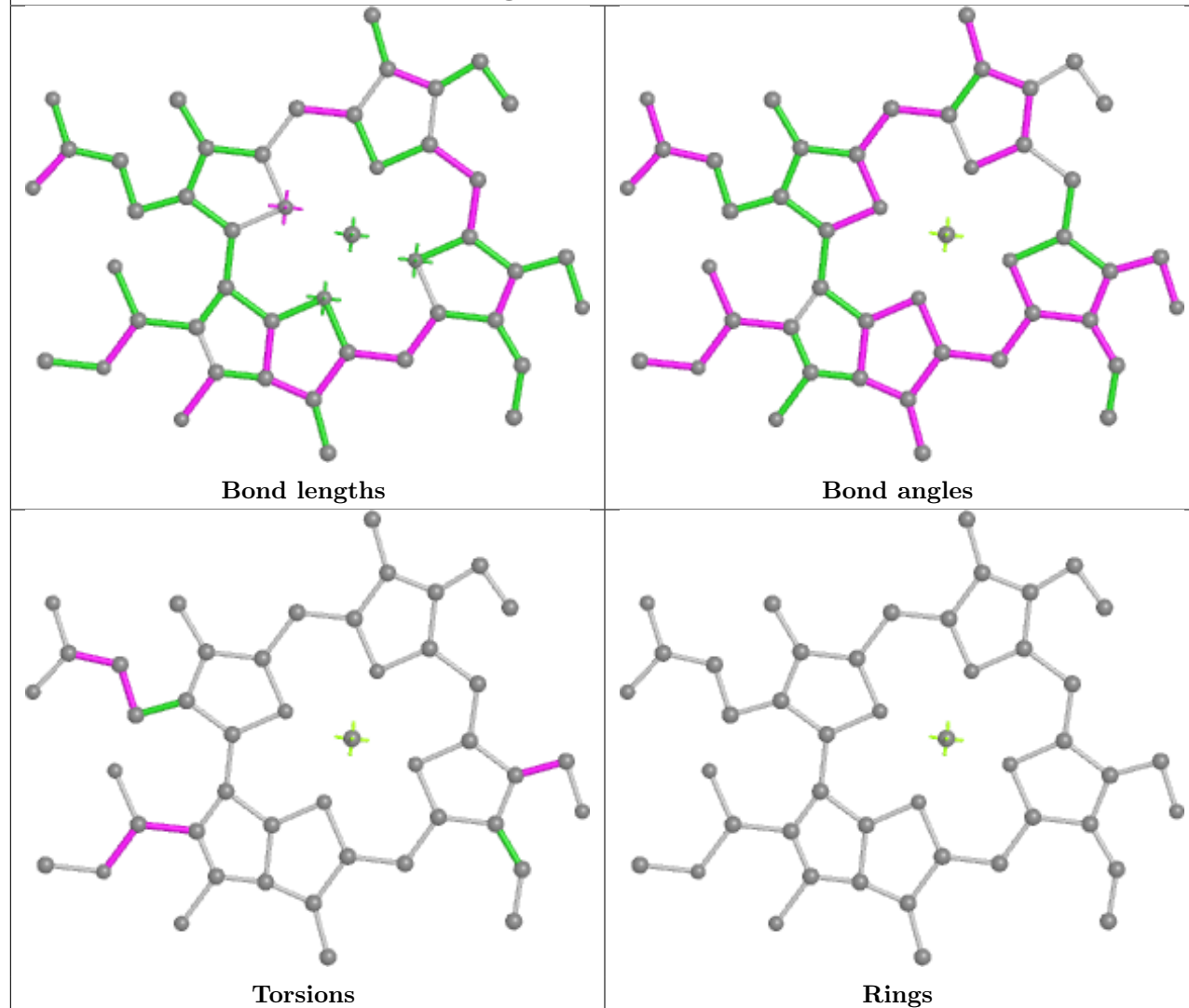


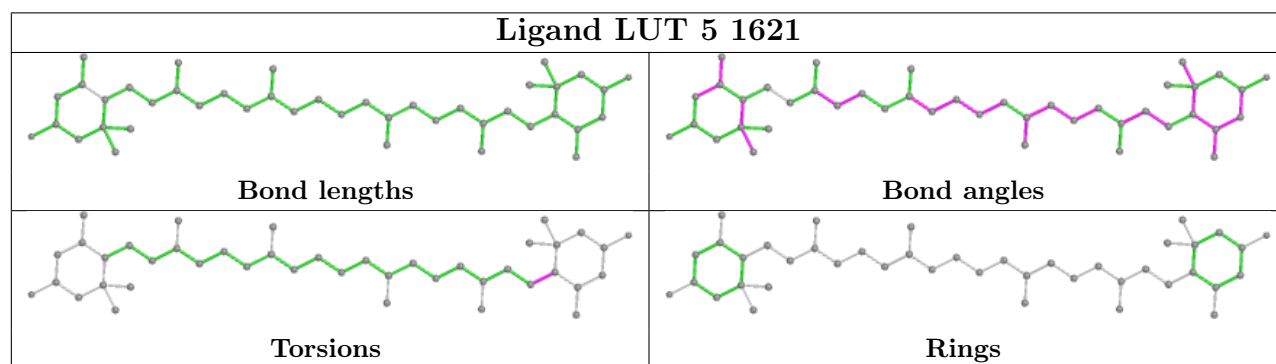
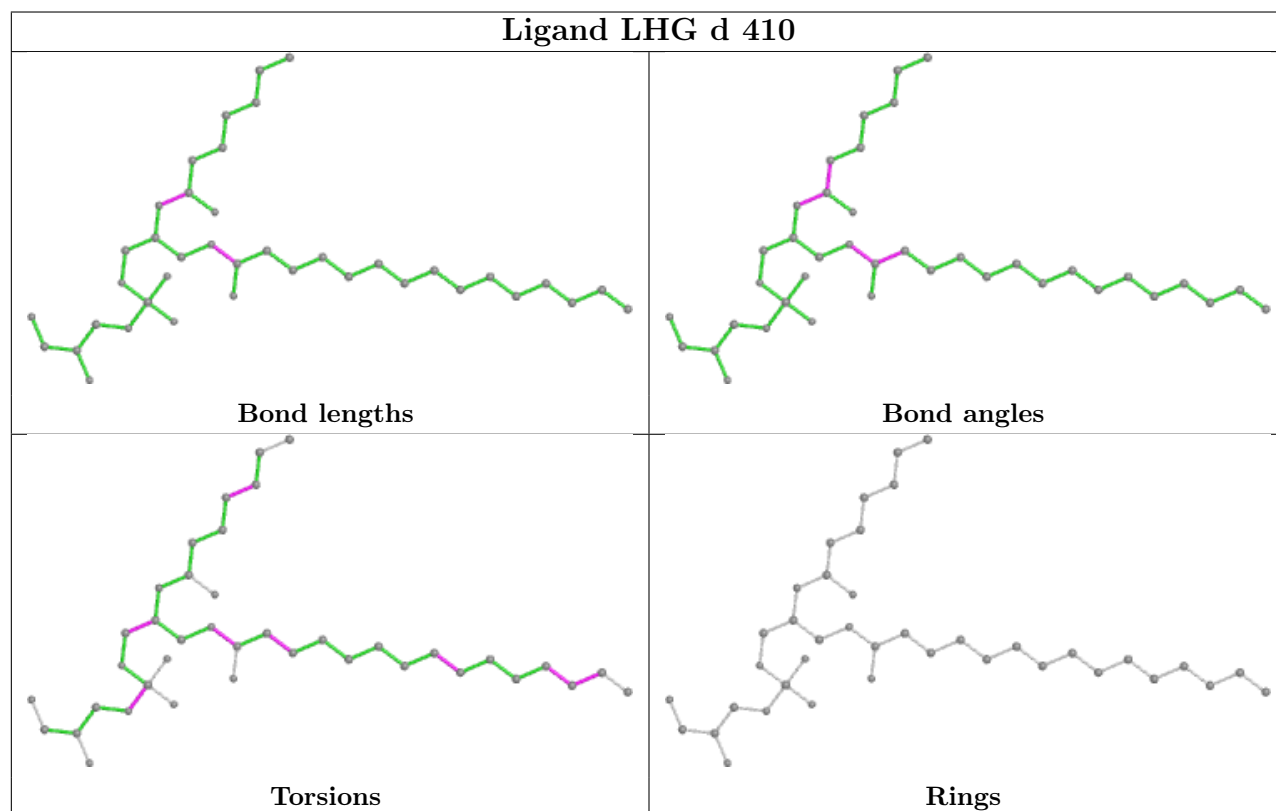
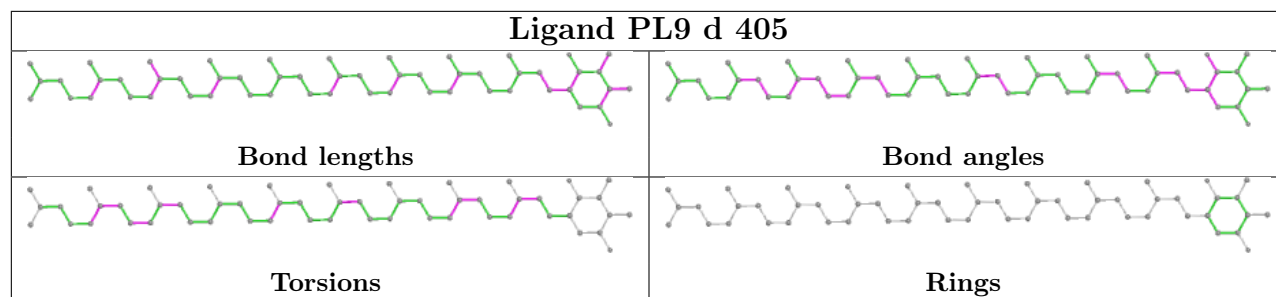
Rings

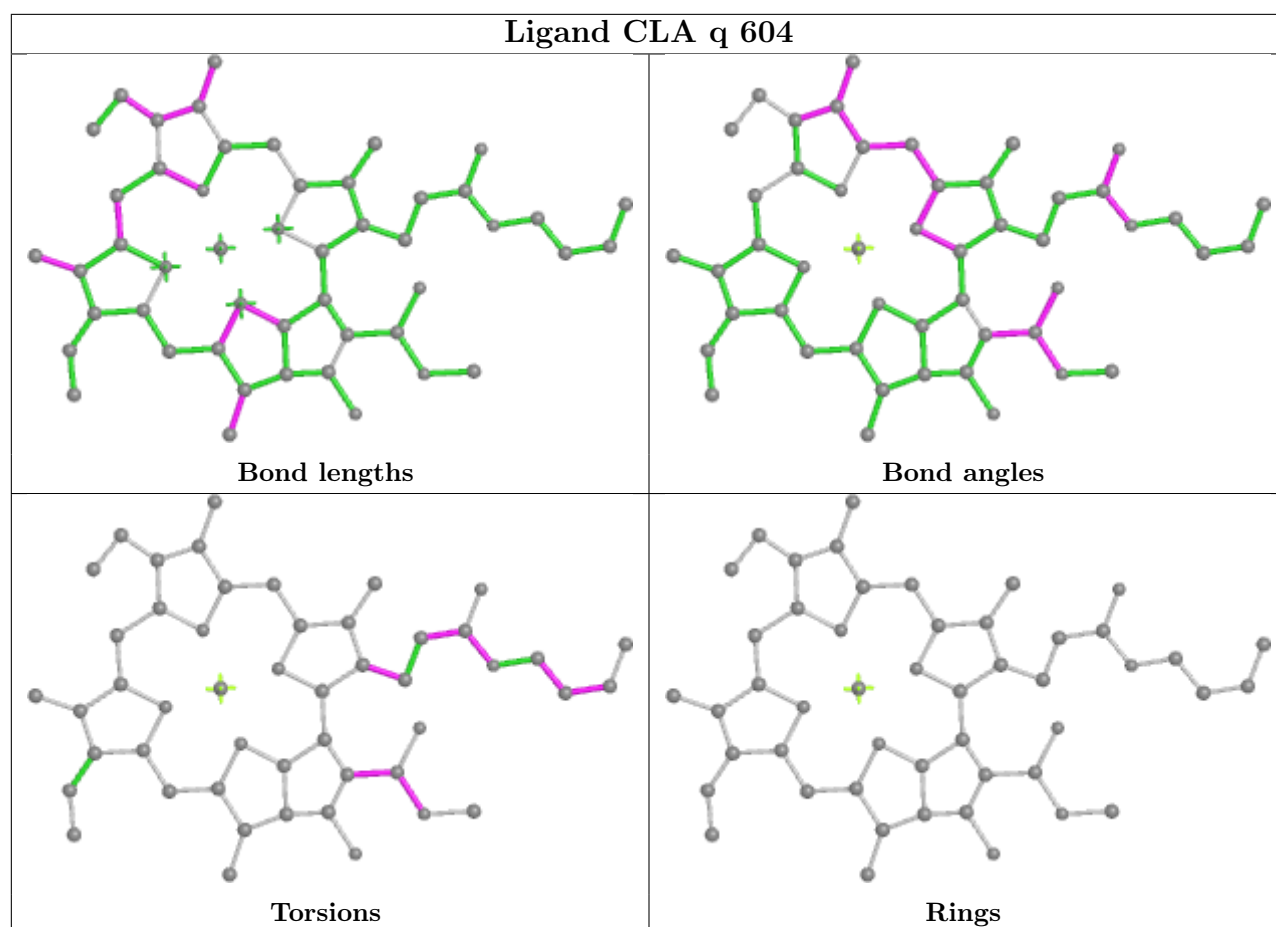
Ligand CLA 5 604

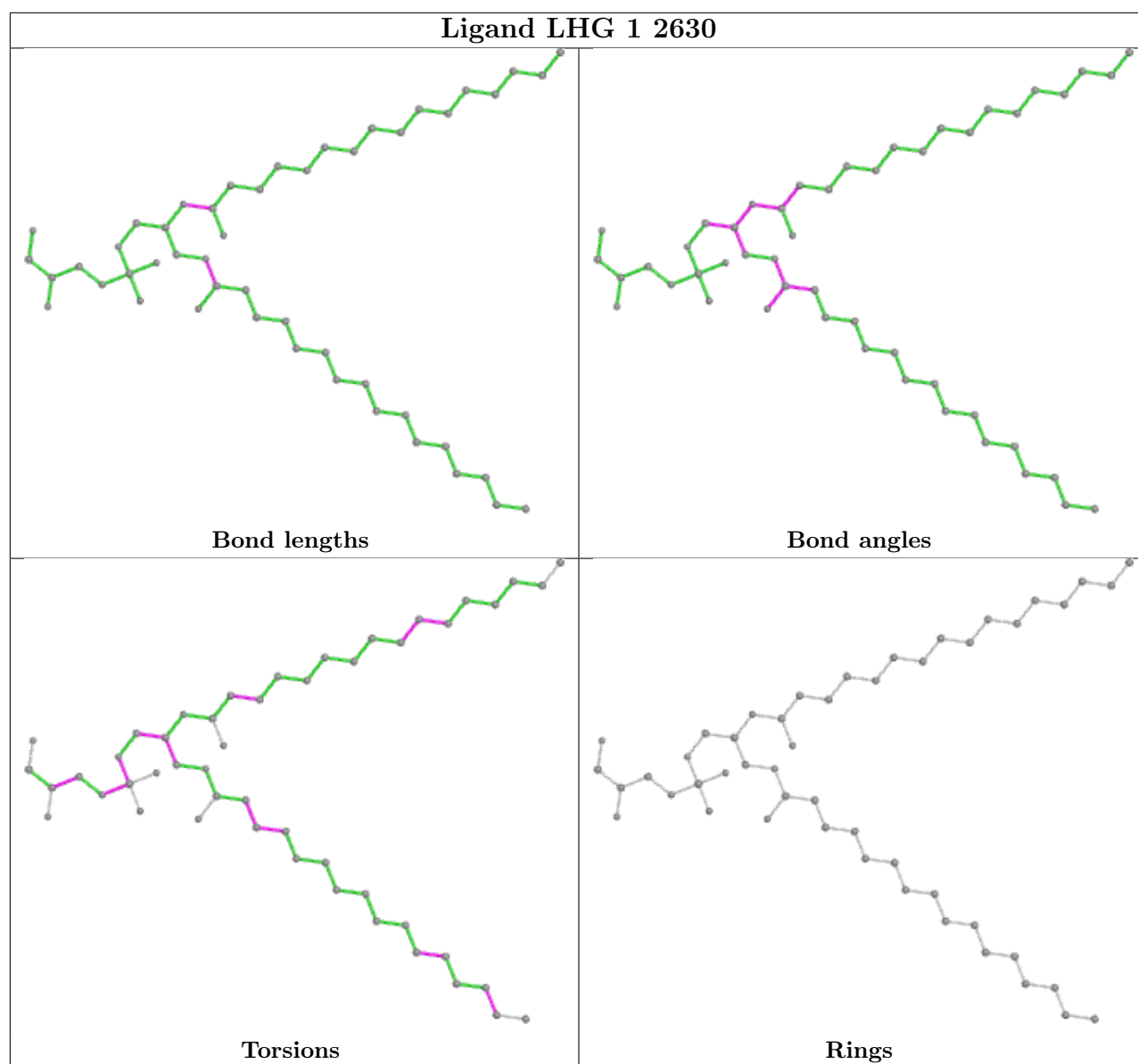


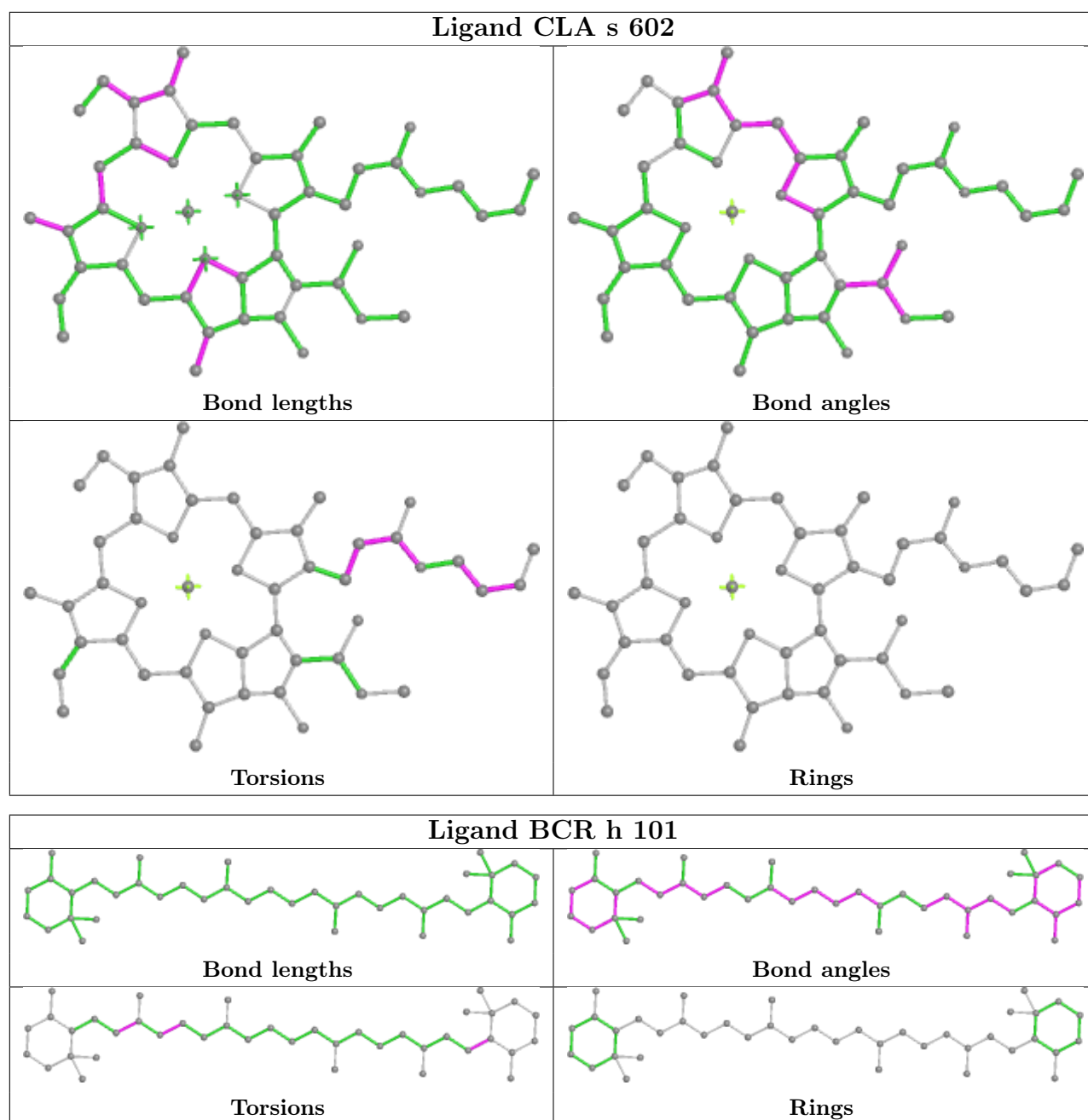
Ligand CHL s 601



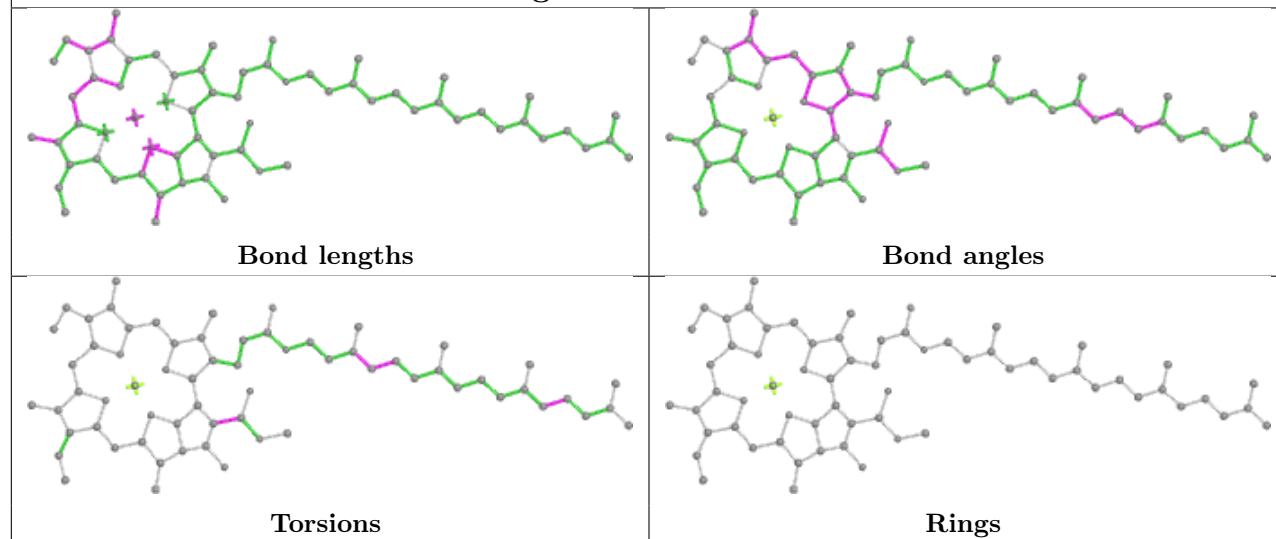




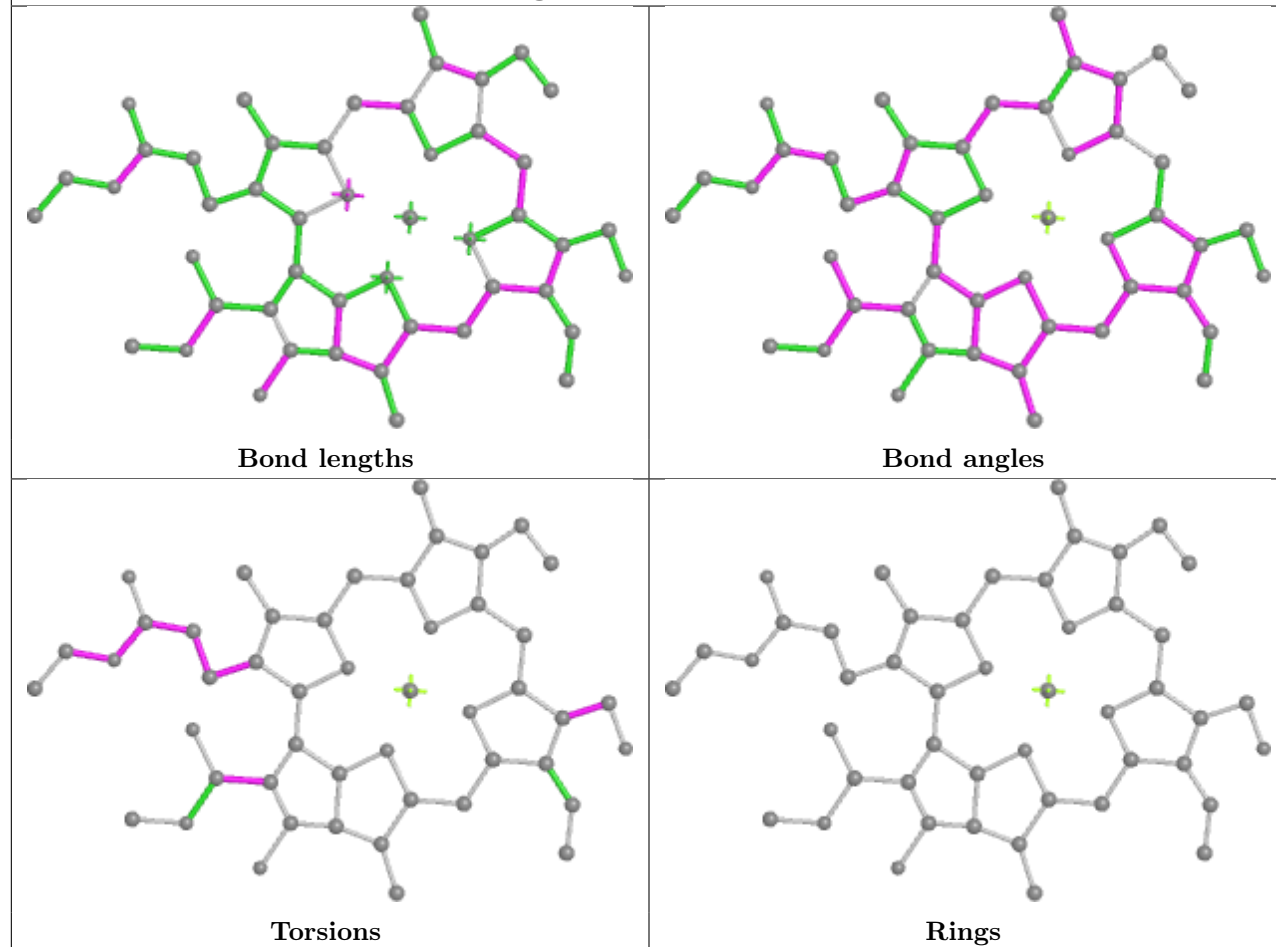


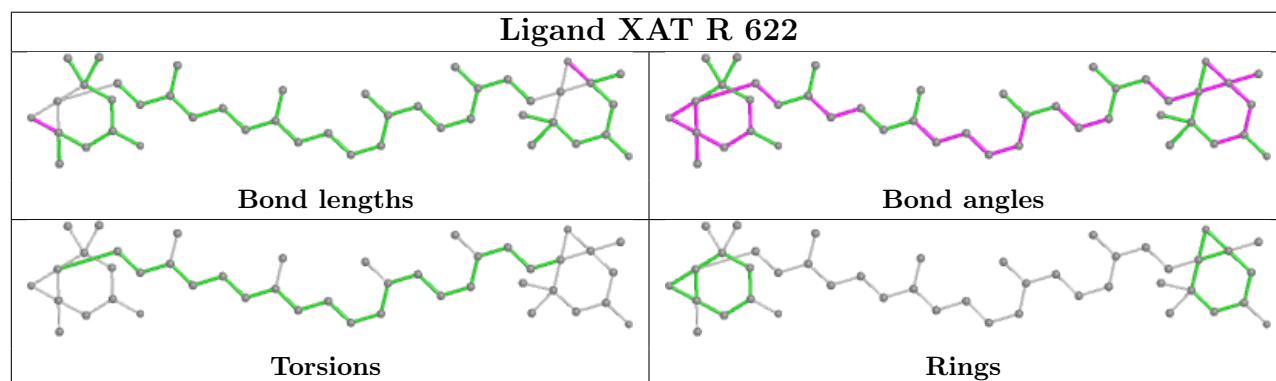
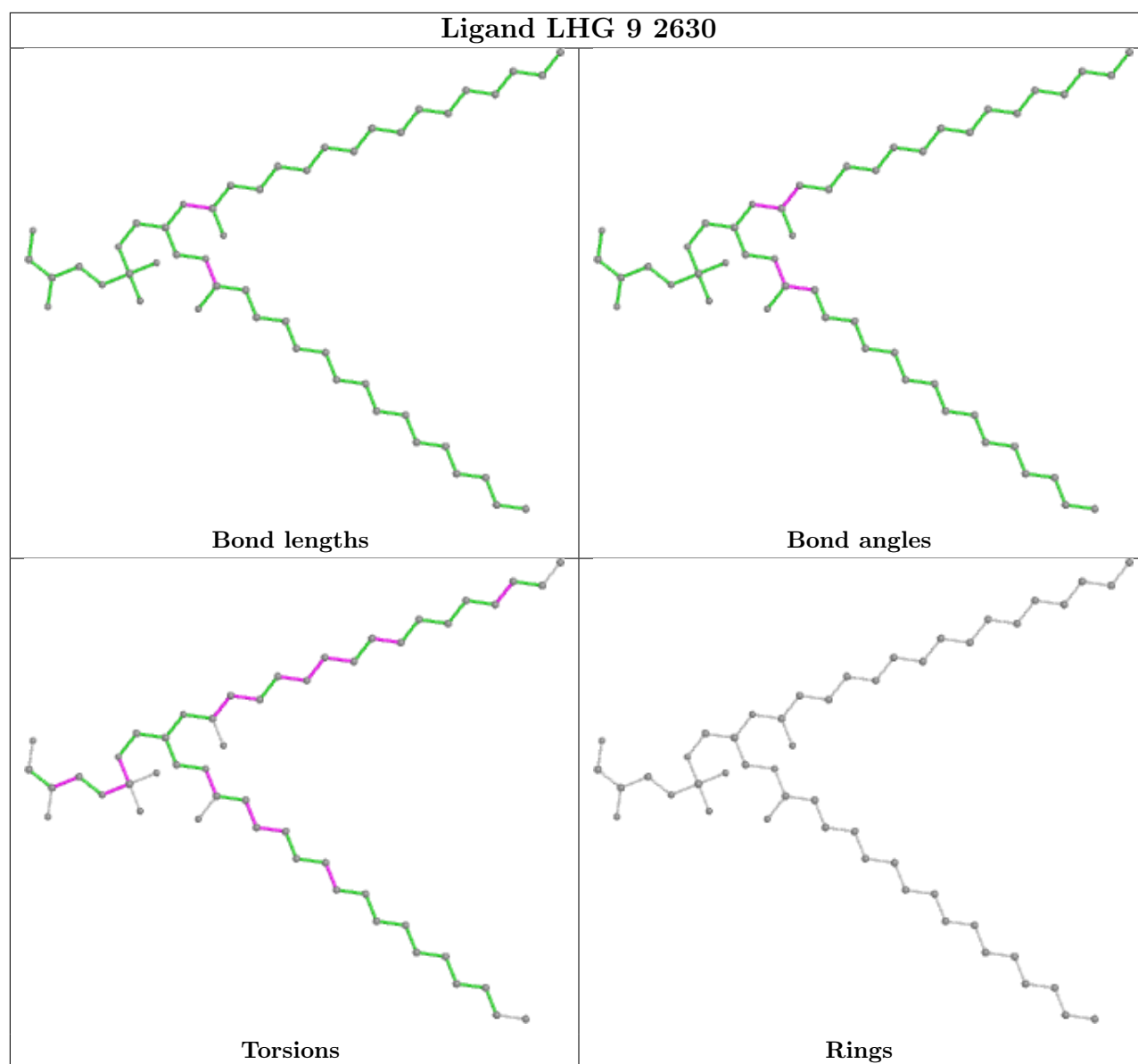


Ligand CLA C 509

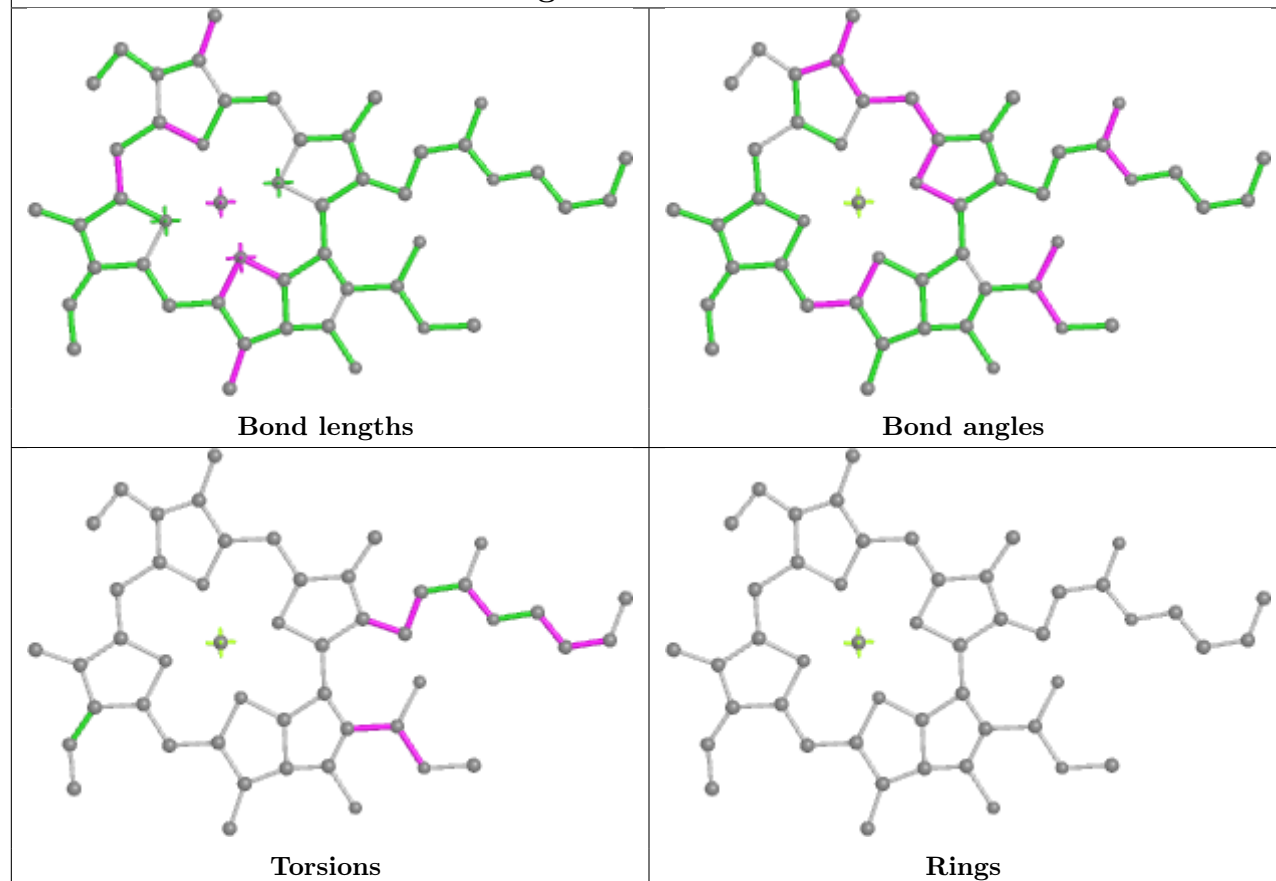


Ligand CHL G 605

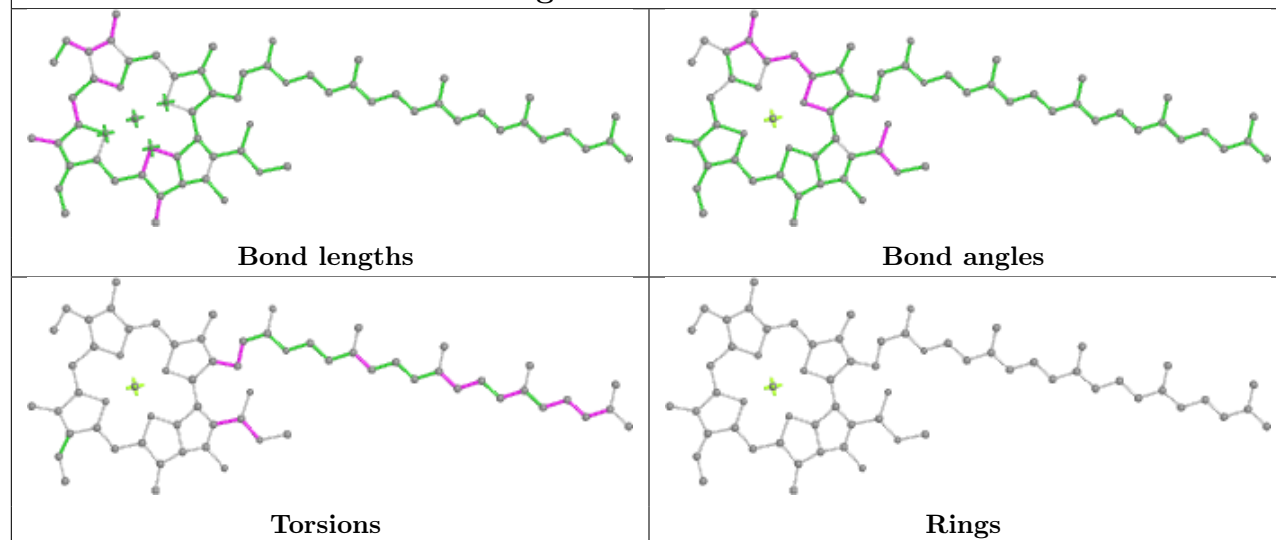


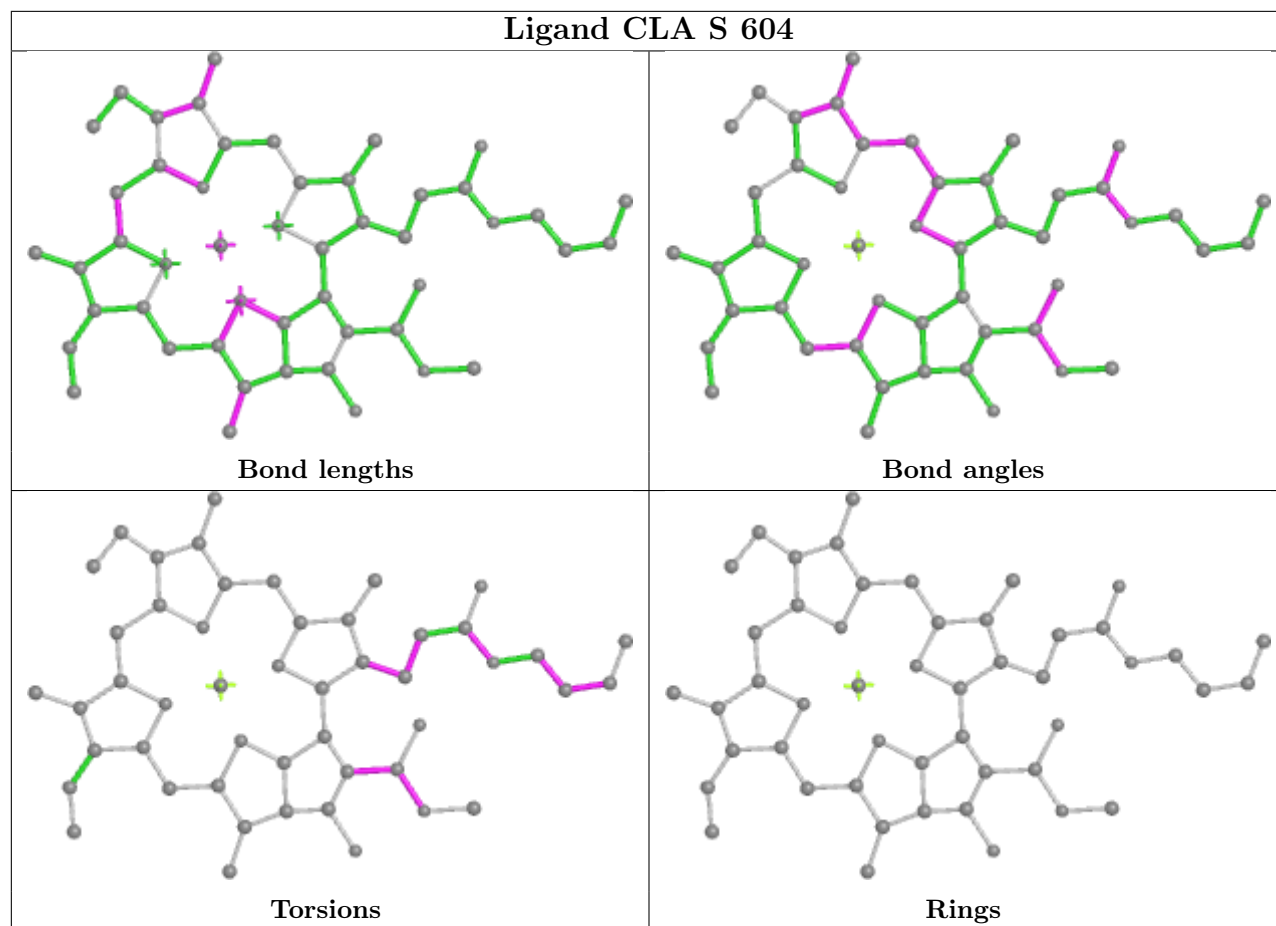


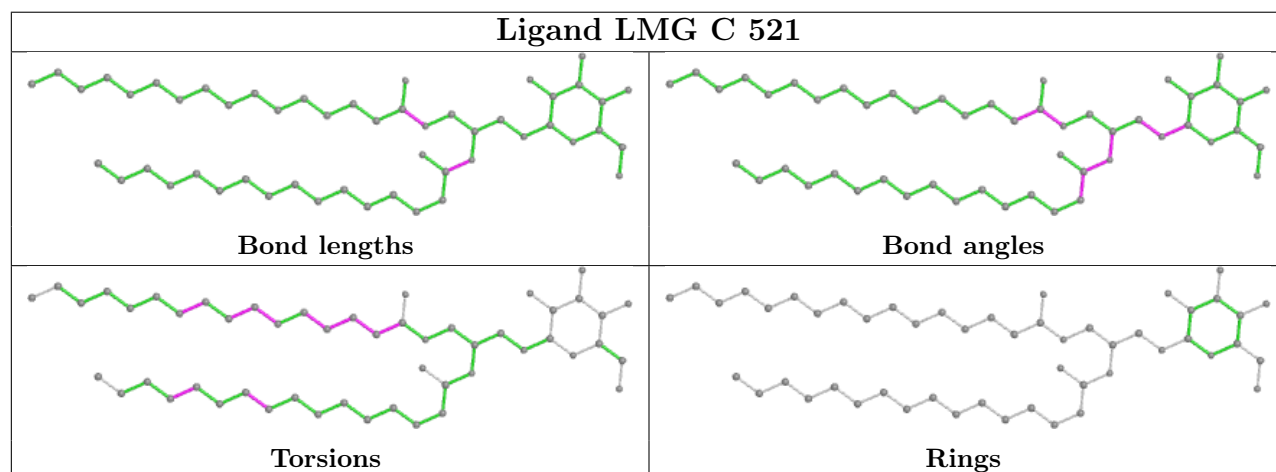
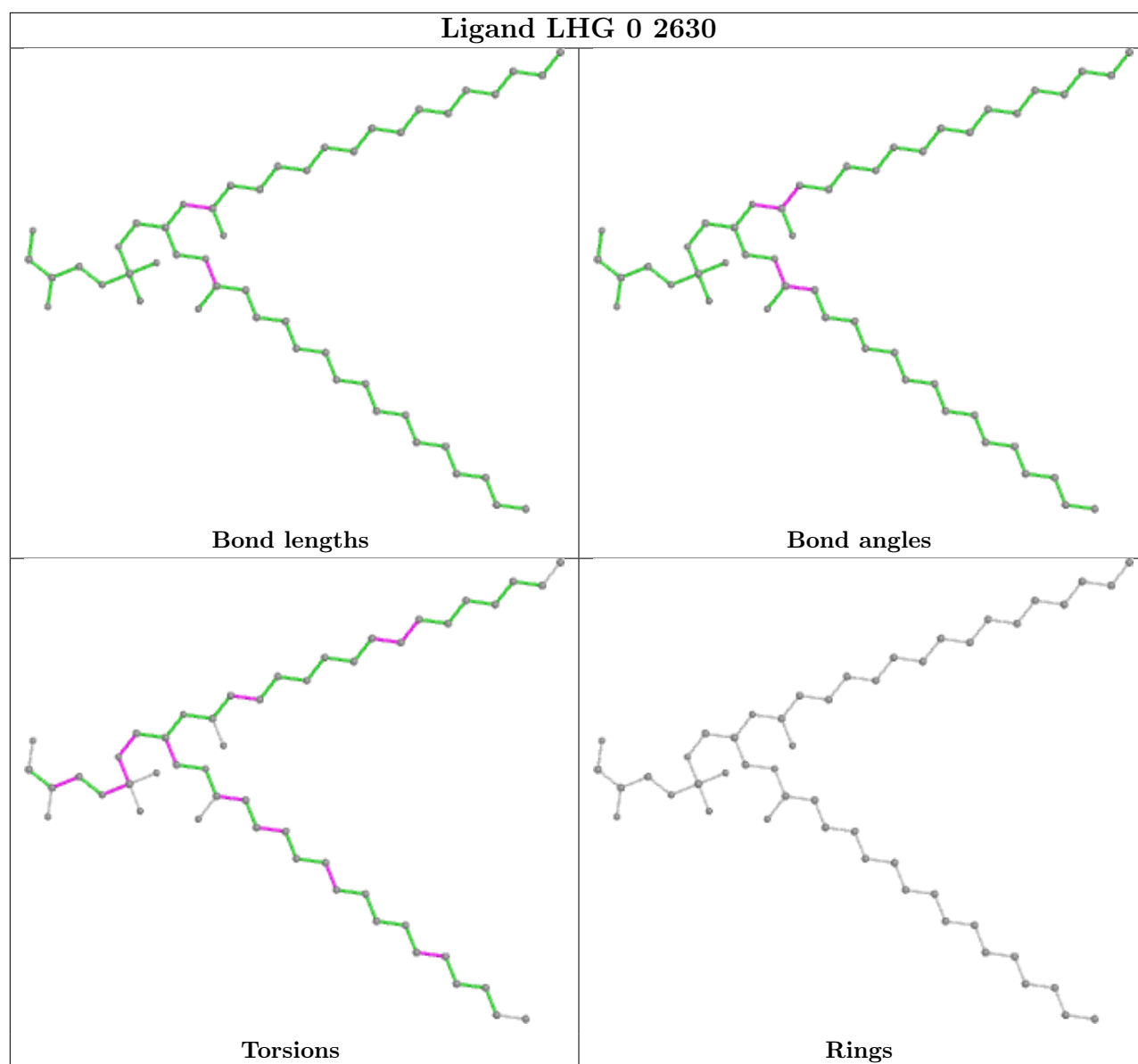
Ligand CLA s 604

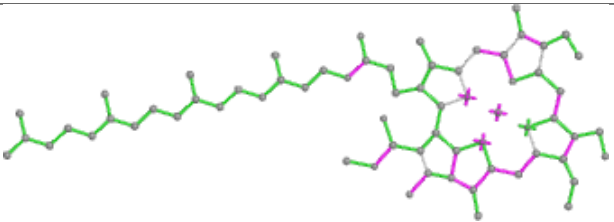
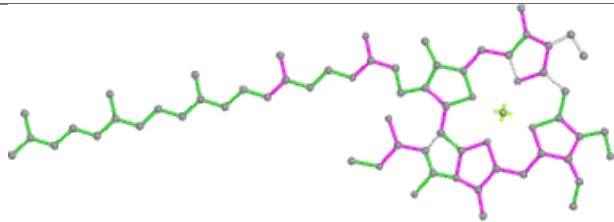
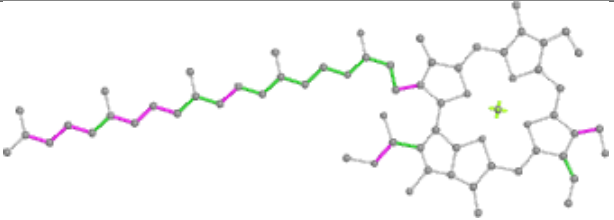
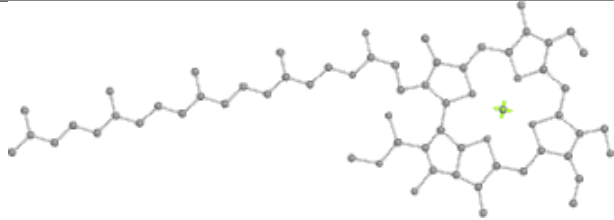


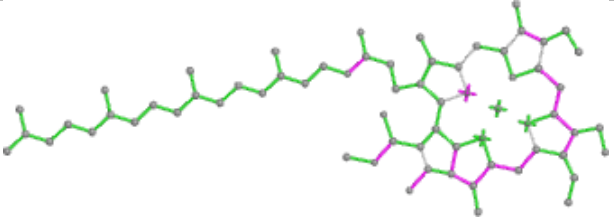
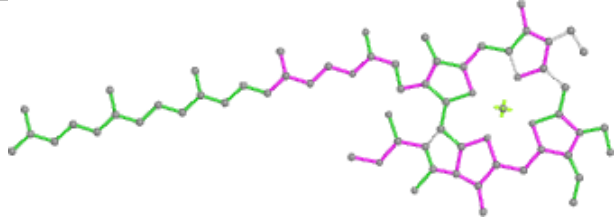
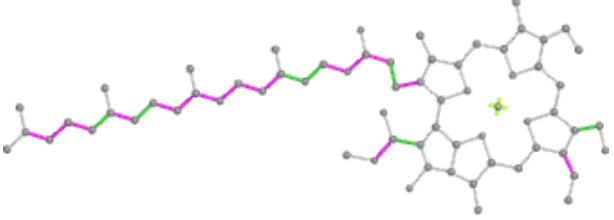
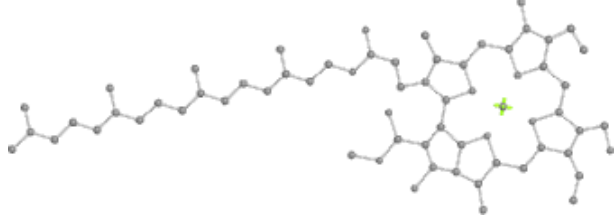
Ligand CLA 6 604

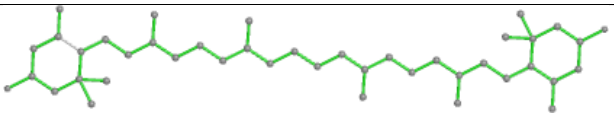
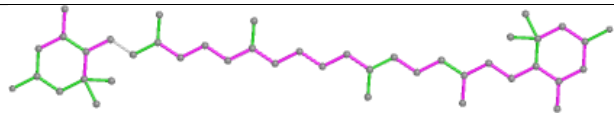
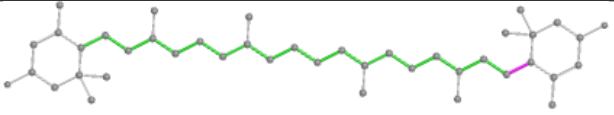
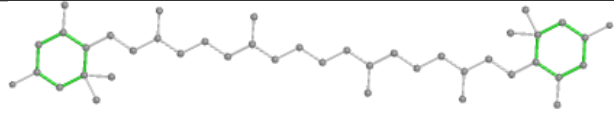




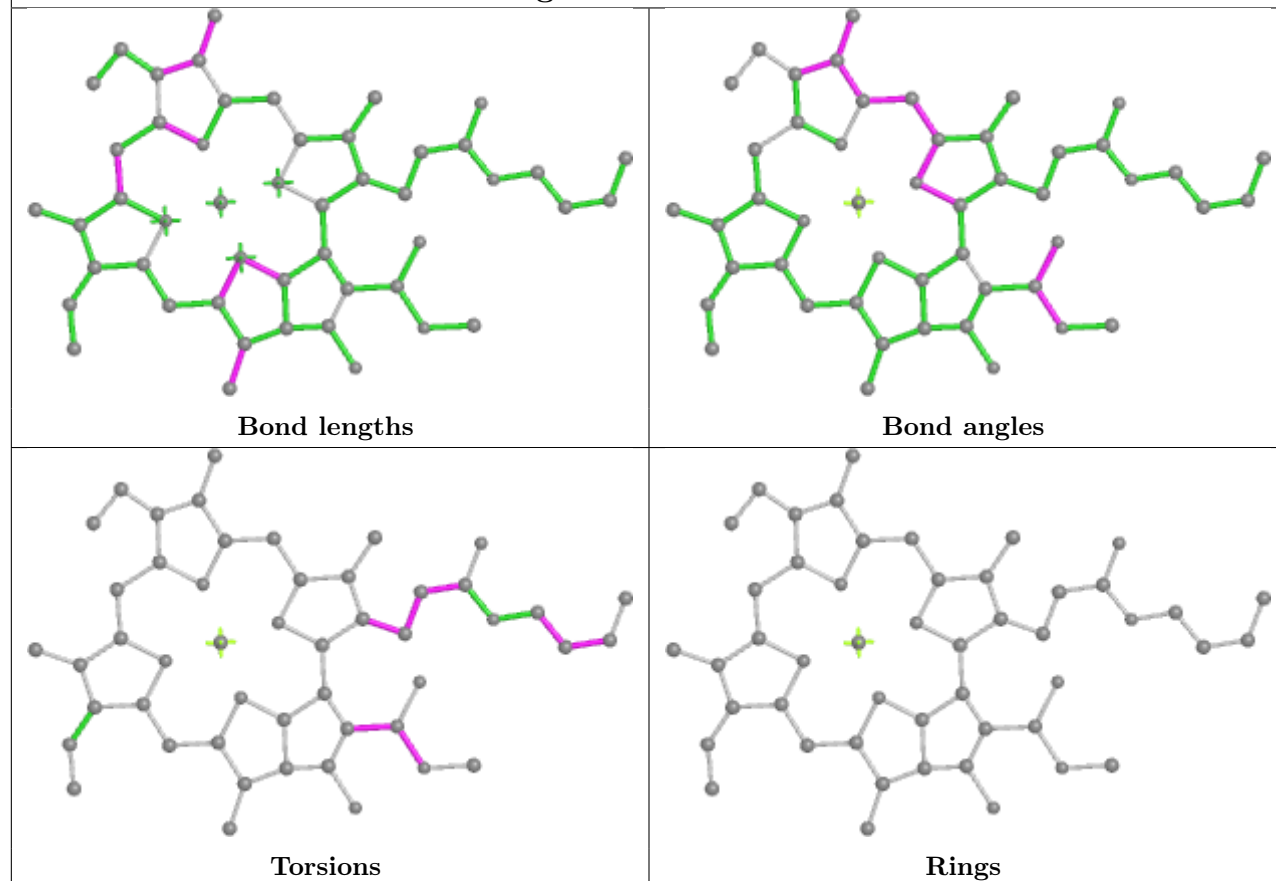


Ligand CHL G 609	
	
Bond lengths	Bond angles
	
Torsions	Rings

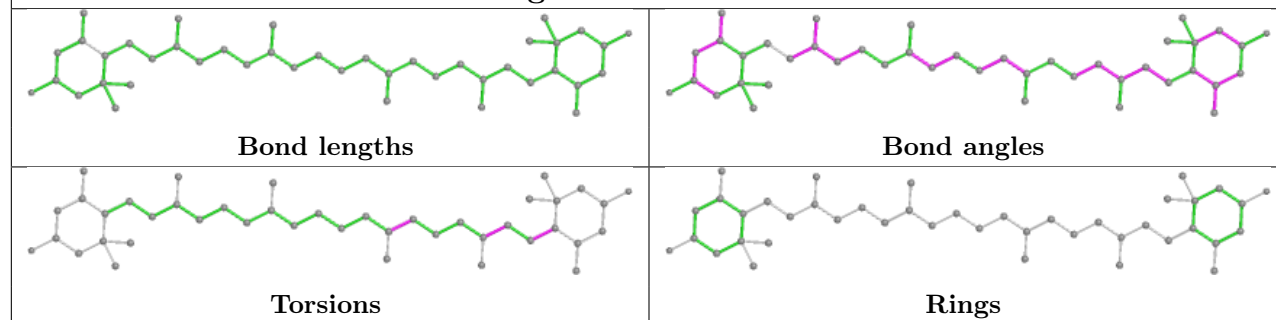
Ligand CHL 3 607	
	
Bond lengths	Bond angles
	
Torsions	Rings

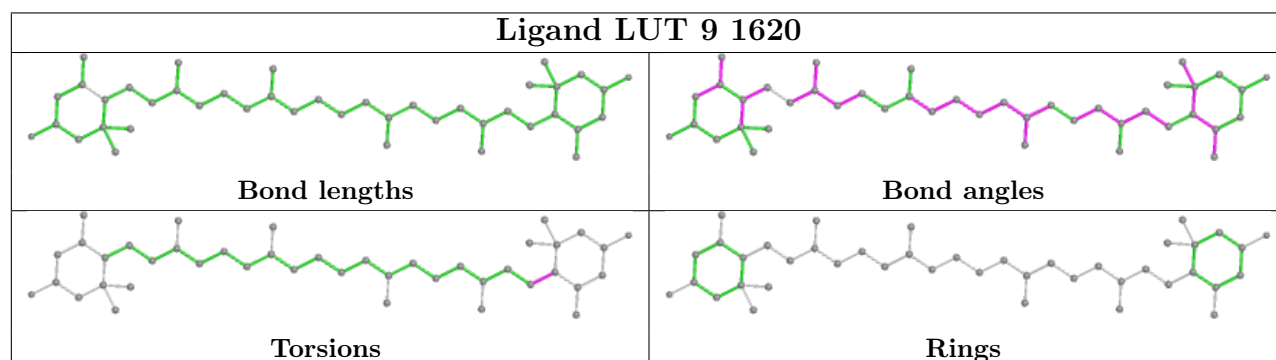
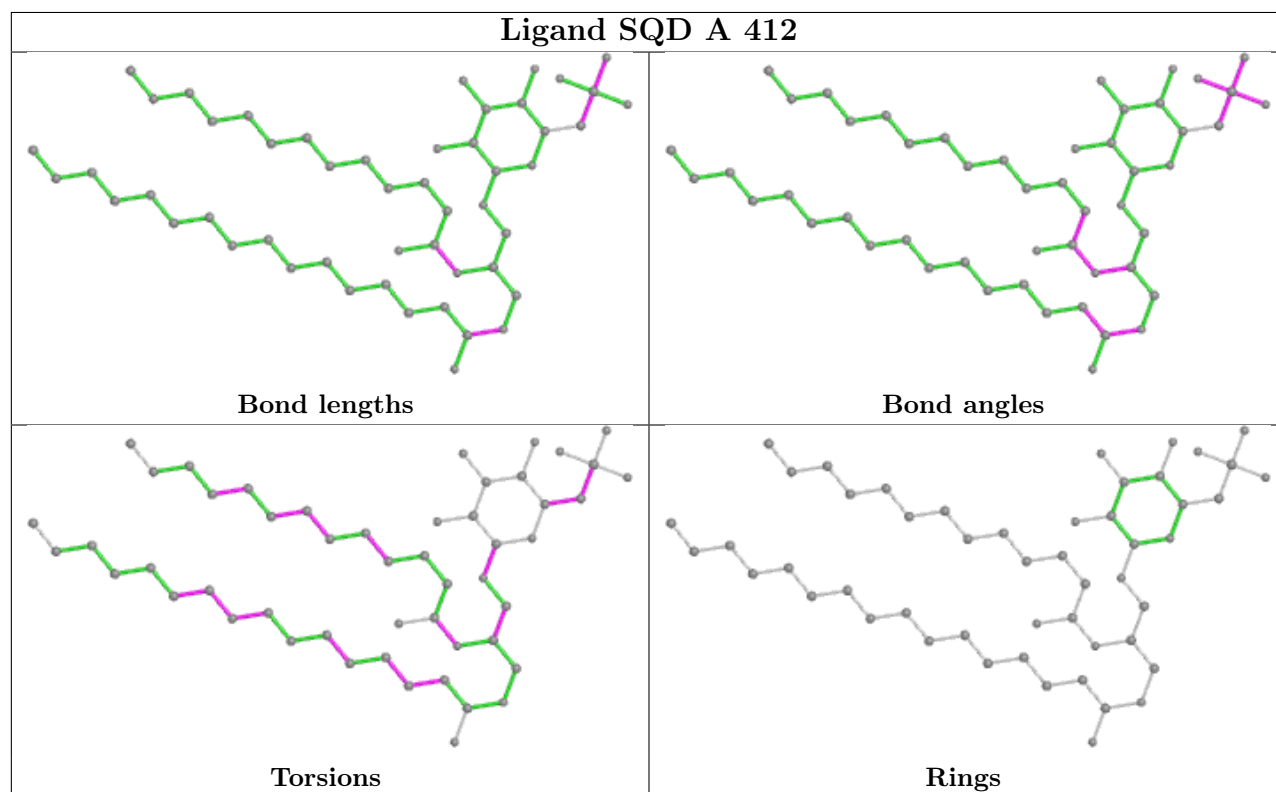
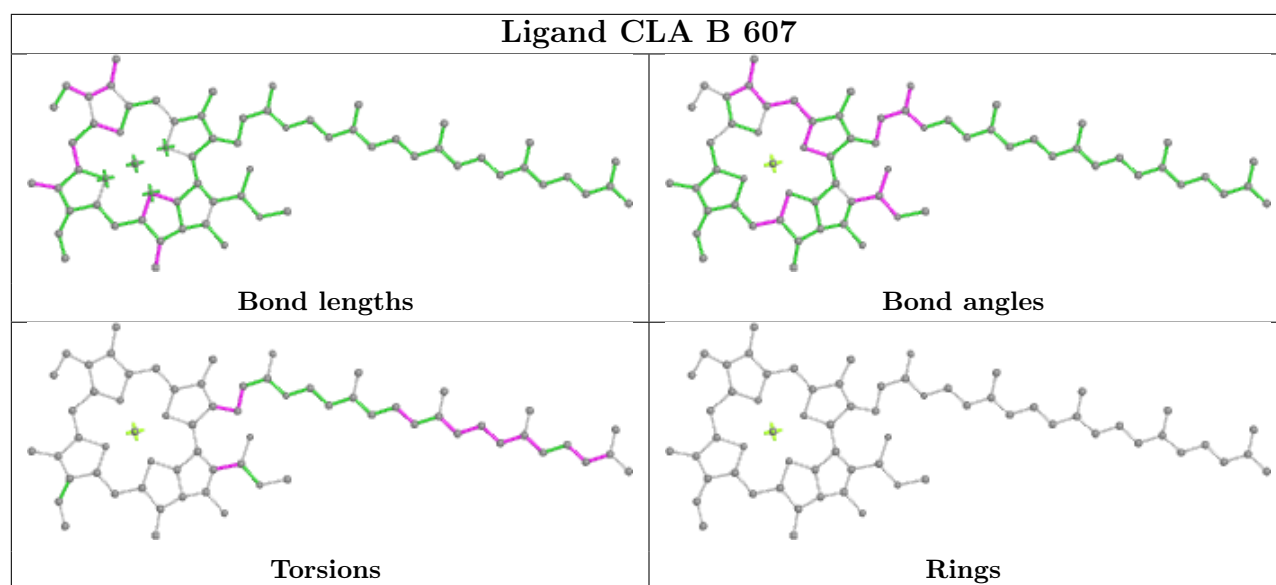
Ligand LUT q 1620	
	
Bond lengths	Bond angles
	
Torsions	Rings

Ligand CLA 5 611

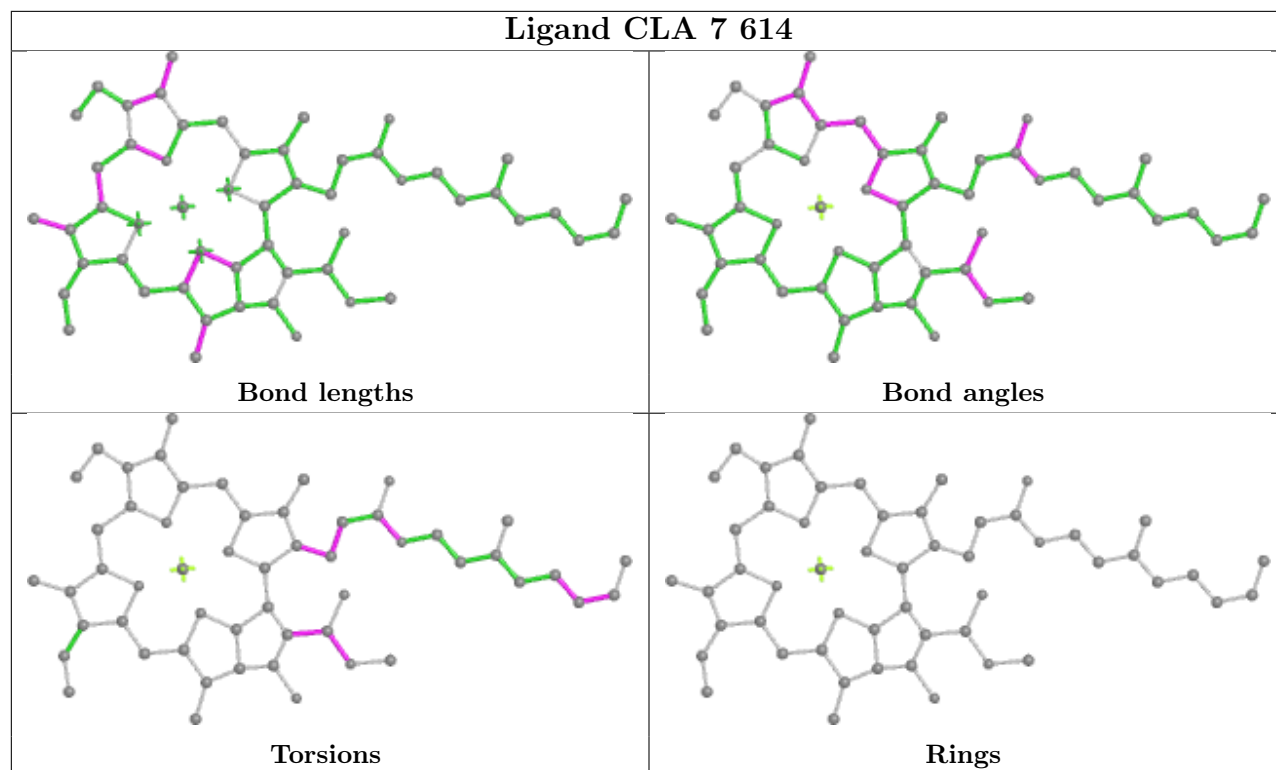


Ligand LUT 2 1621

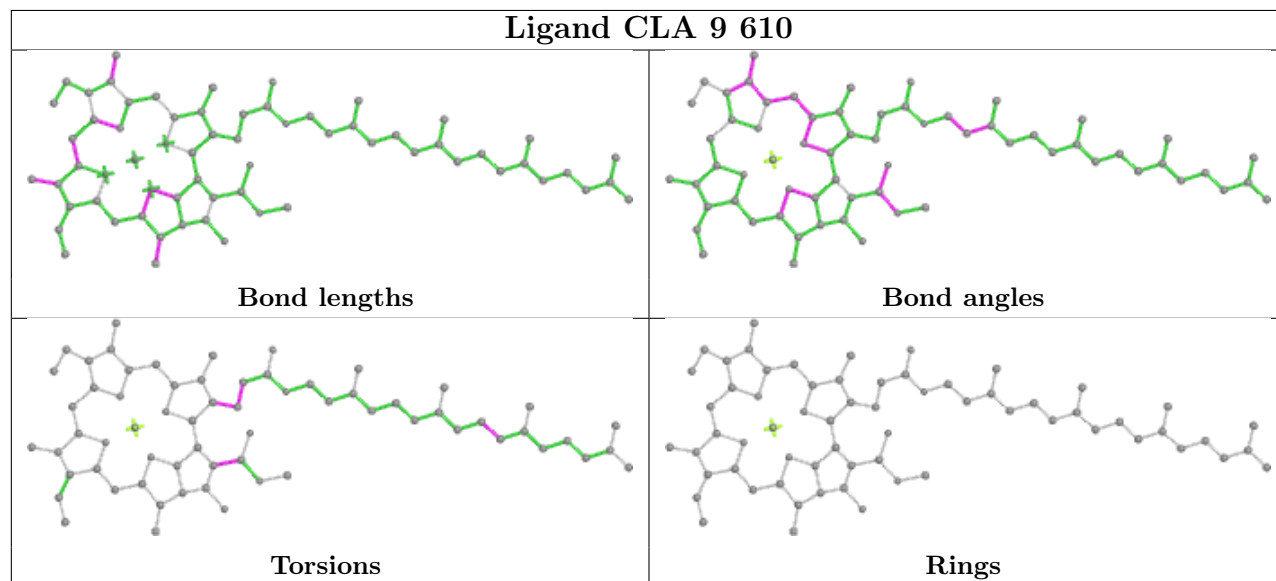




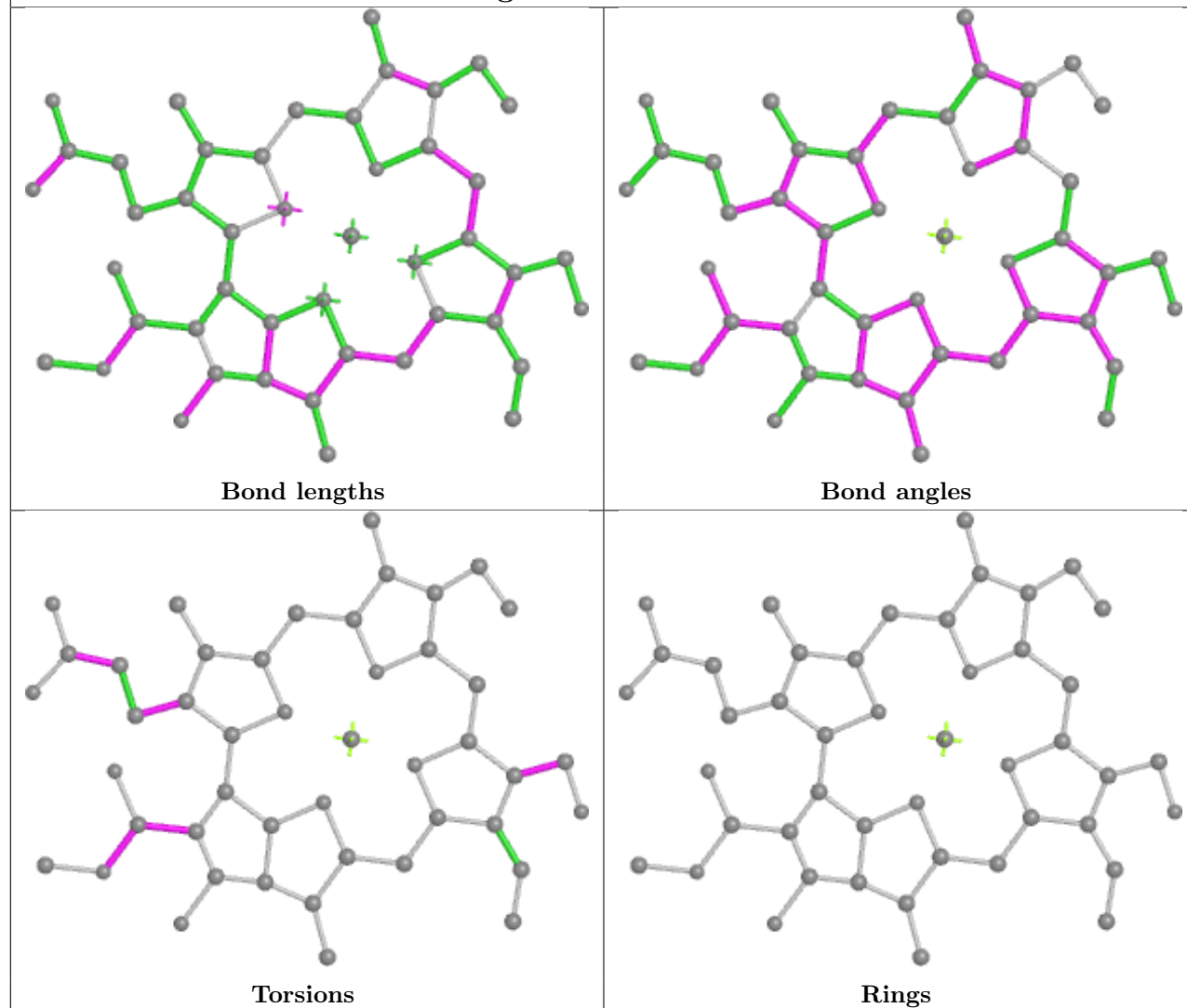
Ligand CLA 7 614

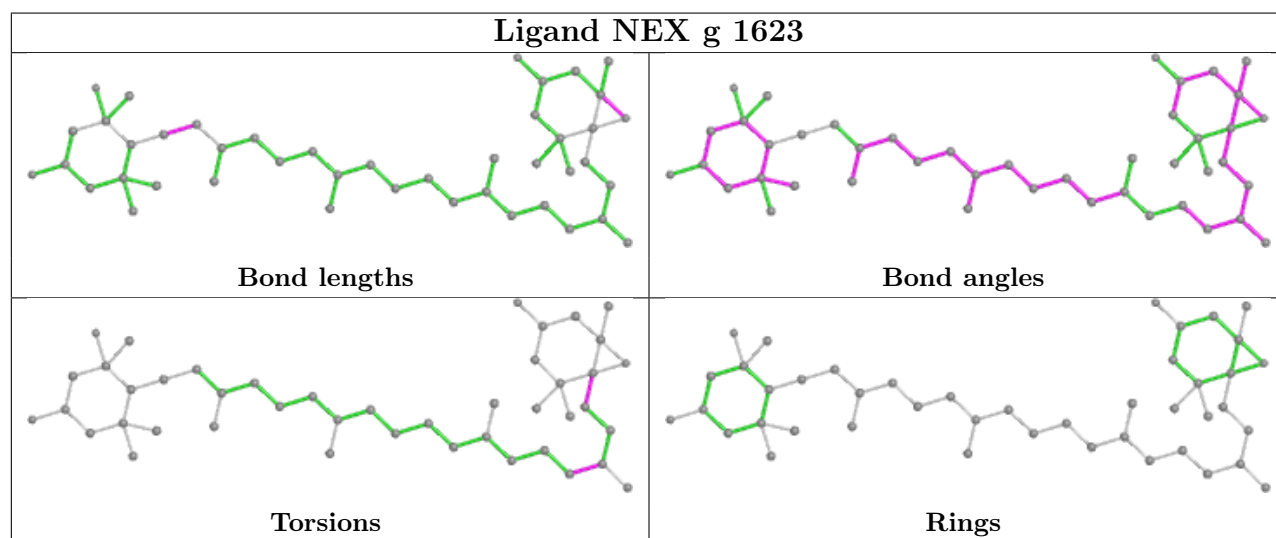
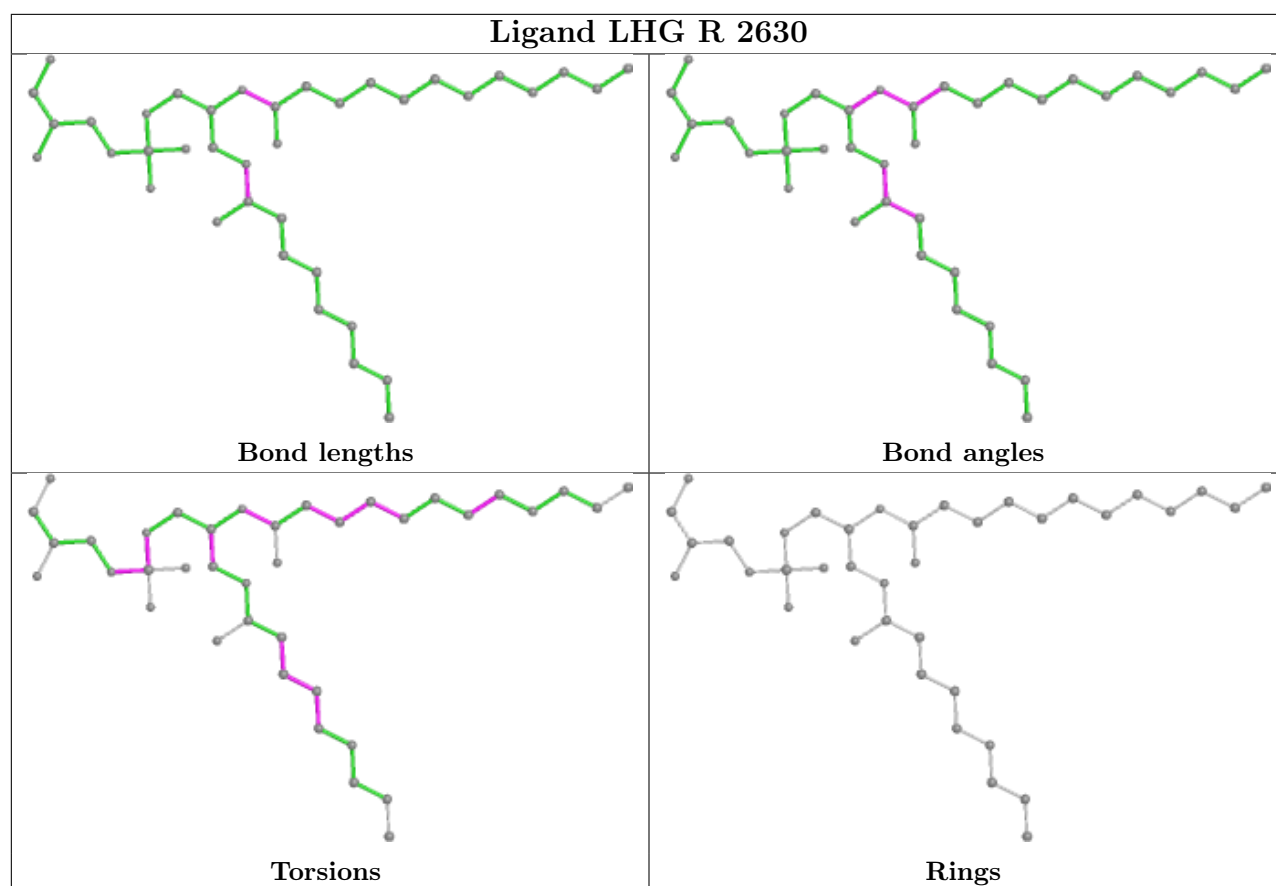


Ligand CLA 9 610

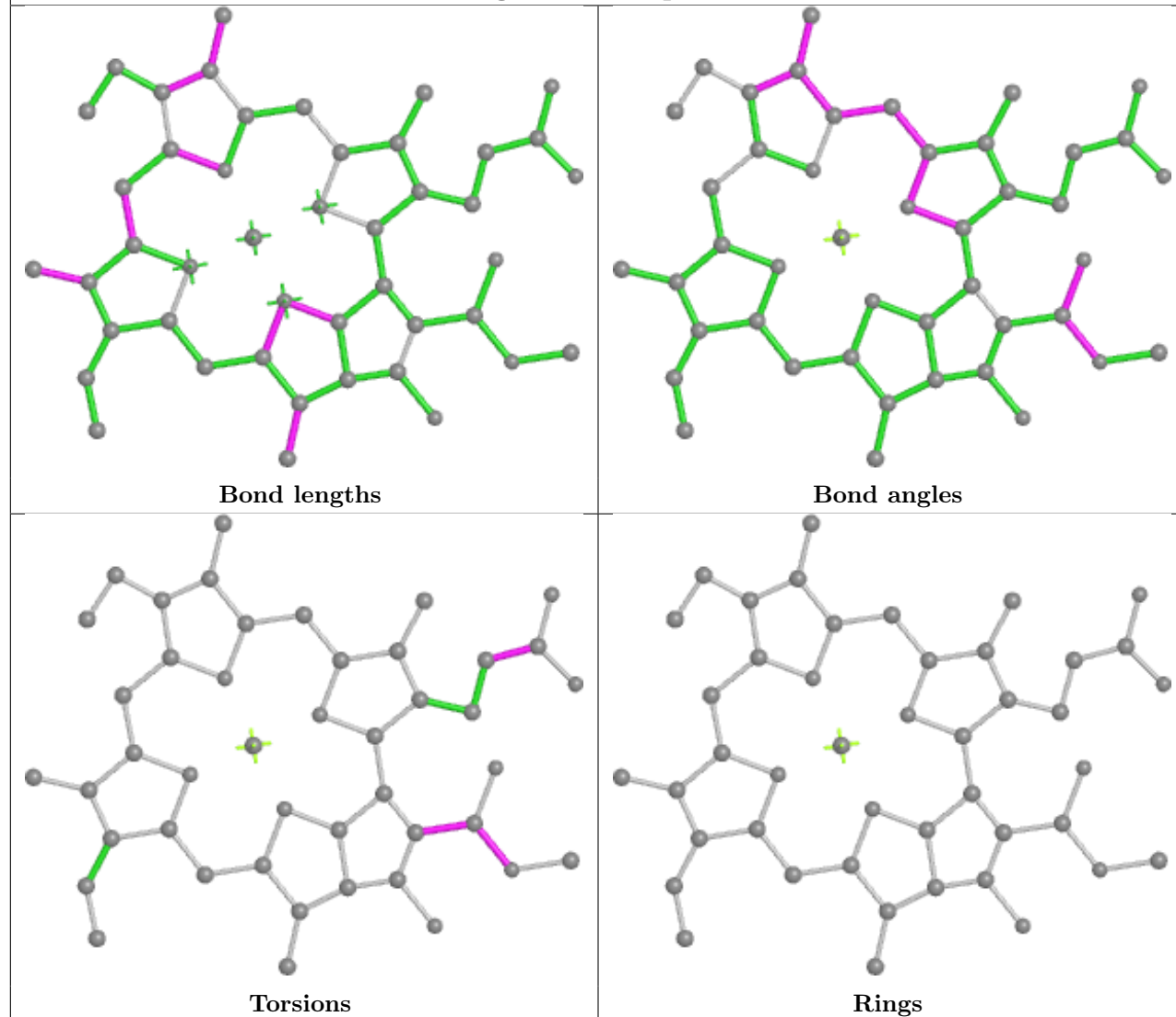


Ligand CHL n 606

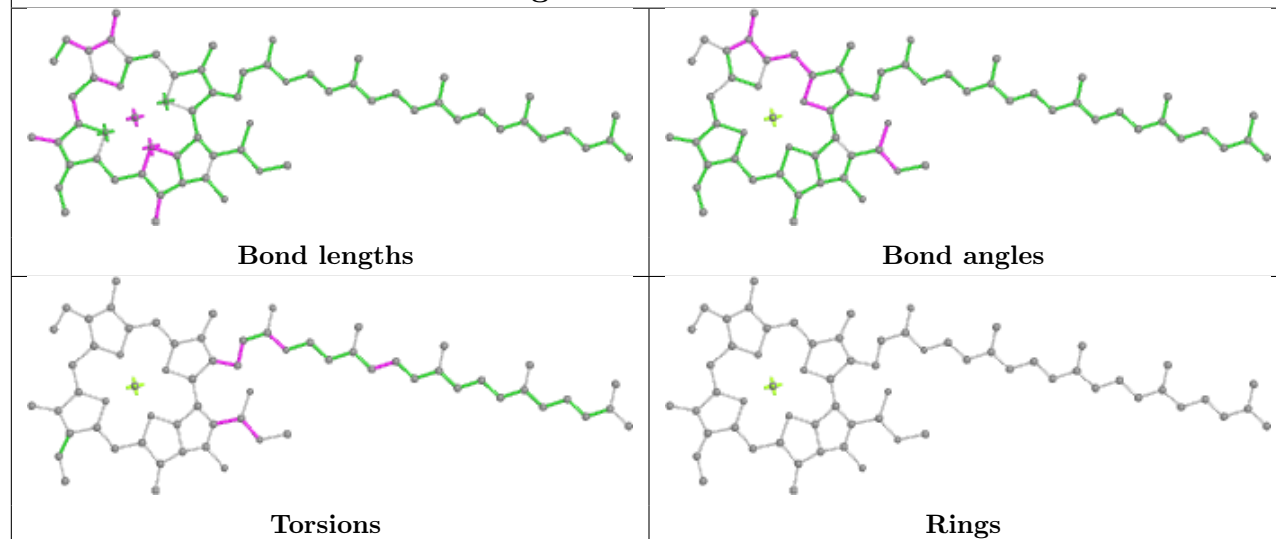


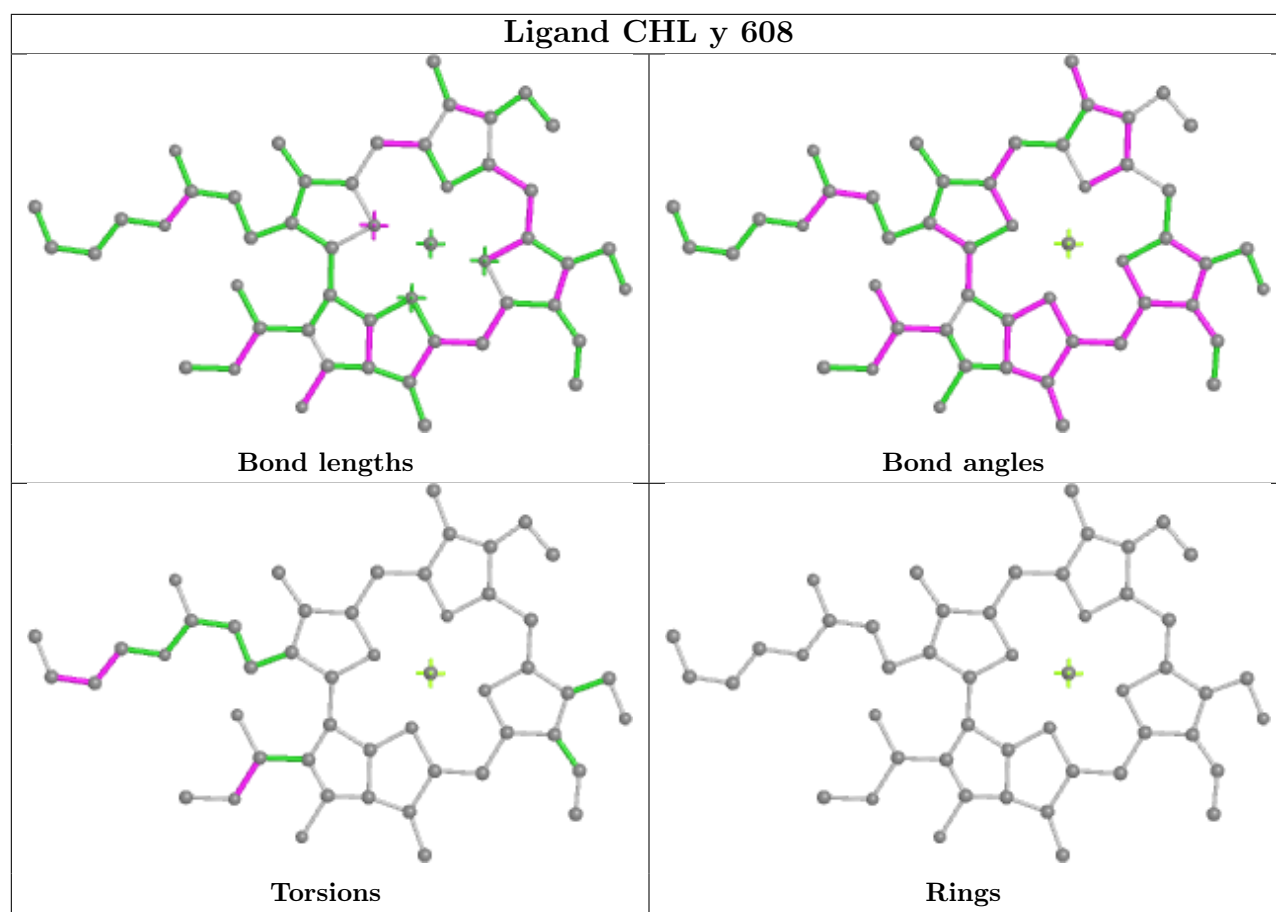


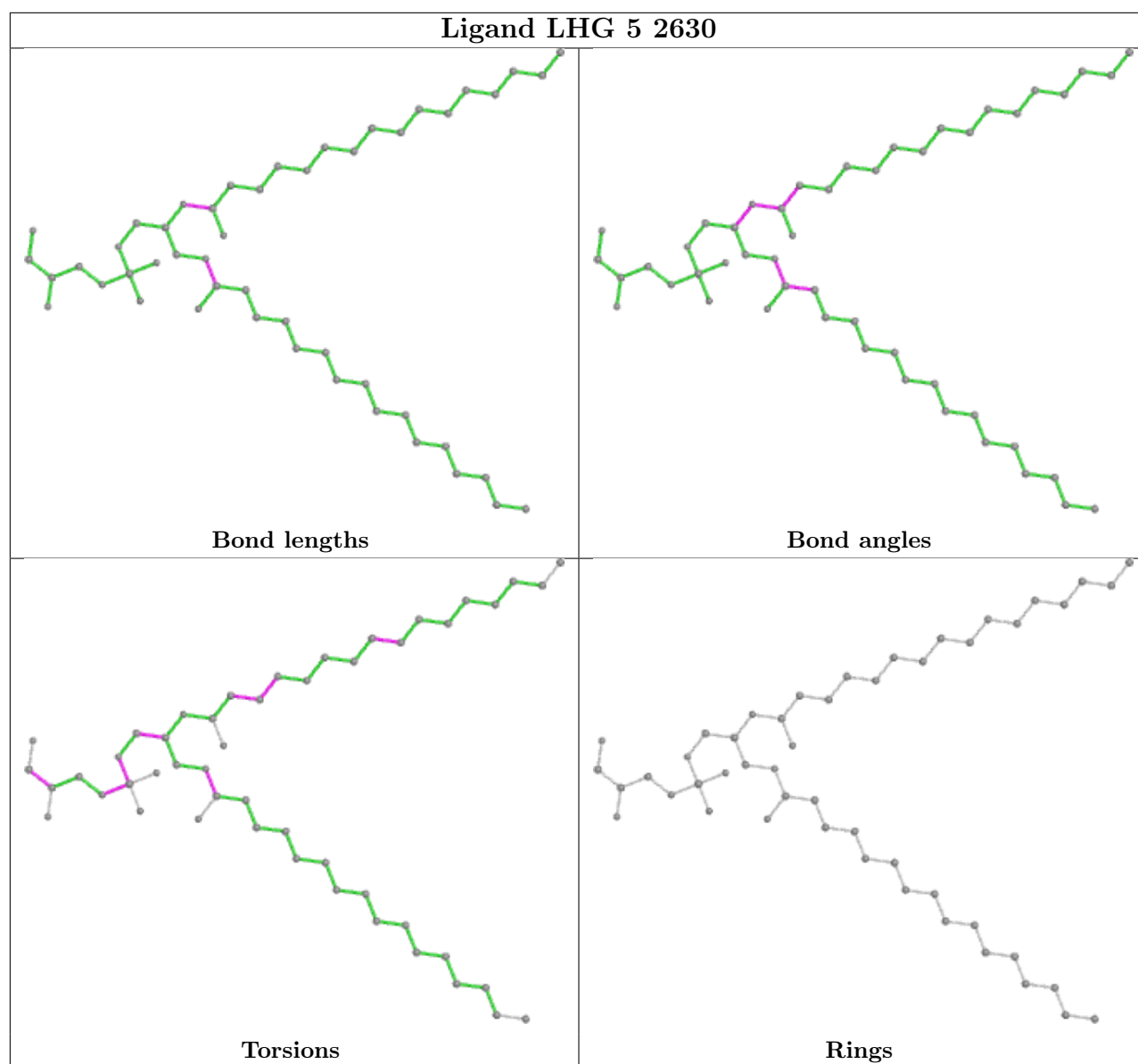
Ligand CLA q 611

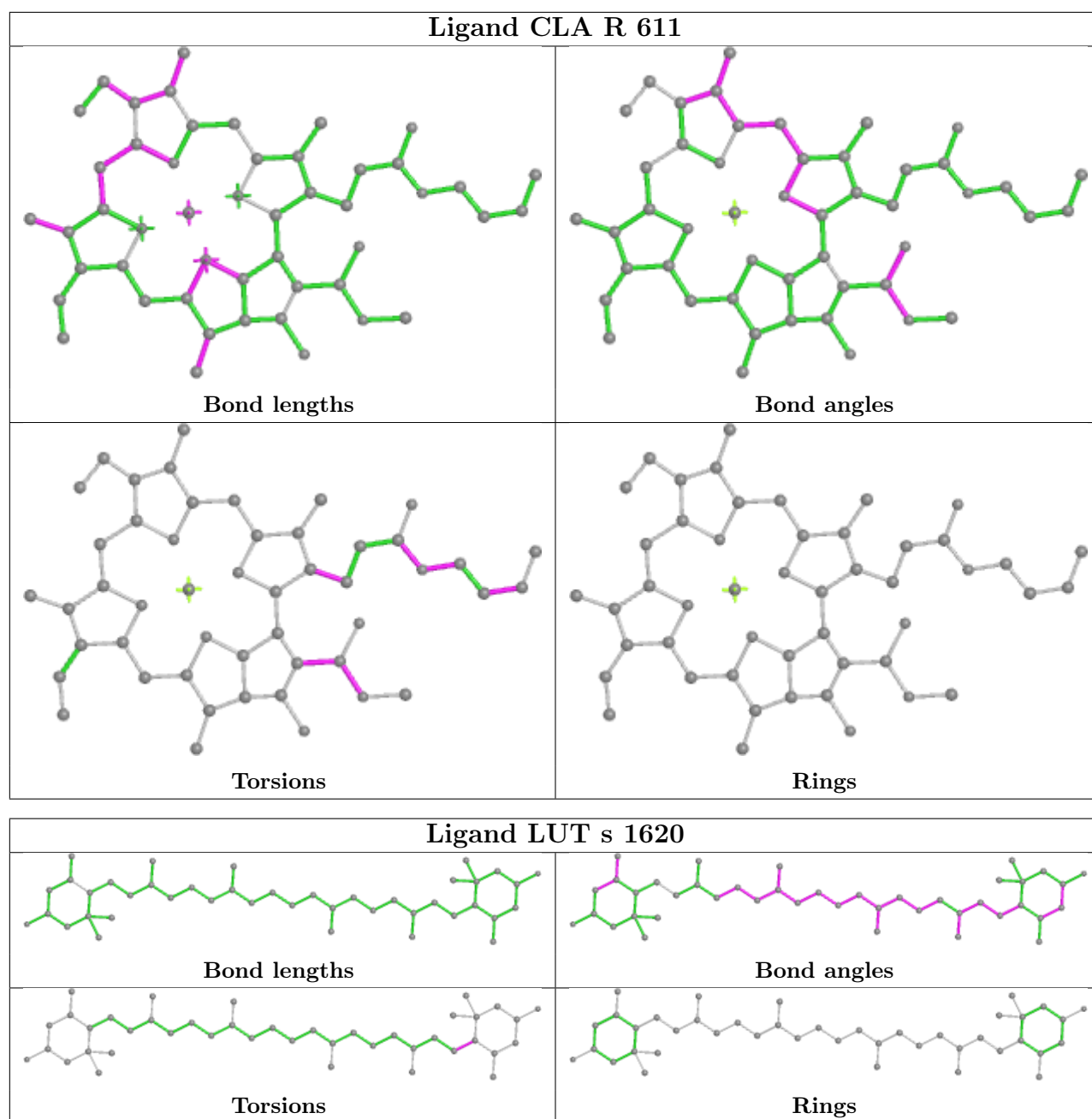


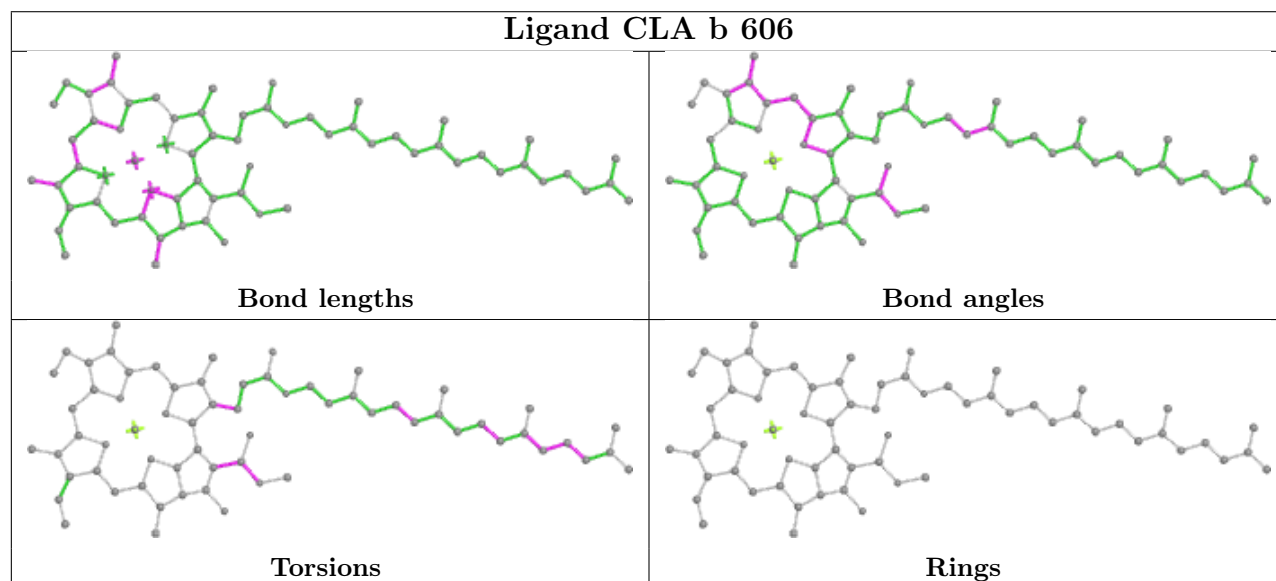
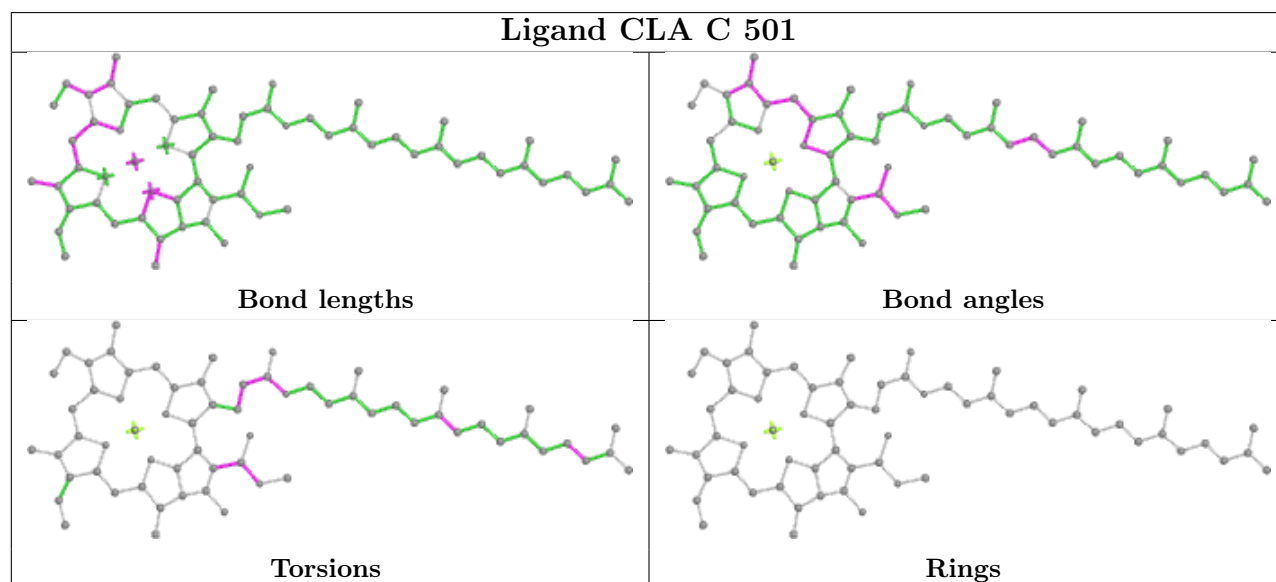
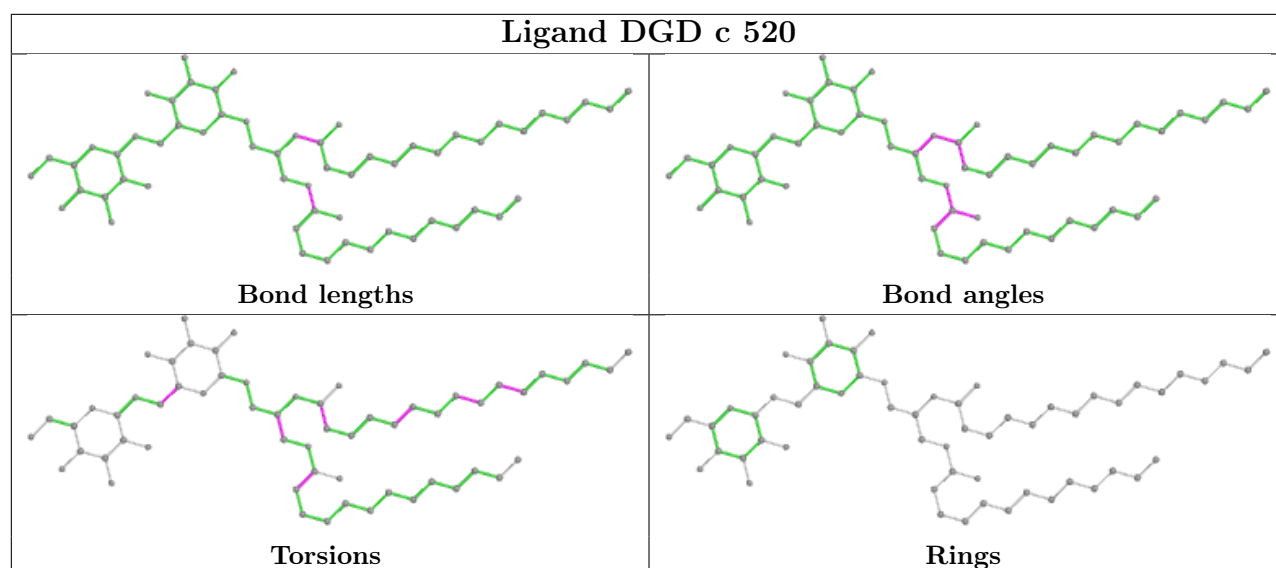
Ligand CLA N 604



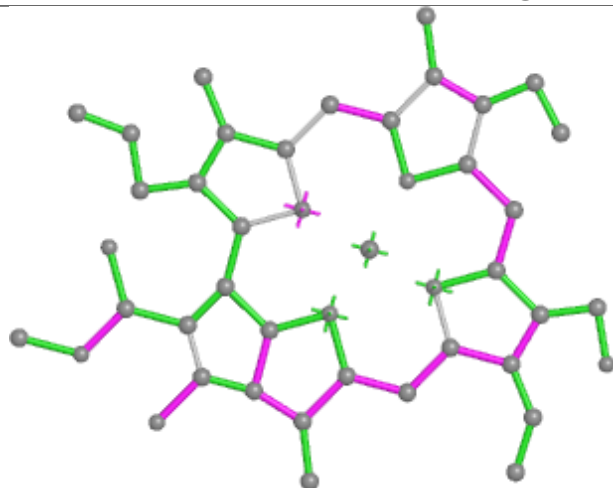




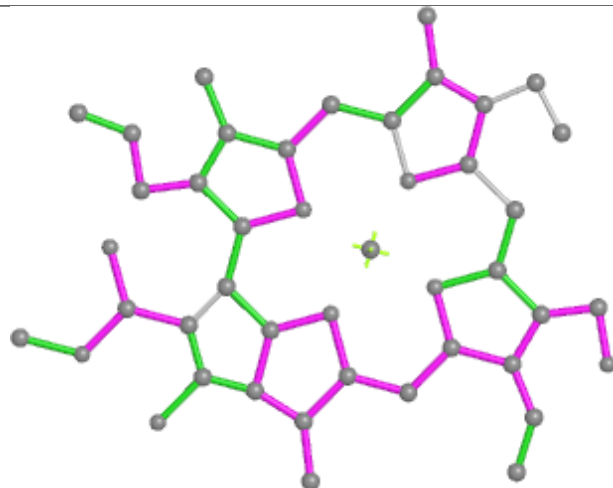




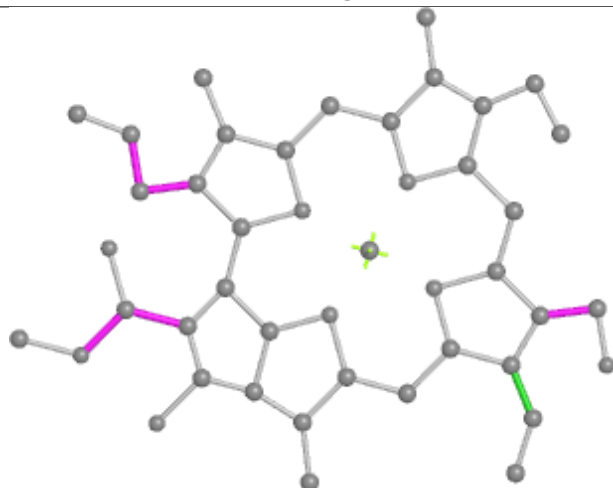
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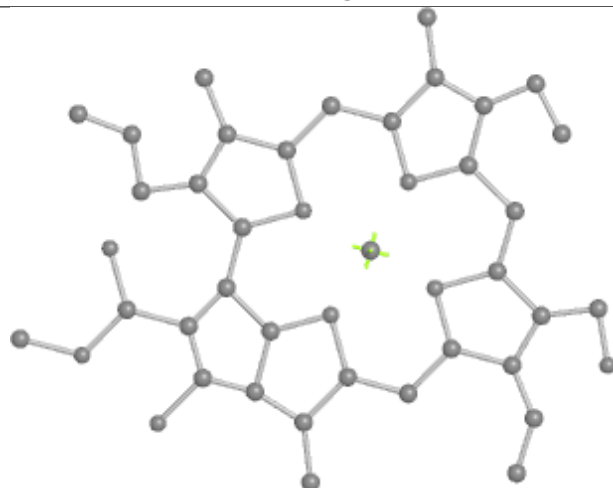
Bond lengths



Bond angles

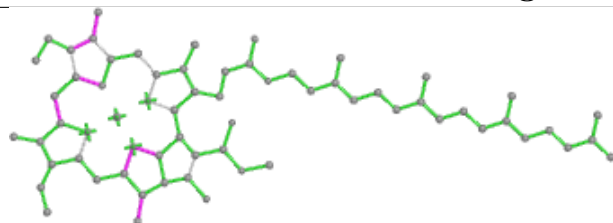


Torsions

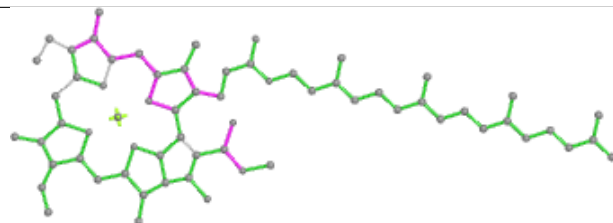


Rings

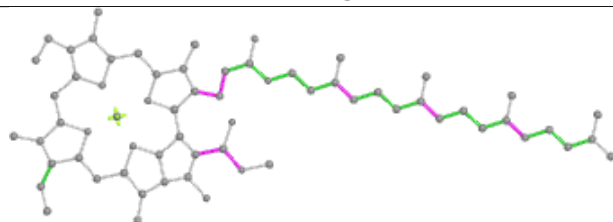
Ligand CLA 5 603



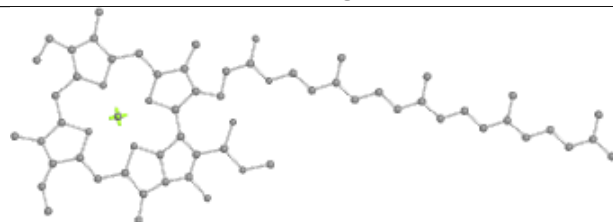
Bond lengths



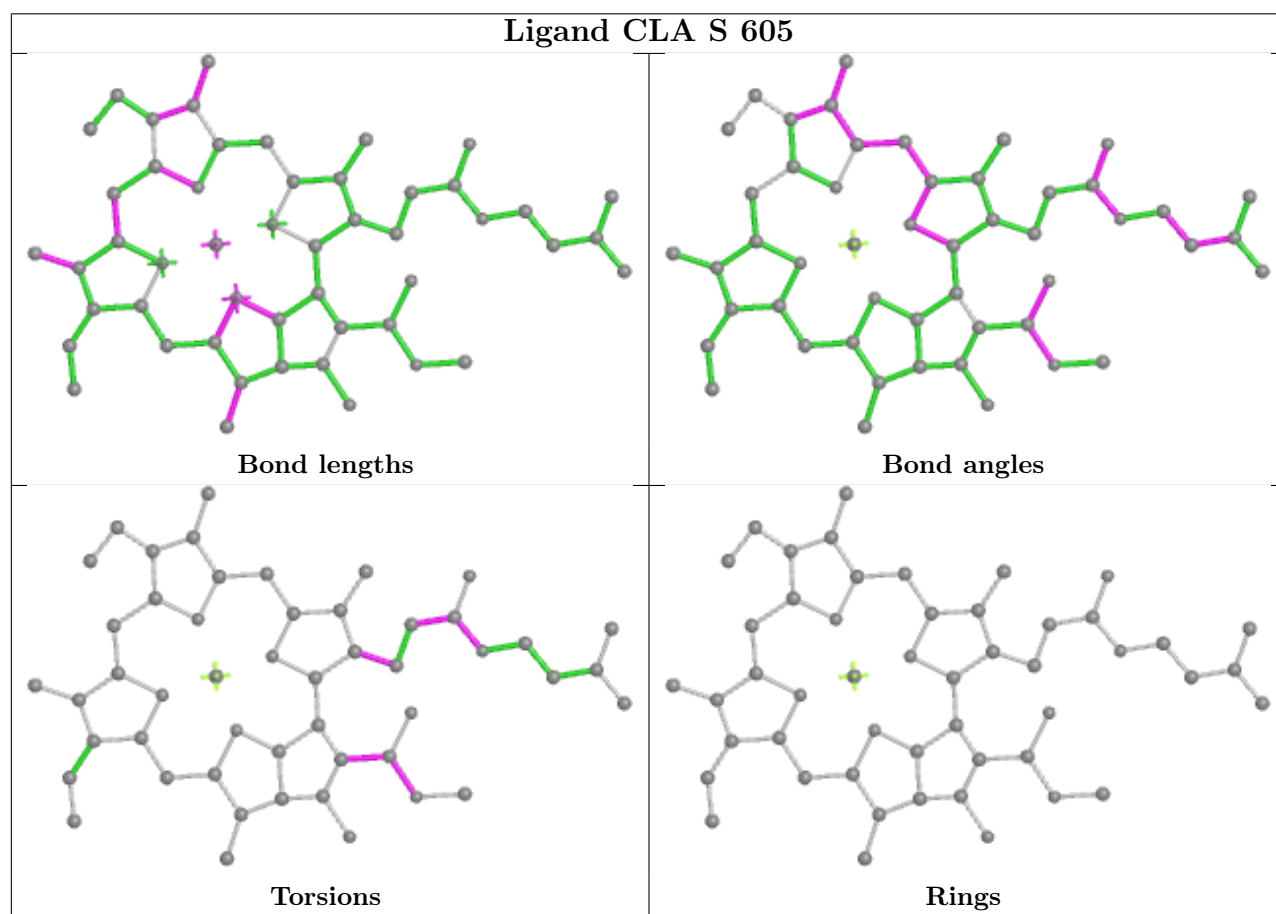
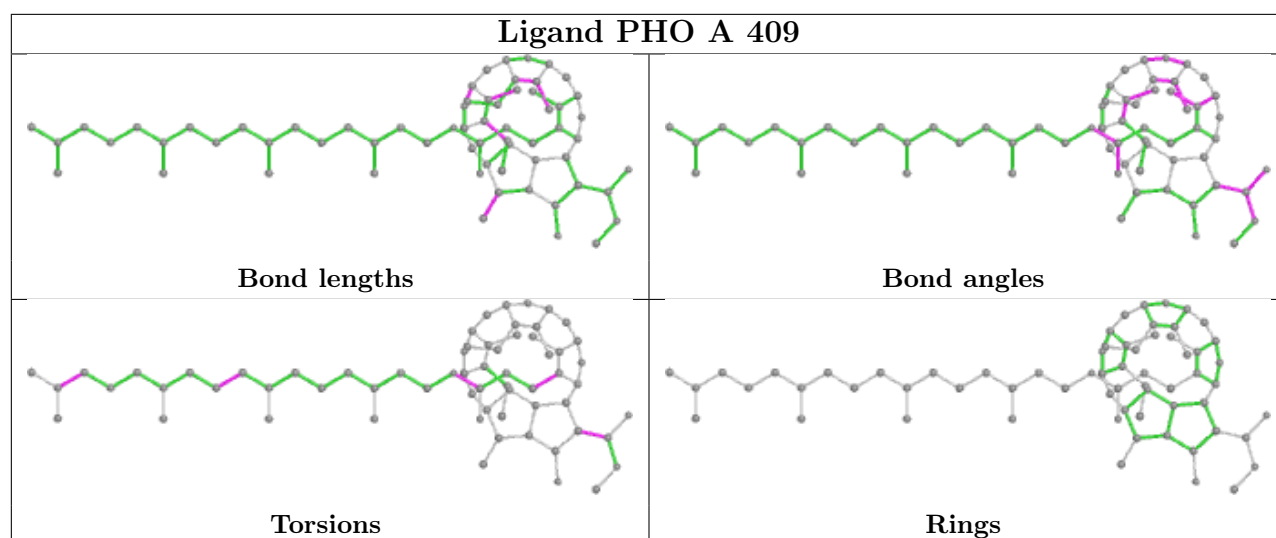
Bond angles

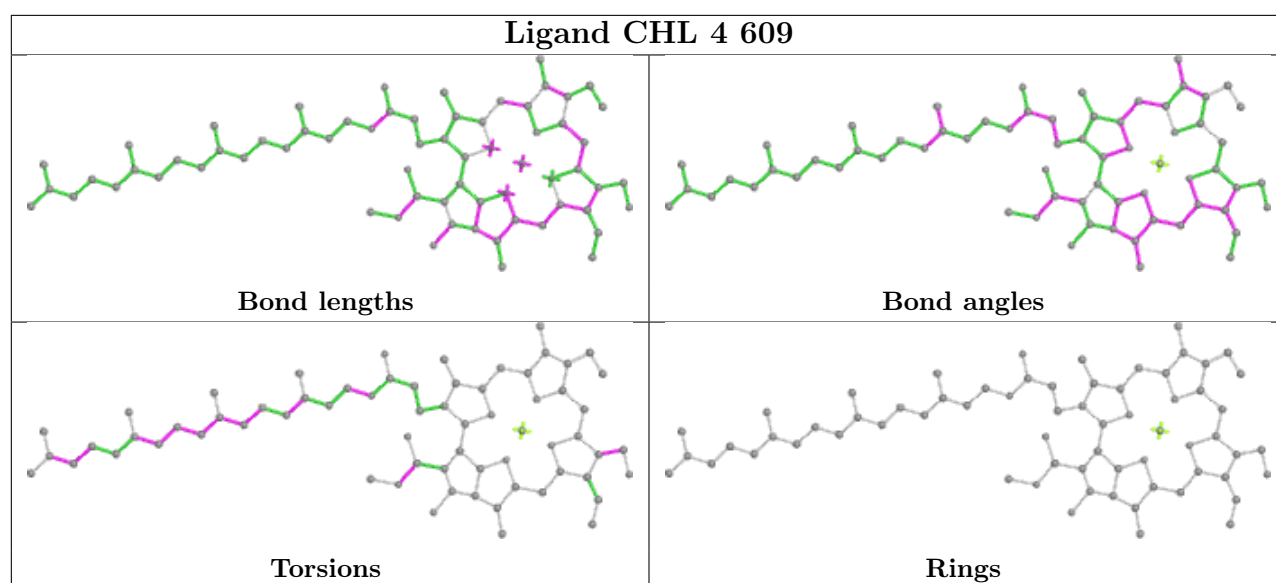
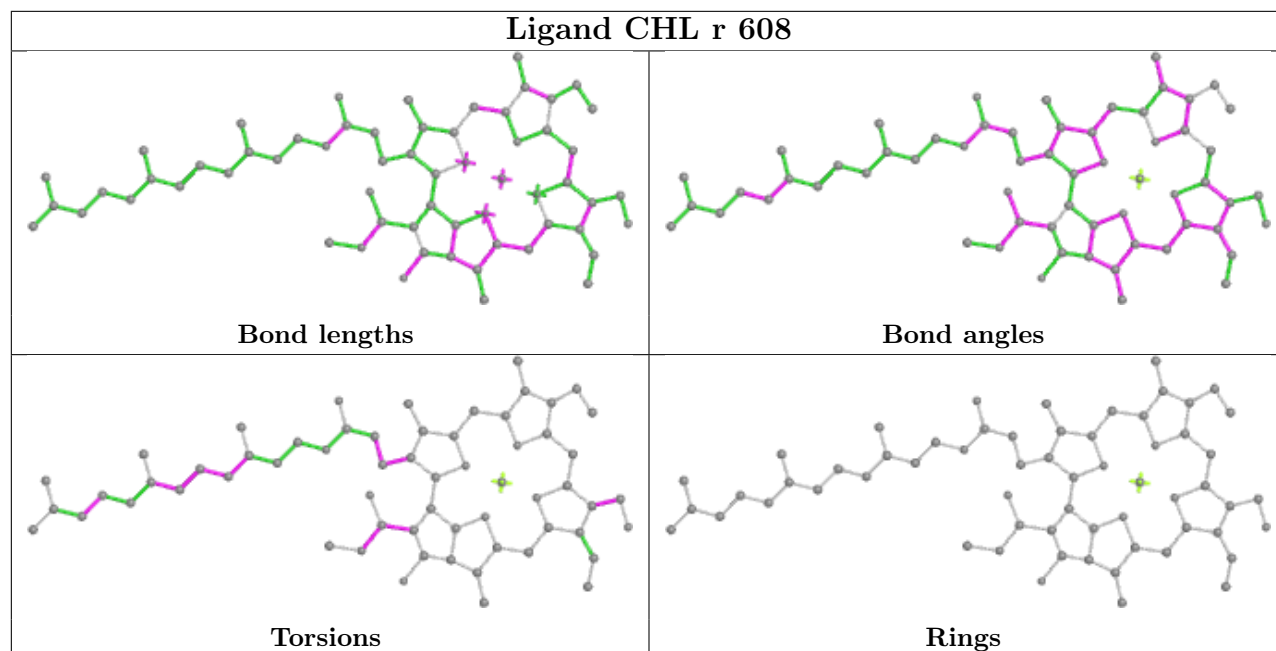
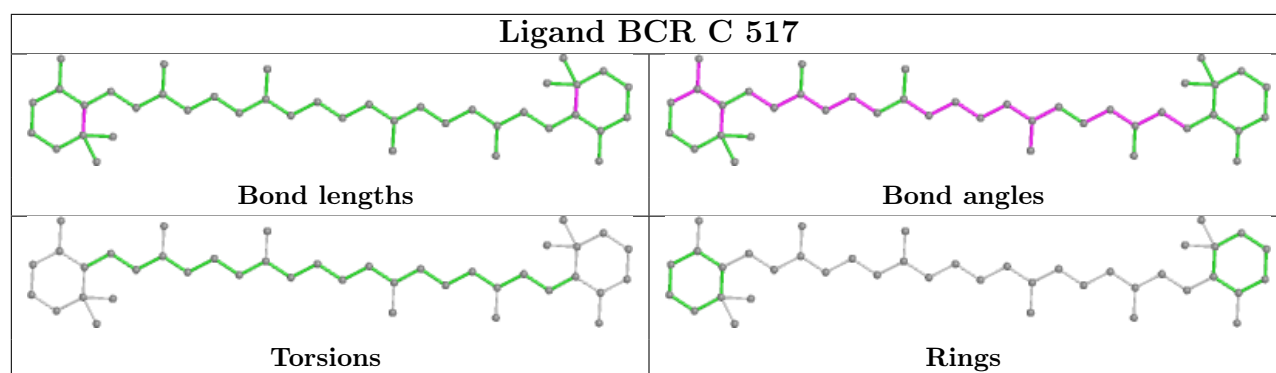


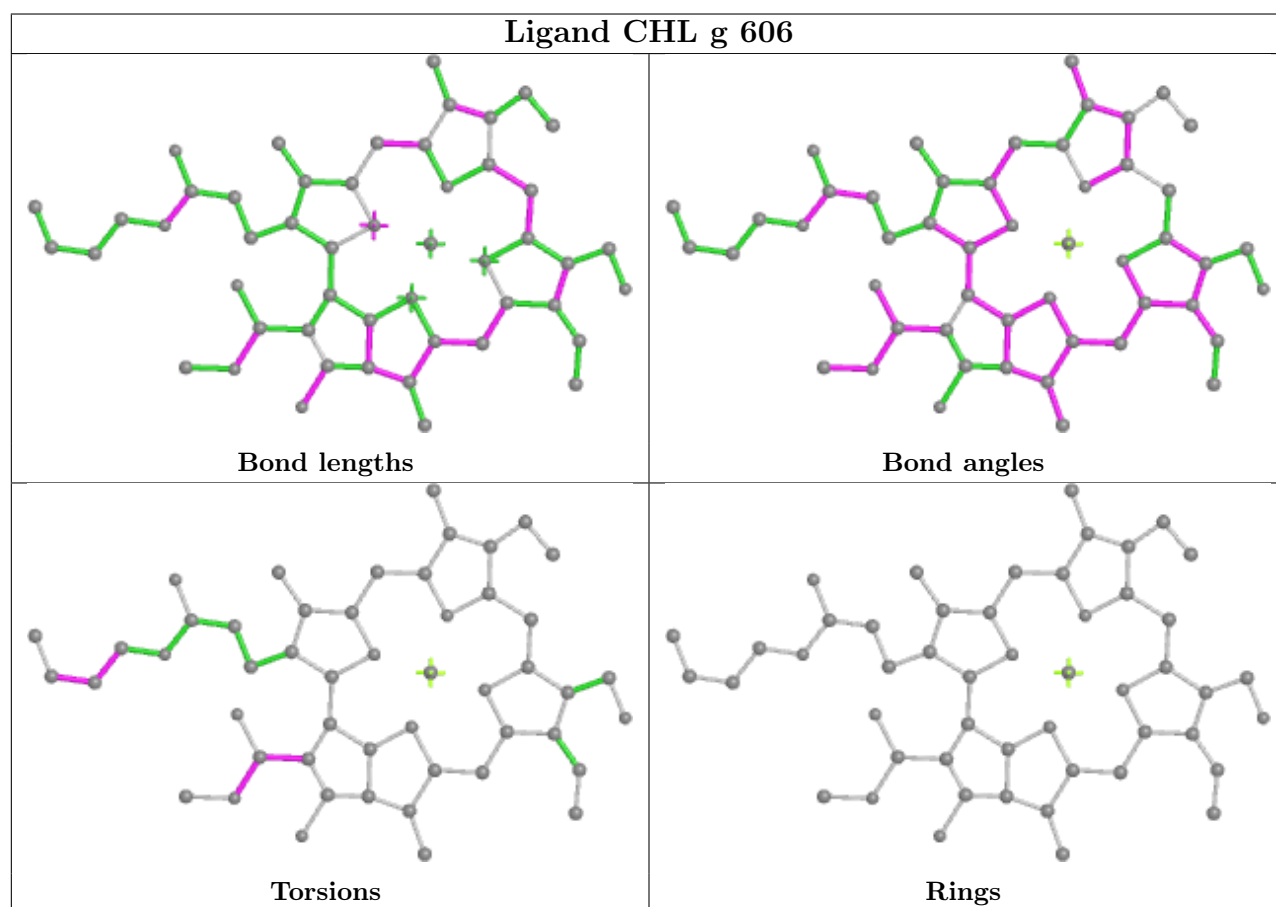
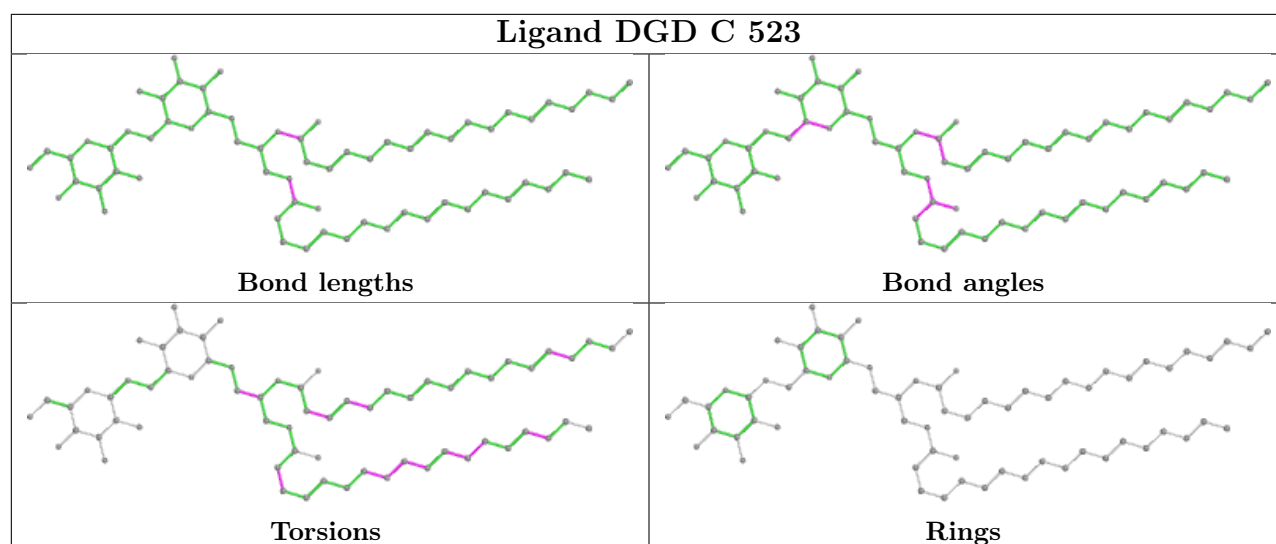
Torsions

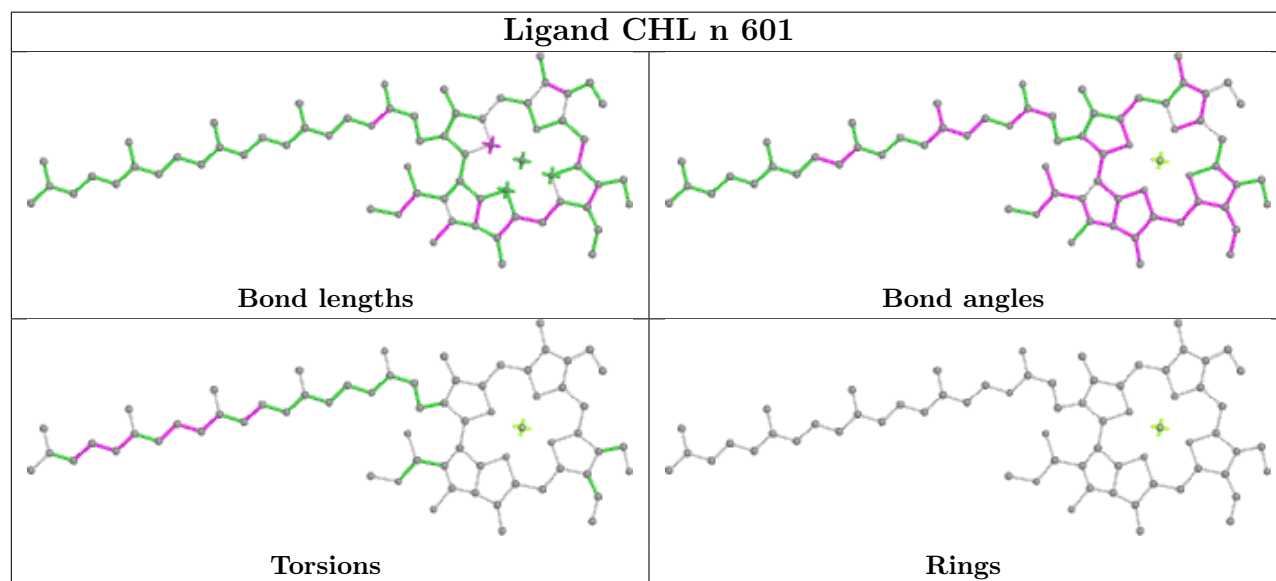
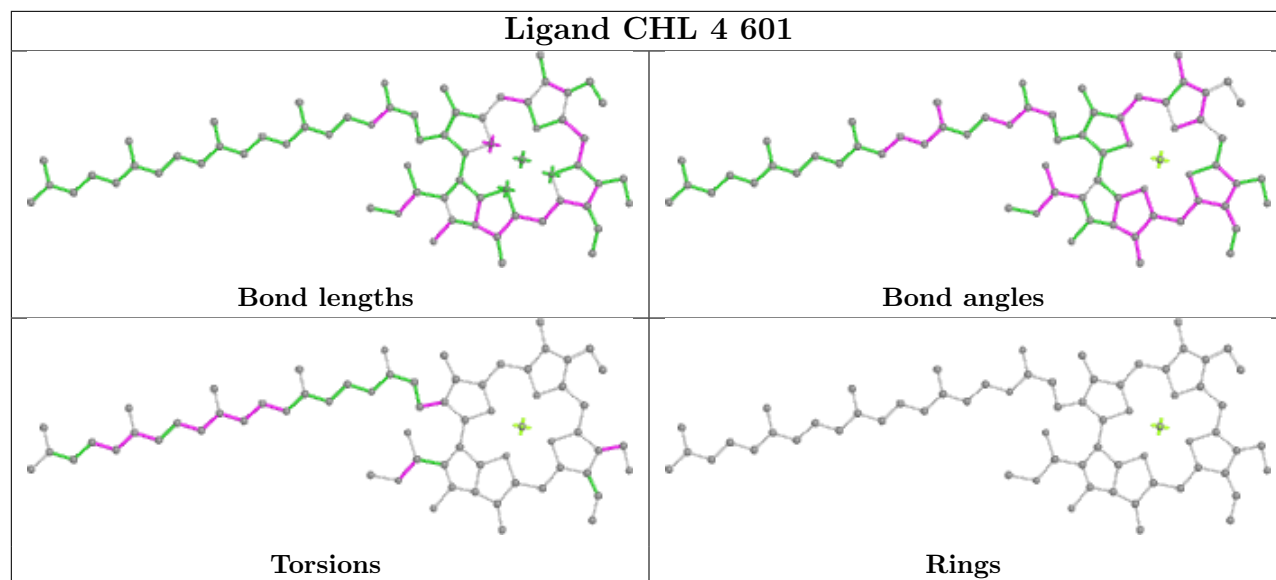


Rings

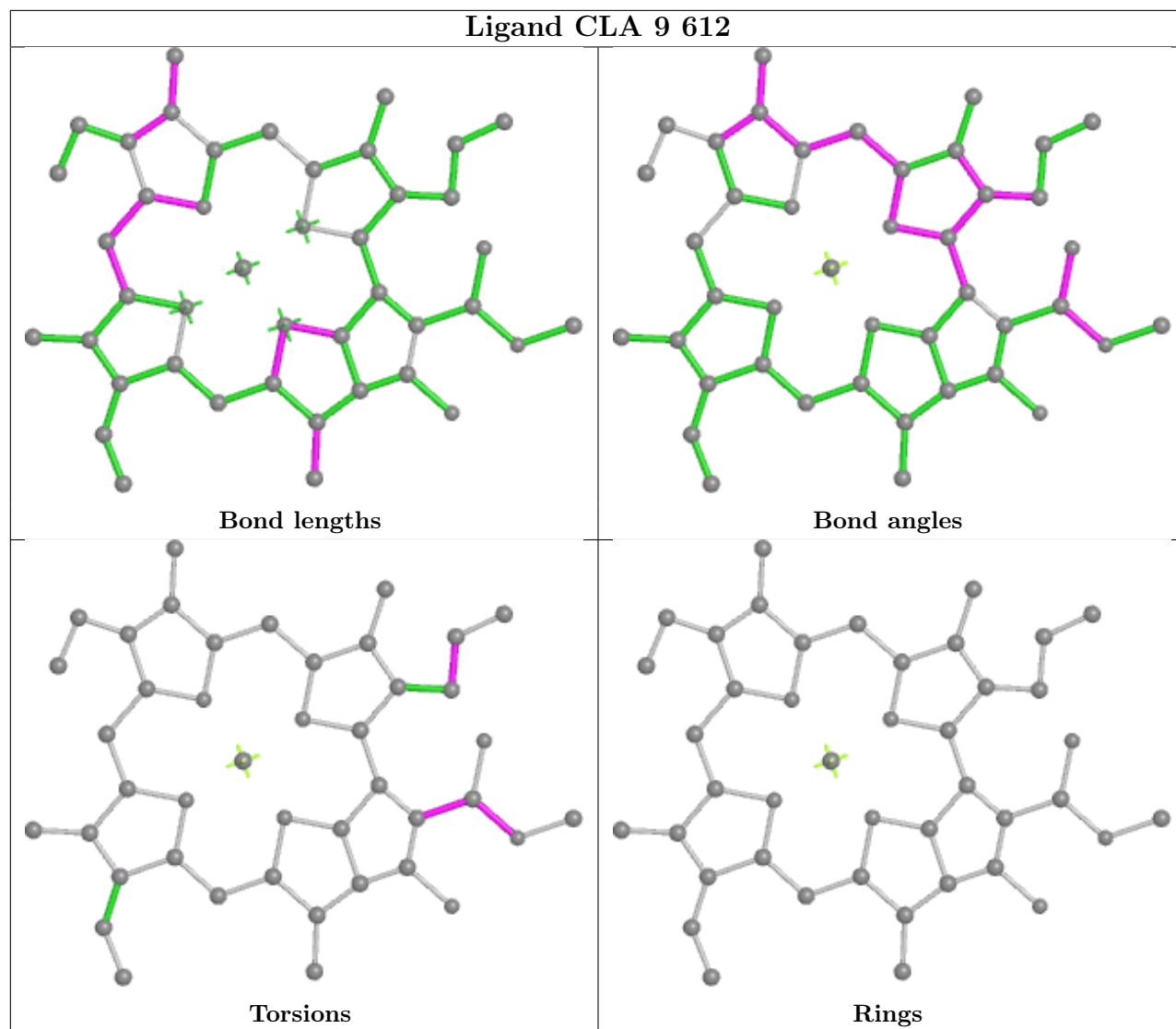




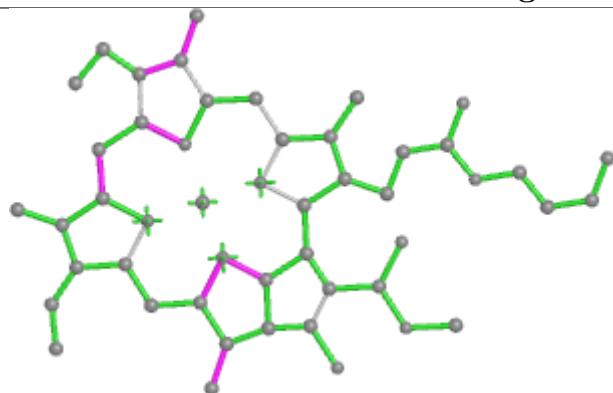




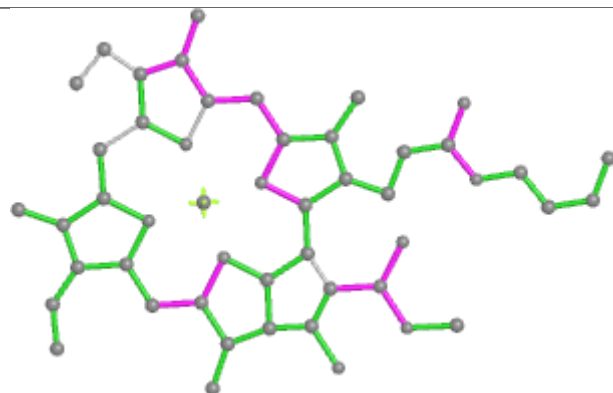
Ligand CLA 9 612



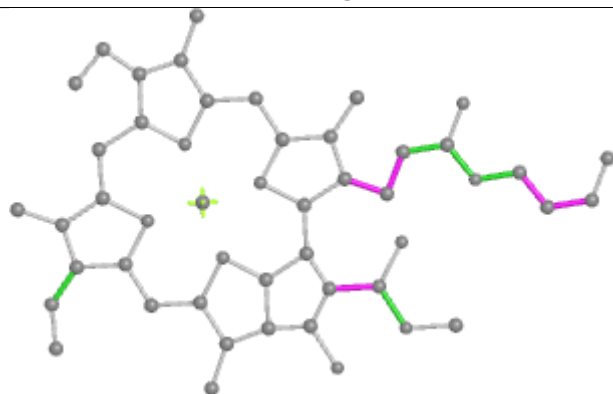
Ligand CLA 3 611



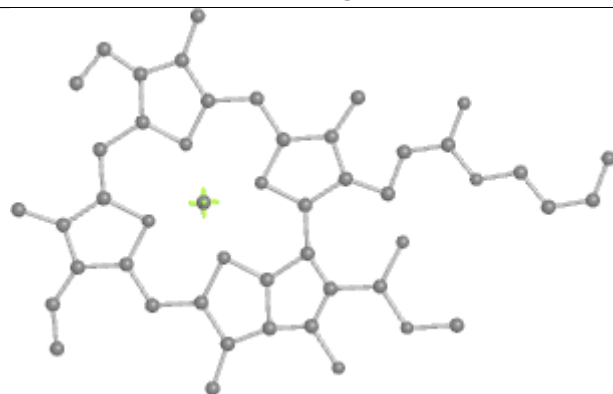
Bond lengths



Bond angles

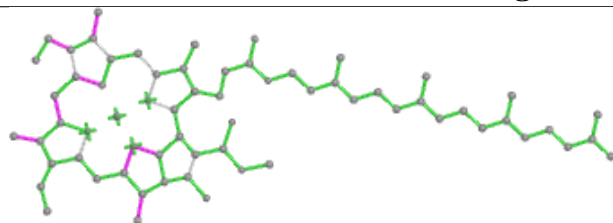


Torsions

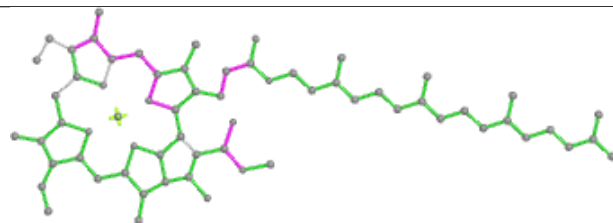


Rings

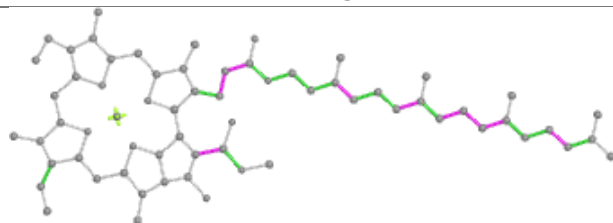
Ligand CLA Y 602



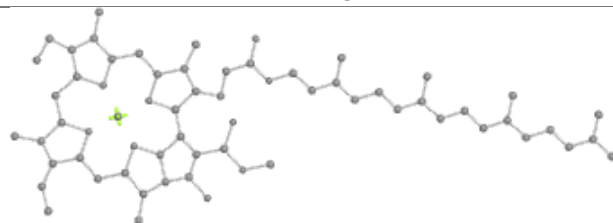
Bond lengths



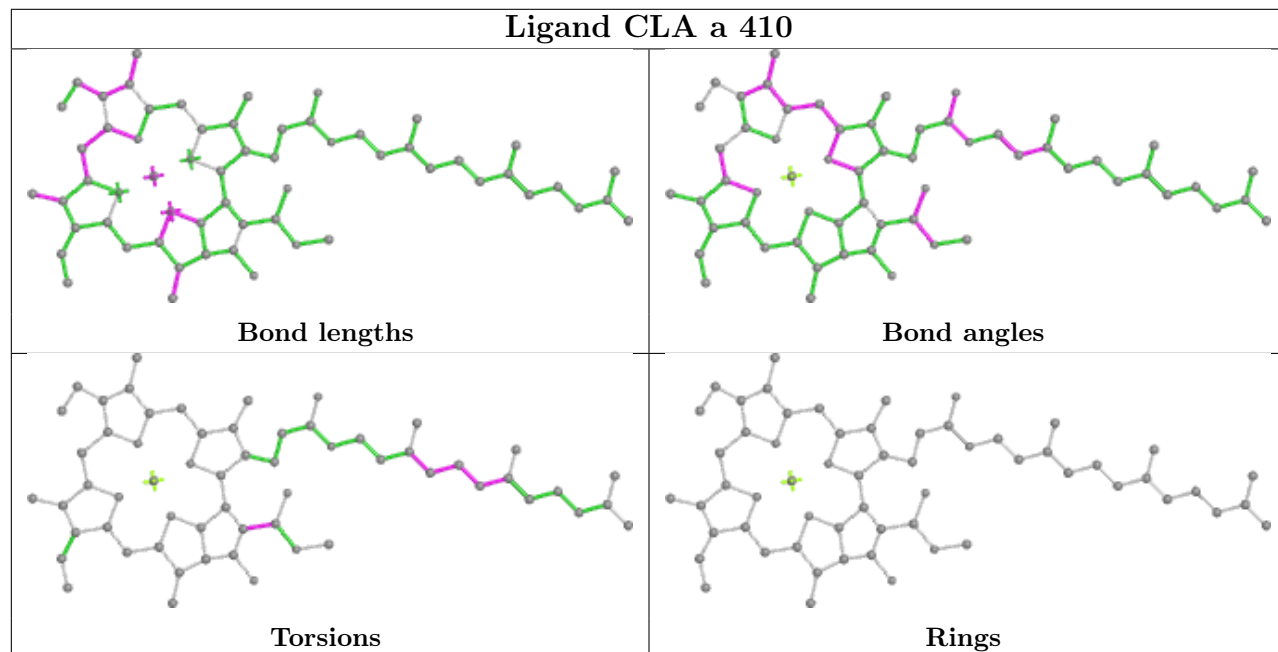
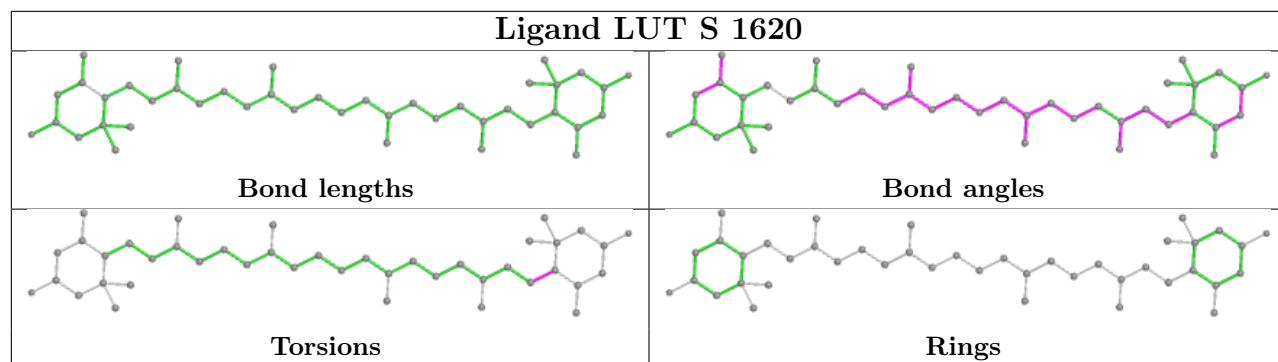
Bond angles



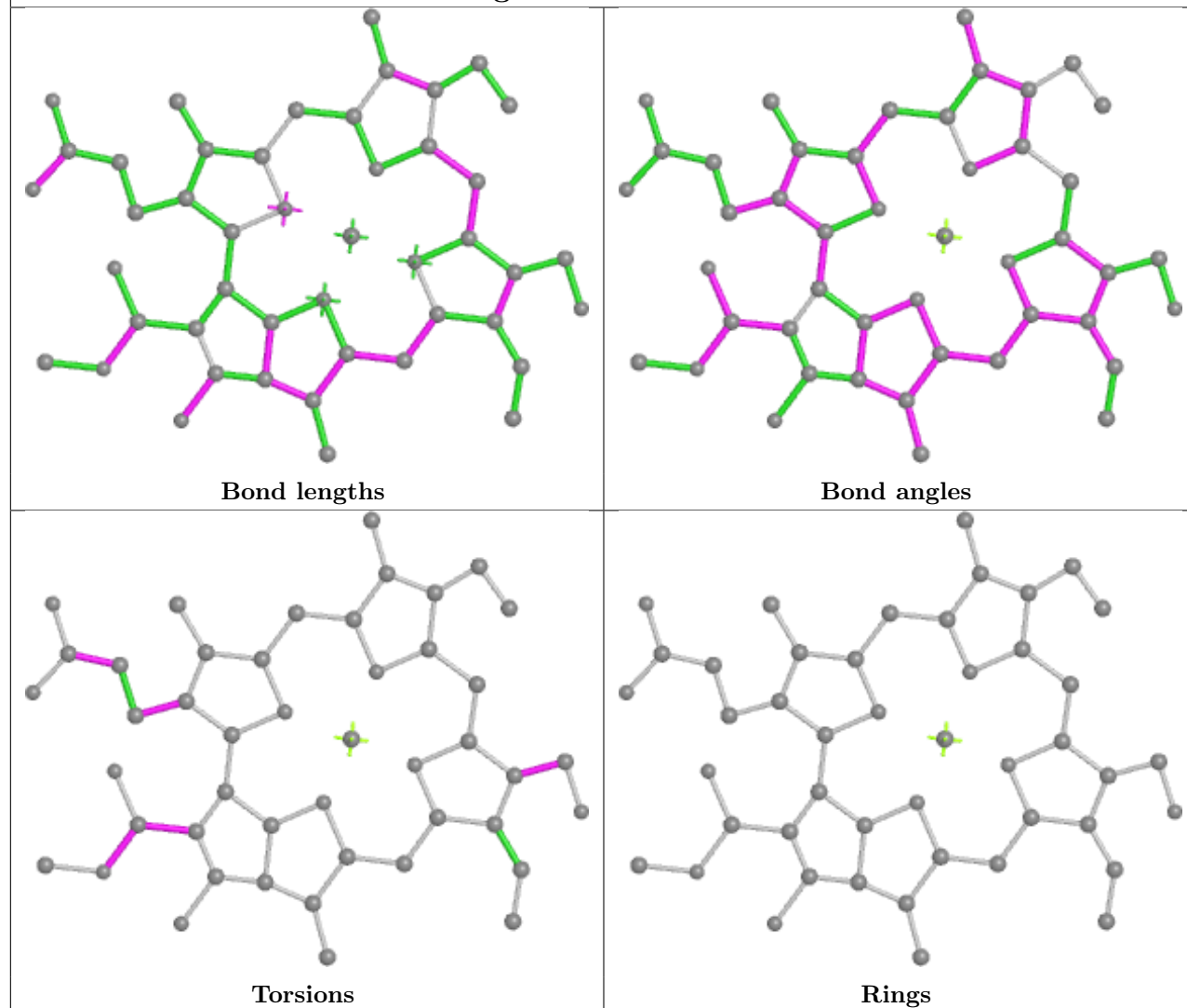
Torsions



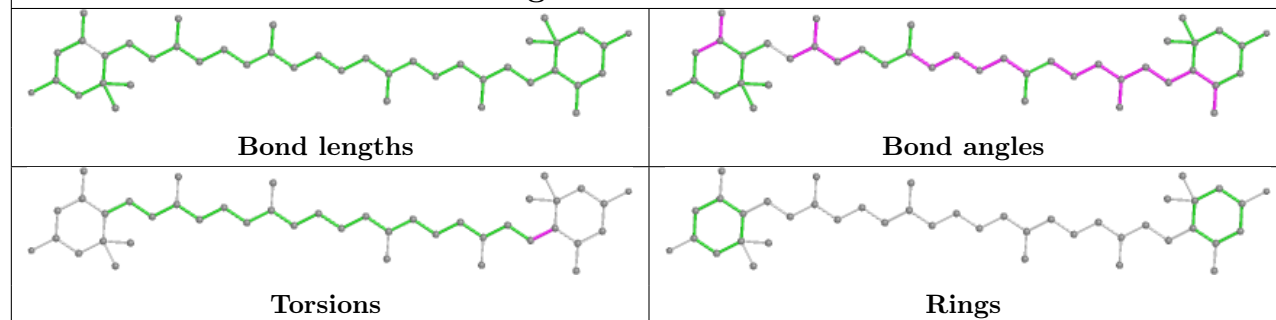
Rings



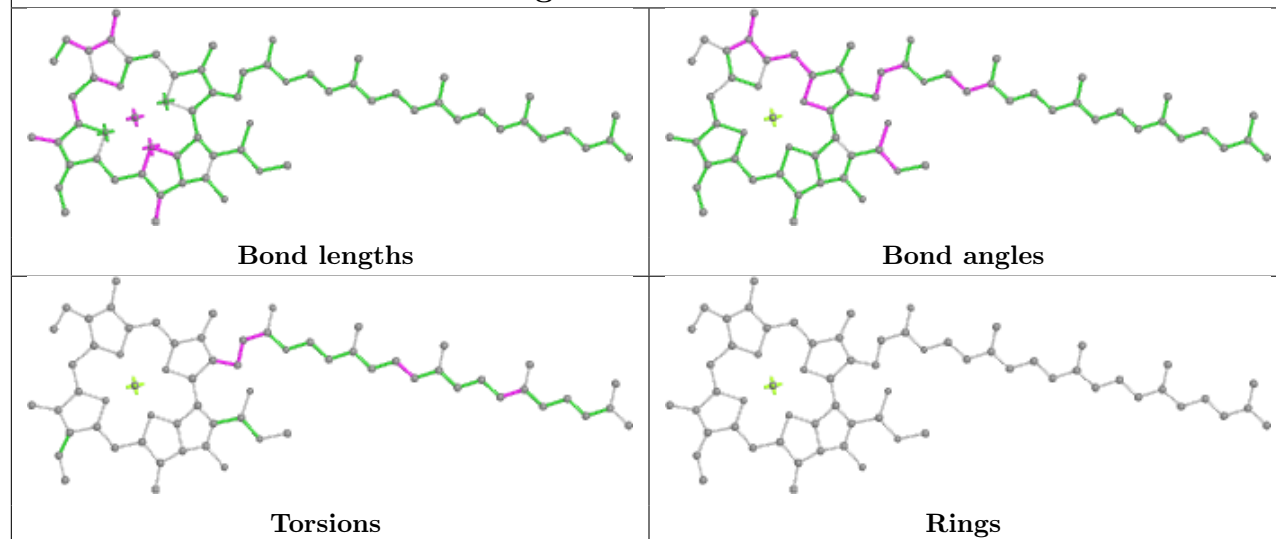
Ligand CHL N 606



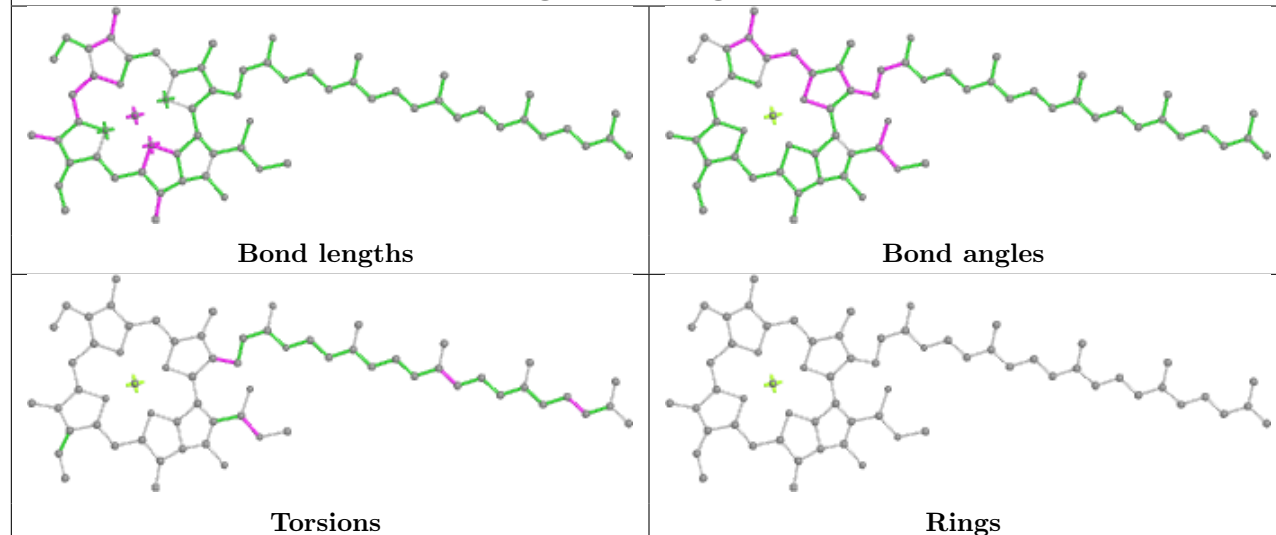
Ligand LUT 0 1620



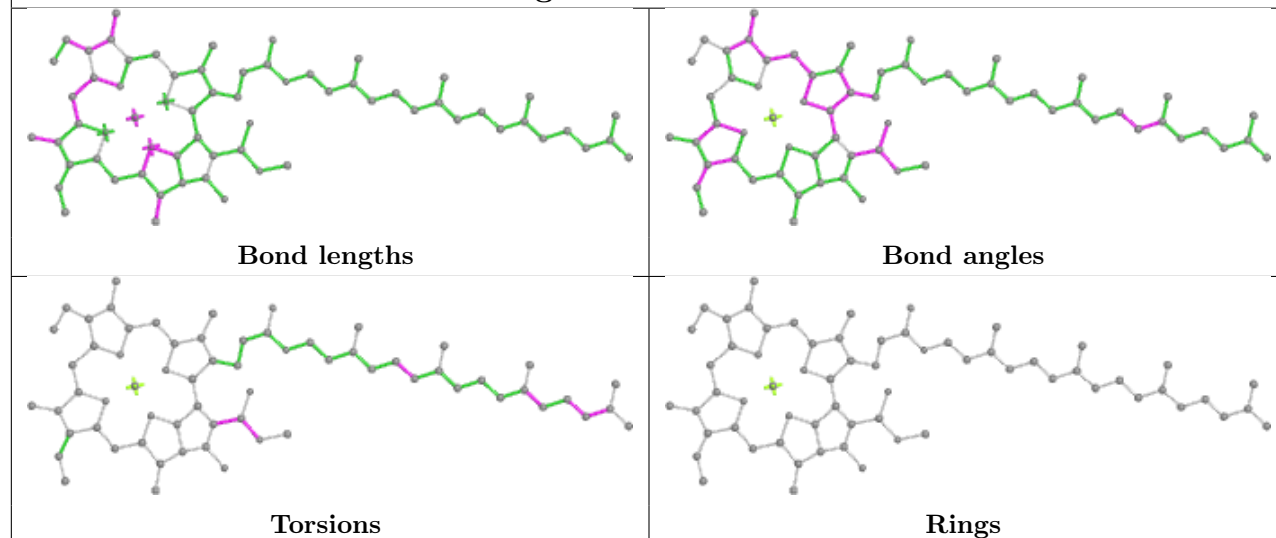
Ligand CLA n 602



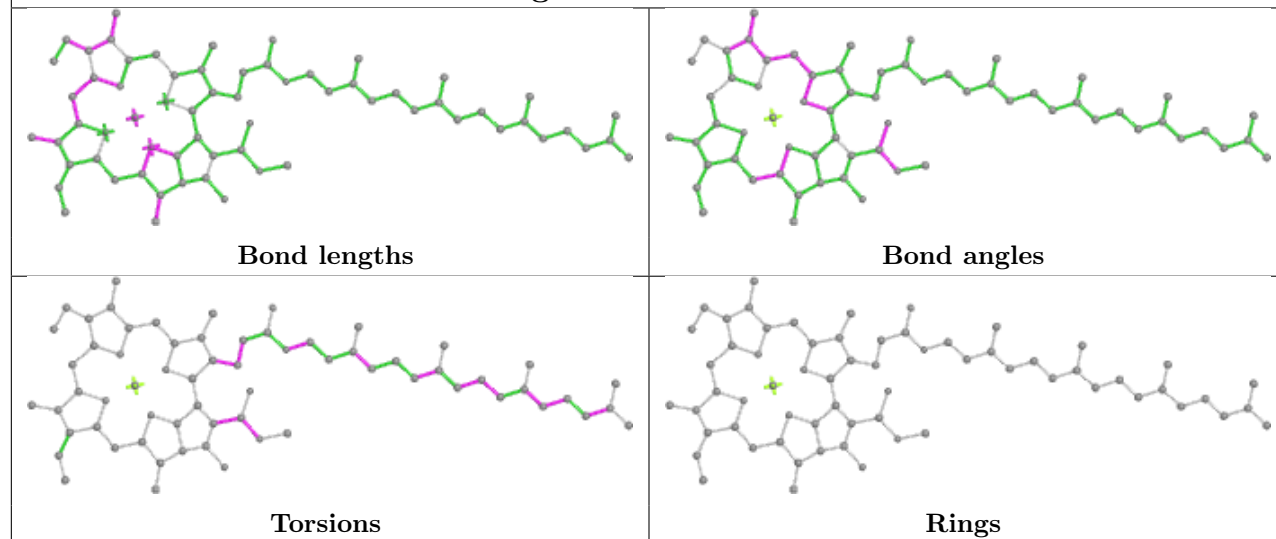
Ligand CLA g 603



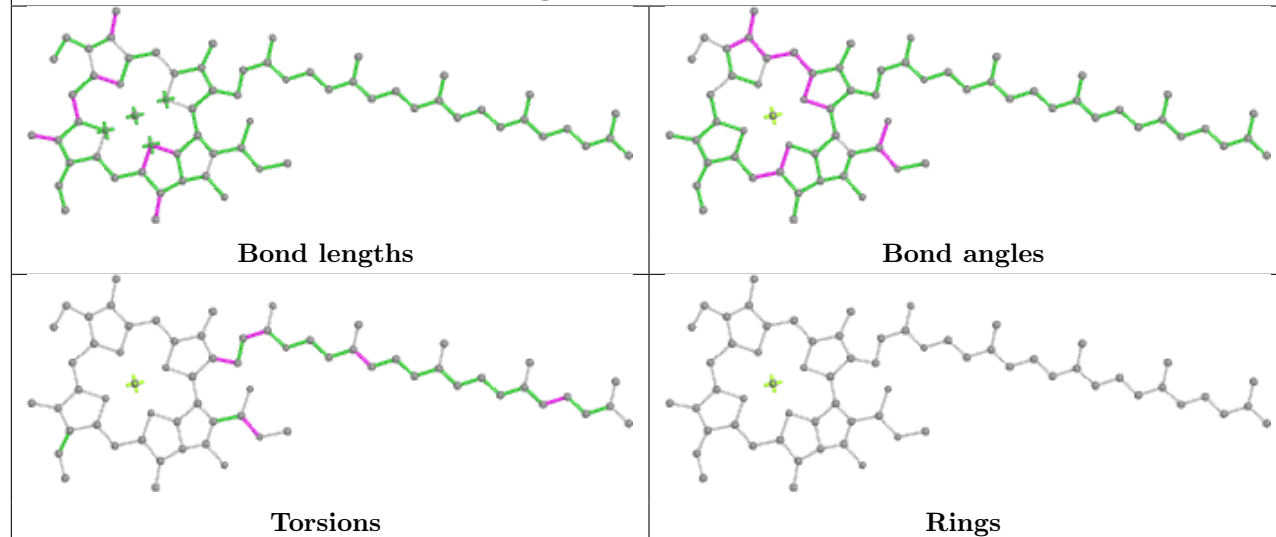
Ligand CLA b 616



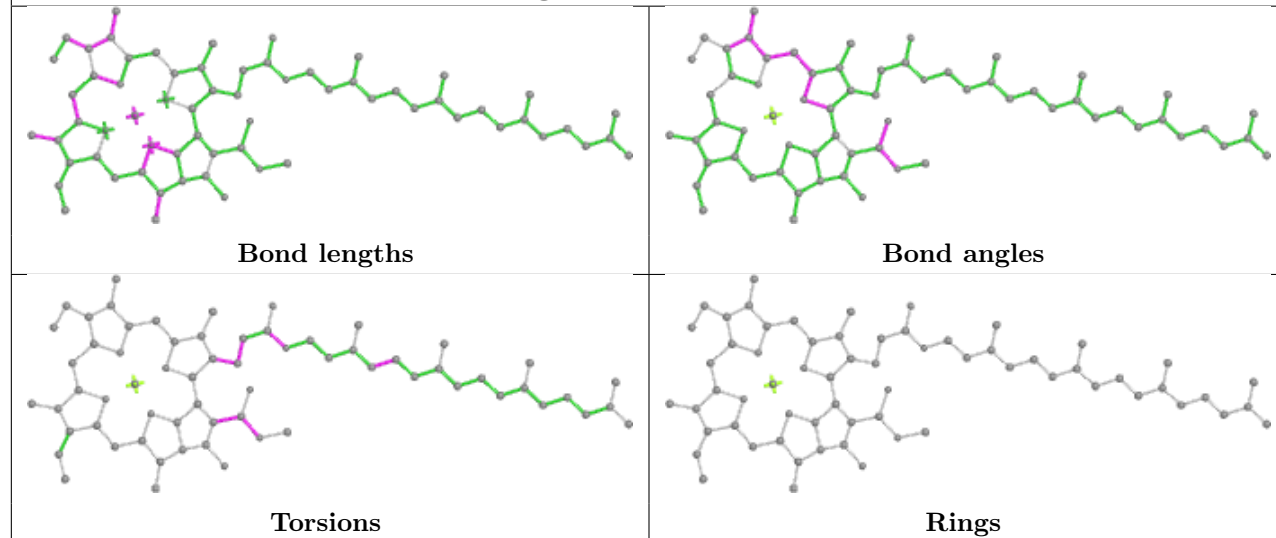
Ligand CLA Y 604



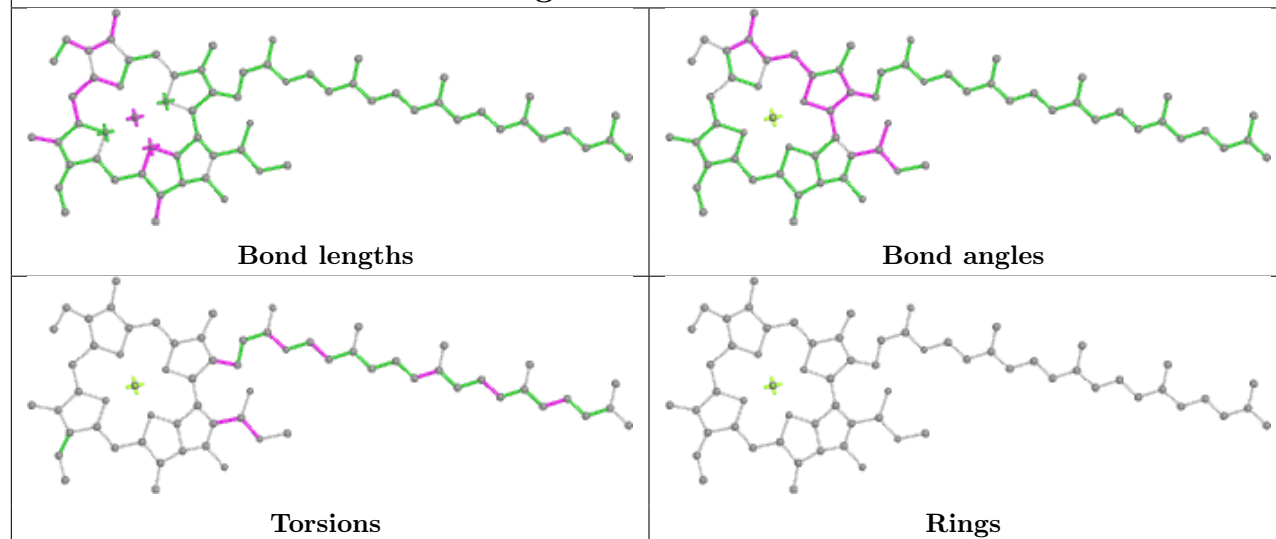
Ligand CLA 3 604



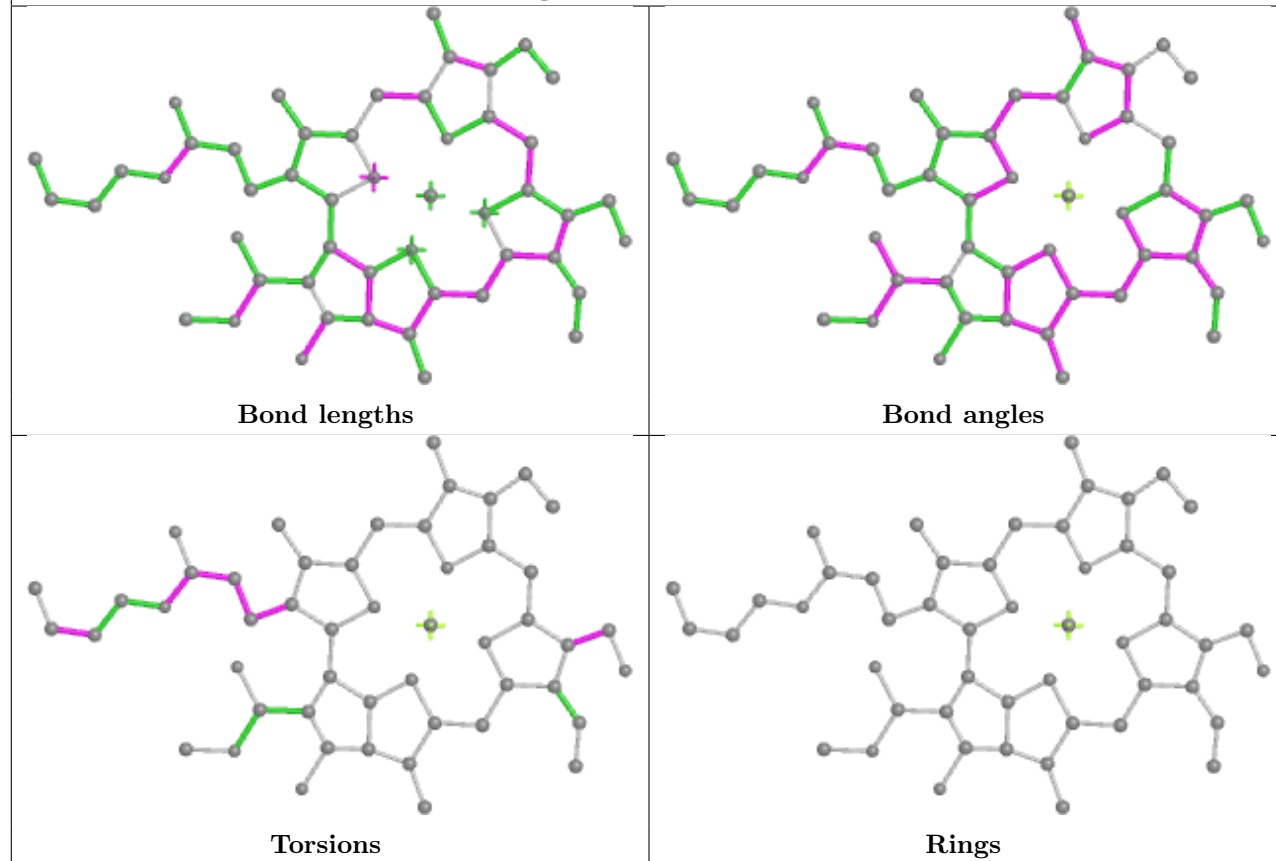
Ligand CLA n 604

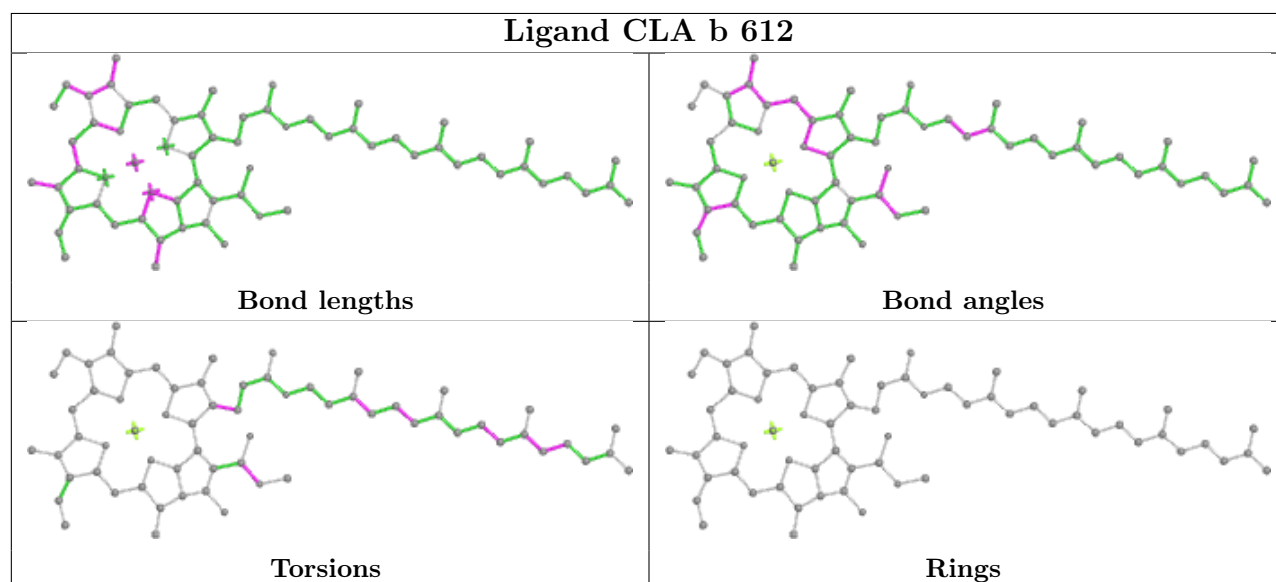
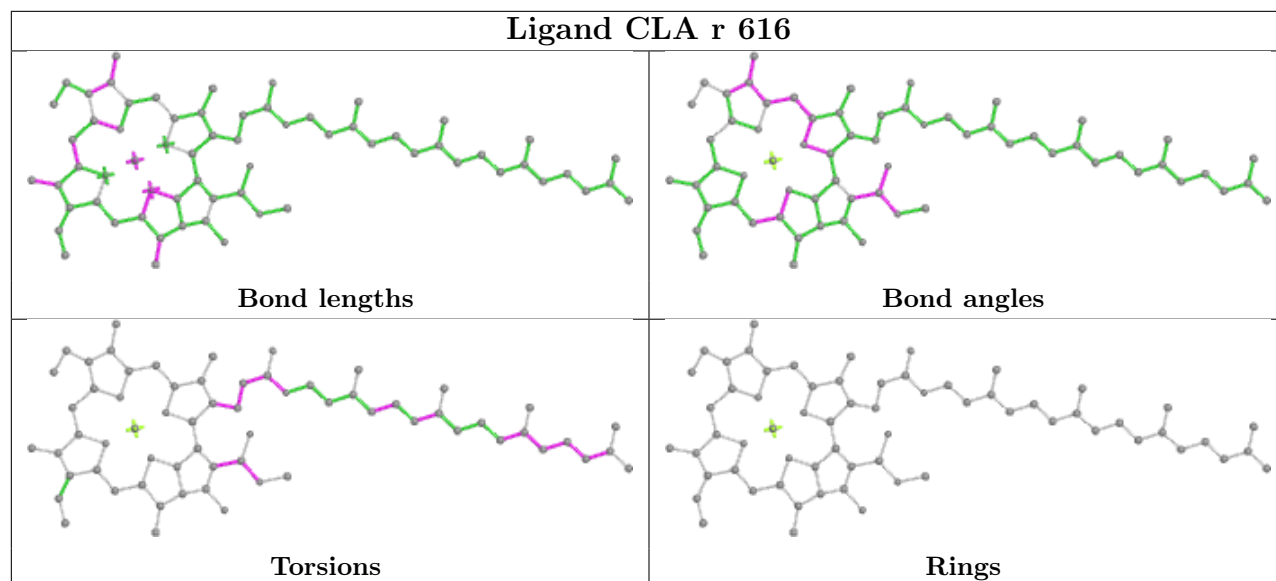
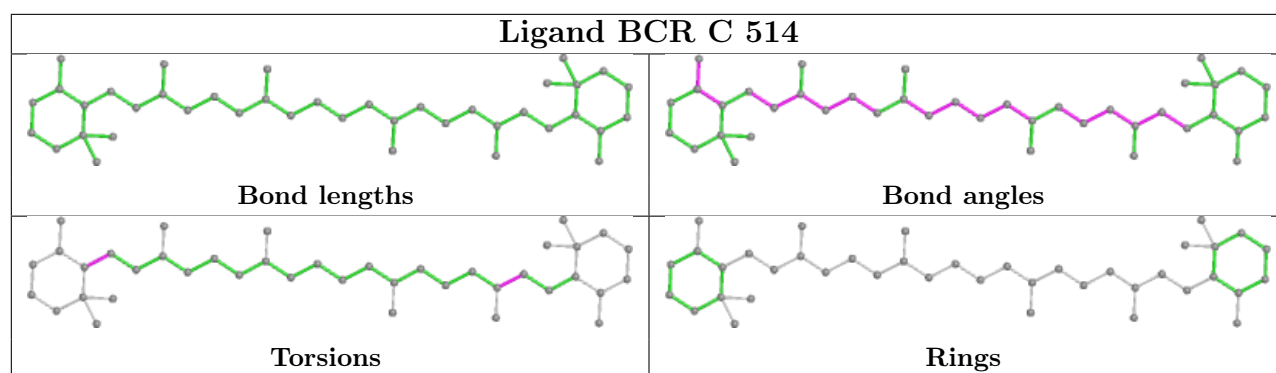


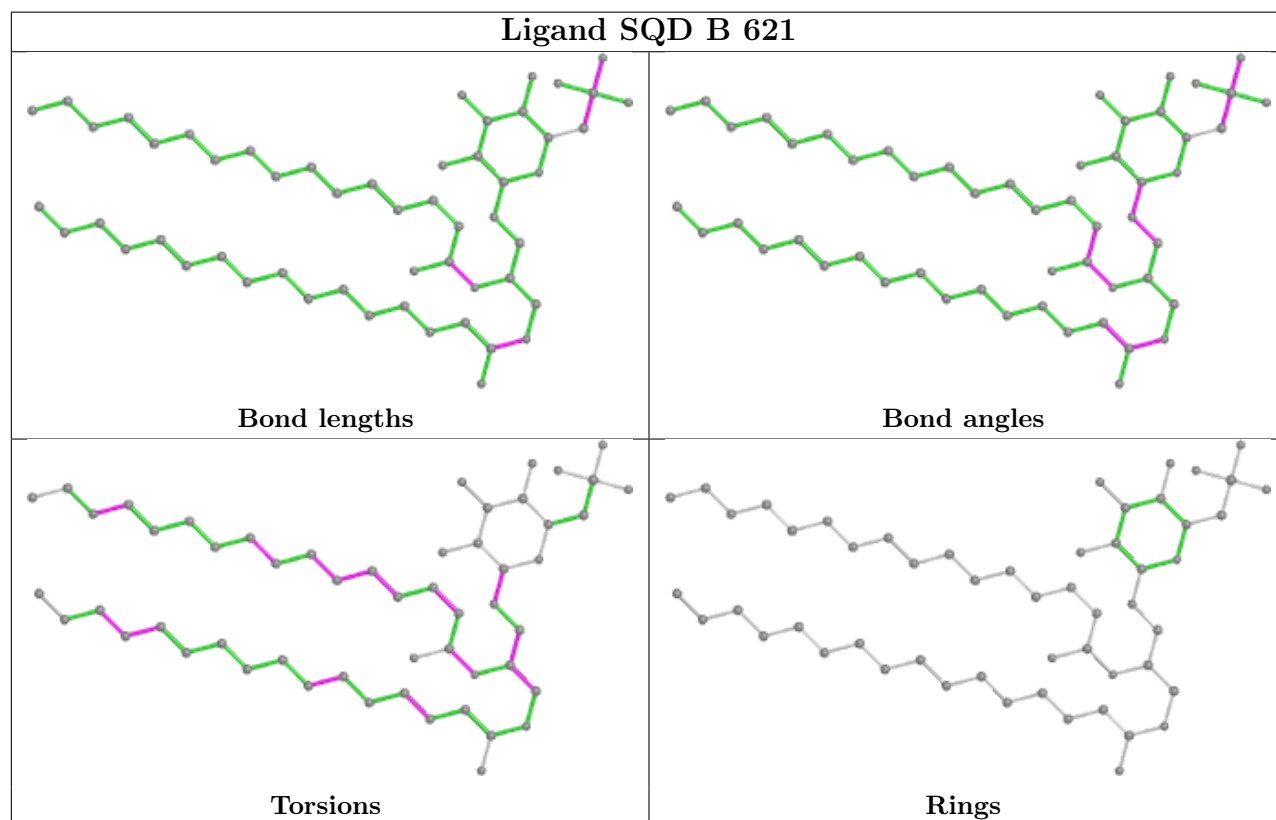
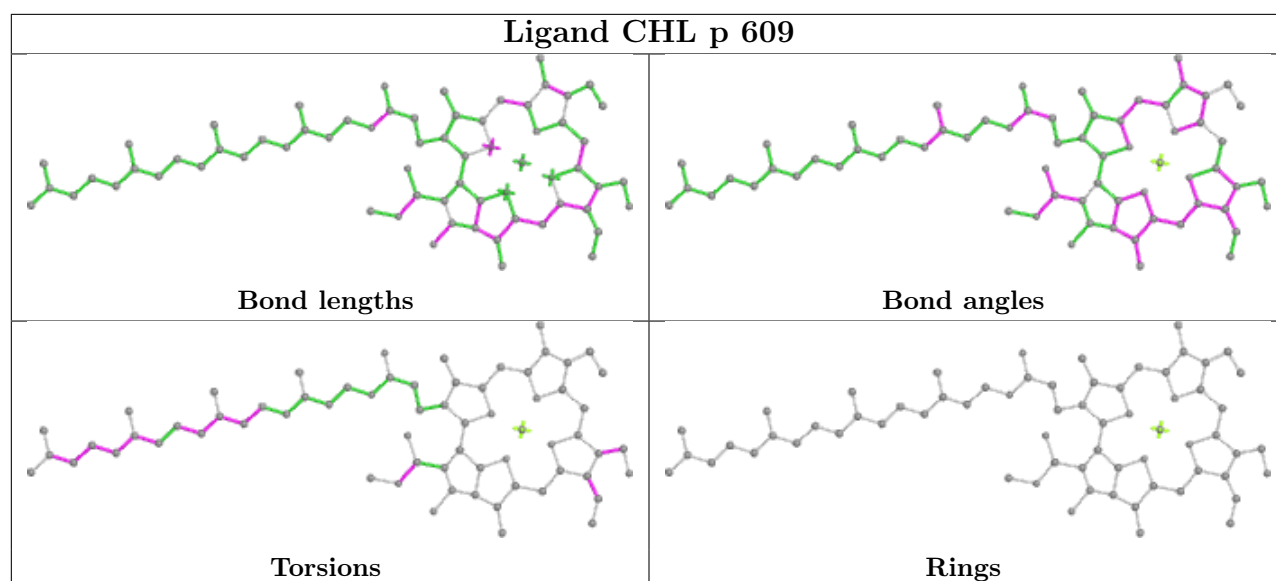
Ligand CLA b 603

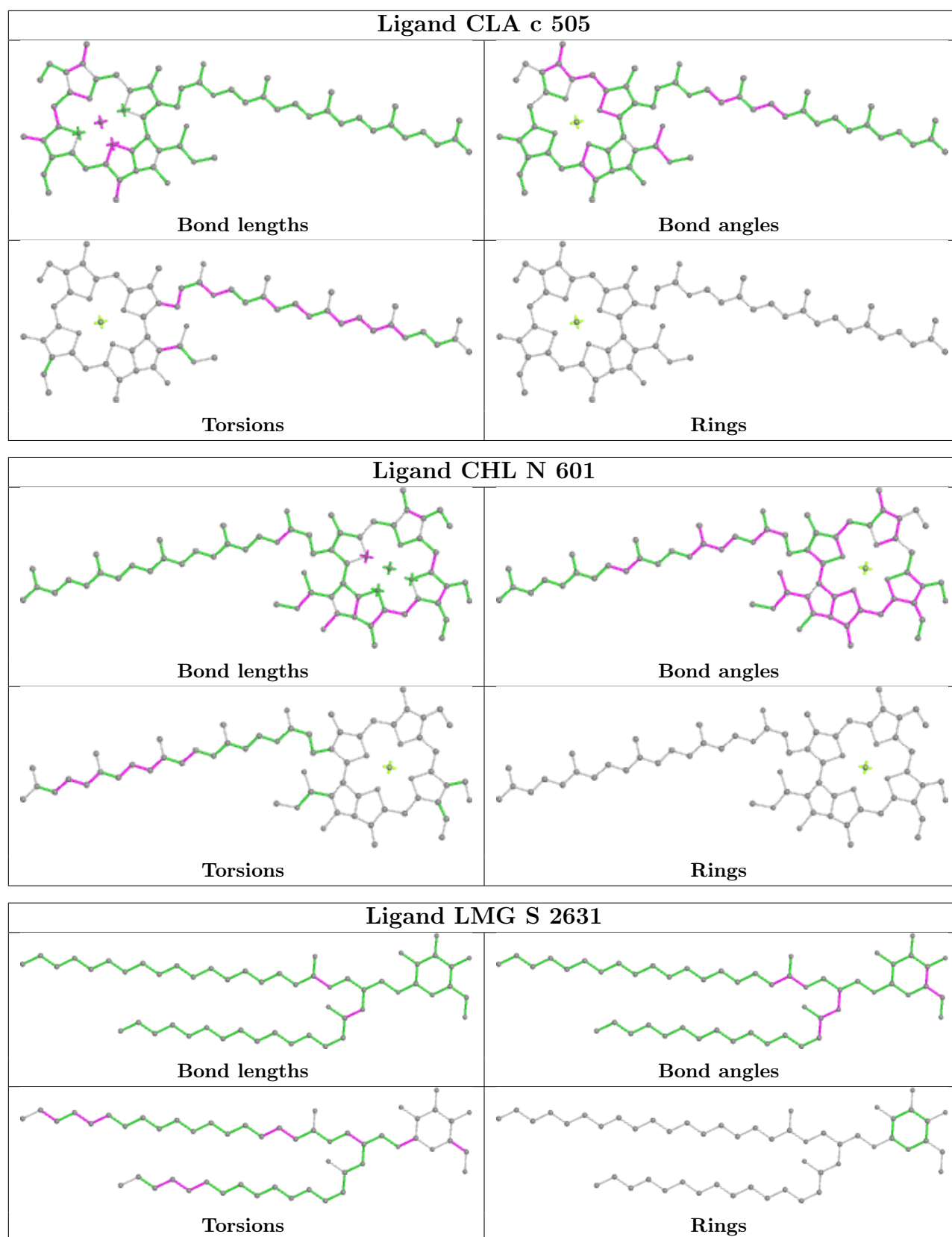


Ligand CHL 2 607

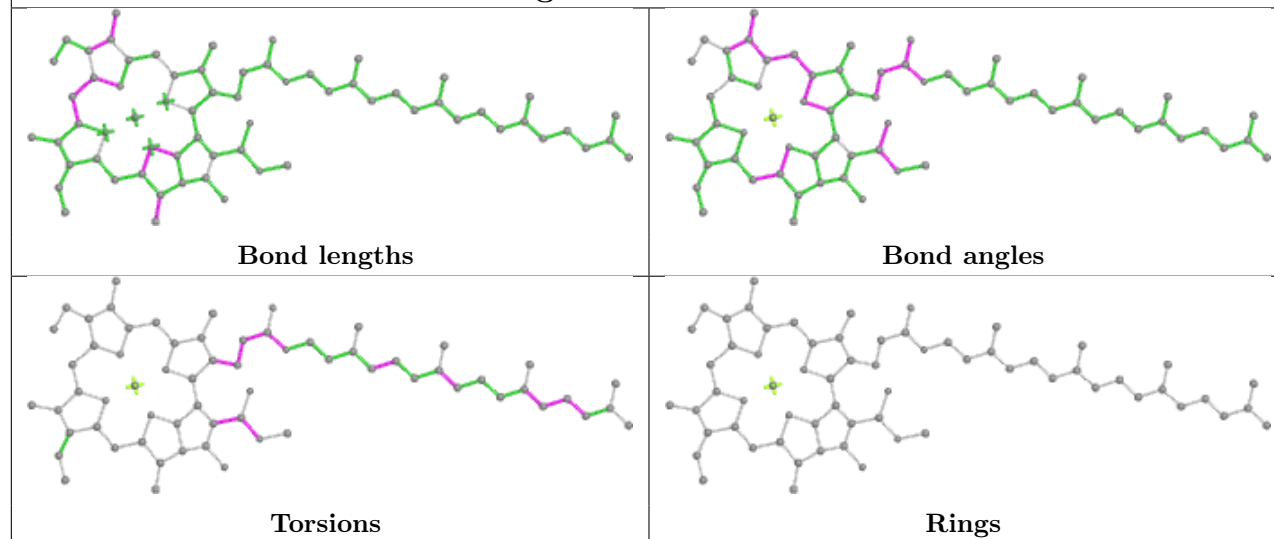




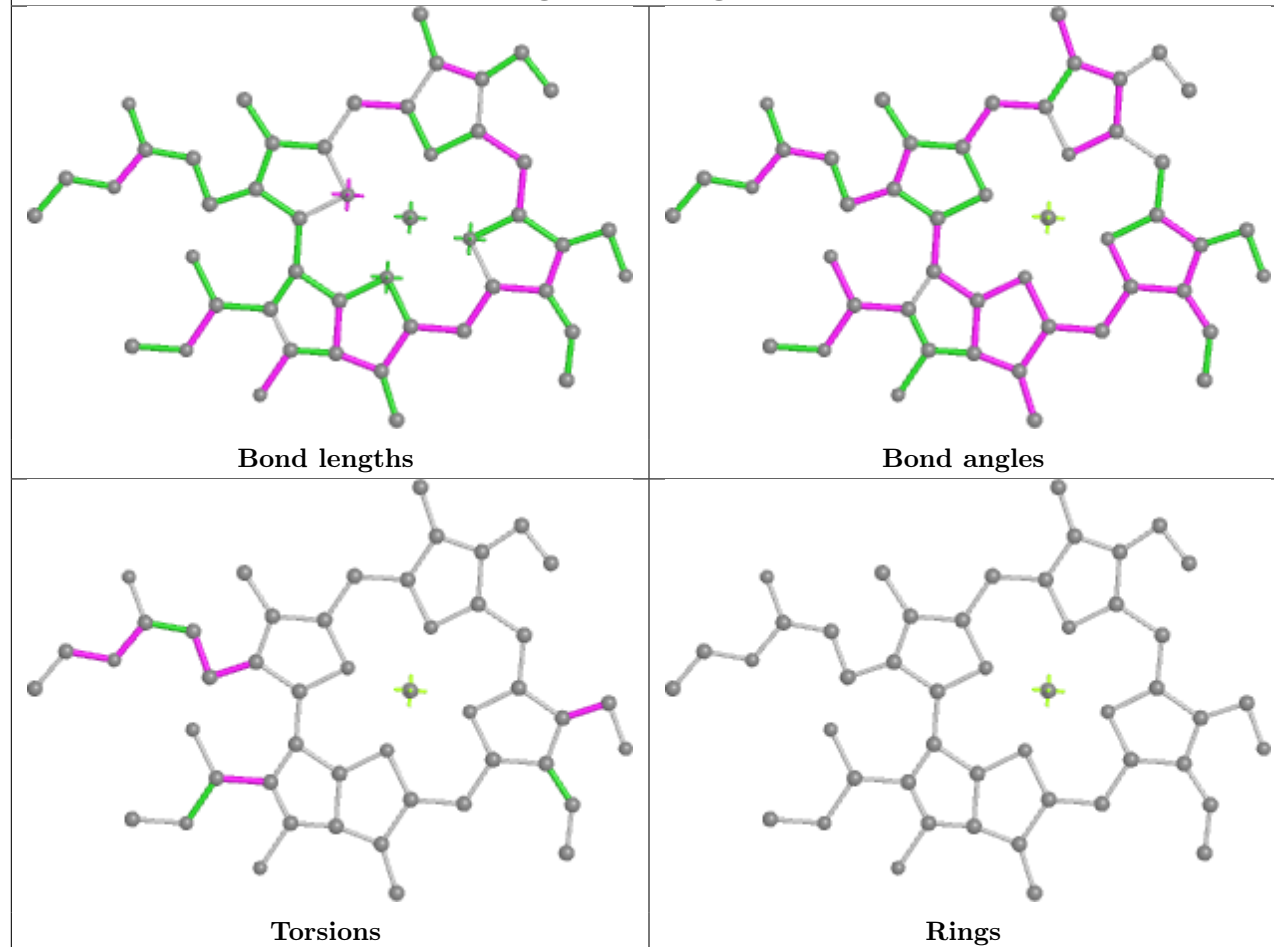




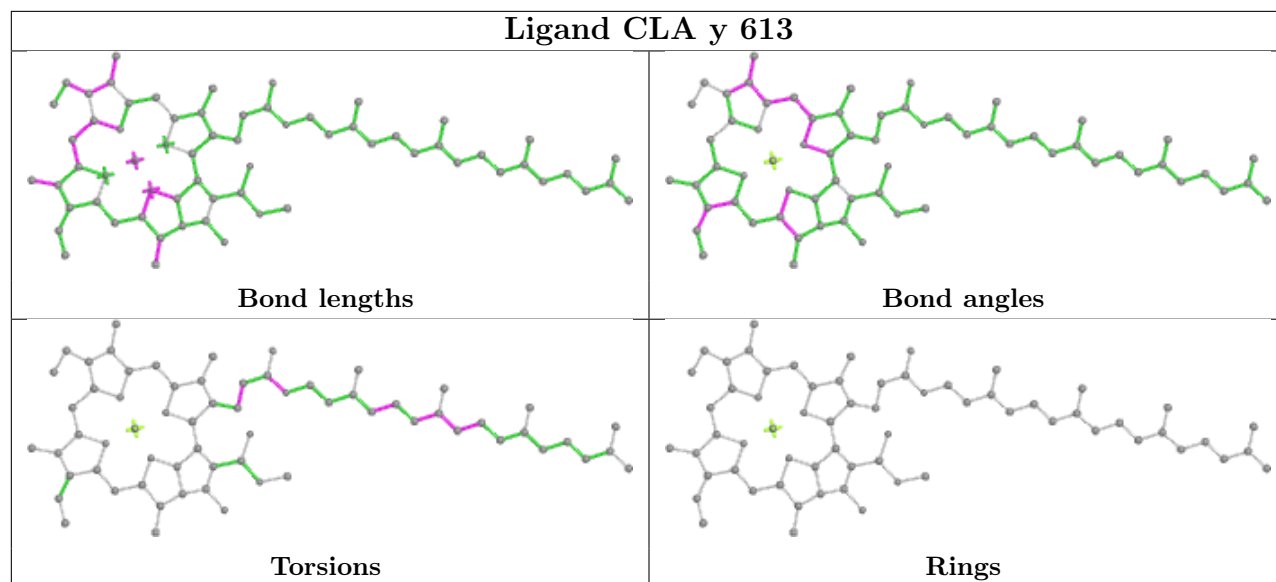
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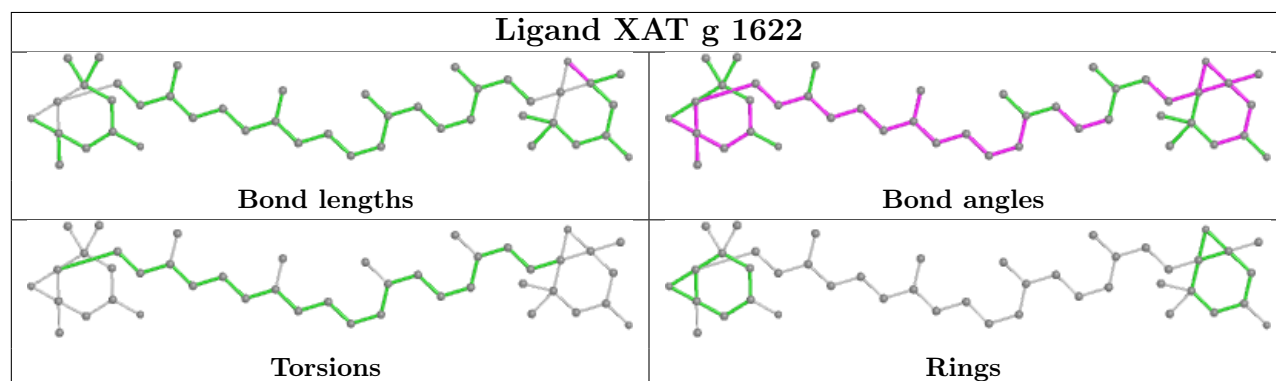
Ligand CHL g 605



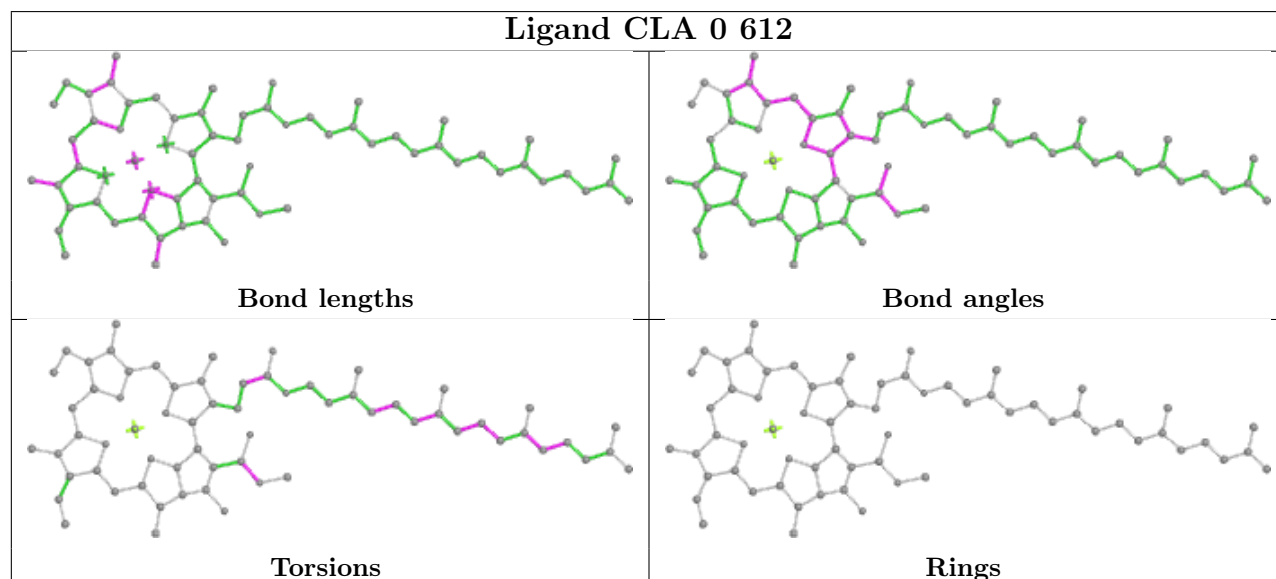
Ligand CLA y 613

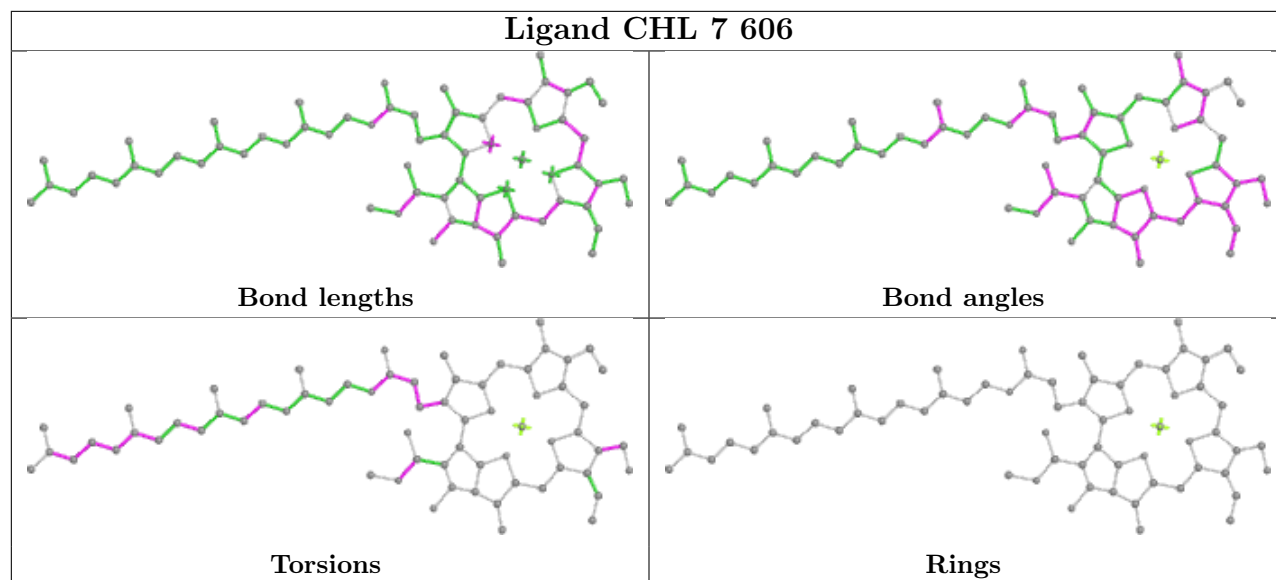
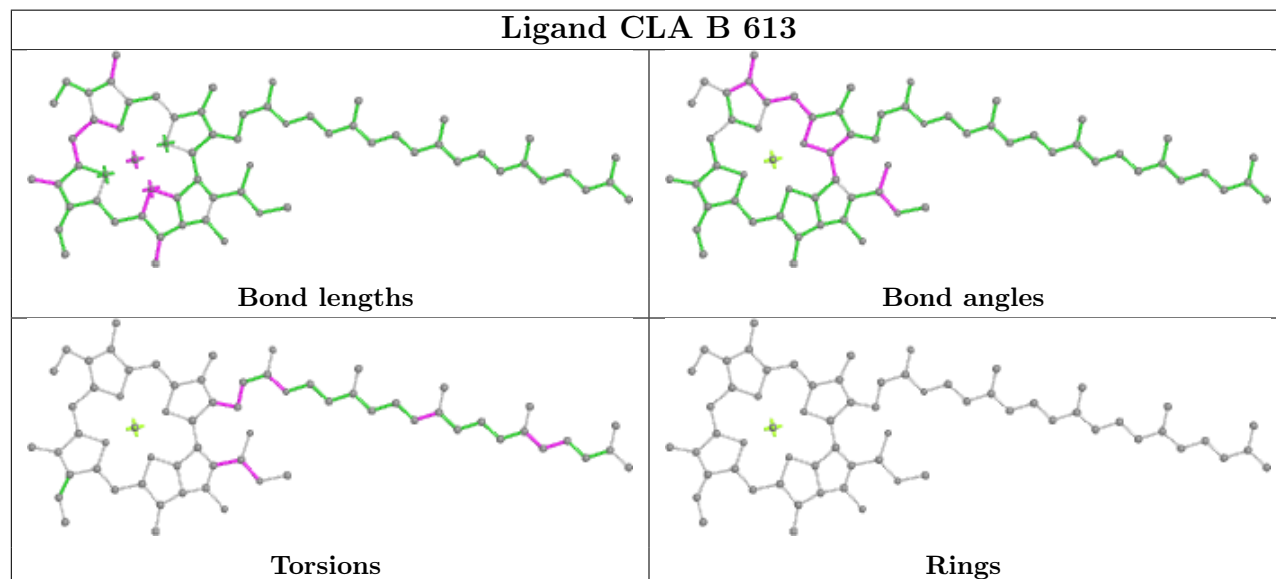
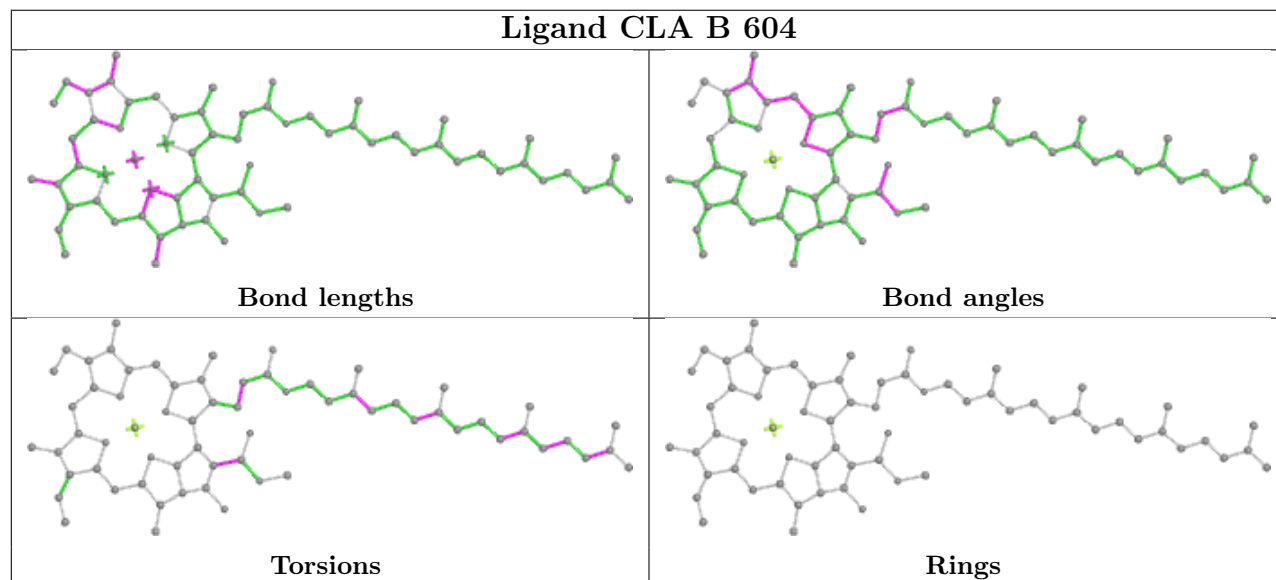


Ligand XAT g 1622

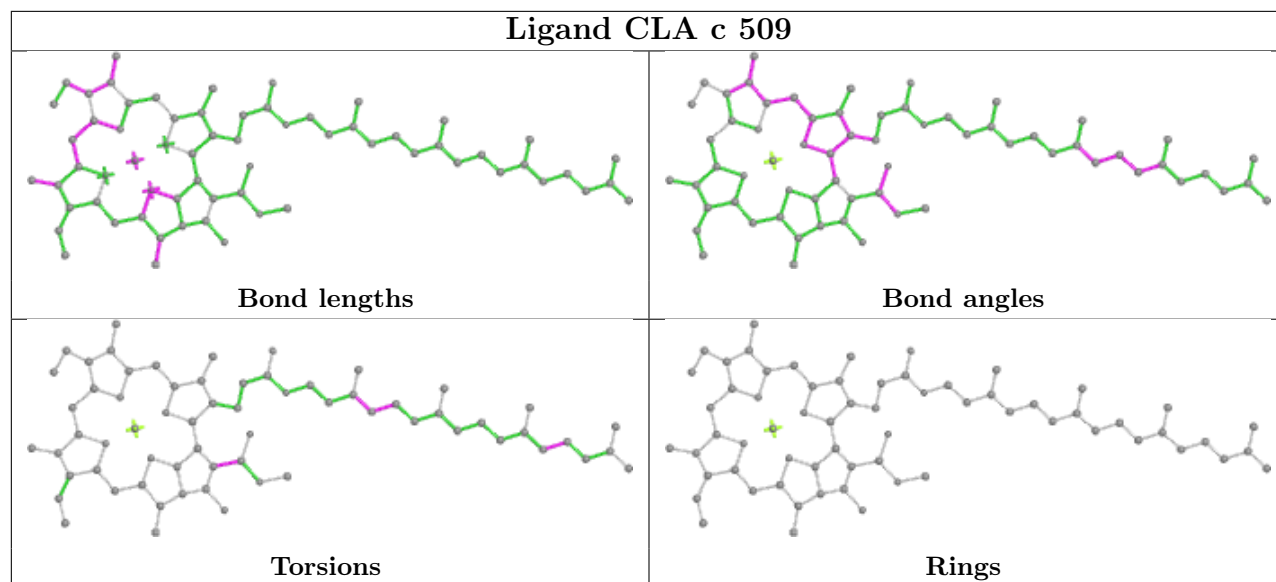


Ligand CLA 0 612

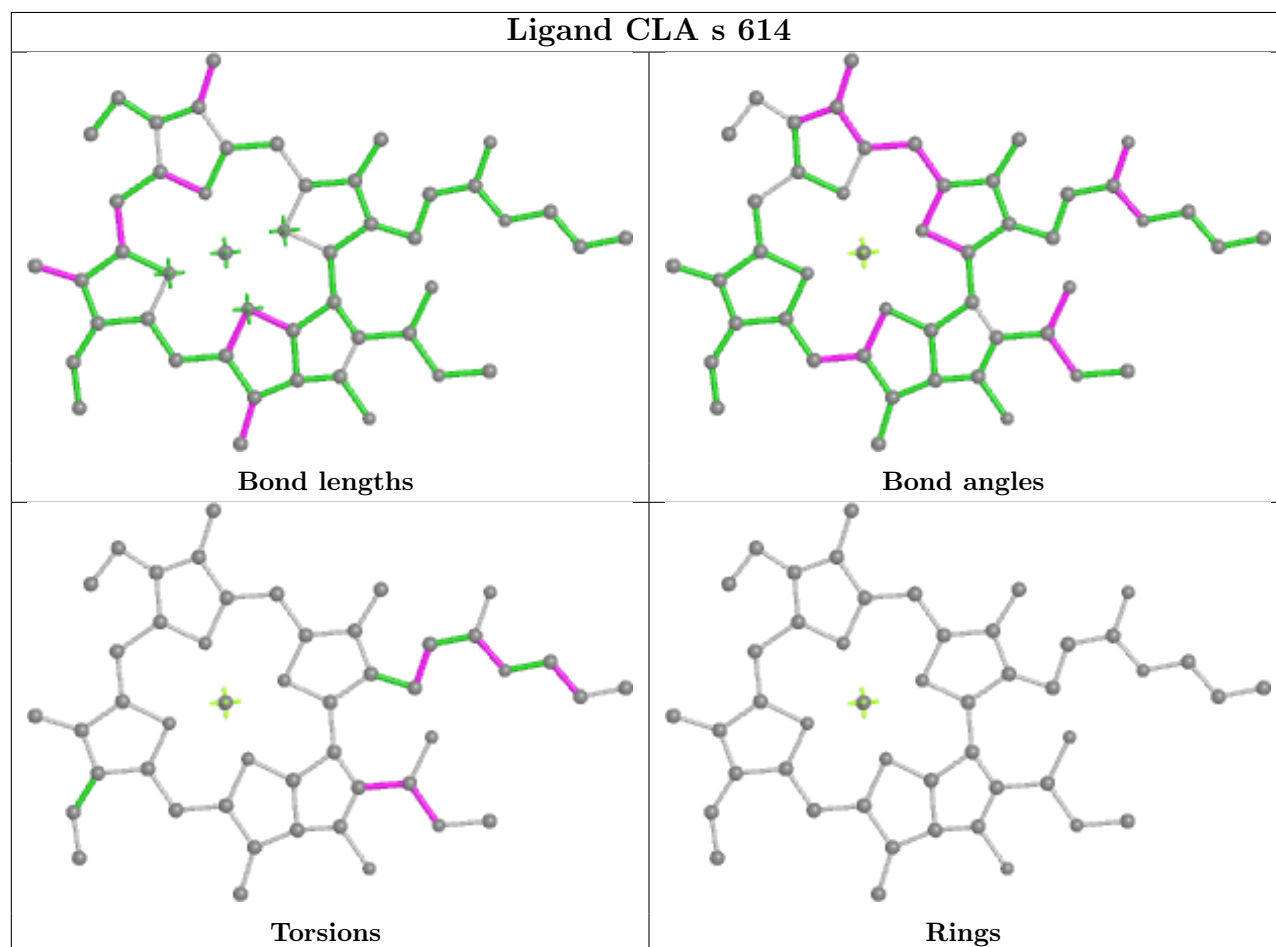


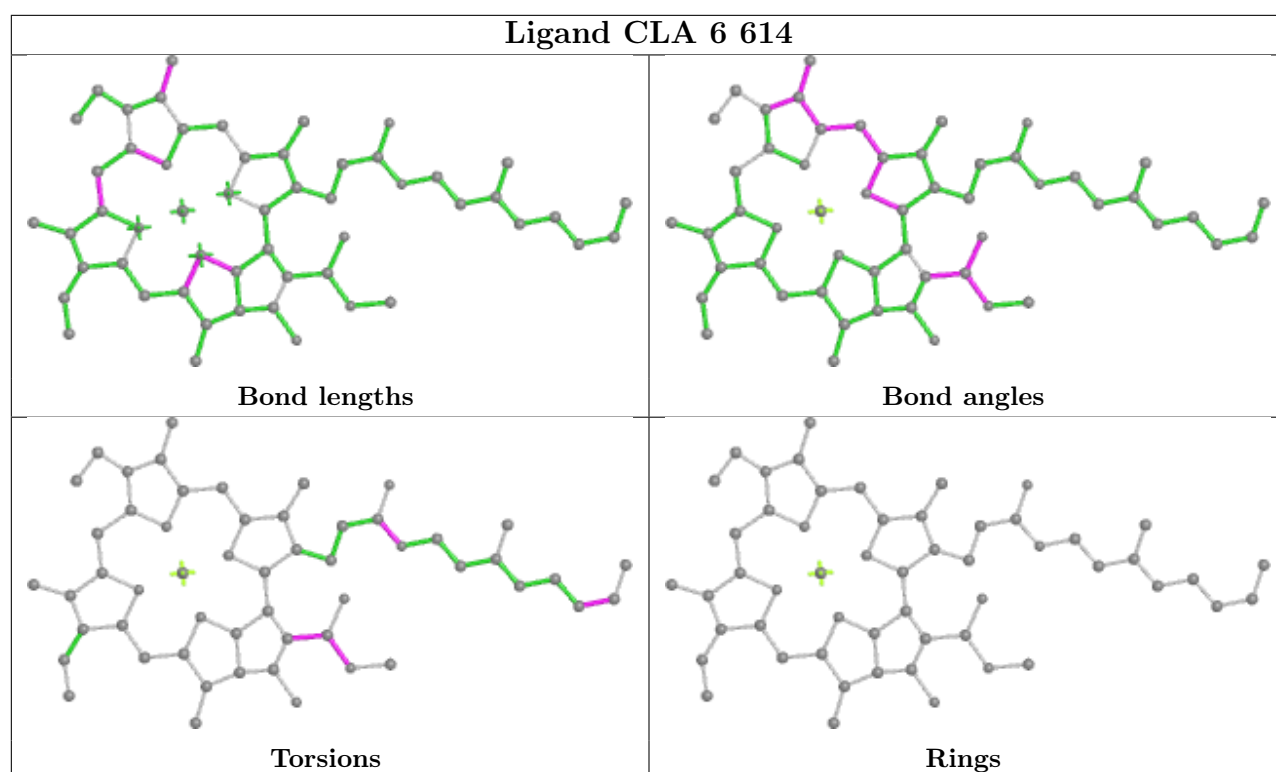
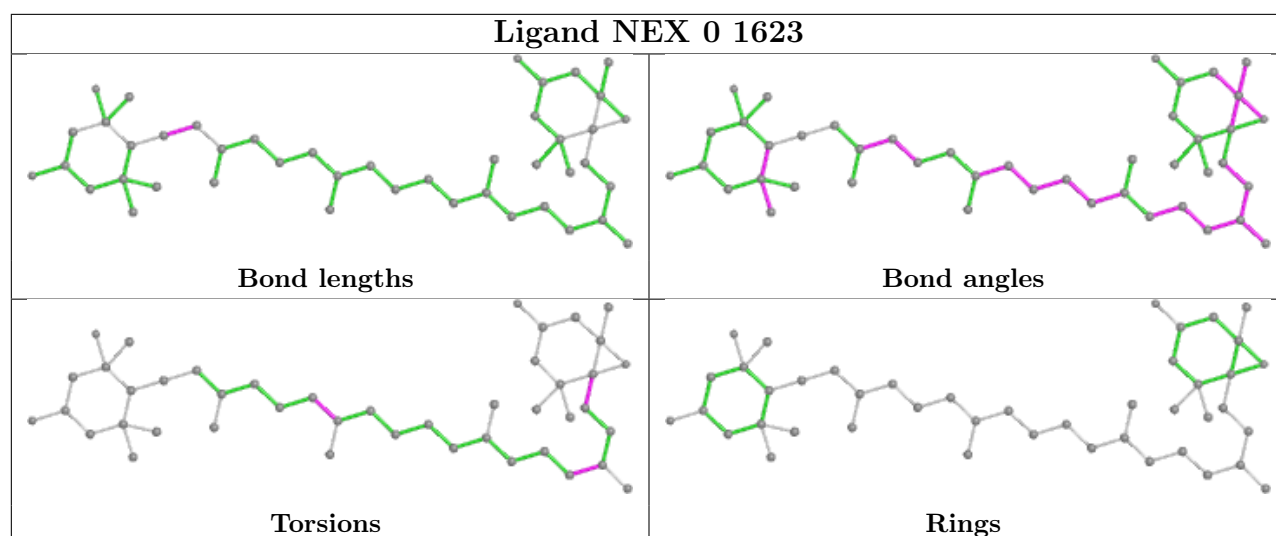
Ligand CHL 7 606**Ligand CLA B 613****Ligand CLA B 604**

Ligand CLA c 509

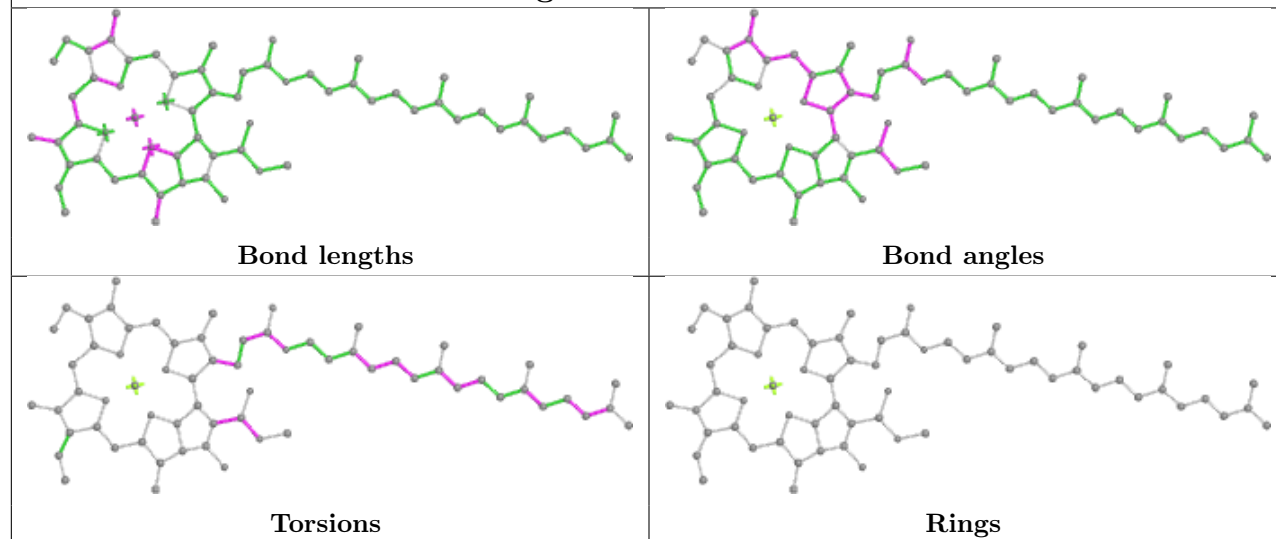


Ligand CLA s 614

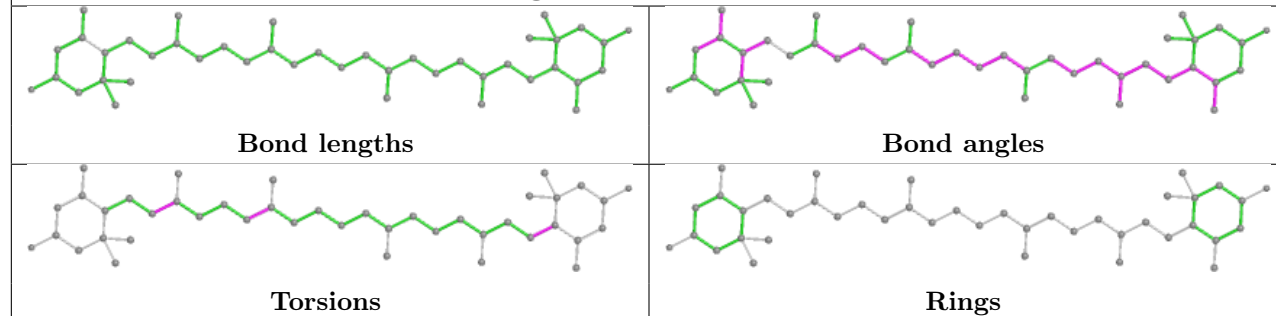




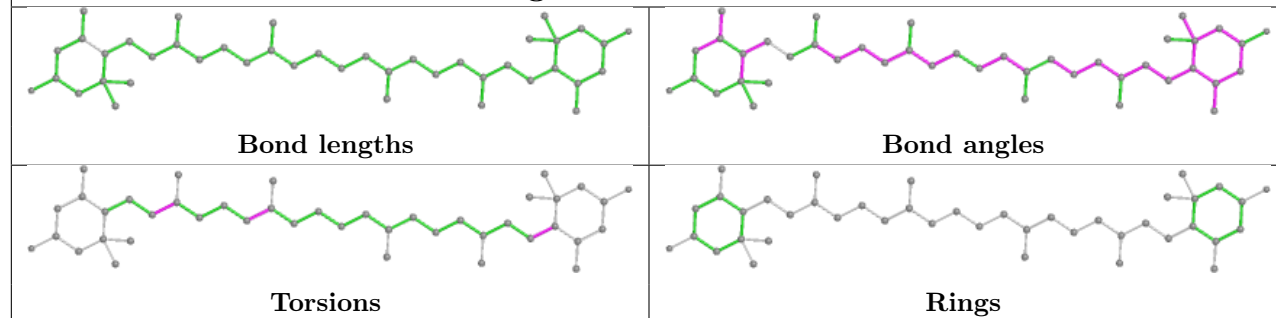
Ligand CLA 9 603



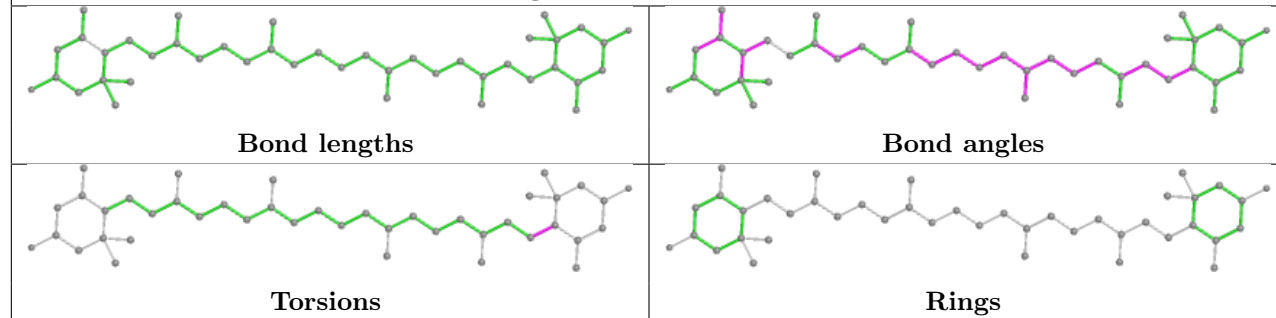
Ligand LUT 3 1620

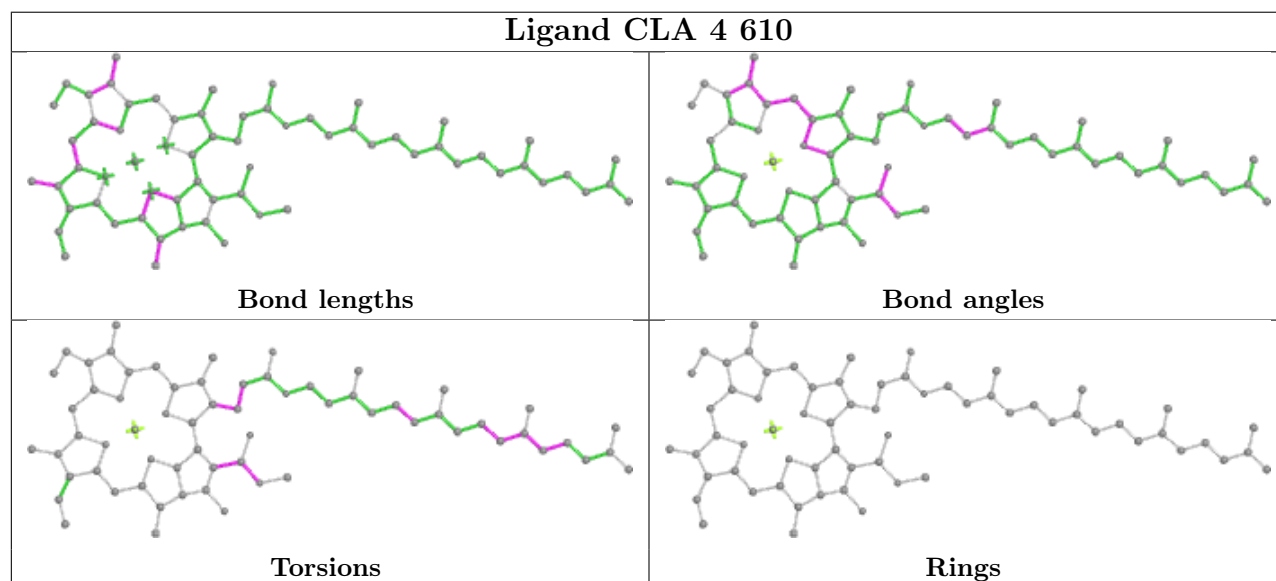
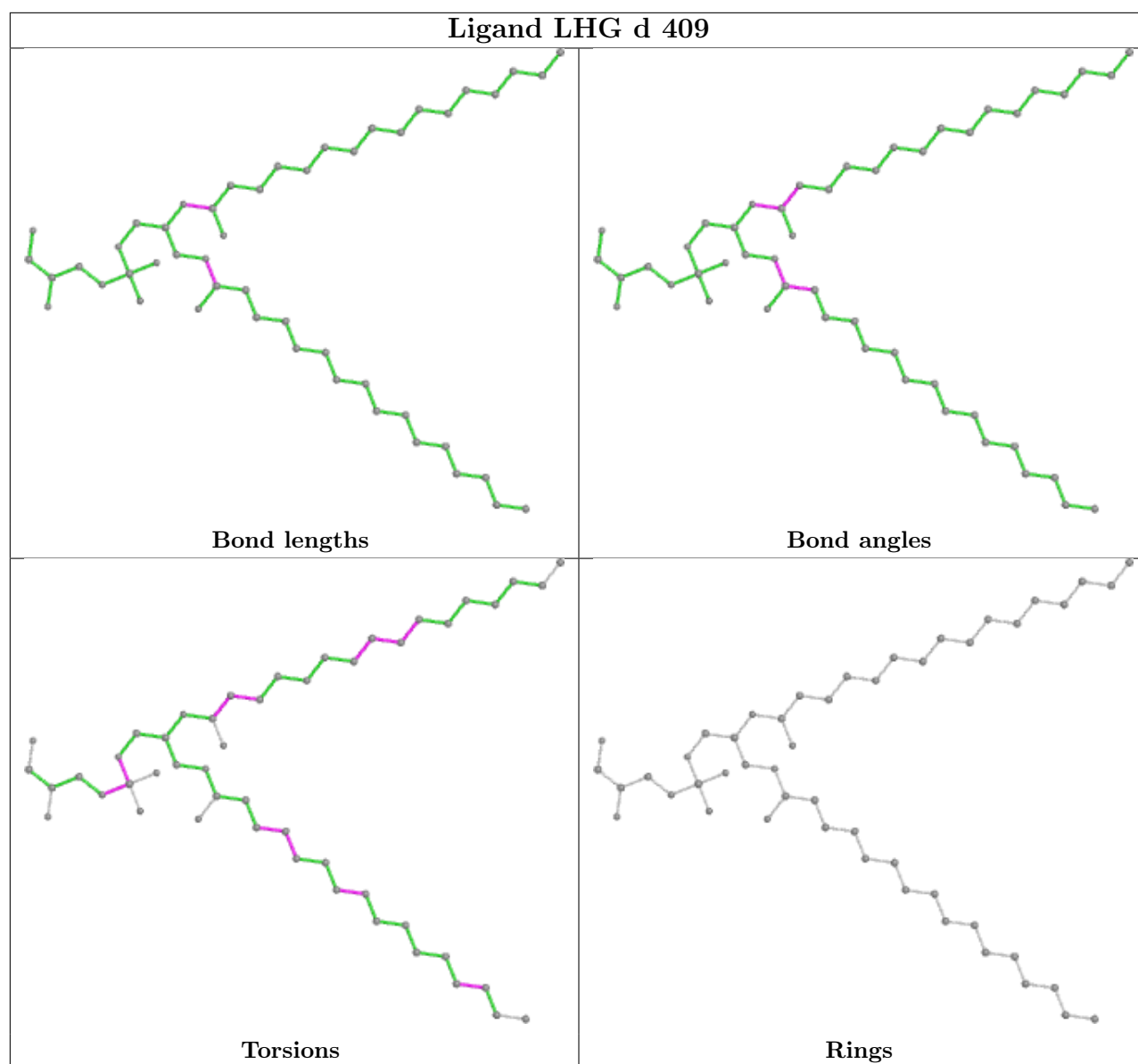


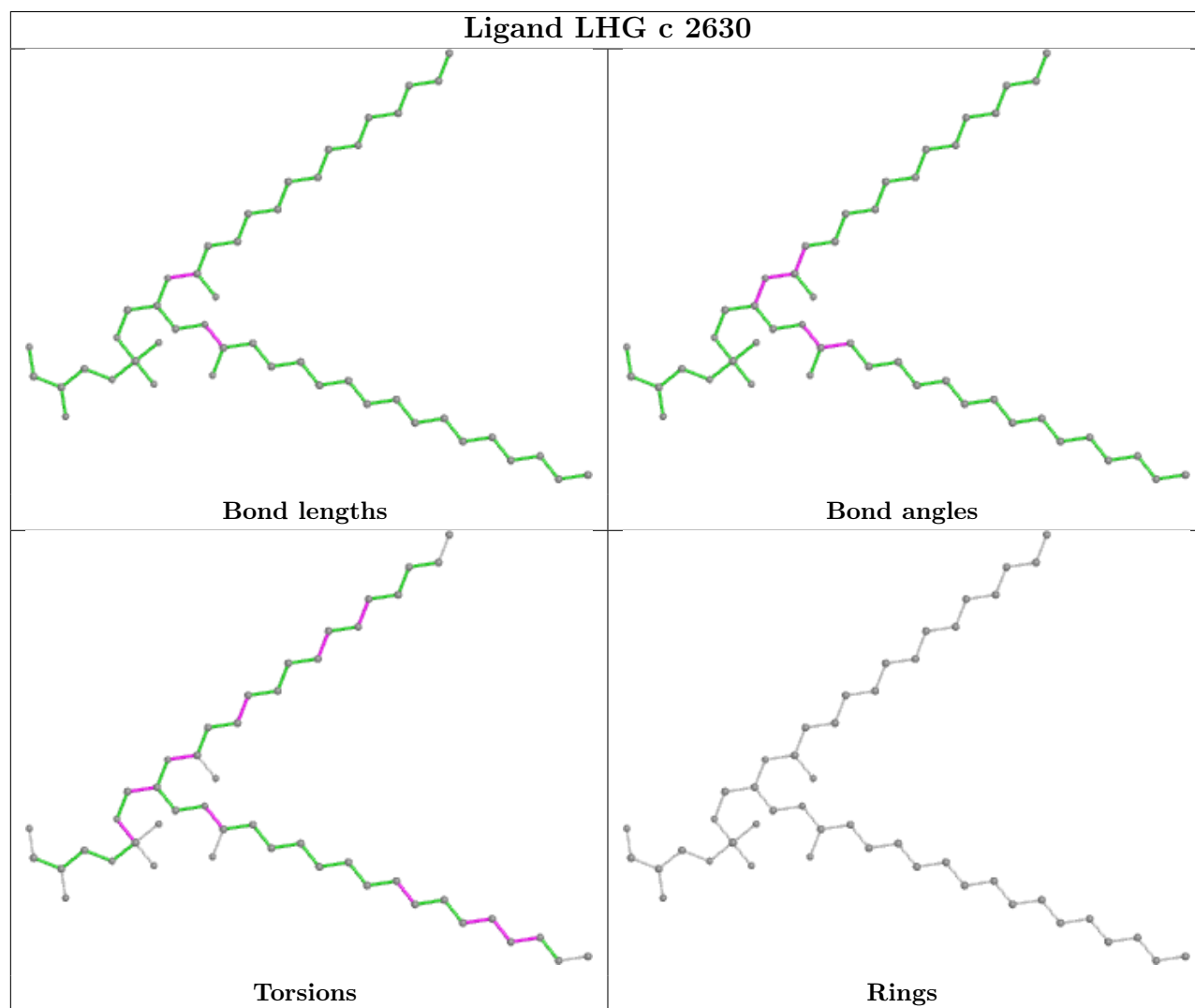
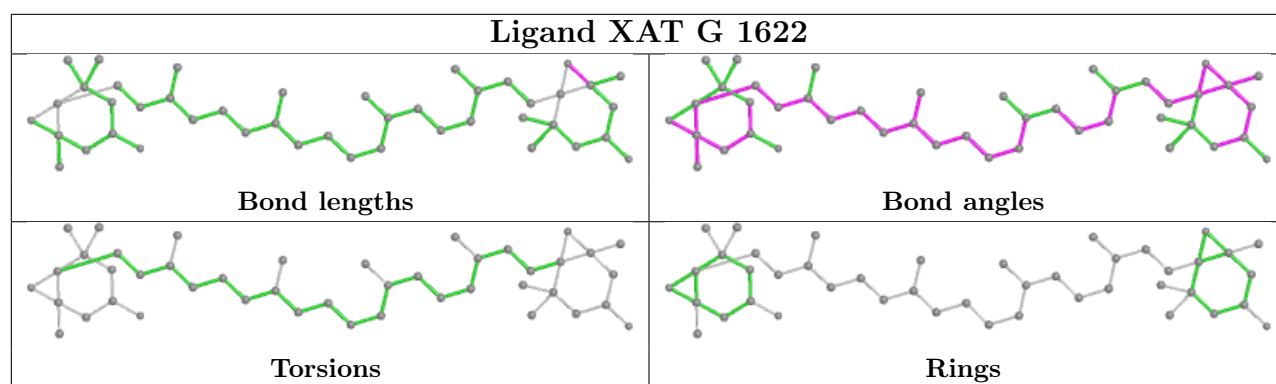
Ligand LUT 4 1620

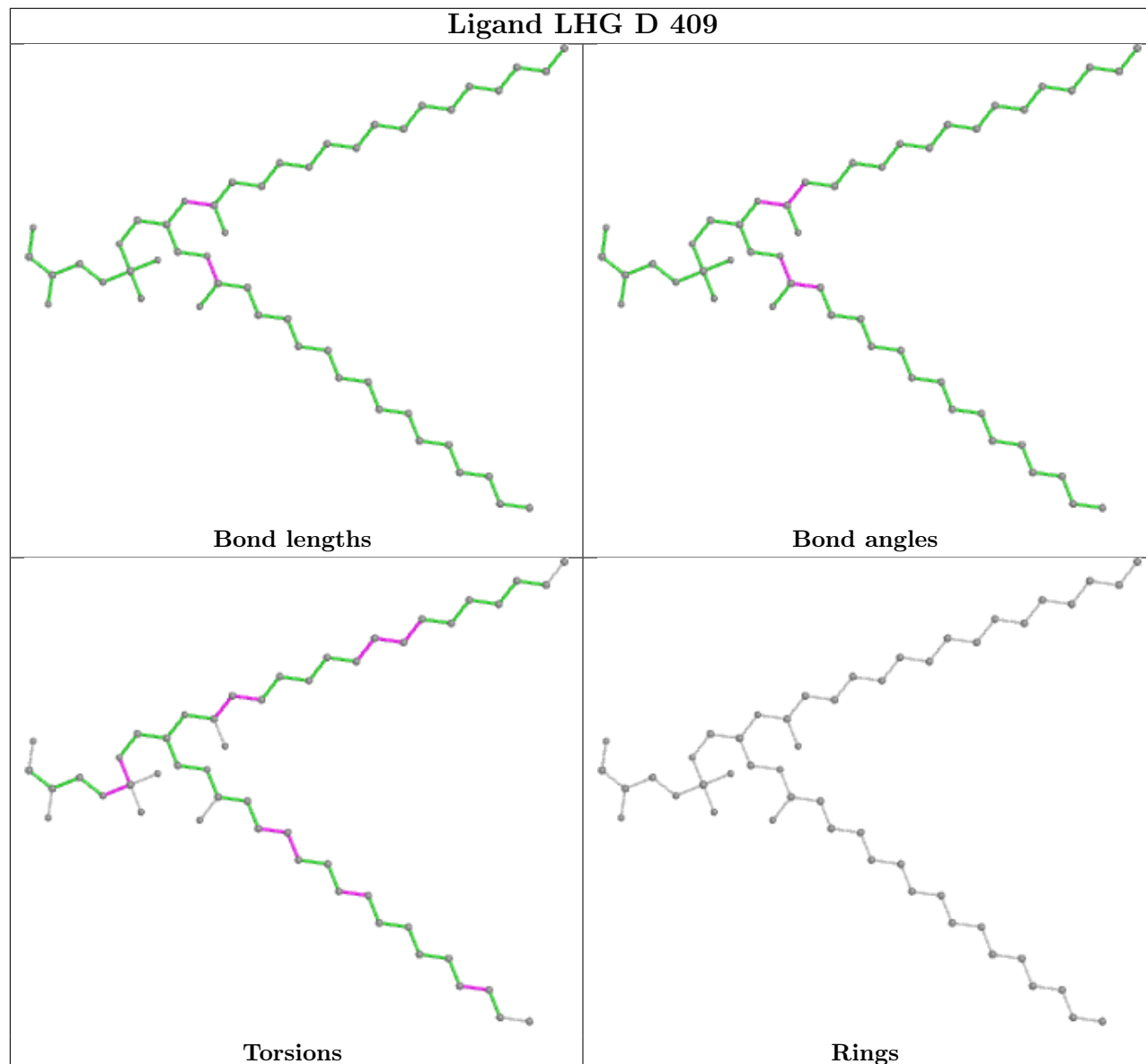
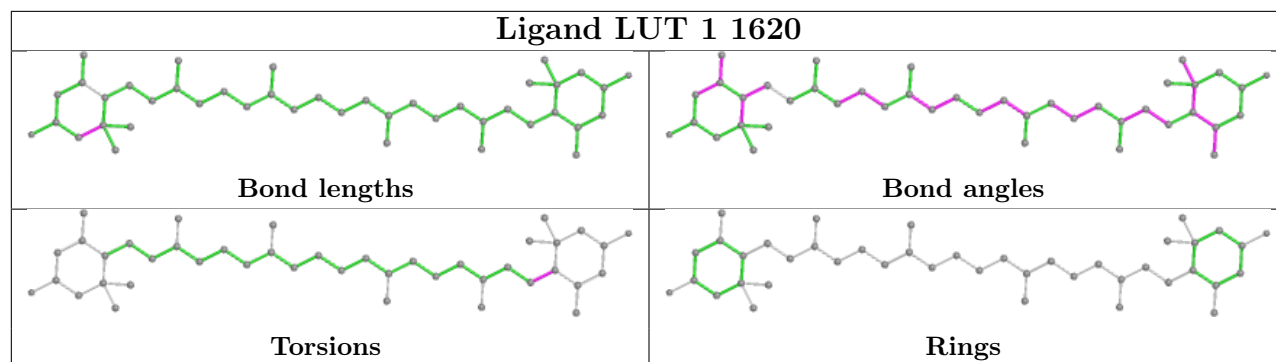


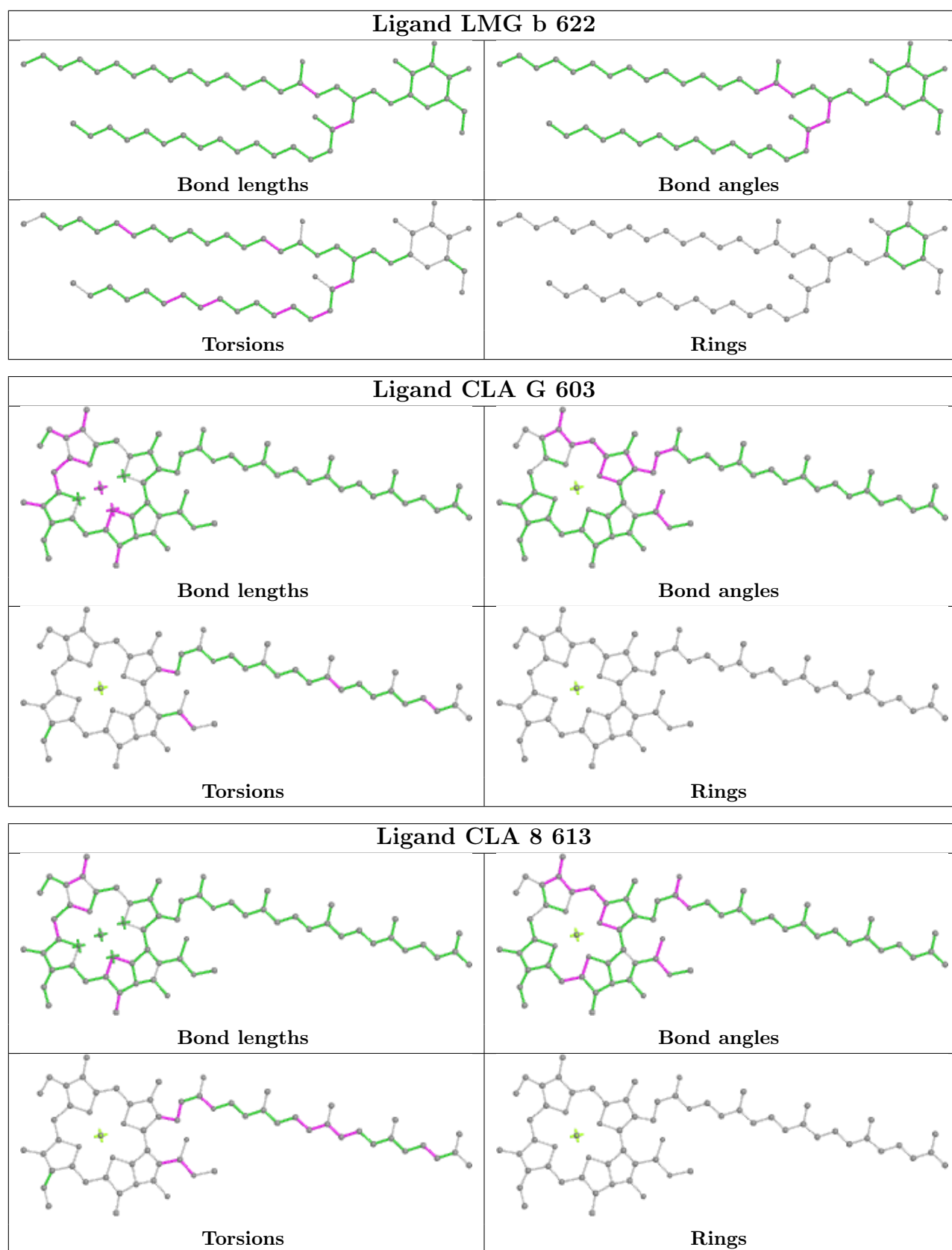
Ligand LUT n 1620

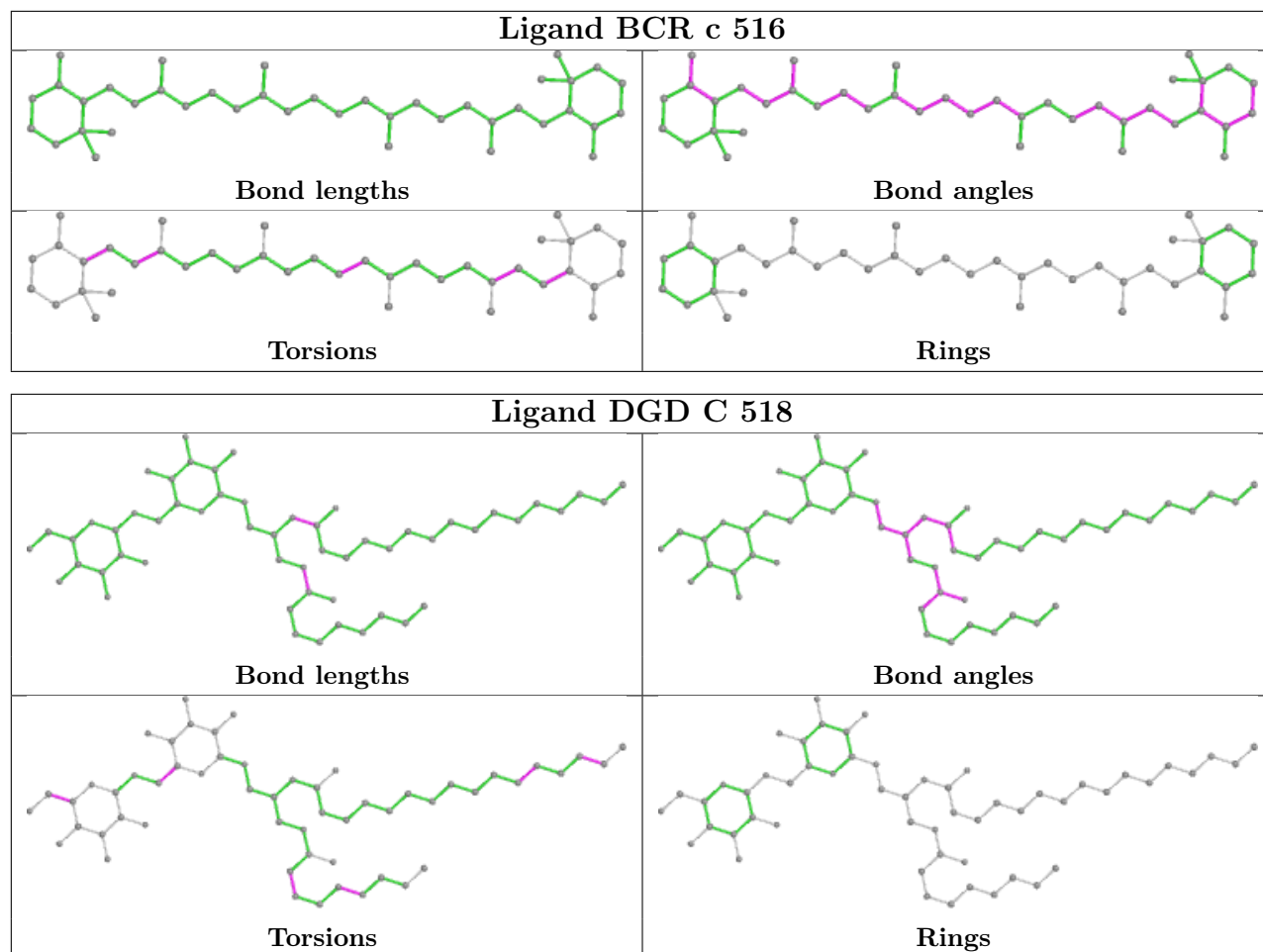




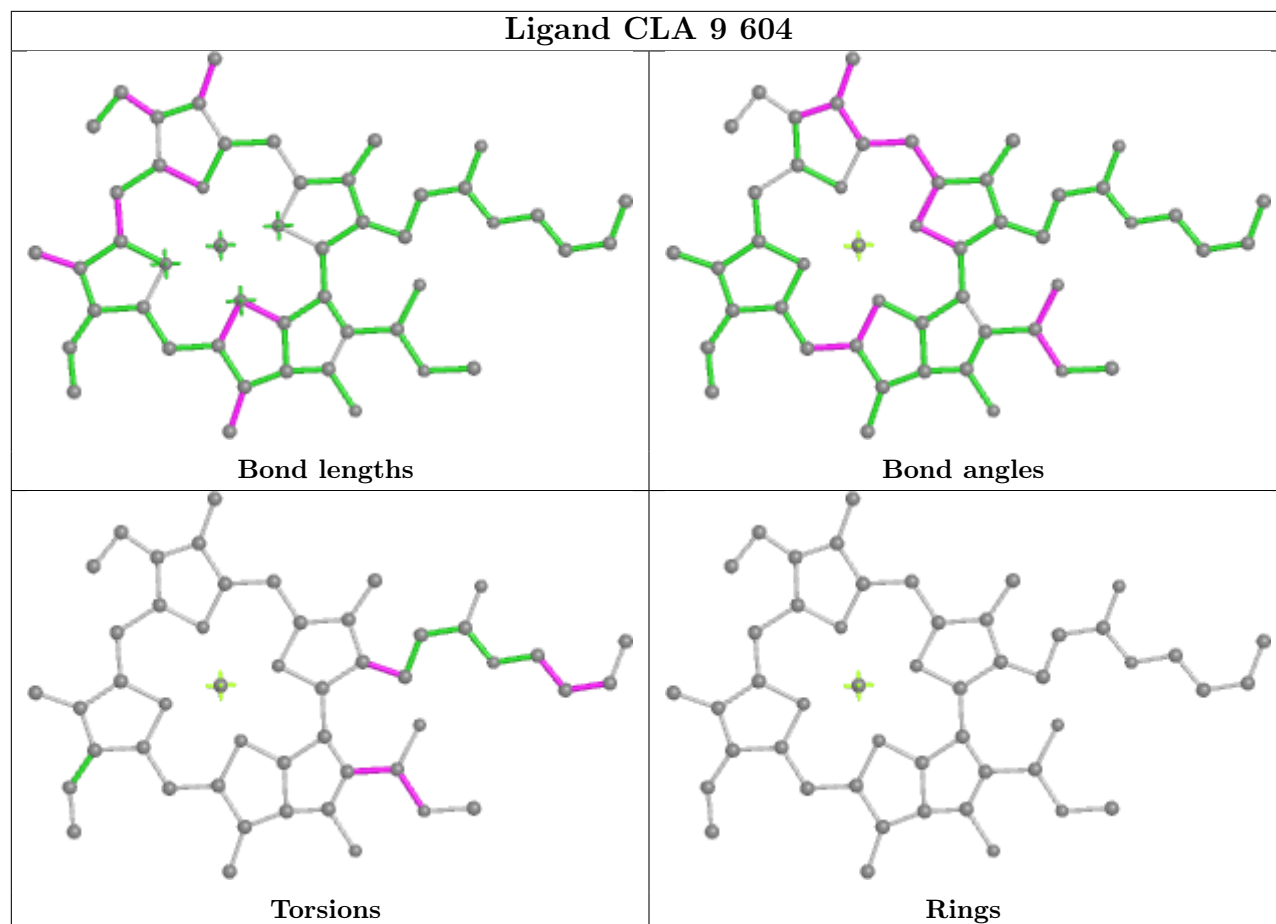


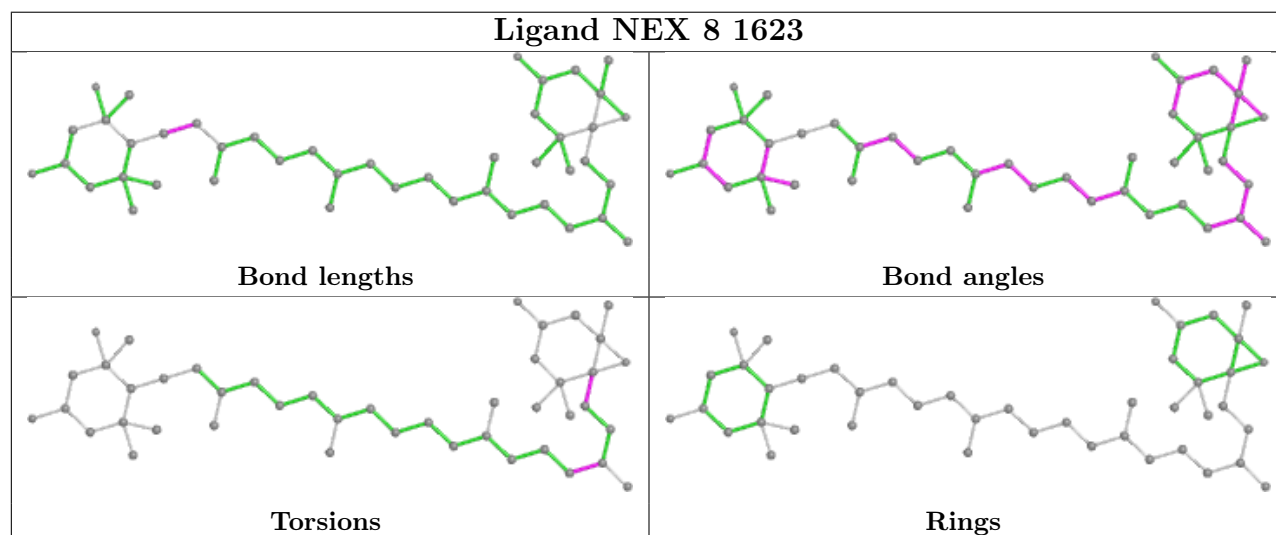
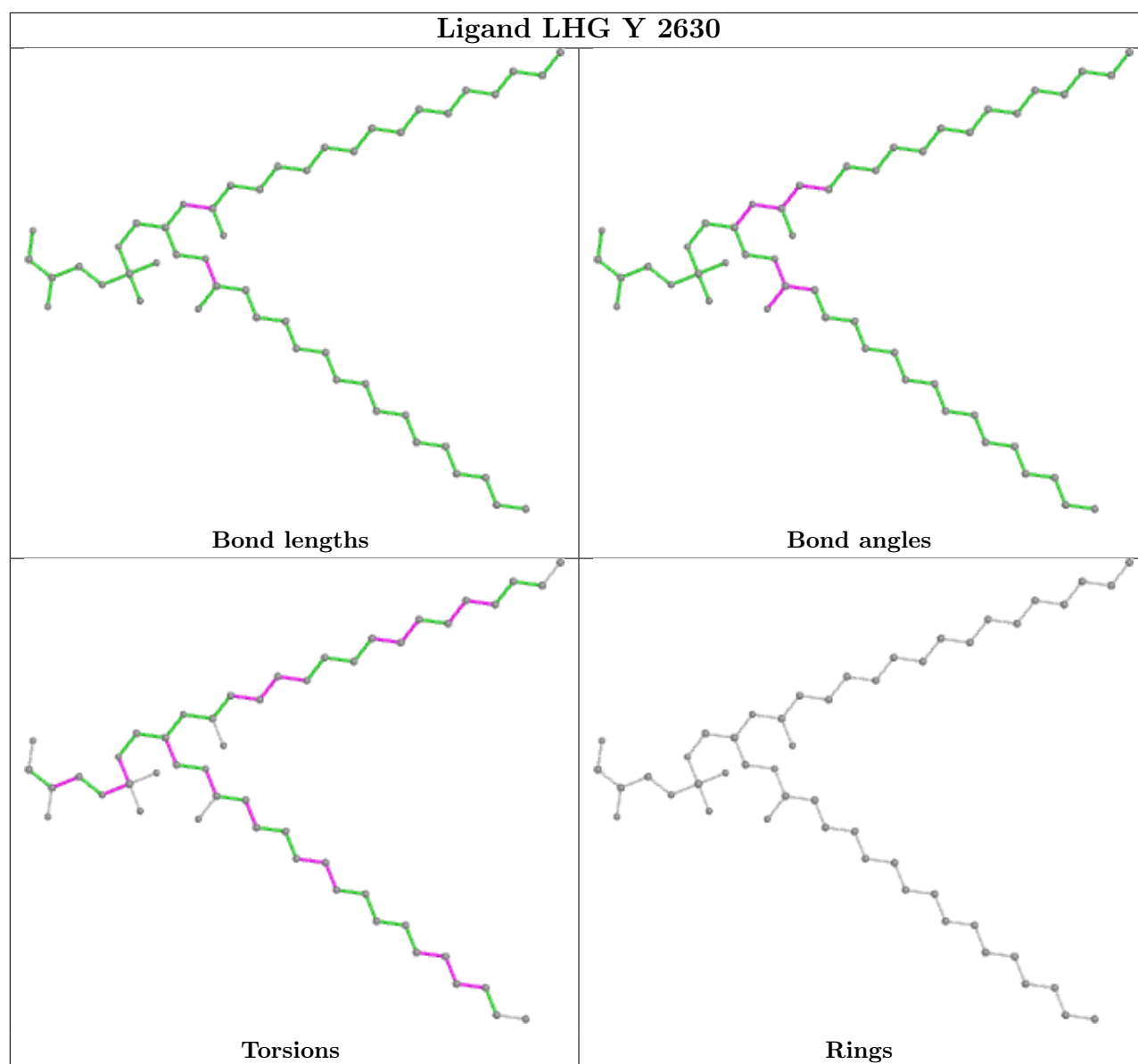


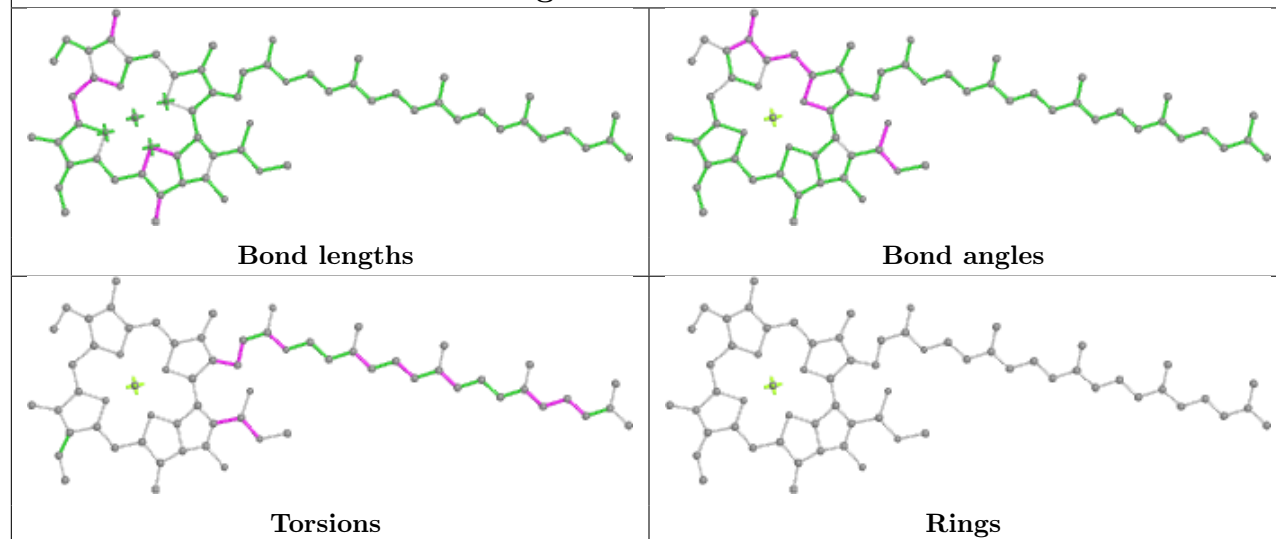
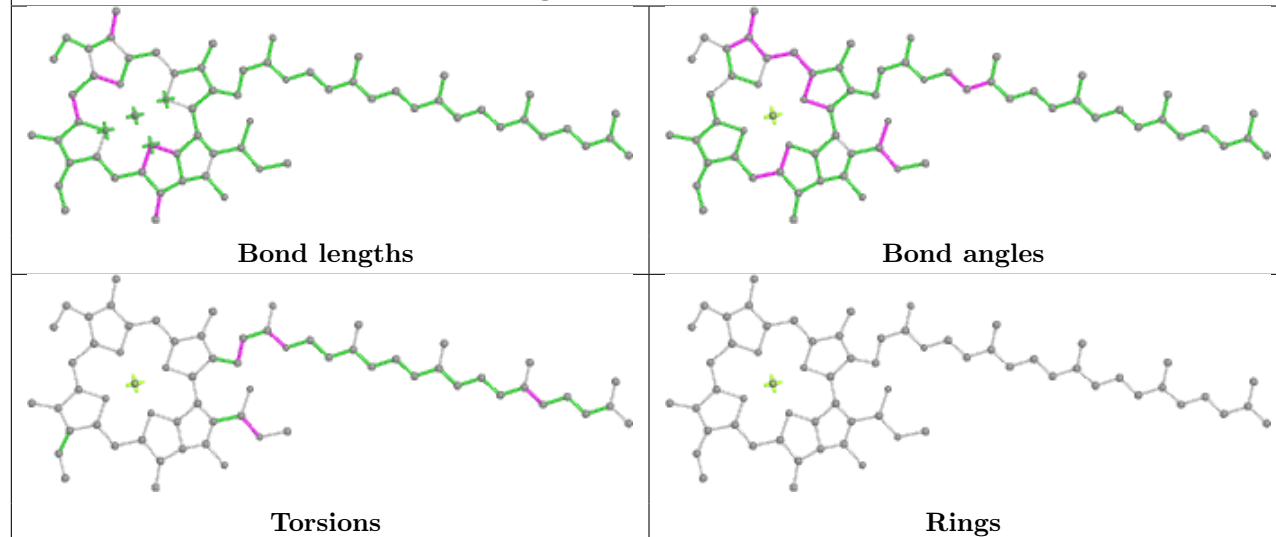


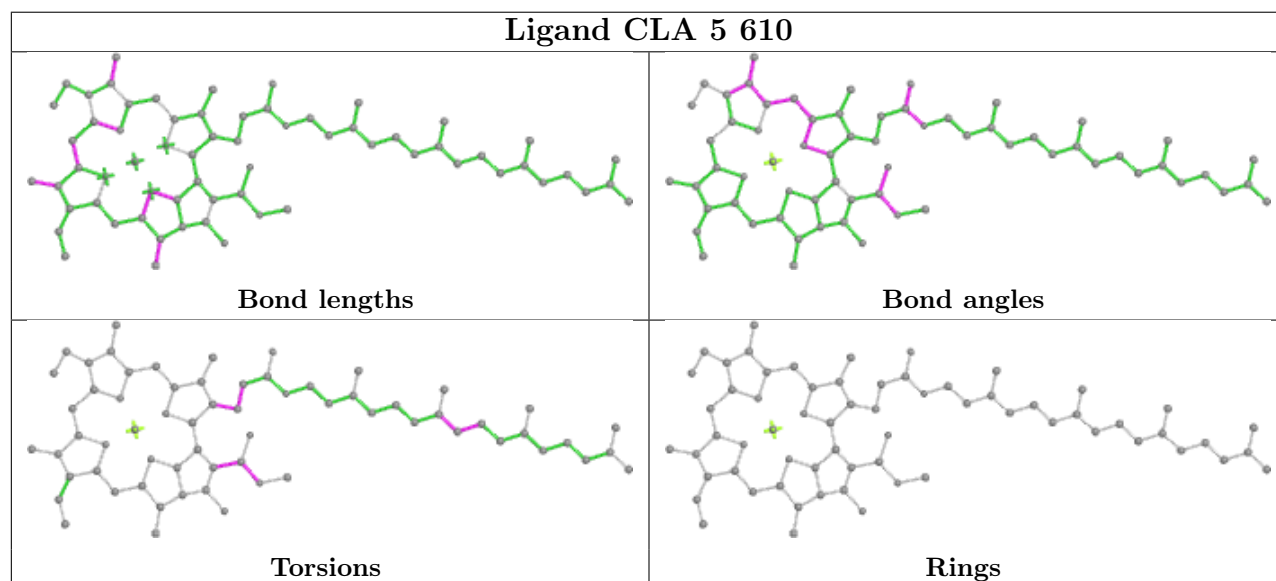
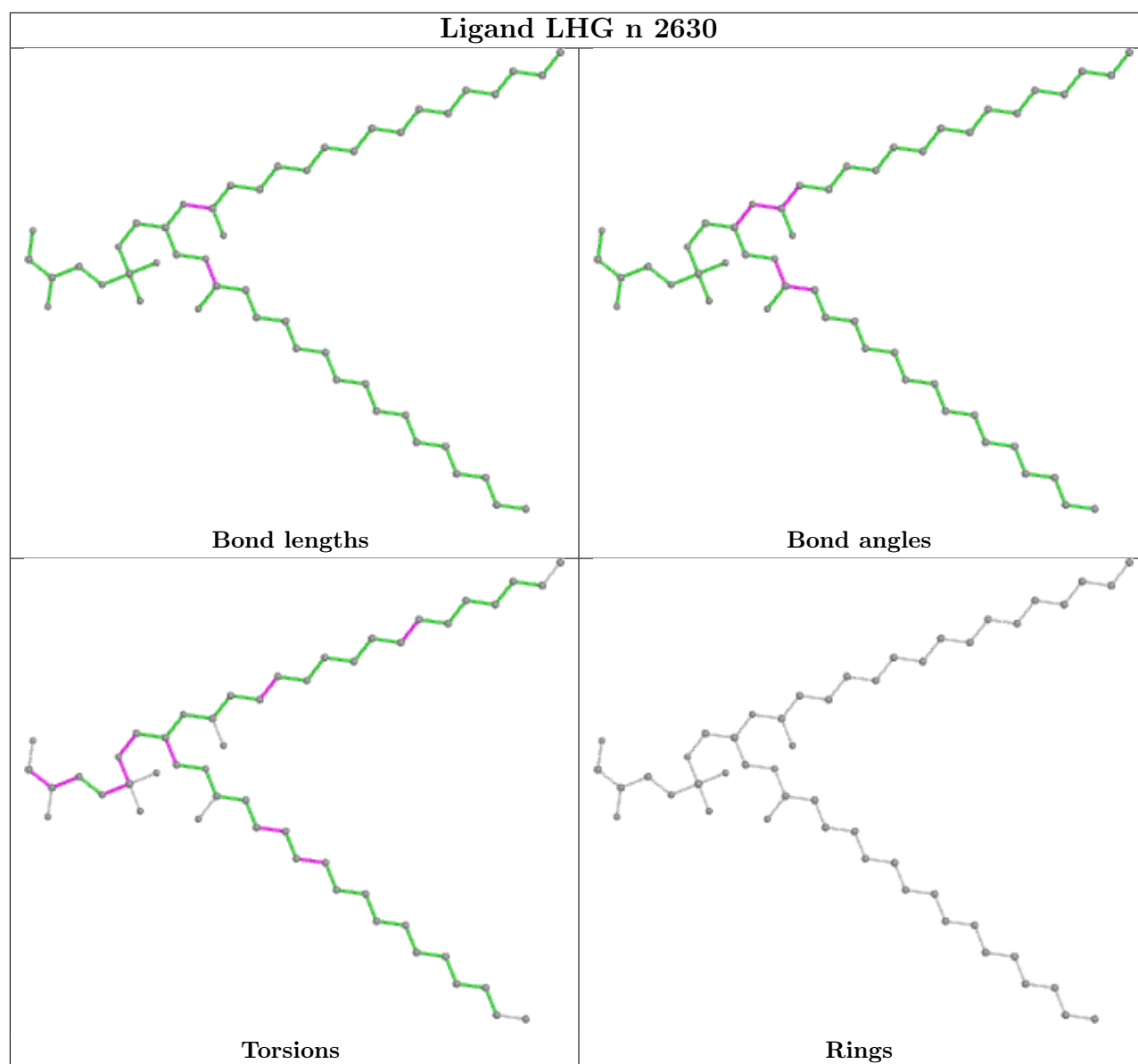


Ligand CLA 9 604

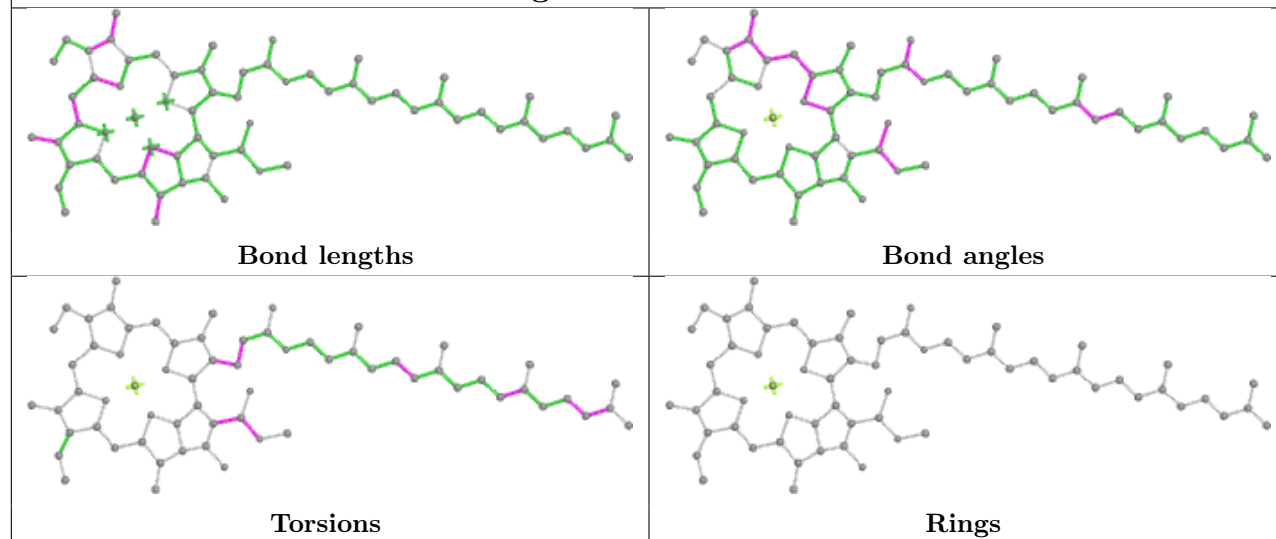




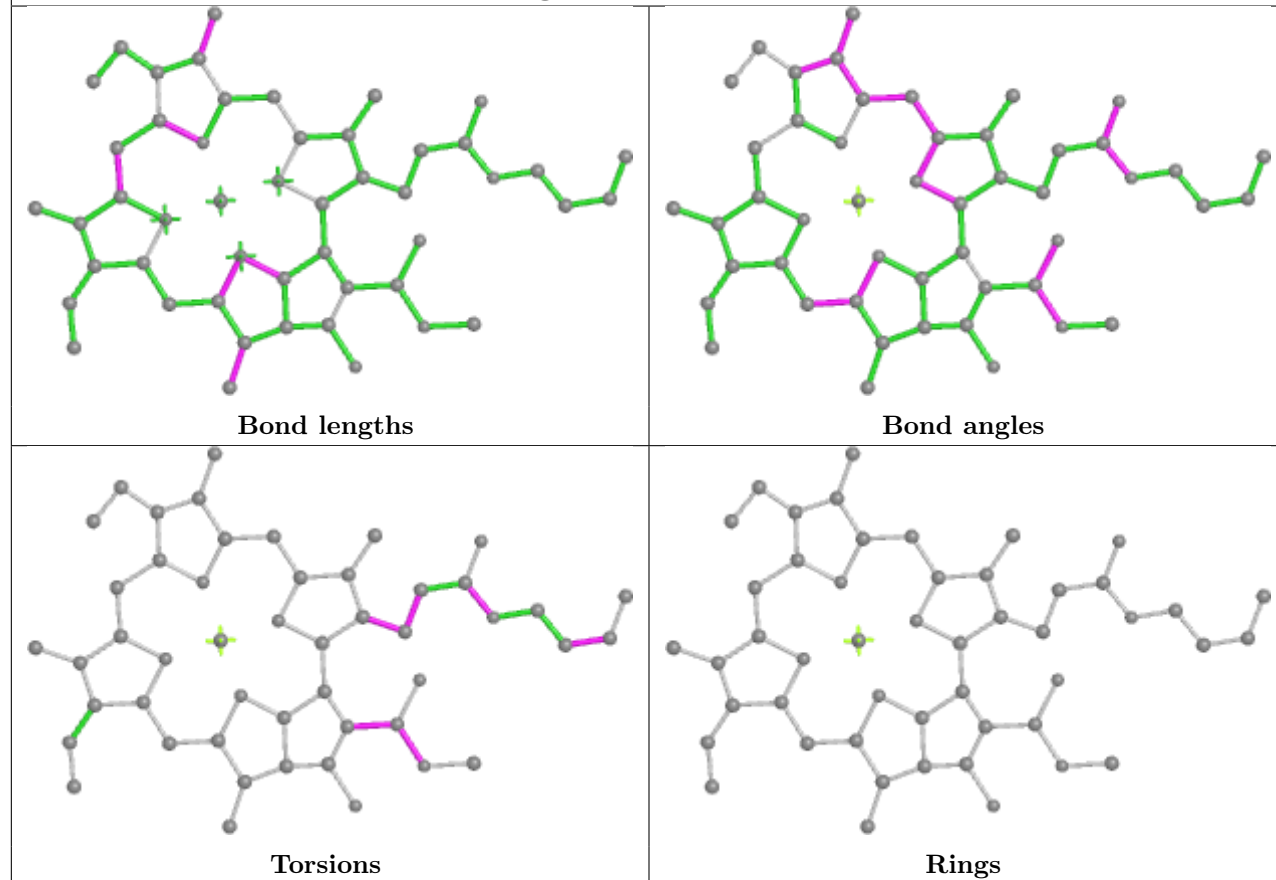
Ligand CLA 4 613**Ligand CLA 0 611**



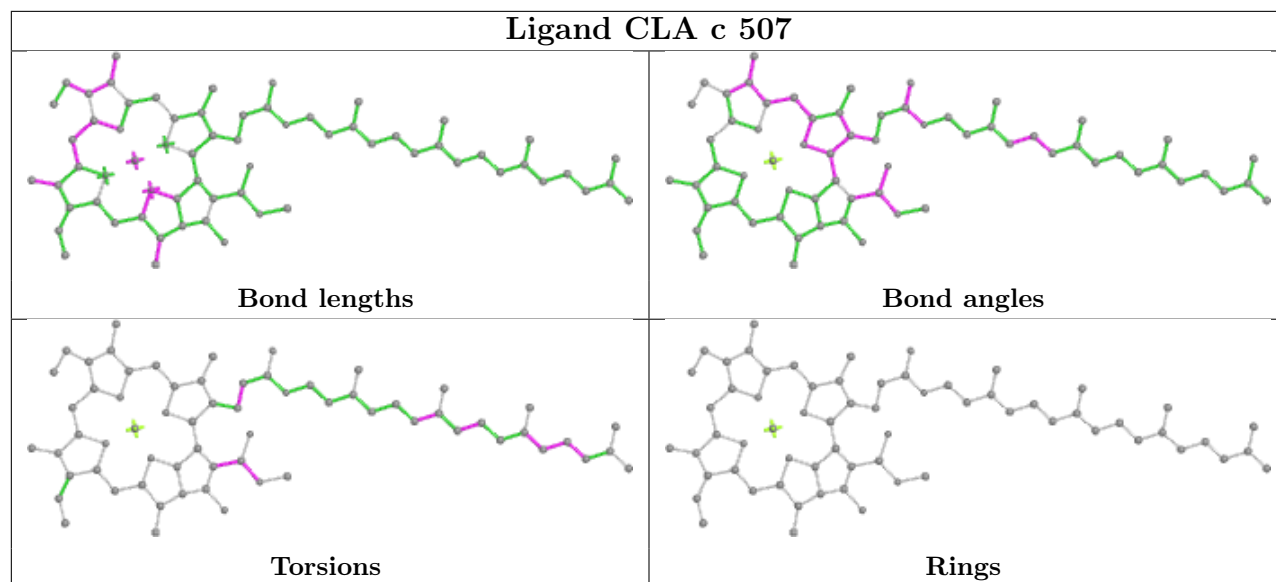
Ligand CLA Y 610



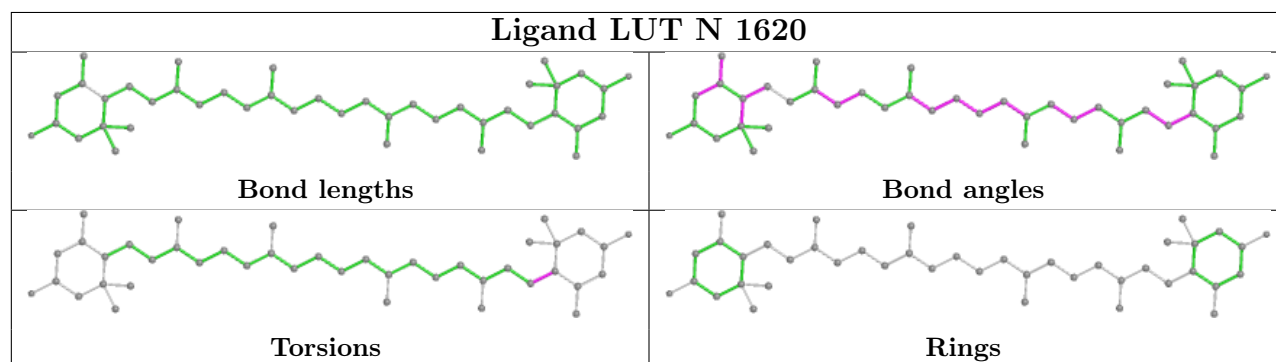
Ligand CLA 3 614



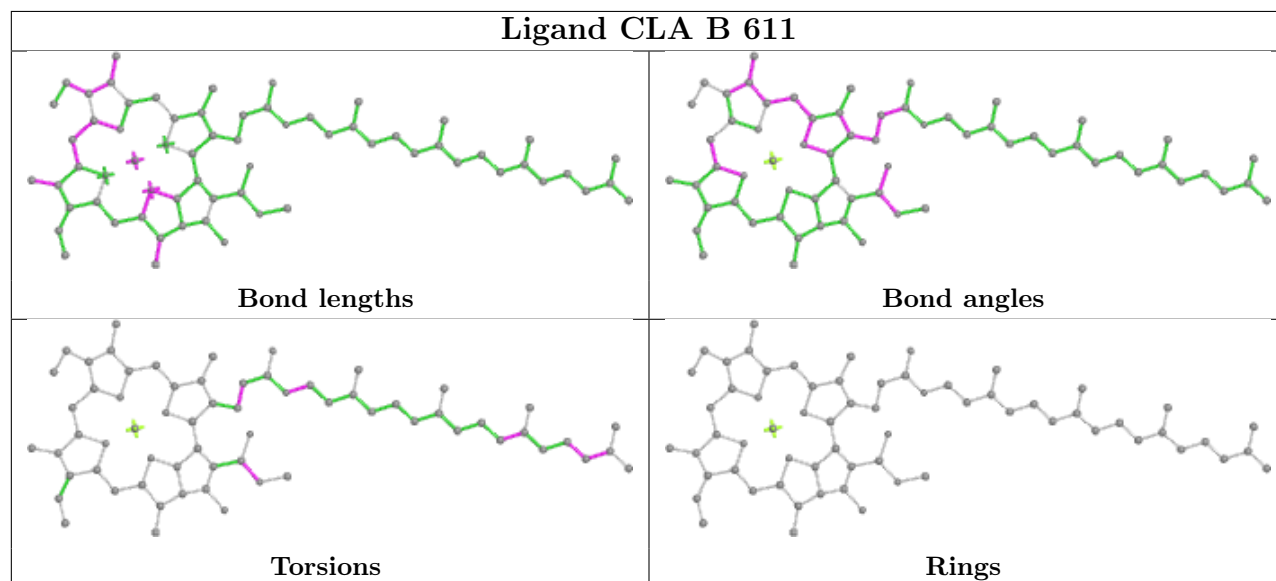
Ligand CLA c 507



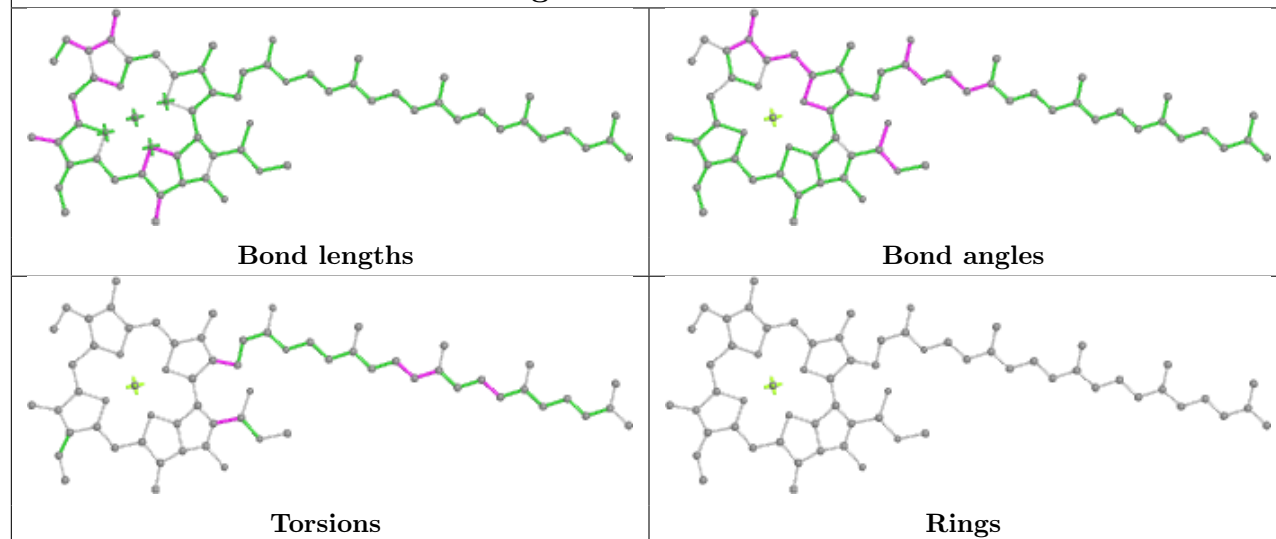
Ligand LUT N 1620



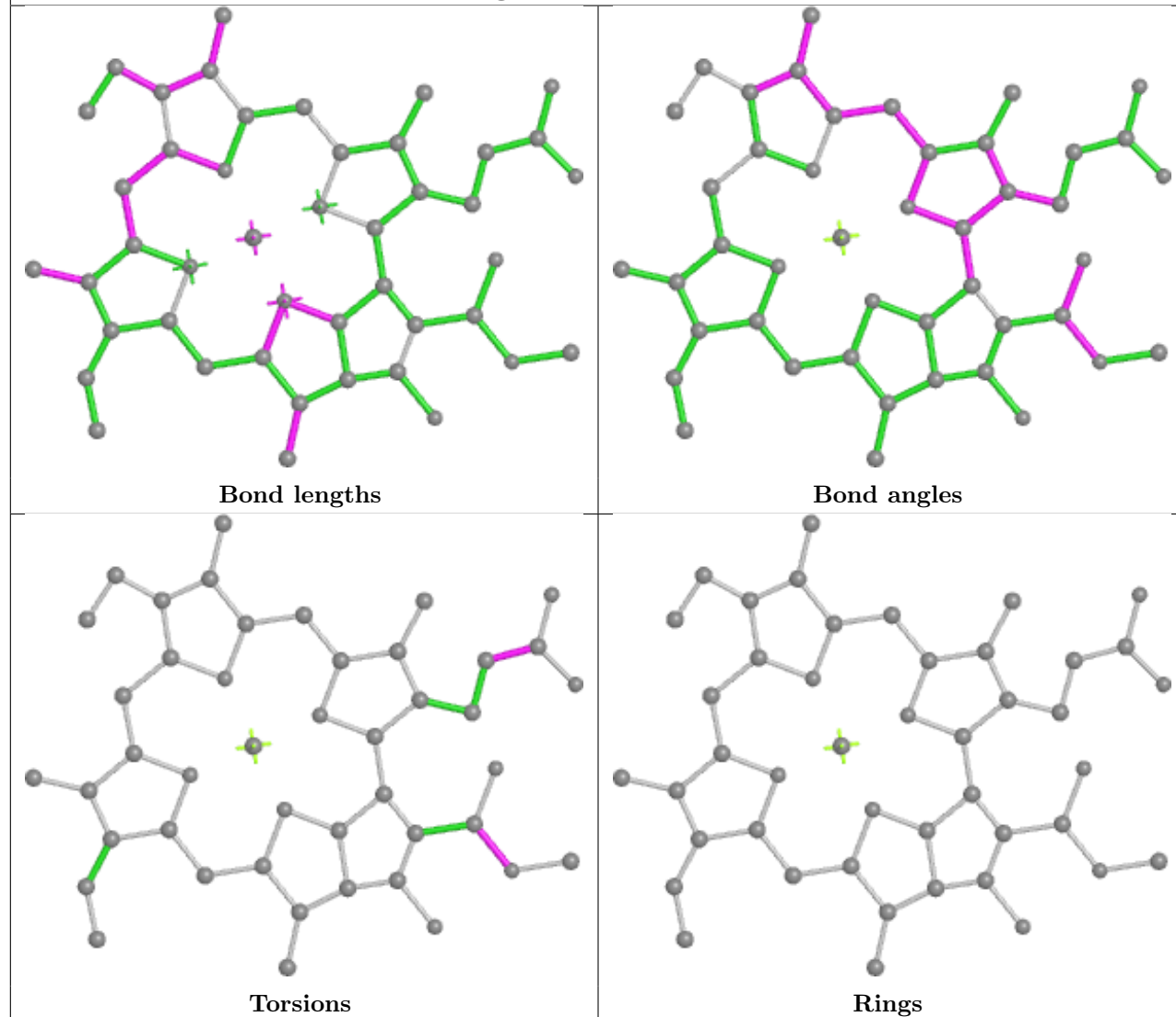
Ligand CLA B 611



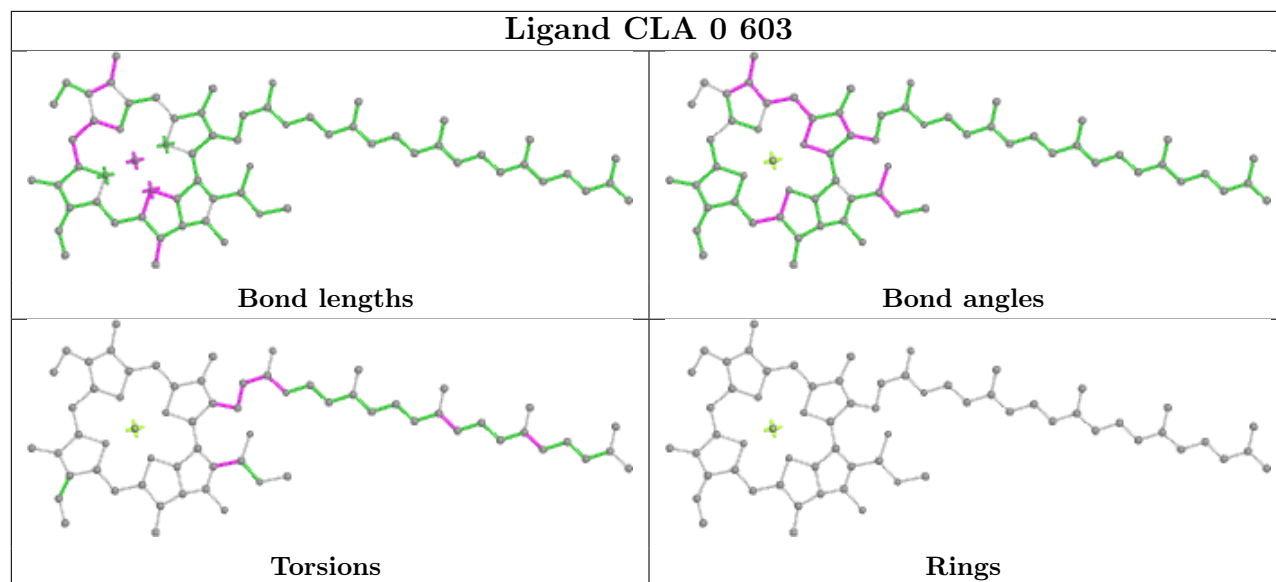
Ligand CLA N 610



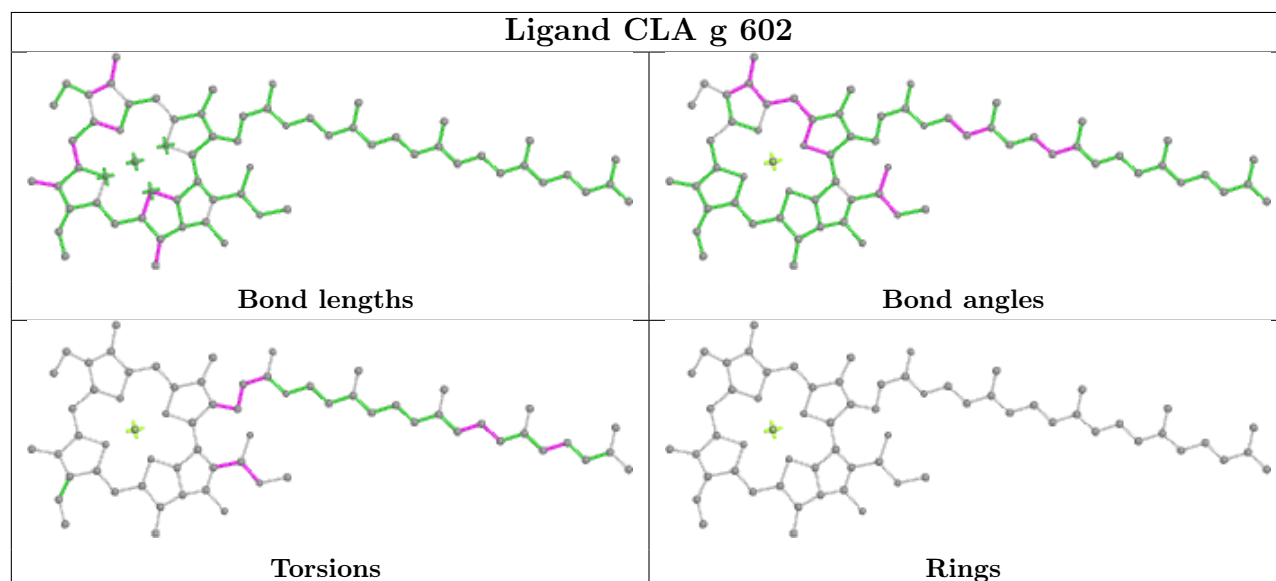
Ligand CLA S 612



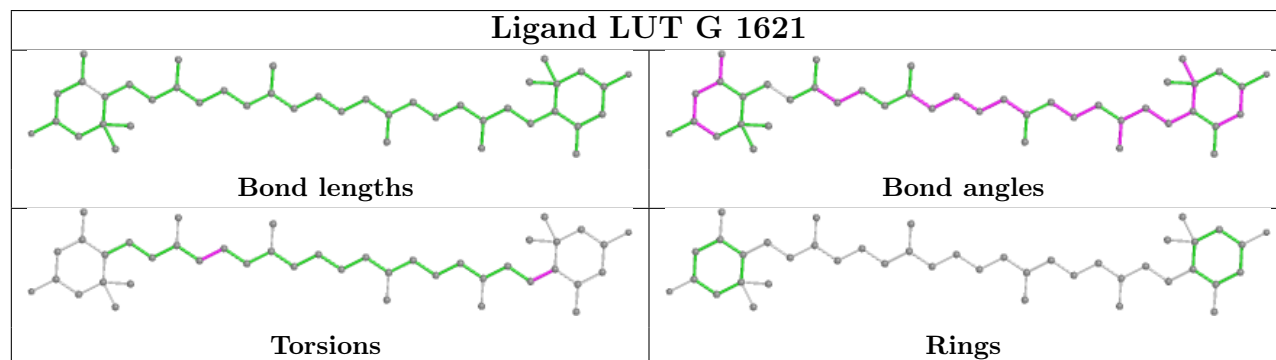
Ligand CLA 0 603



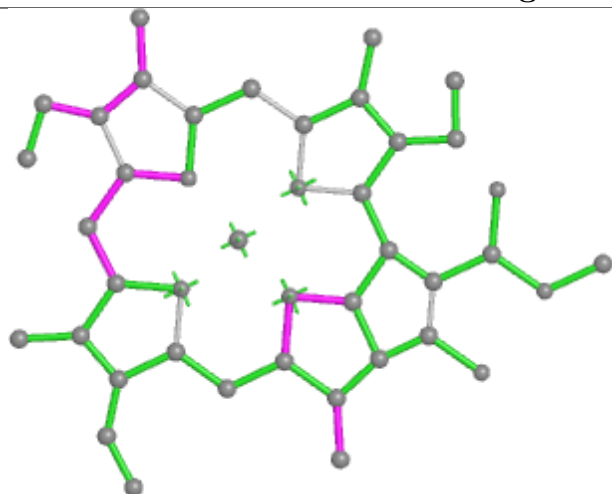
Ligand CLA g 602



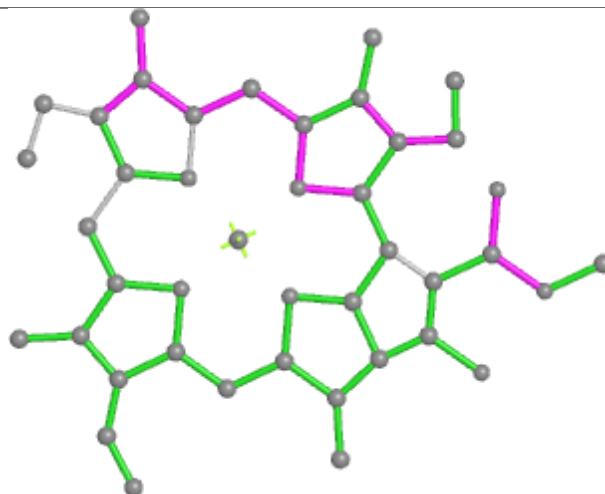
Ligand LUT G 1621



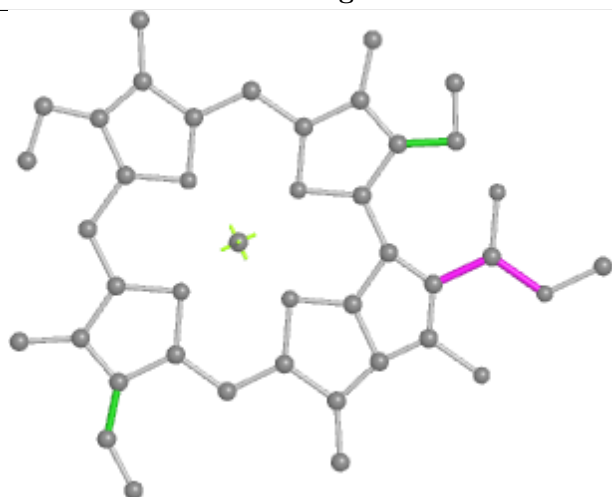
Ligand CLA s 603



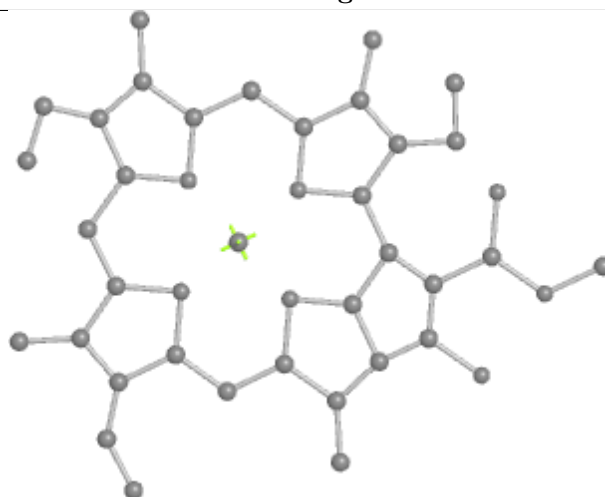
Bond lengths



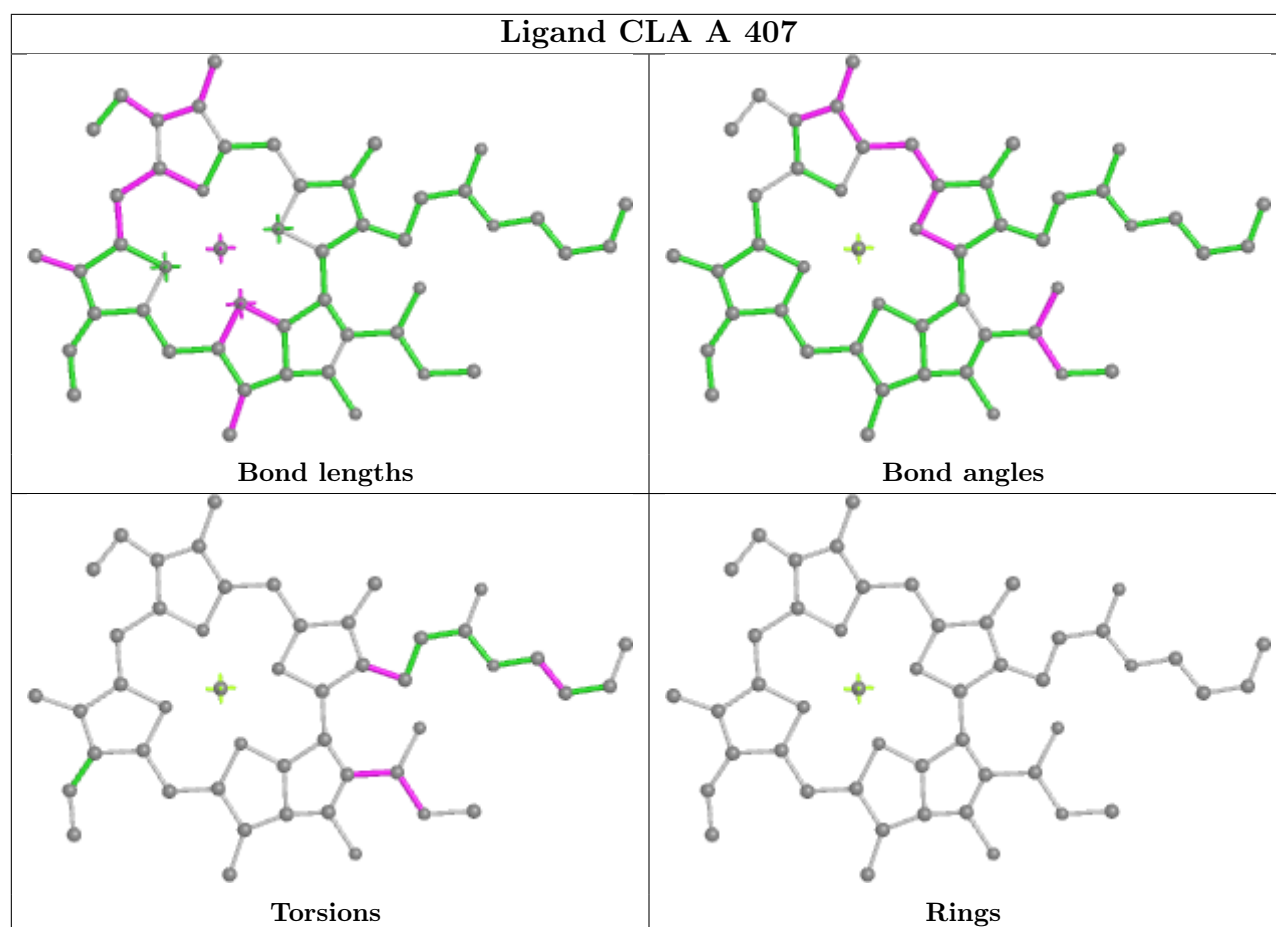
Bond angles



Torsions



Rings



5.7 Other polymers [i](#)

There are no such residues in this entry.

5.8 Polymer linkage issues [i](#)

There are no chain breaks in this entry.

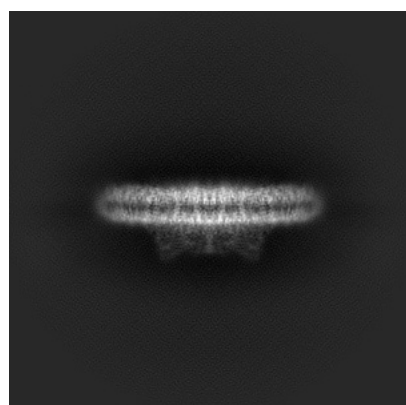
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-9956. These allow visual inspection of the internal detail of the map and identification of artifacts.

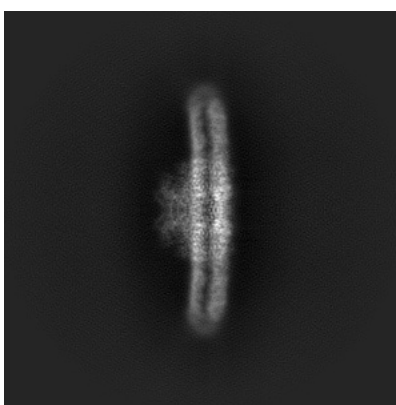
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

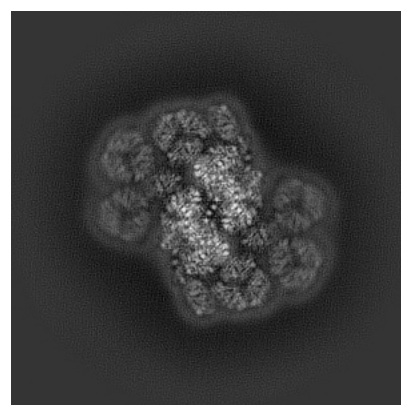
6.1.1 Primary map



X



Y

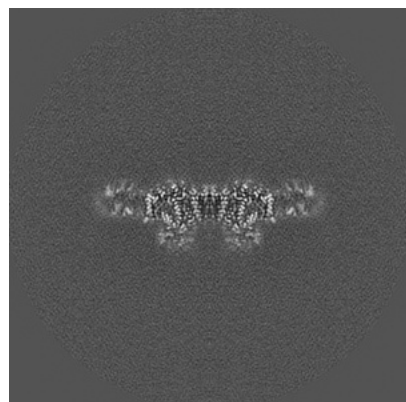


Z

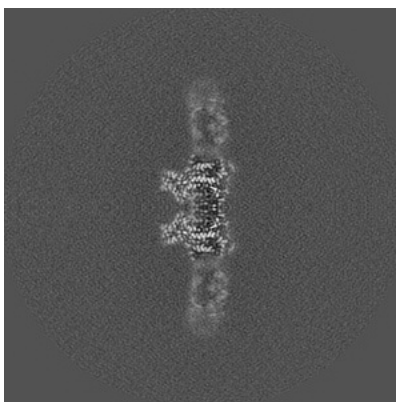
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

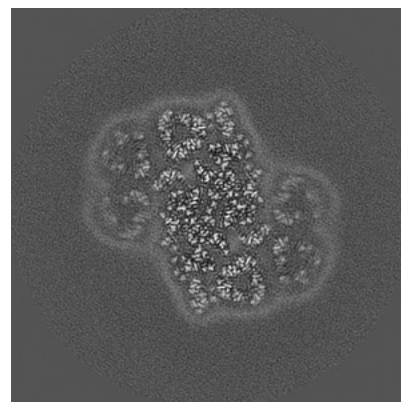
6.2.1 Primary map



X Index: 192



Y Index: 192

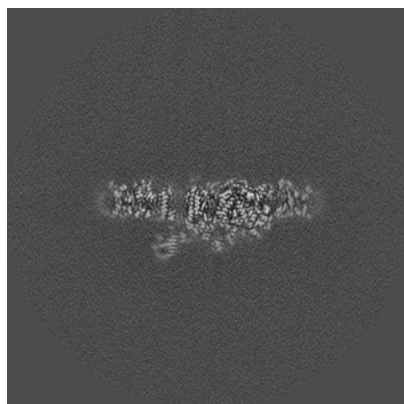


Z Index: 192

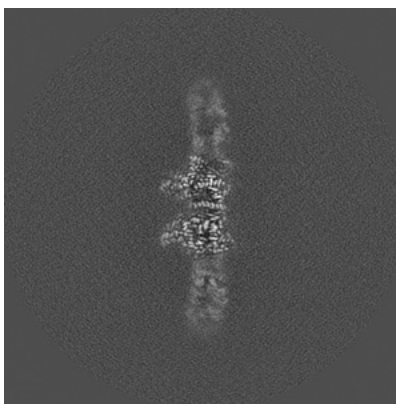
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

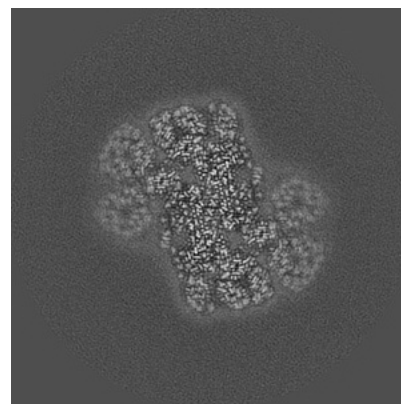
6.3.1 Primary map



X Index: 207



Y Index: 196



Z Index: 204

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

6.4 Orthogonal surface views [i](#)

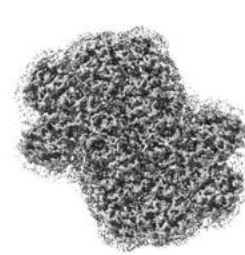
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 0.012. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

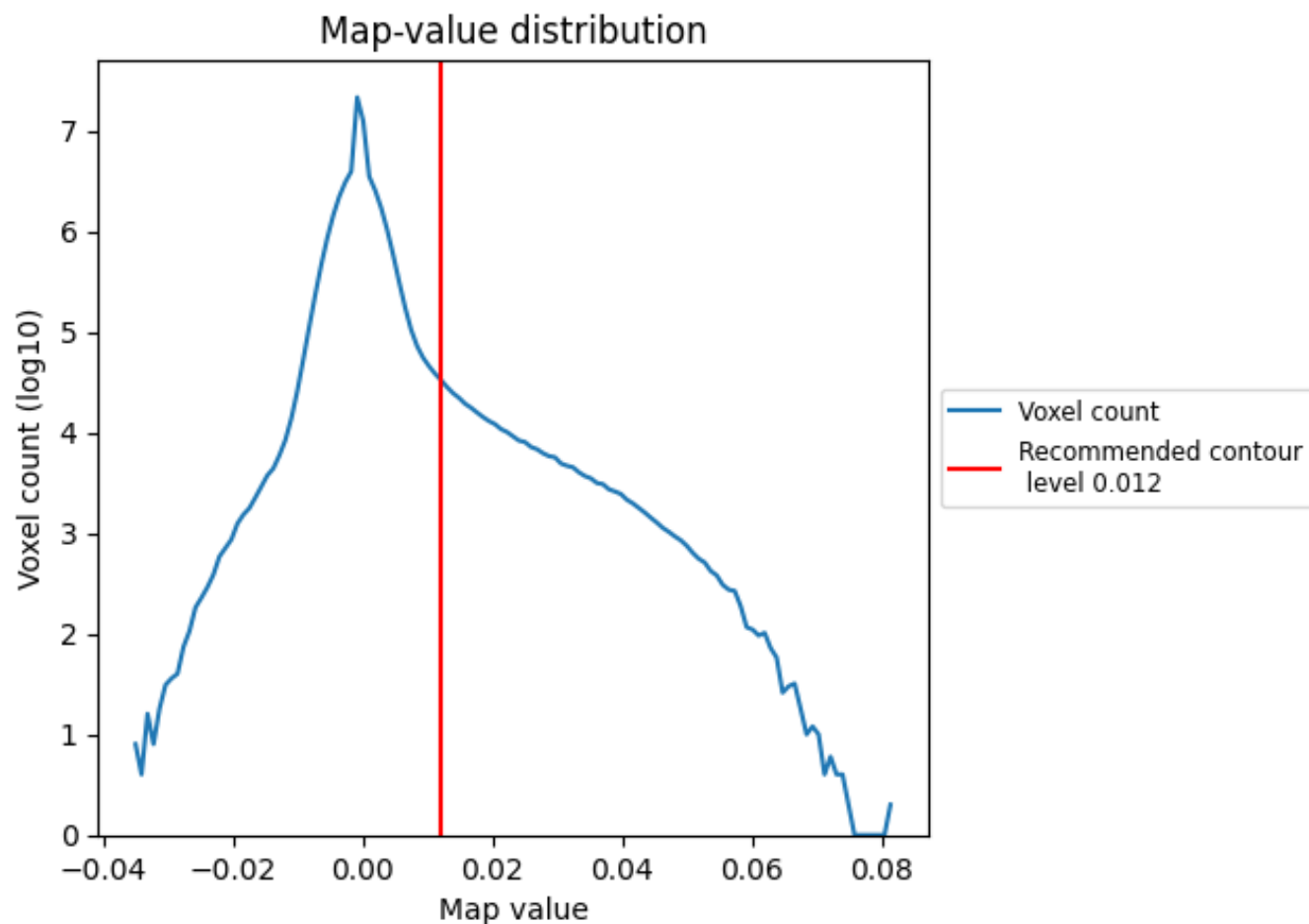
6.5 Mask visualisation

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

7 Map analysis [i](#)

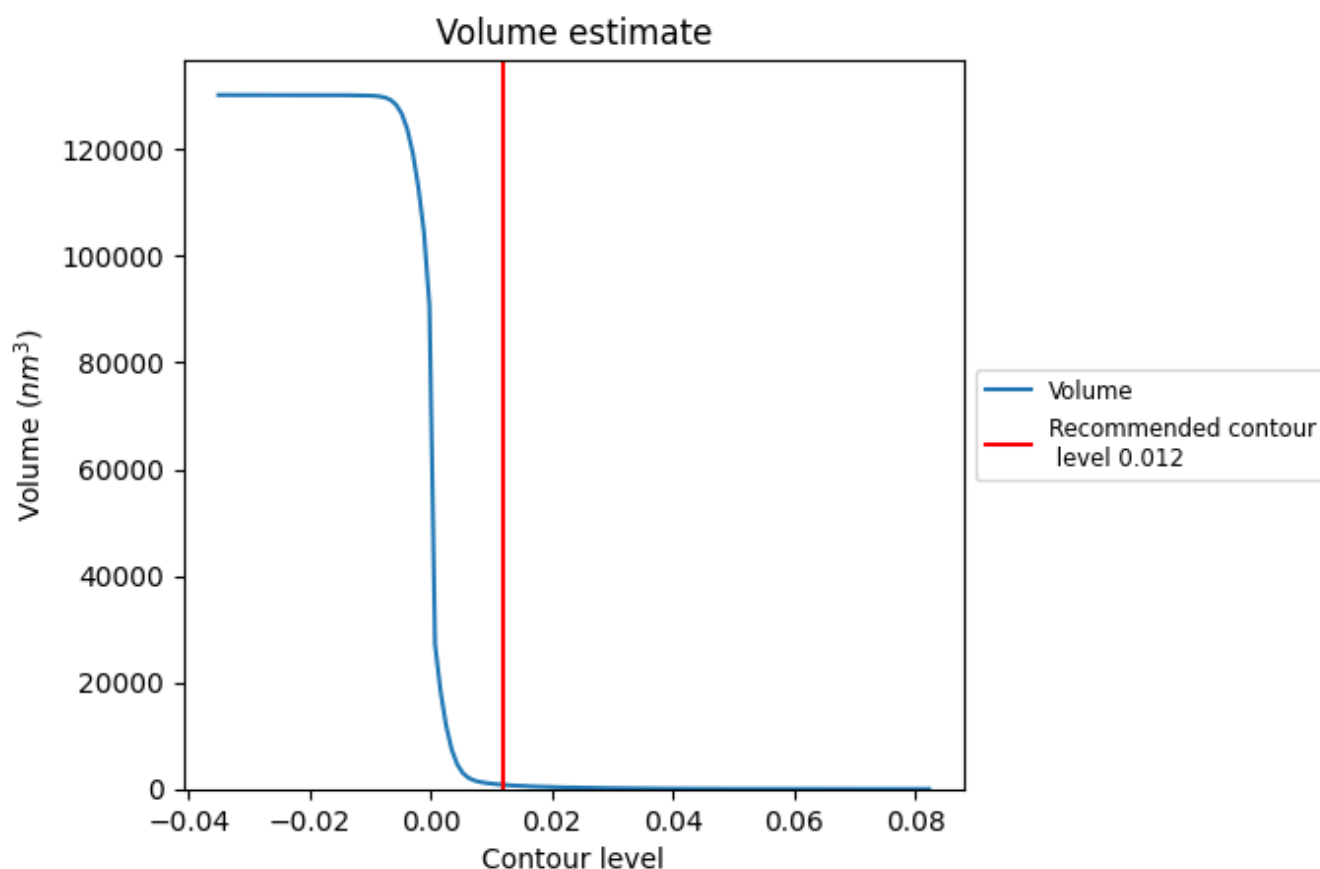
This section contains the results of statistical analysis of the map.

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.

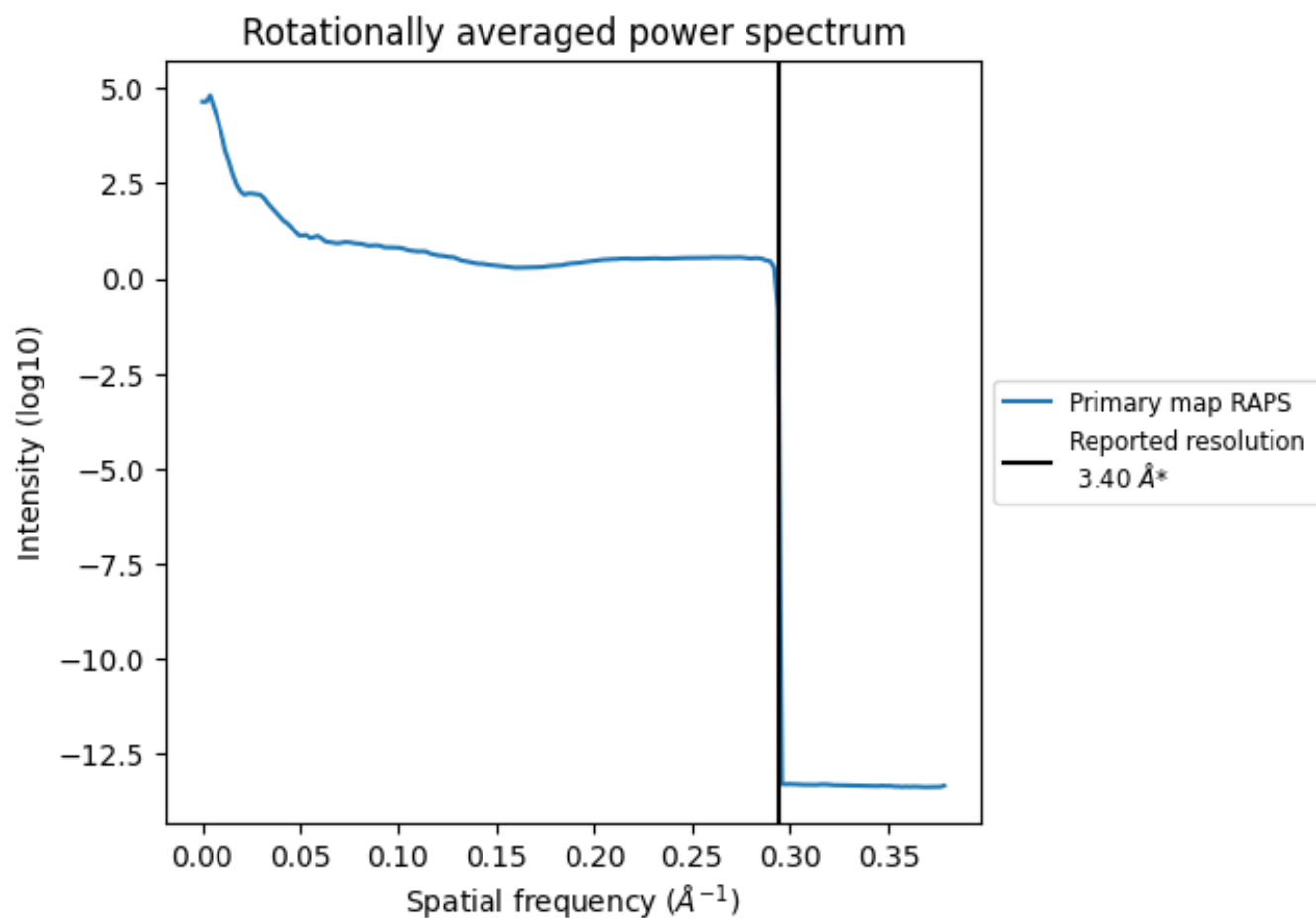
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 778 nm³; this corresponds to an approximate mass of 703 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 ⓘ

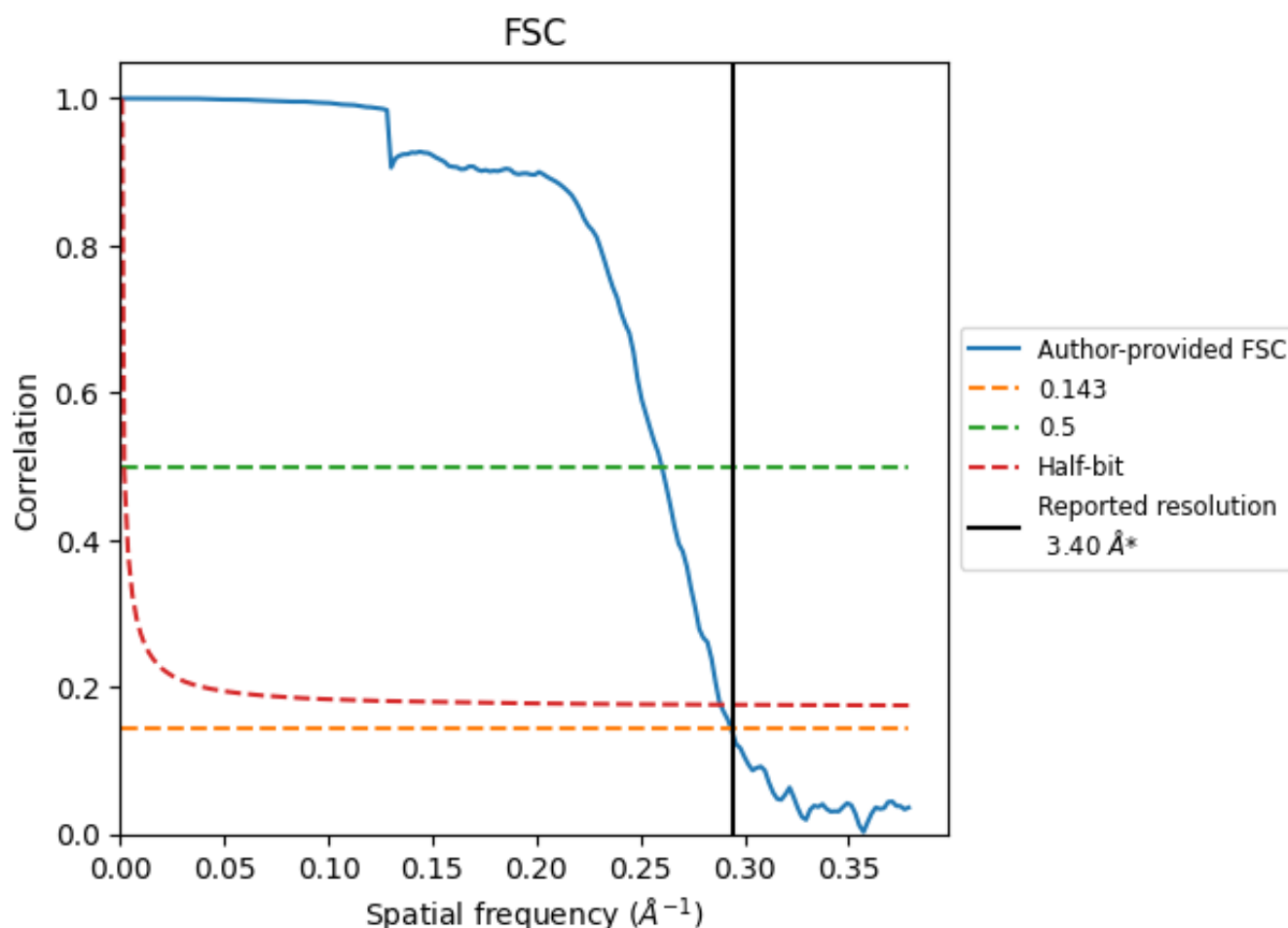


*Reported resolution corresponds to spatial frequency of 0.294 Å⁻¹

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 0.294 \AA^{-1}

8.2 Resolution estimates [i](#)

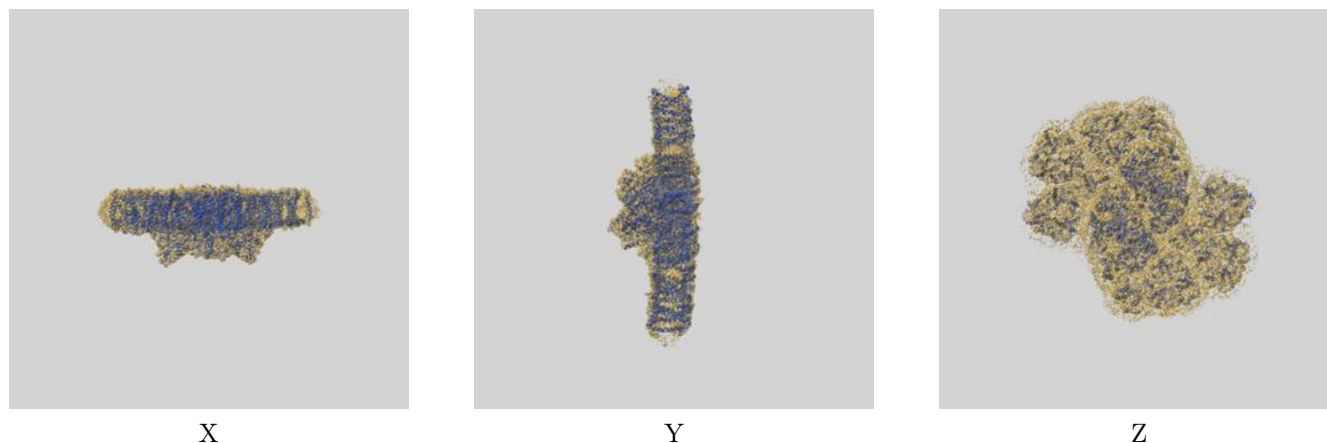
Resolution estimate (Å)	Estimation criterion (FSC cut-off)		
	0.143	0.5	Half-bit
Reported by author	3.40	-	-
Author-provided FSC curve	3.41	3.84	3.47
Unmasked-calculated*	-	-	-

*Resolution estimate based on FSC curve calculated by comparison of deposited half-maps.

9 Map-model fit [i](#)

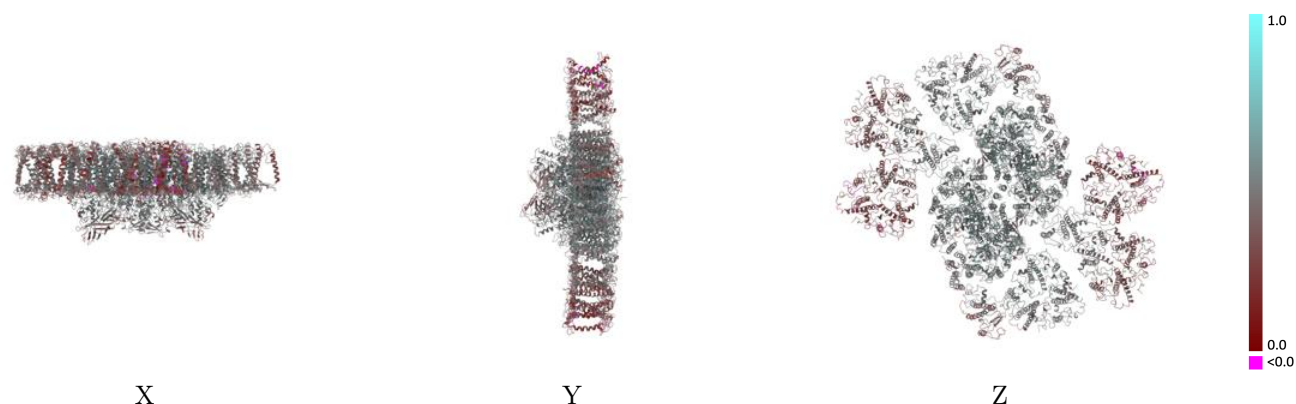
This section contains information regarding the fit between EMDB map EMD-9956 and PDB model 6KAD. Per-residue inclusion information can be found in section [3](#) on page [54](#).

9.1 Map-model overlay [i](#)



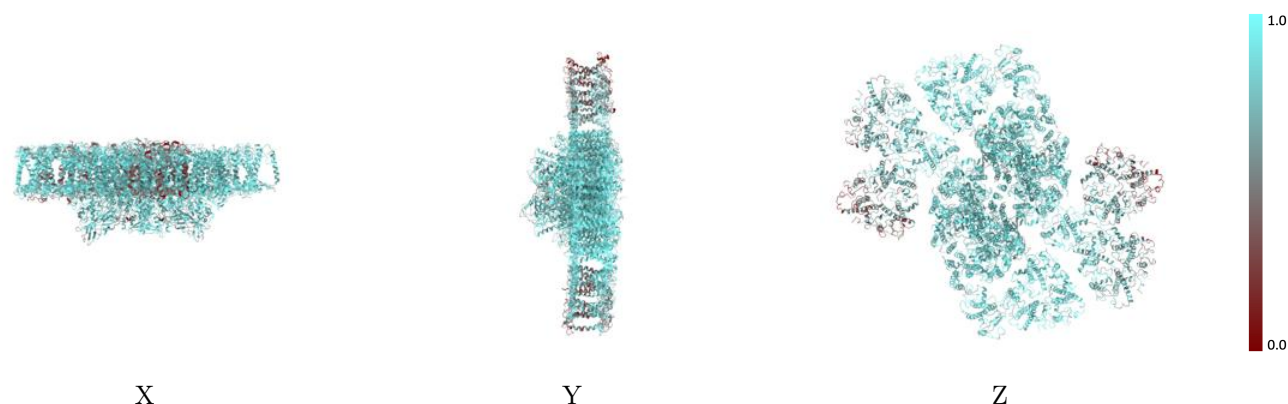
The images above show the 3D surface view of the map at the recommended contour level 0.012 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

9.2 Q-score mapped to coordinate model [i](#)



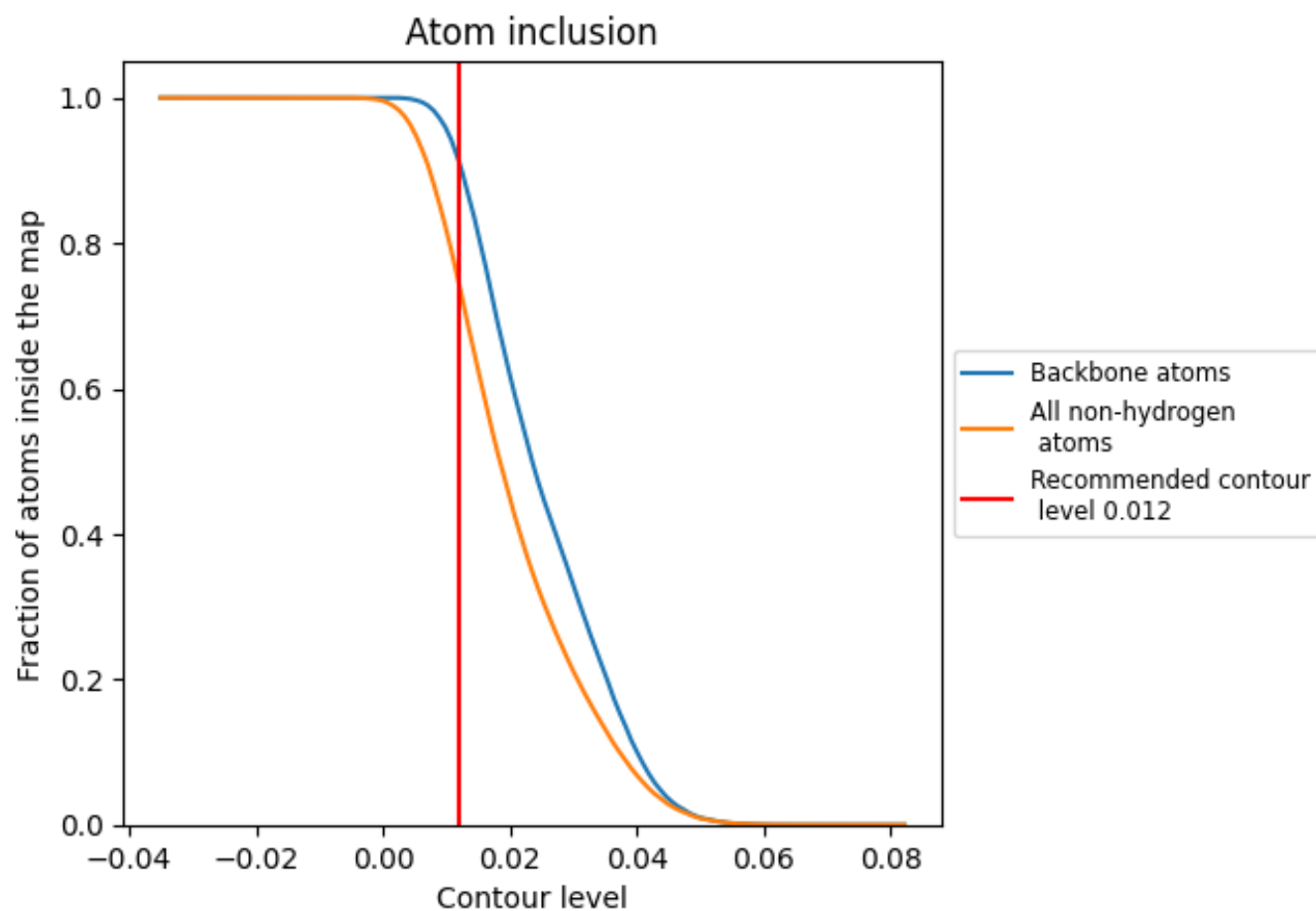
The images above show the model with each residue coloured according its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions at which atoms can be resolved. Low Q-score values may therefore be expected for many entries.

9.3 Atom inclusion mapped to coordinate model [i](#)



The images above show the model with each residue coloured according to its atom inclusion. This shows to what extent they are inside the map at the recommended contour level (0.012).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 91% of all backbone atoms, 74% of all non-hydrogen atoms, are inside the map.

9.5 Map-model fit summary ⓘ

















































The table lists the average atom inclusion at the recommended contour level (0.012) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.7441	 0.4470
0	 0.5846	 0.3510
1	 0.7049	 0.4440
2	 0.5555	 0.3430
3	 0.5778	 0.3480
4	 0.4720	 0.2850
5	 0.3433	 0.2540
6	 0.5790	 0.3470
7	 0.7087	 0.4440
8	 0.5770	 0.3480
9	 0.5535	 0.3450
A	 0.8909	 0.5300
B	 0.8702	 0.5130
C	 0.8510	 0.5210
D	 0.8758	 0.5310
E	 0.8361	 0.4570
F	 0.8246	 0.4730
G	 0.8135	 0.4810
H	 0.8671	 0.5040
I	 0.9179	 0.5410
J	 0.8200	 0.4730
K	 0.8191	 0.4820
L	 0.8621	 0.5240
M	 0.8246	 0.4920
N	 0.8129	 0.4780
O	 0.7010	 0.4070
R	 0.8072	 0.4930
S	 0.7665	 0.4230
T	 0.8264	 0.5120
V	 0.7174	 0.4120
W	 0.8642	 0.5140
X	 0.8455	 0.4760
Y	 0.8583	 0.5270
Z	 0.7478	 0.4270
a	 0.8919	 0.5310



Continued on next page...

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Chain	Atom inclusion	Q-score
b	 0.8710	 0.5120
c	 0.8506	 0.5200
d	 0.8727	 0.5330
e	 0.8328	 0.4510
f	 0.8211	 0.4720
g	 0.8154	 0.4810
h	 0.8455	 0.5020
i	 0.9107	 0.5400
j	 0.8160	 0.4750
k	 0.8225	 0.4810
l	 0.8621	 0.5230
m	 0.8246	 0.4950
n	 0.8152	 0.4800
o	 0.7022	 0.4060
p	 0.3399	 0.2440
q	 0.4669	 0.2820
r	 0.8079	 0.4940
s	 0.7687	 0.4240
t	 0.8264	 0.5120
v	 0.7174	 0.4140
w	 0.8665	 0.5090
x	 0.8412	 0.4710
y	 0.8586	 0.5250
z	 0.7325	 0.4220