



Full wwPDB EM Validation Report ⓘ

Nov 7, 2022 – 03:52 PM JST

PDB ID : 5XNL
EMDB ID : EMD-6741
Title : Structure of stacked C2S2M2-type PSII-LHCII supercomplex from *Pisum sativum*
Authors : Su, X.D.; Ma, J.; Wei, X.P.; Cao, P.; Zhu, D.J.; Chang, W.R.; Liu, Z.F.; Zhang, X.Z.; Li, M.
Deposited on : 2017-05-23
Resolution : 2.70 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:

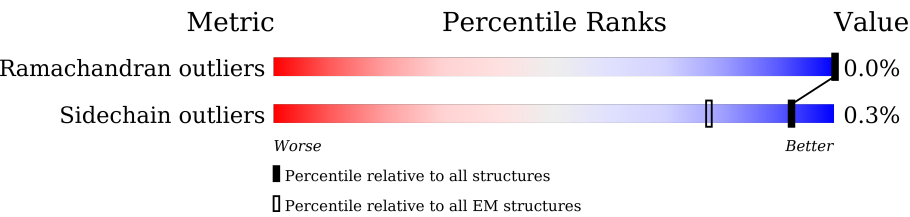
EMDB validation analysis : 0.0.1.dev43
Mogul : 1.8.5 (274361), CSD as541be (2020)
MolProbity : 4.02b-467
buster-report : 1.1.7 (2018)
Percentile statistics : 20191225.v01 (using entries in the PDB archive December 25th 2019)
MapQ : 1.9.9
Ideal geometry (proteins) : Engh & Huber (2001)
Ideal geometry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

1 Overall quality at a glance i

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

The reported resolution of this entry is 2.70 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	1	232	<div><div>93%</div><div><div></div><div></div><div></div><div></div></div><div>94%</div><div>6%</div></div>
1	2	232	<div><div>94%</div><div><div></div><div></div><div></div><div></div></div><div>93%</div><div>• 6%</div></div>
1	5	232	<div><div>94%</div><div><div></div><div></div><div></div><div></div></div><div>94%</div><div>6%</div></div>
1	6	232	<div><div>94%</div><div><div></div><div></div><div></div><div></div></div><div>93%</div><div>• 6%</div></div>
1	G	232	<div><div>27%</div><div><div></div><div></div><div></div><div></div></div><div>94%</div><div>6%</div></div>
1	N	232	<div><div>18%</div><div><div></div><div></div><div></div><div></div></div><div>94%</div><div>6%</div></div>
1	Y	232	<div><div>5%</div><div><div></div><div></div><div></div><div></div></div><div>94%</div><div>6%</div></div>
1	g	232	<div><div>26%</div><div><div></div><div></div><div></div><div></div></div><div>94%</div><div>6%</div></div>
1	n	232	<div><div>18%</div><div><div></div><div></div><div></div><div></div></div><div>94%</div><div>6%</div></div>

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Mol	Chain	Length	Quality of chain
1	y	232	
2	3	243	
2	7	243	
3	4	210	
3	8	210	
4	A	344	
4	a	344	
5	B	507	
5	b	507	
6	C	473	
6	c	473	
7	D	353	
7	d	353	
8	E	83	
8	e	83	
9	F	39	
9	f	39	
10	H	73	
10	h	73	
11	I	36	
11	i	36	
12	J	40	
12	j	40	
13	K	61	
13	k	61	

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Mol	Chain	Length	Quality of chain
14	L	38	
14	l	38	
15	M	34	
15	m	34	
16	O	248	
16	o	248	
17	P	186	
17	p	186	
18	Q	148	
18	q	148	
19	R	246	
19	r	246	
20	S	244	
20	s	244	
21	T	35	
21	t	35	
22	W	54	
22	w	54	
23	X	86	
23	x	86	
24	Z	62	
24	z	62	

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

Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
25	CHL	1	601	X	-	-	-
25	CHL	1	605	X	-	-	-
25	CHL	1	606	X	-	-	-
25	CHL	1	607	X	-	-	-
25	CHL	1	608	X	-	-	-
25	CHL	1	609	X	-	-	-
25	CHL	2	601	X	-	-	-
25	CHL	2	605	X	-	-	-
25	CHL	2	606	X	-	-	-
25	CHL	2	607	X	-	-	-
25	CHL	2	608	X	-	-	-
25	CHL	2	609	X	-	-	-
25	CHL	3	601	X	-	-	-
25	CHL	3	605	X	-	-	-
25	CHL	3	606	X	-	-	-
25	CHL	3	607	X	-	-	-
25	CHL	3	608	X	-	-	-
25	CHL	3	609	X	-	-	-
25	CHL	4	601	X	-	-	-
25	CHL	4	606	X	-	-	-
25	CHL	4	607	X	-	-	-
25	CHL	4	608	X	-	-	-
25	CHL	4	609	X	-	-	-
25	CHL	5	601	X	-	-	-
25	CHL	5	605	X	-	-	-
25	CHL	5	606	X	-	-	-
25	CHL	5	607	X	-	-	-
25	CHL	5	608	X	-	-	-
25	CHL	5	609	X	-	-	-
25	CHL	6	601	X	-	-	-
25	CHL	6	605	X	-	-	-
25	CHL	6	606	X	-	-	-
25	CHL	6	607	X	-	-	-
25	CHL	6	608	X	-	-	-
25	CHL	6	609	X	-	-	-
25	CHL	7	601	X	-	-	-
25	CHL	7	605	X	-	-	-
25	CHL	7	606	X	-	-	-
25	CHL	7	607	X	-	-	-
25	CHL	7	608	X	-	-	-
25	CHL	7	609	X	-	-	-
25	CHL	8	601	X	-	-	-
25	CHL	8	606	X	-	-	-

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

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

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	5	612	X	-	-	-
26	CLA	5	614	X	-	-	-
26	CLA	6	602	X	-	-	-
26	CLA	6	603	X	-	-	-
26	CLA	6	604	X	-	-	-
26	CLA	6	610	X	-	-	-
26	CLA	6	612	X	-	-	-
26	CLA	6	614	X	-	-	-
26	CLA	7	602	X	-	-	-
26	CLA	7	603	X	-	-	-
26	CLA	7	604	X	-	-	-
26	CLA	7	610	X	-	-	-
26	CLA	7	611	X	-	-	-
26	CLA	7	612	X	-	-	-
26	CLA	7	613	X	-	-	-
26	CLA	7	614	X	-	-	-
26	CLA	8	602	X	-	-	-
26	CLA	8	603	X	-	-	-
26	CLA	8	610	X	-	-	-
26	CLA	8	611	X	-	-	-
26	CLA	8	612	X	-	-	-
26	CLA	A	405	X	-	-	-
26	CLA	A	406	X	-	-	-
26	CLA	A	410	X	-	-	-
26	CLA	B	602	X	-	-	-
26	CLA	B	603	X	-	-	-
26	CLA	B	604	X	-	-	-
26	CLA	B	605	X	-	-	-
26	CLA	B	606	X	-	-	-
26	CLA	B	607	X	-	-	-
26	CLA	B	608	X	-	-	-
26	CLA	B	611	X	-	-	-
26	CLA	B	612	X	-	-	-
26	CLA	B	613	X	-	-	-
26	CLA	B	614	X	-	-	-
26	CLA	B	615	X	-	-	-
26	CLA	B	616	X	-	-	-
26	CLA	B	617	X	-	-	-
26	CLA	C	501	X	-	-	-
26	CLA	C	502	X	-	-	-
26	CLA	C	503	X	-	-	-
26	CLA	C	504	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	C	505	X	-	-	-
26	CLA	C	506	X	-	-	-
26	CLA	C	507	X	-	-	-
26	CLA	C	508	X	-	-	-
26	CLA	C	509	X	-	-	-
26	CLA	C	510	X	-	-	-
26	CLA	C	511	X	-	-	-
26	CLA	C	512	X	-	-	-
26	CLA	D	402	X	-	-	-
26	CLA	G	602	X	-	-	-
26	CLA	G	603	X	-	-	-
26	CLA	G	604	X	-	-	-
26	CLA	G	610	X	-	-	-
26	CLA	G	611	X	-	-	-
26	CLA	G	612	X	-	-	-
26	CLA	G	613	X	-	-	-
26	CLA	G	614	X	-	-	-
26	CLA	N	602	X	-	-	-
26	CLA	N	603	X	-	-	-
26	CLA	N	604	X	-	-	-
26	CLA	N	610	X	-	-	-
26	CLA	N	611	X	-	-	-
26	CLA	N	612	X	-	-	-
26	CLA	N	613	X	-	-	-
26	CLA	N	614	X	-	-	-
26	CLA	R	601	X	-	-	-
26	CLA	R	602	X	-	-	-
26	CLA	R	603	X	-	-	-
26	CLA	R	604	X	-	-	-
26	CLA	R	609	X	-	-	-
26	CLA	R	610	X	-	-	-
26	CLA	R	611	X	-	-	-
26	CLA	R	612	X	-	-	-
26	CLA	R	613	X	-	-	-
26	CLA	S	602	X	-	-	-
26	CLA	S	603	X	-	-	-
26	CLA	S	604	X	-	-	-
26	CLA	S	609	X	-	-	-
26	CLA	S	610	X	-	-	-
26	CLA	S	611	X	-	-	-
26	CLA	S	612	X	-	-	-
26	CLA	S	613	X	-	-	-

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Mol	Type	Chain	Res	Chirality	Geometry	Clashes	Electron density
26	CLA	S	614	X	-	-	-
26	CLA	Y	602	X	-	-	-
26	CLA	Y	603	X	-	-	-
26	CLA	Y	604	X	-	-	-
26	CLA	Y	610	X	-	-	-
26	CLA	Y	611	X	-	-	-
26	CLA	Y	612	X	-	-	-
26	CLA	Y	613	X	-	-	-
26	CLA	Y	614	X	-	-	-
26	CLA	a	405	X	-	-	-
26	CLA	a	406	X	-	-	-
26	CLA	a	410	X	-	-	-
26	CLA	b	602	X	-	-	-
26	CLA	b	603	X	-	-	-
26	CLA	b	604	X	-	-	-
26	CLA	b	605	X	-	-	-
26	CLA	b	606	X	-	-	-
26	CLA	b	607	X	-	-	-
26	CLA	b	608	X	-	-	-
26	CLA	b	611	X	-	-	-
26	CLA	b	612	X	-	-	-
26	CLA	b	613	X	-	-	-
26	CLA	b	614	X	-	-	-
26	CLA	b	615	X	-	-	-
26	CLA	b	616	X	-	-	-
26	CLA	b	617	X	-	-	-
26	CLA	c	501	X	-	-	-
26	CLA	c	502	X	-	-	-
26	CLA	c	503	X	-	-	-
26	CLA	c	504	X	-	-	-
26	CLA	c	505	X	-	-	-
26	CLA	c	506	X	-	-	-
26	CLA	c	507	X	-	-	-
26	CLA	c	508	X	-	-	-
26	CLA	c	509	X	-	-	-
26	CLA	c	510	X	-	-	-
26	CLA	c	511	X	-	-	-
26	CLA	c	512	X	-	-	-
26	CLA	d	402	X	-	-	-
26	CLA	g	602	X	-	-	-
26	CLA	g	603	X	-	-	-
26	CLA	g	604	X	-	-	-

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

2 Entry composition [i](#)

There are 42 unique types of molecules in this entry. The entry contains 98986 atoms, of which 0 are hydrogens and 0 are deuteriums.

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

- Molecule 1 is a protein called Chlorophyll a-b binding protein 8, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
1	1	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	2	218	Total	C	N	O	S	0	0
			1664	1079	269	311	5		
1	G	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	N	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	Y	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	5	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	6	218	Total	C	N	O	S	0	0
			1664	1079	269	311	5		
1	g	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	n	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		
1	y	219	Total	C	N	O	S	0	0
			1668	1081	270	312	5		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
2	3	220	Total	C	N	O	S	0	0
			1707	1116	277	309	5		
2	7	220	Total	C	N	O	S	0	0
			1707	1116	277	309	5		

- Molecule 3 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24.

Mol	Chain	Residues	Atoms					AltConf	Trace
3	4	197	Total	C	N	O	S	0	0
			1534	1009	247	274	4		

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Mol	Chain	Residues	Atoms					AltConf	Trace
3	8	197	Total	C	N	O	S	0	0
			1534	1009	247	274	4		

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

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

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

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

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
7	D	341	Total	C	N	O	S	0	0
			2712	1790	444	466	12		
7	d	341	Total	C	N	O	S	0	0
			2712	1790	444	466	12		

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

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

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

Mol	Chain	Residues	Atoms					AltConf	Trace
9	F	30	Total	C	N	O	S	0	0
			241	162	41	37	1		
9	f	30	Total	C	N	O	S	0	0
			241	162	41	37	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
10	H	60	Total	C	N	O	S	0	0
			452	296	72	81	3		
10	h	60	Total	C	N	O	S	0	0
			452	296	72	81	3		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
11	I	34	Total	C	N	O	S	0	0
			278	191	43	43	1		
11	i	34	Total	C	N	O	S	0	0
			278	191	43	43	1		

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

Mol	Chain	Residues	Atoms				AltConf	Trace
12	J	35	Total	C	N	O	0	0
			256	174	39	43		
12	j	35	Total	C	N	O	0	0
			256	174	39	43		

- 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
			306	215	44	46		
13	k	37	Total	C	N	O	0	0
			306	215	44	46		

- 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
			311	205	49	57		
14	l	37	Total	C	N	O	0	0
			311	205	49	57		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
15	M	33	Total	C	N	O	S	0	0
			256	176	36	43	1		
15	m	33	Total	C	N	O	S	0	0
			256	176	36	43	1		

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

Mol	Chain	Residues	Atoms					AltConf	Trace
16	O	248	Total	C	N	O	S	0	0
			1870	1179	306	382	3		
16	o	248	Total	C	N	O	S	0	0
			1870	1179	306	382	3		

- Molecule 17 is a protein called Oxygen-evolving enhancer protein 2, chloroplastic.

Mol	Chain	Residues	Atoms					AltConf	Trace
17	P	186	Total	C	N	O	S	0	0
			1434	909	238	286	1		
17	p	186	Total	C	N	O	S	0	0
			1434	909	238	286	1		

- Molecule 18 is a protein called Oxygen-evolving enhancer protein 3.

Mol	Chain	Residues	Atoms				AltConf	Trace
18	Q	129	Total	C	N	O	0	0
			1034	661	177	196		
18	q	129	Total	C	N	O	0	0
			1034	661	177	196		

- Molecule 19 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29.

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

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

- Molecule 20 is a protein called Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26.

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

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

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

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

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

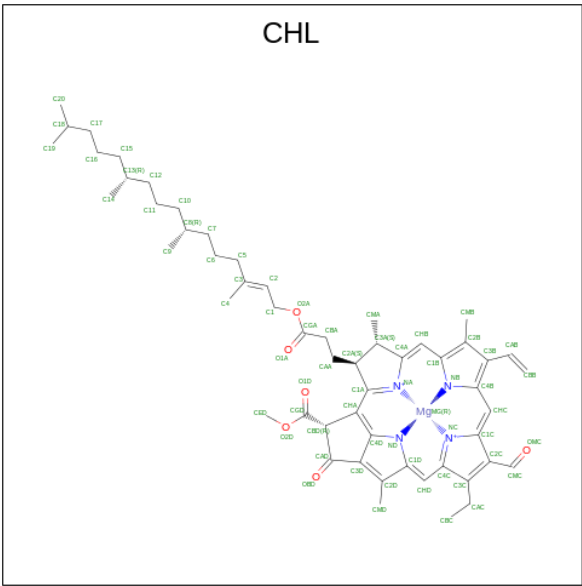
- Molecule 23 is a protein called Photosystem II reaction center protein X.

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

- Molecule 24 is a protein called Photosystem II reaction center protein Z.

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

- Molecule 25 is CHLOROPHYLL B (three-letter code: CHL) (formula: C₅₅H₇₀MgN₄O₆).



Mol	Chain	Residues	Atoms					AltConf
25	1	1	Total	C	Mg	N	O	0
			309	243	6	24	36	
			Total	C	Mg	N	O	
			309	243	6	24	36	
			Total	C	Mg	N	O	
25	1	1	309	243	6	24	36	0
			Total	C	Mg	N	O	
			309	243	6	24	36	
			Total	C	Mg	N	O	
			309	243	6	24	36	
25	2	1	Total	C	Mg	N	O	0
			306	240	6	24	36	
			Total	C	Mg	N	O	
			306	240	6	24	36	
			Total	C	Mg	N	O	
25	2	1	306	240	6	24	36	0
			Total	C	Mg	N	O	
			306	240	6	24	36	
			Total	C	Mg	N	O	
			306	240	6	24	36	
25	3	1	Total	C	Mg	N	O	0
			316	250	6	24	36	
			Total	C	Mg	N	O	
			316	250	6	24	36	
			Total	C	Mg	N	O	

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Mol	Chain	Residues	Atoms					AltConf
25	3	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	3	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	3	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	3	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	3	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	4	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	4	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	4	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	4	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	4	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	G	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	G	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	G	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	G	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	G	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	G	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	N	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	N	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	N	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	N	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	N	1	Total 362	C 296	Mg 6	N 24	O 36	0

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Mol	Chain	Residues	Atoms					AltConf
25	N	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	R	1	Total 225	C 183	Mg 4	N 16	O 22	0
25	R	1	Total 225	C 183	Mg 4	N 16	O 22	0
25	R	1	Total 225	C 183	Mg 4	N 16	O 22	0
25	R	1	Total 225	C 183	Mg 4	N 16	O 22	0
25	S	1	Total 196	C 152	Mg 4	N 16	O 24	0
25	S	1	Total 196	C 152	Mg 4	N 16	O 24	0
25	S	1	Total 196	C 152	Mg 4	N 16	O 24	0
25	S	1	Total 196	C 152	Mg 4	N 16	O 24	0
25	Y	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	Y	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	Y	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	Y	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	Y	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	Y	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	5	1	Total 309	C 243	Mg 6	N 24	O 36	0
25	5	1	Total 309	C 243	Mg 6	N 24	O 36	0
25	5	1	Total 309	C 243	Mg 6	N 24	O 36	0
25	5	1	Total 309	C 243	Mg 6	N 24	O 36	0
25	5	1	Total 309	C 243	Mg 6	N 24	O 36	0
25	5	1	Total 309	C 243	Mg 6	N 24	O 36	0

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Mol	Chain	Residues	Atoms					AltConf
25	6	1	Total 306	C 240	Mg 6	N 24	O 36	0
25	6	1	Total 306	C 240	Mg 6	N 24	O 36	0
25	6	1	Total 306	C 240	Mg 6	N 24	O 36	0
25	6	1	Total 306	C 240	Mg 6	N 24	O 36	0
25	6	1	Total 306	C 240	Mg 6	N 24	O 36	0
25	6	1	Total 306	C 240	Mg 6	N 24	O 36	0
25	7	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	7	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	7	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	7	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	7	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	7	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	7	1	Total 316	C 250	Mg 6	N 24	O 36	0
25	8	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	8	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	8	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	8	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	8	1	Total 229	C 174	Mg 5	N 20	O 30	0
25	g	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	g	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	g	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	g	1	Total 355	C 289	Mg 6	N 24	O 36	0

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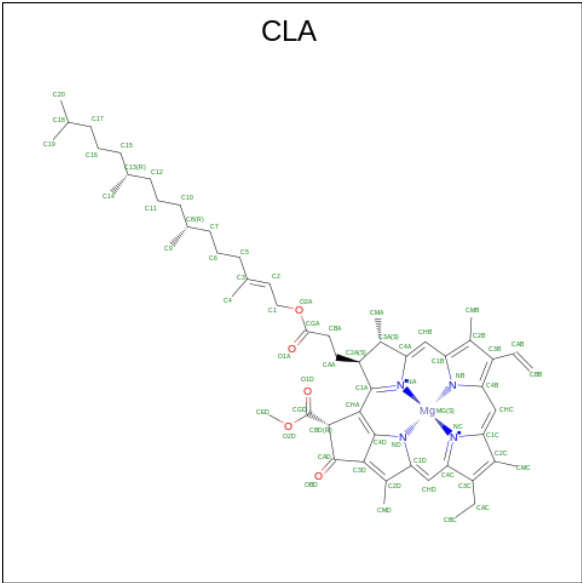
Mol	Chain	Residues	Atoms					AltConf
25	g	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	g	1	Total 355	C 289	Mg 6	N 24	O 36	0
25	n	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	n	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	n	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	n	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	n	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	n	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	r	1	Total 225	C 183	Mg 4	N 16	O 22	0
25	r	1	Total 225	C 183	Mg 4	N 16	O 22	0
25	r	1	Total 225	C 183	Mg 4	N 16	O 22	0
25	r	1	Total 225	C 183	Mg 4	N 16	O 22	0
25	s	1	Total 196	C 152	Mg 4	N 16	O 24	0
25	s	1	Total 196	C 152	Mg 4	N 16	O 24	0
25	s	1	Total 196	C 152	Mg 4	N 16	O 24	0
25	s	1	Total 196	C 152	Mg 4	N 16	O 24	0
25	y	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	y	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	y	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	y	1	Total 362	C 296	Mg 6	N 24	O 36	0
25	y	1	Total 362	C 296	Mg 6	N 24	O 36	0

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Mol	Chain	Residues	Atoms					AltConf
25	y	1	Total	C	Mg	N	O	0
			362	296	6	24	36	

- Molecule 26 is CHLOROPHYLL A (three-letter code: CLA) (formula: C₅₅H₇₂MgN₄O₅).



Mol	Chain	Residues	Atoms					AltConf
26	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
26	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
26	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
26	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
26	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
26	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
26	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
26	1	1	Total	C	Mg	N	O	0
			412	332	8	32	40	
26	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	
26	2	1	Total	C	Mg	N	O	0
			391	311	8	32	40	

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Mol	Chain	Residues	Atoms					AltConf
26	2	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	2	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	2	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	2	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	2	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	2	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	3	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	3	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	3	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	3	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	3	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	3	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	3	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	3	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	3	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	4	1	Total 270	C 210	Mg 6	N 24	O 30	0
26	4	1	Total 270	C 210	Mg 6	N 24	O 30	0
26	4	1	Total 270	C 210	Mg 6	N 24	O 30	0
26	4	1	Total 270	C 210	Mg 6	N 24	O 30	0
26	4	1	Total 270	C 210	Mg 6	N 24	O 30	0
26	4	1	Total 270	C 210	Mg 6	N 24	O 30	0
26	A	1	Total 240	C 200	Mg 4	N 16	O 20	0

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

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Mol	Chain	Residues	Atoms					AltConf
26	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
26	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
26	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
26	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
26	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
26	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
26	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
26	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
26	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
26	C	1	Total 845	C 715	Mg 13	N 52	O 65	0
26	D	1	Total 130	C 110	Mg 2	N 8	O 10	0
26	D	1	Total 130	C 110	Mg 2	N 8	O 10	0
26	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
26	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
26	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
26	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
26	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
26	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
26	G	1	Total 477	C 397	Mg 8	N 32	O 40	0
26	G	1	Total 477	C 397	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
26	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	N	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	R	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0

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Mol	Chain	Residues	Atoms					AltConf
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	S	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	Y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
26	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
26	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
26	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
26	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
26	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
26	5	1	Total 412	C 332	Mg 8	N 32	O 40	0

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Mol	Chain	Residues	Atoms					AltConf
26	5	1	Total 412	C 332	Mg 8	N 32	O 40	0
26	6	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	6	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	6	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	6	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	6	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	6	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	6	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	6	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	6	1	Total 391	C 311	Mg 8	N 32	O 40	0
26	7	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	7	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	7	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	7	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	7	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	7	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	7	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	7	1	Total 426	C 346	Mg 8	N 32	O 40	0
26	8	1	Total 270	C 210	Mg 6	N 24	O 30	0
26	8	1	Total 270	C 210	Mg 6	N 24	O 30	0
26	8	1	Total 270	C 210	Mg 6	N 24	O 30	0
26	8	1	Total 270	C 210	Mg 6	N 24	O 30	0

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Mol	Chain	Residues	Atoms					AltConf
26	8	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
26	8	1	Total	C	Mg	N	O	0
			270	210	6	24	30	
26	a	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
26	a	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
26	a	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
26	a	1	Total	C	Mg	N	O	0
			240	200	4	16	20	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	

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Mol	Chain	Residues	Atoms					AltConf
26	b	1	Total	C	Mg	N	O	0
			1040	880	16	64	80	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	c	1	Total	C	Mg	N	O	0
			845	715	13	52	65	
26	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
26	d	1	Total	C	Mg	N	O	0
			130	110	2	8	10	
26	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
26	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
26	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
26	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	
26	g	1	Total	C	Mg	N	O	0
			477	397	8	32	40	

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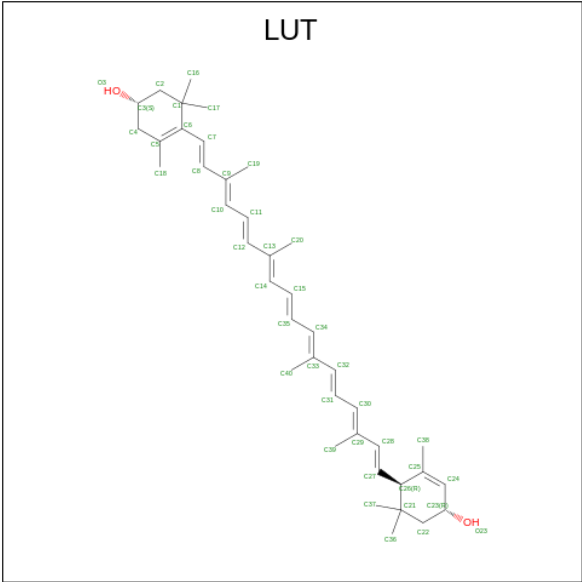
Mol	Chain	Residues	Atoms					AltConf
26	g	1	Total 477	C 397	Mg 8	N 32	O 40	0
26	g	1	Total 477	C 397	Mg 8	N 32	O 40	0
26	g	1	Total 477	C 397	Mg 8	N 32	O 40	0
26	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	n	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	r	1	Total 543	C 443	Mg 10	N 40	O 50	0
26	r	1	Total 543	C 443	Mg 10	N 40	O 50	0

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Mol	Chain	Residues	Atoms					AltConf
26	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	s	1	Total 465	C 375	Mg 9	N 36	O 45	0
26	y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	y	1	Total 473	C 393	Mg 8	N 32	O 40	0
26	y	1	Total 473	C 393	Mg 8	N 32	O 40	0

- Molecule 27 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
27	1	1	Total	C	O	0
			84	80	4	
27	1	1	Total	C	O	0
			84	80	4	
27	2	1	Total	C	O	0
			84	80	4	
27	2	1	Total	C	O	0
			84	80	4	
27	3	1	Total	C	O	0
			84	80	4	
27	3	1	Total	C	O	0
			84	80	4	
27	4	1	Total	C	O	0
			42	40	2	
27	G	1	Total	C	O	0
			84	80	4	
27	G	1	Total	C	O	0
			84	80	4	
27	N	1	Total	C	O	0
			84	80	4	
27	N	1	Total	C	O	0
			84	80	4	
27	R	1	Total	C	O	0
			42	40	2	
27	S	1	Total	C	O	0
			84	80	4	
27	S	1	Total	C	O	0
			84	80	4	

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Mol	Chain	Residues	Atoms			AltConf
27	Y	1	Total	C	O	0
			84	80	4	
27	Y	1	Total	C	O	0
			84	80	4	
27	5	1	Total	C	O	0
			84	80	4	
27	5	1	Total	C	O	0
			84	80	4	
27	6	1	Total	C	O	0
			84	80	4	
27	6	1	Total	C	O	0
			84	80	4	
27	7	1	Total	C	O	0
			84	80	4	
27	7	1	Total	C	O	0
			84	80	4	
27	8	1	Total	C	O	0
			42	40	2	
27	g	1	Total	C	O	0
			84	80	4	
27	g	1	Total	C	O	0
			84	80	4	
27	n	1	Total	C	O	0
			84	80	4	
27	n	1	Total	C	O	0
			84	80	4	
27	r	1	Total	C	O	0
			42	40	2	
27	s	1	Total	C	O	0
			84	80	4	
27	s	1	Total	C	O	0
			84	80	4	
27	y	1	Total	C	O	0
			84	80	4	
27	y	1	Total	C	O	0
			84	80	4	

- Molecule 28 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).

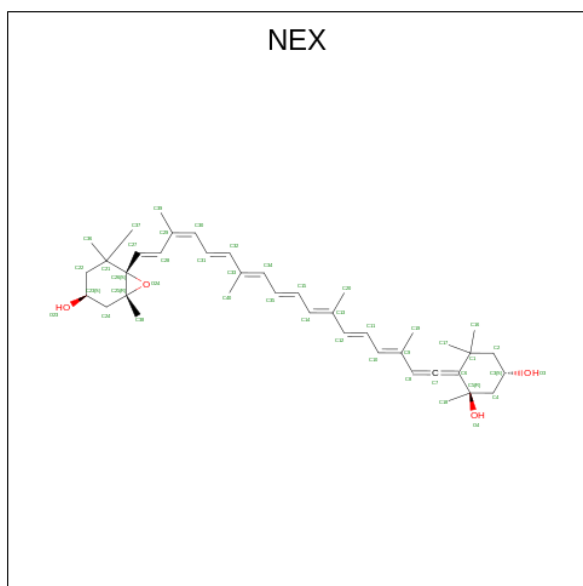


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Mol	Chain	Residues	Atoms			AltConf
28	r	1	Total	C	O	0
			44	40	4	
28	y	1	Total	C	O	0
			44	40	4	

- Molecule 29 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-TETRAMETHYLOCTADEC-1,3,5,7,9,11,13,15,17-NONAENYLIDENE]-1,5,5-TRIMETHYLCYCLOHEXANE-1,3-DIOL (three-letter code: NEX) (formula: C₄₀H₅₆O₄).



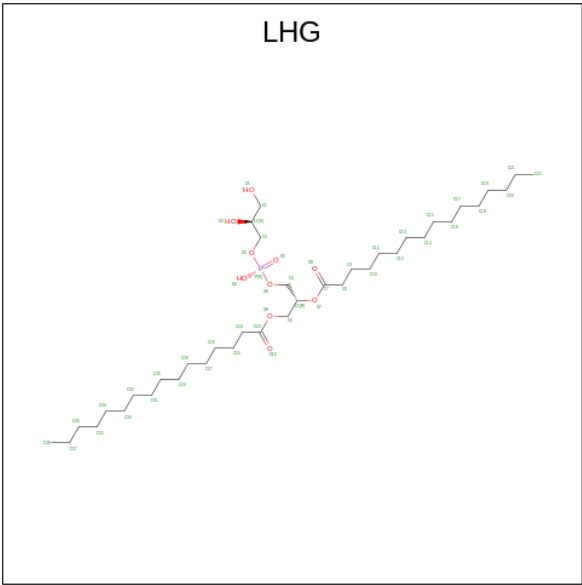
Mol	Chain	Residues	Atoms			AltConf
29	1	1	Total	C	O	0
			44	40	4	
29	2	1	Total	C	O	0
			44	40	4	
29	3	1	Total	C	O	0
			44	40	4	
29	G	1	Total	C	O	0
			44	40	4	
29	N	1	Total	C	O	0
			44	40	4	
29	R	1	Total	C	O	0
			44	40	4	
29	S	1	Total	C	O	0
			44	40	4	
29	Y	1	Total	C	O	0
			44	40	4	

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Mol	Chain	Residues	Atoms			AltConf
29	5	1	Total	C	O	0
			44	40	4	
29	6	1	Total	C	O	0
			44	40	4	
29	7	1	Total	C	O	0
			44	40	4	
29	g	1	Total	C	O	0
			44	40	4	
29	n	1	Total	C	O	0
			44	40	4	
29	r	1	Total	C	O	0
			44	40	4	
29	s	1	Total	C	O	0
			44	40	4	
29	y	1	Total	C	O	0
			44	40	4	

- Molecule 30 is 1,2-DIPALMITOYL-PHOSPHATIDYL-GLYCEROLE (three-letter code: LHG) (formula: C₃₈H₇₅O₁₀P).



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

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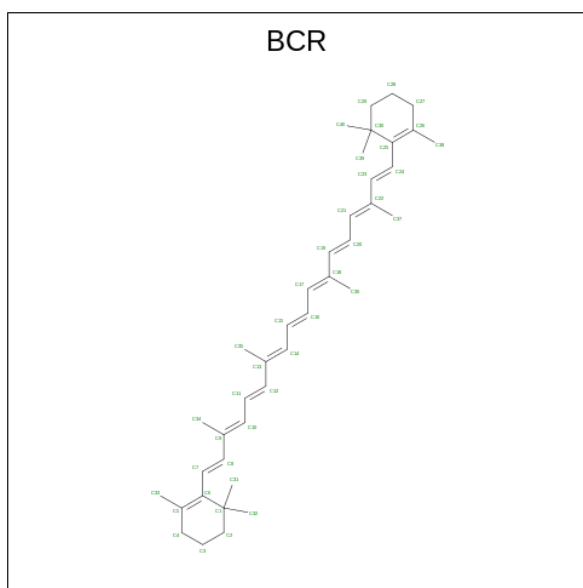
Mol	Chain	Residues	Atoms				AltConf
30	4	1	Total	C	O	P	0
			21	10	10	1	
30	B	1	Total	C	O	P	0
			96	74	20	2	
30	B	1	Total	C	O	P	0
			96	74	20	2	
30	C	1	Total	C	O	P	0
			147	114	30	3	
30	C	1	Total	C	O	P	0
			147	114	30	3	
30	C	1	Total	C	O	P	0
			147	114	30	3	
30	D	1	Total	C	O	P	0
			138	105	30	3	
30	D	1	Total	C	O	P	0
			138	105	30	3	
30	D	1	Total	C	O	P	0
			138	105	30	3	
30	G	1	Total	C	O	P	0
			49	38	10	1	
30	L	1	Total	C	O	P	0
			49	38	10	1	
30	N	1	Total	C	O	P	0
			49	38	10	1	
30	R	1	Total	C	O	P	0
			42	31	10	1	
30	S	1	Total	C	O	P	0
			49	38	10	1	
30	Y	1	Total	C	O	P	0
			49	38	10	1	
30	5	1	Total	C	O	P	0
			41	30	10	1	
30	6	1	Total	C	O	P	0
			37	26	10	1	
30	7	1	Total	C	O	P	0
			47	36	10	1	
30	8	1	Total	C	O	P	0
			21	10	10	1	
30	b	1	Total	C	O	P	0
			96	74	20	2	
30	b	1	Total	C	O	P	0
			96	74	20	2	

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Mol	Chain	Residues	Atoms				AltConf
30	c	1	Total	C	O	P	0
			147	114	30	3	
30	c	1	Total	C	O	P	0
			147	114	30	3	
30	c	1	Total	C	O	P	0
			147	114	30	3	
30	d	1	Total	C	O	P	0
			138	105	30	3	
30	d	1	Total	C	O	P	0
			138	105	30	3	
30	d	1	Total	C	O	P	0
			138	105	30	3	
30	g	1	Total	C	O	P	0
			49	38	10	1	
30	l	1	Total	C	O	P	0
			49	38	10	1	
30	n	1	Total	C	O	P	0
			49	38	10	1	
30	r	1	Total	C	O	P	0
			42	31	10	1	
30	s	1	Total	C	O	P	0
			49	38	10	1	
30	y	1	Total	C	O	P	0
			49	38	10	1	

- Molecule 31 is BETA-CAROTENE (three-letter code: BCR) (formula: $C_{40}H_{56}$).



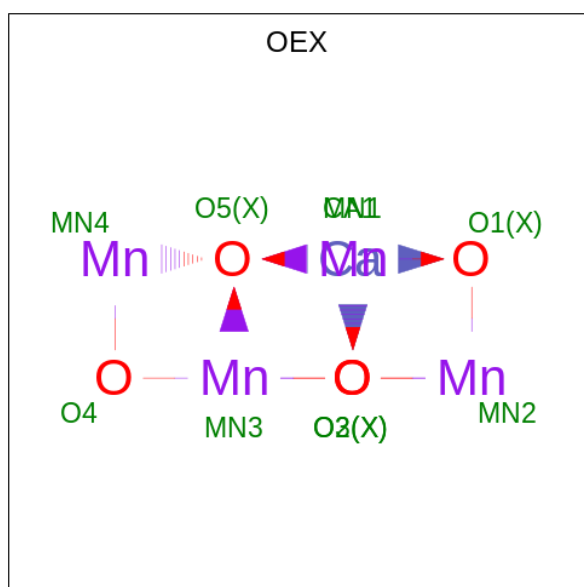
Mol	Chain	Residues	Atoms	AltConf
31	4	1	Total C 40 40	0
31	A	1	Total C 40 40	0
31	B	1	Total C 120 120	0
31	B	1	Total C 120 120	0
31	B	1	Total C 120 120	0
31	C	1	Total C 160 160	0
31	C	1	Total C 160 160	0
31	C	1	Total C 160 160	0
31	C	1	Total C 160 160	0
31	D	1	Total C 40 40	0
31	H	1	Total C 40 40	0
31	T	1	Total C 40 40	0
31	8	1	Total C 40 40	0
31	a	1	Total C 40 40	0
31	b	1	Total C 120 120	0
31	b	1	Total C 120 120	0
31	b	1	Total C 120 120	0
31	c	1	Total C 160 160	0
31	c	1	Total C 160 160	0
31	c	1	Total C 160 160	0
31	c	1	Total C 160 160	0
31	d	1	Total C 40 40	0

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

- Molecule 32 is CA-MN4-O5 CLUSTER (three-letter code: OEX) (formula: CaMn_4O_5).



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

- Molecule 33 is FE (II) ION (three-letter code: FE2) (formula: Fe).

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

- Molecule 34 is CHLORIDE ION (three-letter code: CL) (formula: Cl).

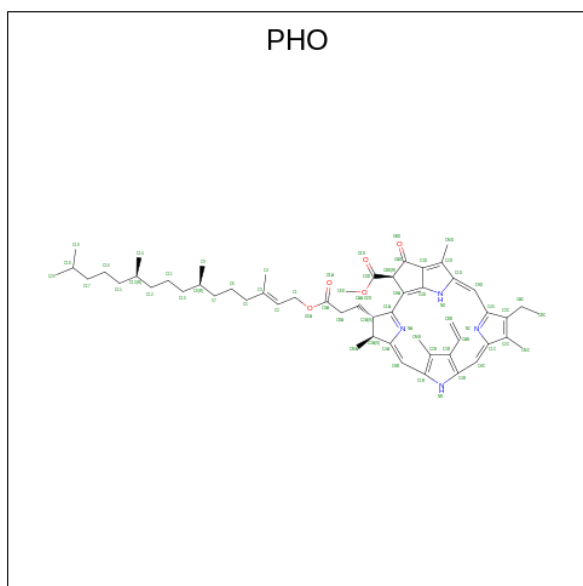
Mol	Chain	Residues	Atoms		AltConf
34	A	2	Total	Cl	0
			2	2	

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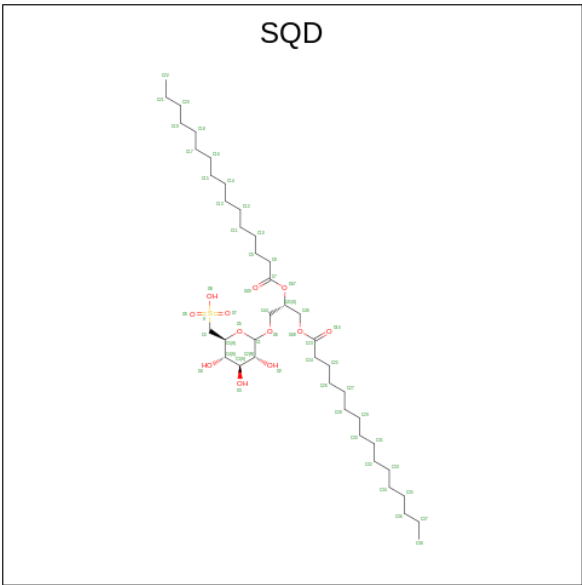
Mol	Chain	Residues	Atoms		AltConf
34	a	2	Total	Cl	0
			2	2	

- Molecule 35 is PHEOPHYTIN A (three-letter code: PHO) (formula: $C_{55}H_{74}N_4O_5$).



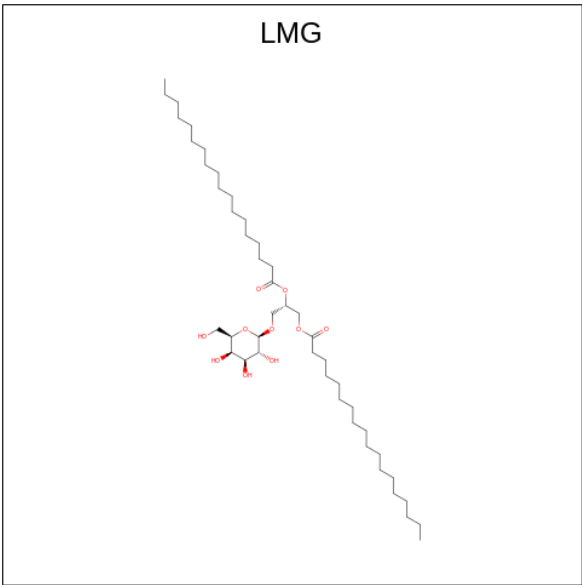
Mol	Chain	Residues	Atoms				AltConf
35	A	1	Total	C	N	O	0
			128	110	8	10	
35	A	1	Total	C	N	O	0
			128	110	8	10	
35	a	1	Total	C	N	O	0
			128	110	8	10	
35	a	1	Total	C	N	O	0
			128	110	8	10	

- Molecule 36 is 1,2-DI-O-ACYL-3-O-[6-DEOXY-6-SULFO-ALPHA-D-GLUCOPYRANOSYL]-SN-GLYCEROL (three-letter code: SQD) (formula: $C_{41}H_{78}O_{12}S$).



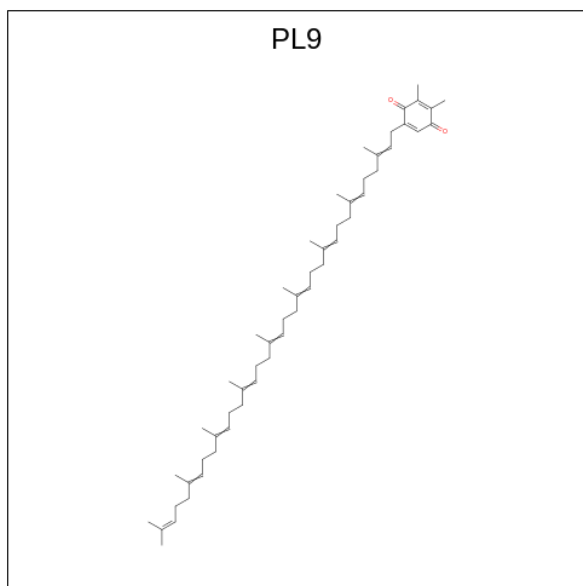
Mol	Chain	Residues	Atoms				AltConf
36	A	1	Total	C	O	S	0
			104	78	24	2	
36	A	1	Total	C	O	S	0
			104	78	24	2	
36	B	1	Total	C	O	S	0
			96	70	24	2	
36	B	1	Total	C	O	S	0
			96	70	24	2	
36	a	1	Total	C	O	S	0
			104	78	24	2	
36	a	1	Total	C	O	S	0
			104	78	24	2	
36	b	1	Total	C	O	S	0
			96	70	24	2	
36	b	1	Total	C	O	S	0
			96	70	24	2	

- Molecule 37 is 1,2-DISTEAROYL-MONOGALACTOSYL-DIGLYCERIDE (three-letter code: LMG) (formula: C₄₅H₈₆O₁₀).



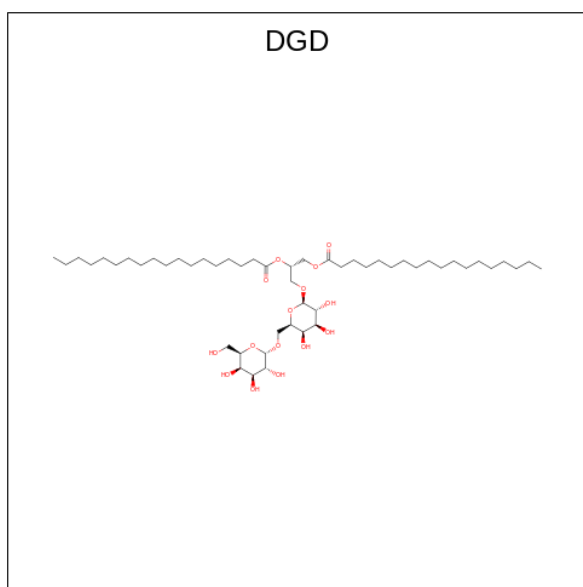
Mol	Chain	Residues	Atoms			AltConf
37	A	1	Total	C	O	0
			88	68	20	
37	A	1	Total	C	O	0
			88	68	20	
37	B	1	Total	C	O	0
			106	86	20	
37	B	1	Total	C	O	0
			106	86	20	
37	C	1	Total	C	O	0
			51	41	10	
37	D	1	Total	C	O	0
			46	36	10	
37	Z	1	Total	C	O	0
			51	41	10	
37	a	1	Total	C	O	0
			88	68	20	
37	a	1	Total	C	O	0
			88	68	20	
37	b	1	Total	C	O	0
			106	86	20	
37	b	1	Total	C	O	0
			106	86	20	
37	c	1	Total	C	O	0
			51	41	10	
37	d	1	Total	C	O	0
			46	36	10	
37	z	1	Total	C	O	0
			51	41	10	

- Molecule 38 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: $C_{53}H_{80}O_2$).



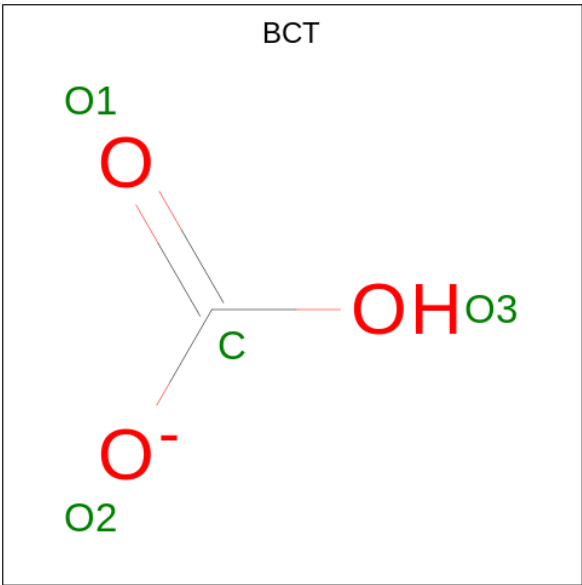
Mol	Chain	Residues	Atoms			AltConf
38	A	1	Total	C	O	0
			13	11	2	
38	D	1	Total	C	O	0
			55	53	2	
38	a	1	Total	C	O	0
			13	11	2	
38	d	1	Total	C	O	0
			55	53	2	

- Molecule 39 is DIGALACTOSYL DIACYL GLYCEROL (DGDG) (three-letter code: DGD) (formula: $C_{51}H_{96}O_{15}$).



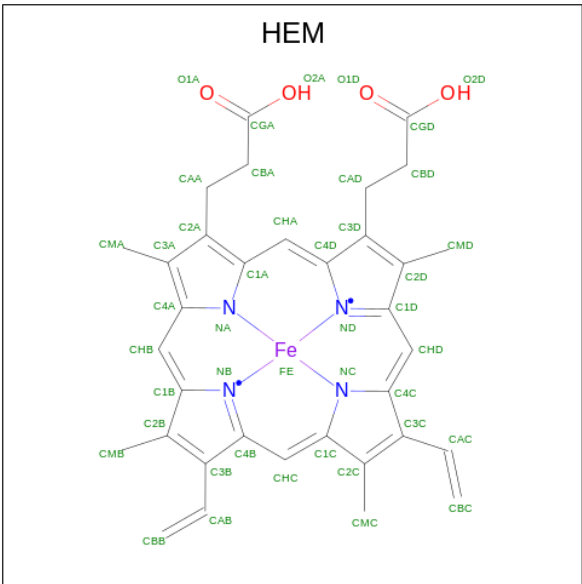
Mol	Chain	Residues	Atoms			AltConf
39	B	1	Total	C	O	0
			59	44	15	
39	C	1	Total	C	O	0
			177	132	45	
39	C	1	Total	C	O	0
			177	132	45	
39	C	1	Total	C	O	0
			177	132	45	
39	H	1	Total	C	O	0
			62	47	15	
39	b	1	Total	C	O	0
			59	44	15	
39	c	1	Total	C	O	0
			177	132	45	
39	c	1	Total	C	O	0
			177	132	45	
39	c	1	Total	C	O	0
			177	132	45	
39	h	1	Total	C	O	0
			62	47	15	

- Molecule 40 is BICARBONATE ION (three-letter code: BCT) (formula: CHO_3).



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

- Molecule 41 is PROTOPORPHYRIN IX CONTAINING FE (three-letter code: HEM) (formula: C₃₄H₃₂FeN₄O₄).



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

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

- Molecule 42 is water.

Mol	Chain	Residues	Atoms		AltConf
42	A	96	Total	O	0
			96	96	
42	B	89	Total	O	0
			89	89	
42	C	68	Total	O	0
			68	68	
42	D	58	Total	O	0
			58	58	
42	E	10	Total	O	0
			10	10	
42	F	2	Total	O	0
			2	2	
42	G	15	Total	O	0
			15	15	
42	H	16	Total	O	0
			16	16	
42	J	3	Total	O	0
			3	3	
42	K	2	Total	O	0
			2	2	
42	L	10	Total	O	0
			10	10	
42	M	4	Total	O	0
			4	4	
42	N	20	Total	O	0
			20	20	
42	O	31	Total	O	0
			31	31	
42	P	16	Total	O	0
			16	16	
42	R	30	Total	O	0
			30	30	
42	S	14	Total	O	0
			14	14	
42	T	2	Total	O	0
			2	2	

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Mol	Chain	Residues	Atoms	AltConf
42	W	4	Total O 4 4	0
42	X	5	Total O 5 5	0
42	Y	39	Total O 39 39	0
42	Z	4	Total O 4 4	0
42	a	96	Total O 96 96	0
42	b	89	Total O 89 89	0
42	c	68	Total O 68 68	0
42	d	58	Total O 58 58	0
42	e	10	Total O 10 10	0
42	f	2	Total O 2 2	0
42	g	15	Total O 15 15	0
42	h	16	Total O 16 16	0
42	j	3	Total O 3 3	0
42	k	2	Total O 2 2	0
42	l	10	Total O 10 10	0
42	m	4	Total O 4 4	0
42	n	20	Total O 20 20	0
42	o	31	Total O 31 31	0
42	p	16	Total O 16 16	0
42	r	30	Total O 30 30	0
42	s	14	Total O 14 14	0

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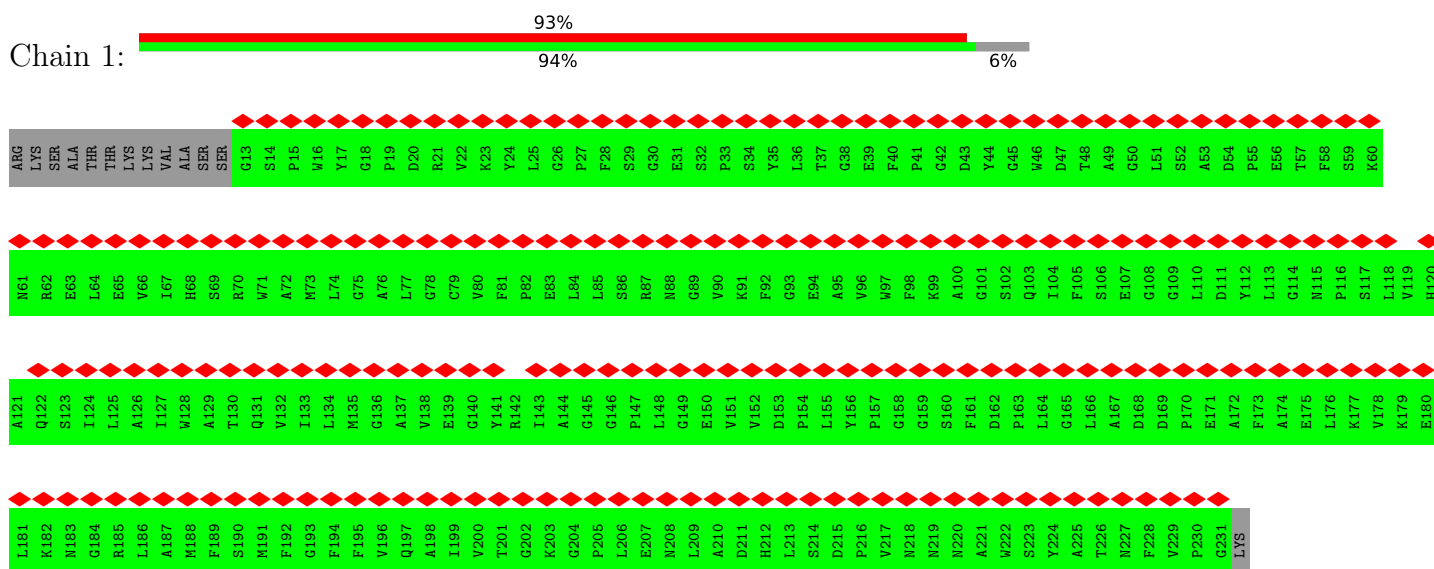
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Mol	Chain	Residues	Atoms		AltConf
42	t	2	Total 2	O 2	0
42	w	4	Total 4	O 4	0
42	x	5	Total 5	O 5	0
42	y	39	Total 39	O 39	0
42	z	4	Total 4	O 4	0

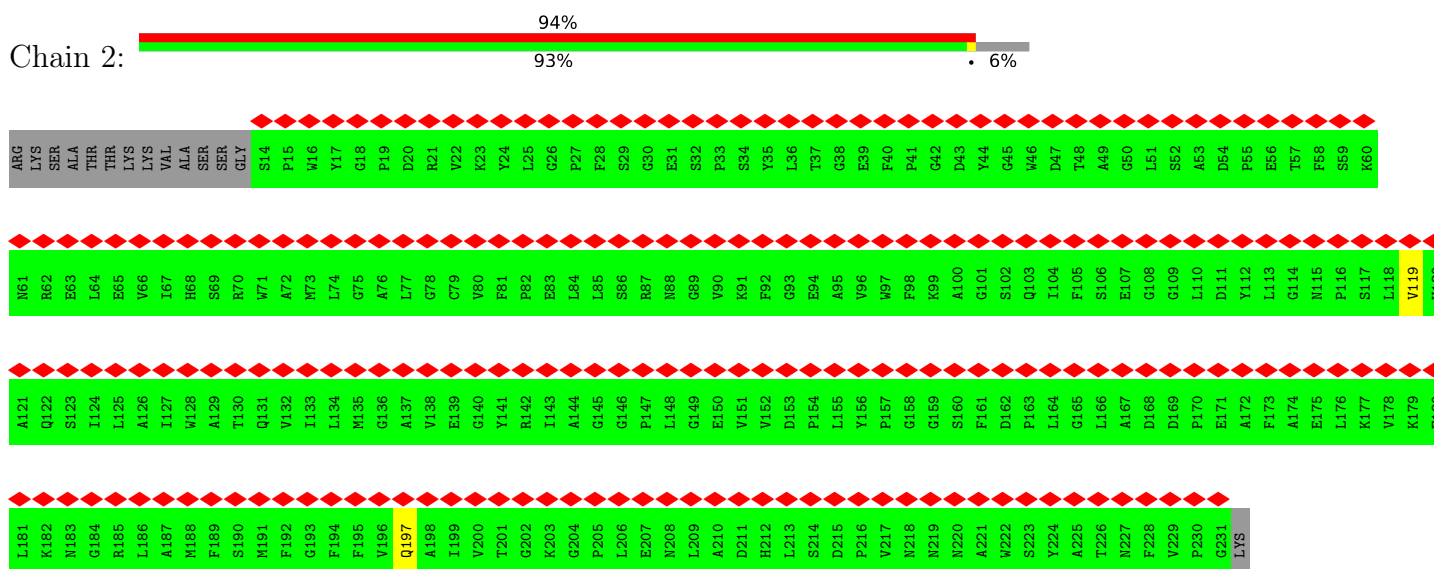
3 Residue-property plots

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

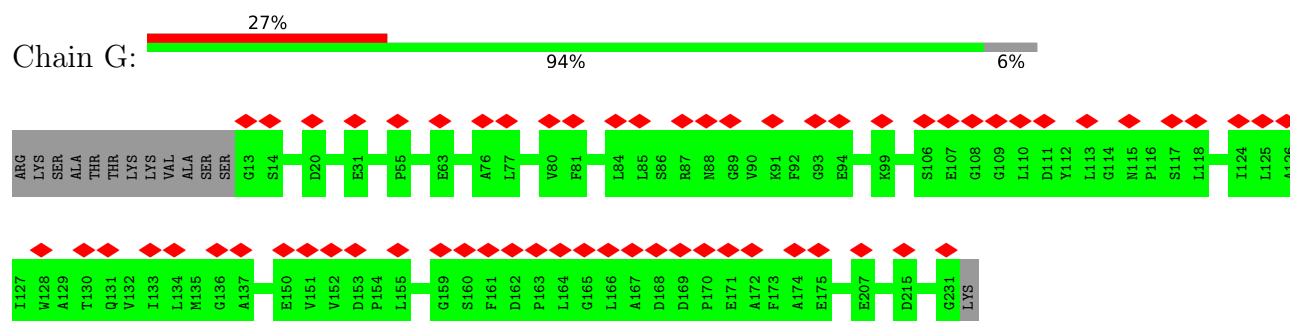
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



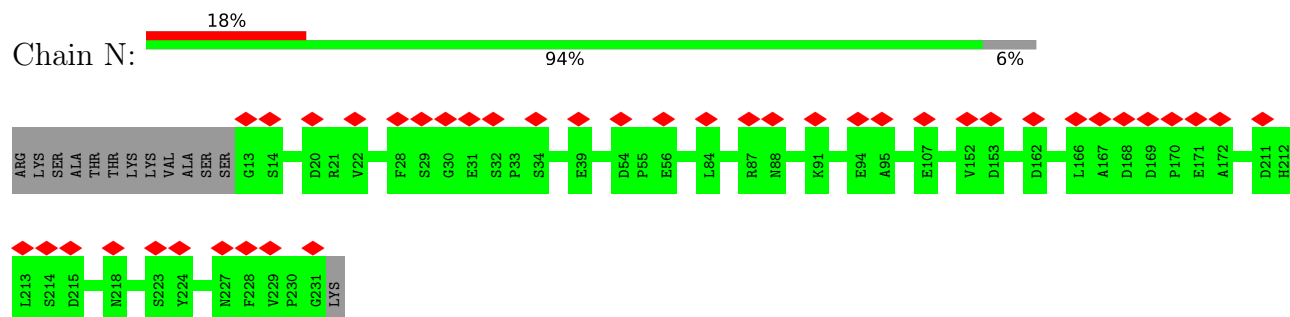
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



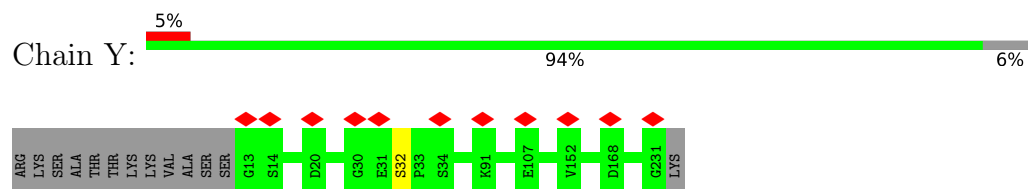
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



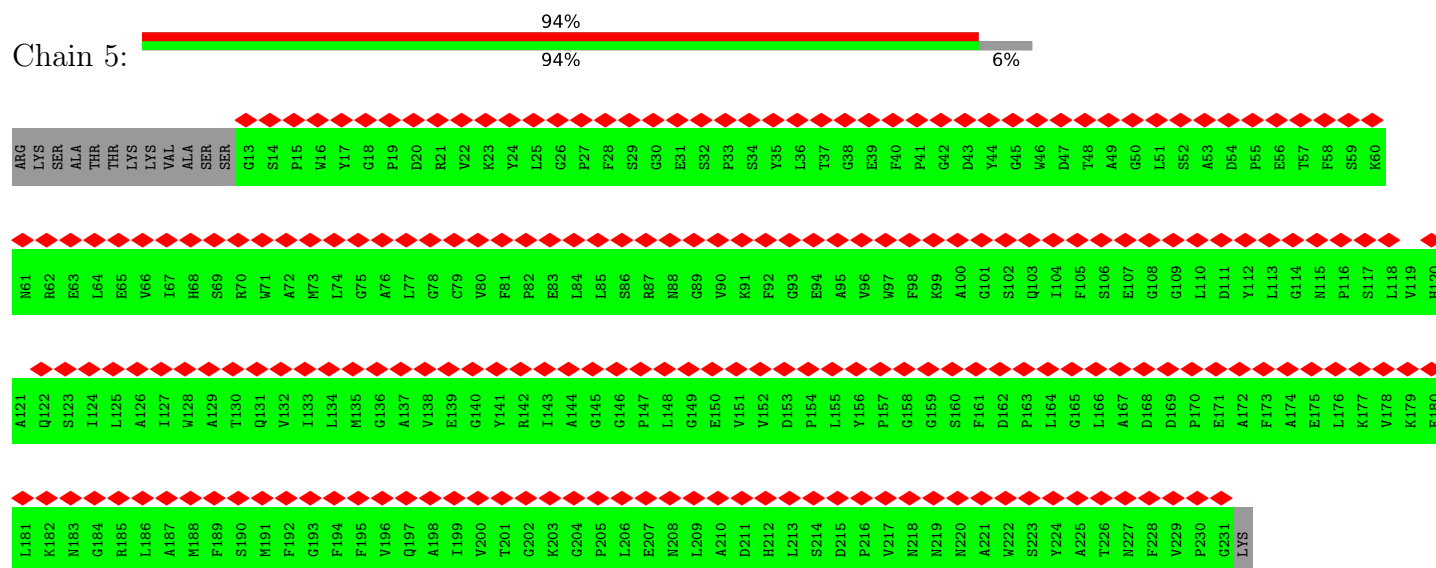
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



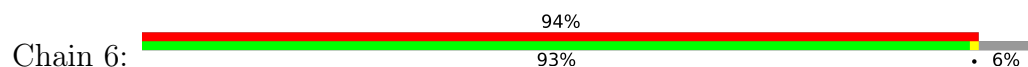
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

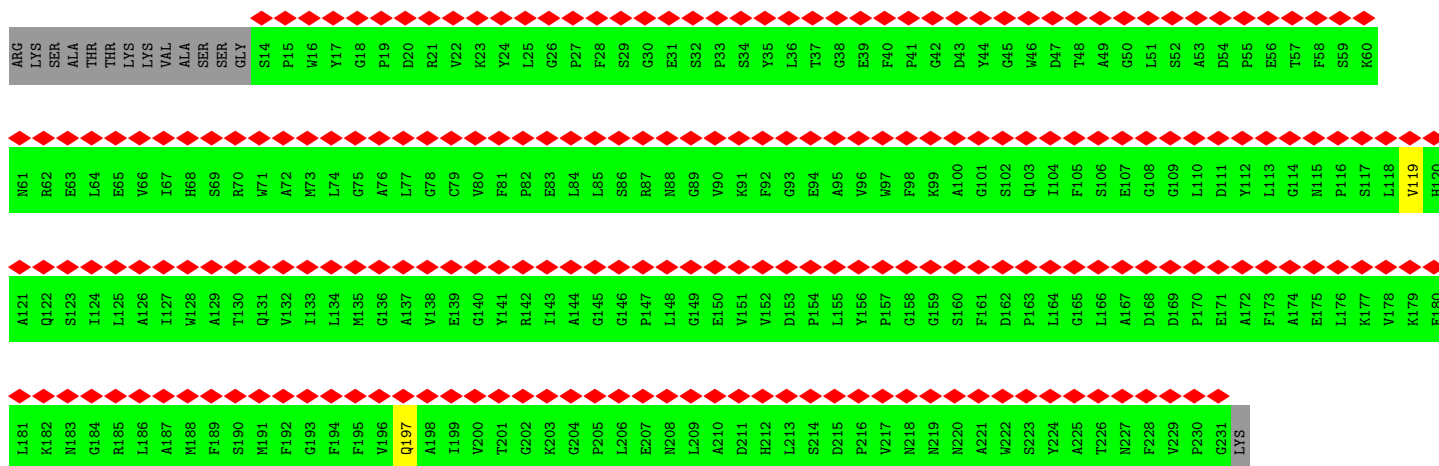


- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

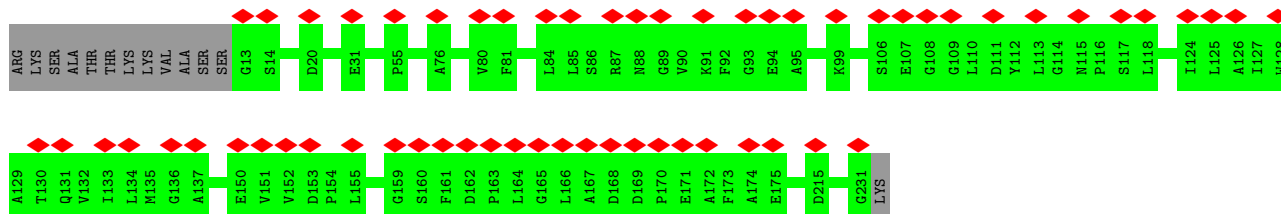
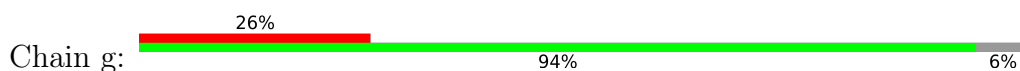


- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

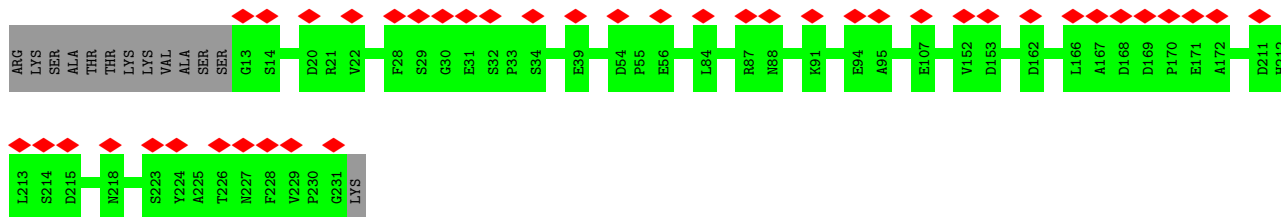




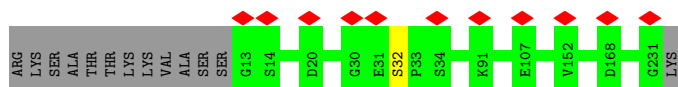
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic



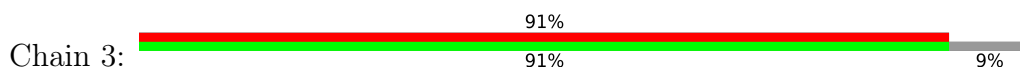
- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

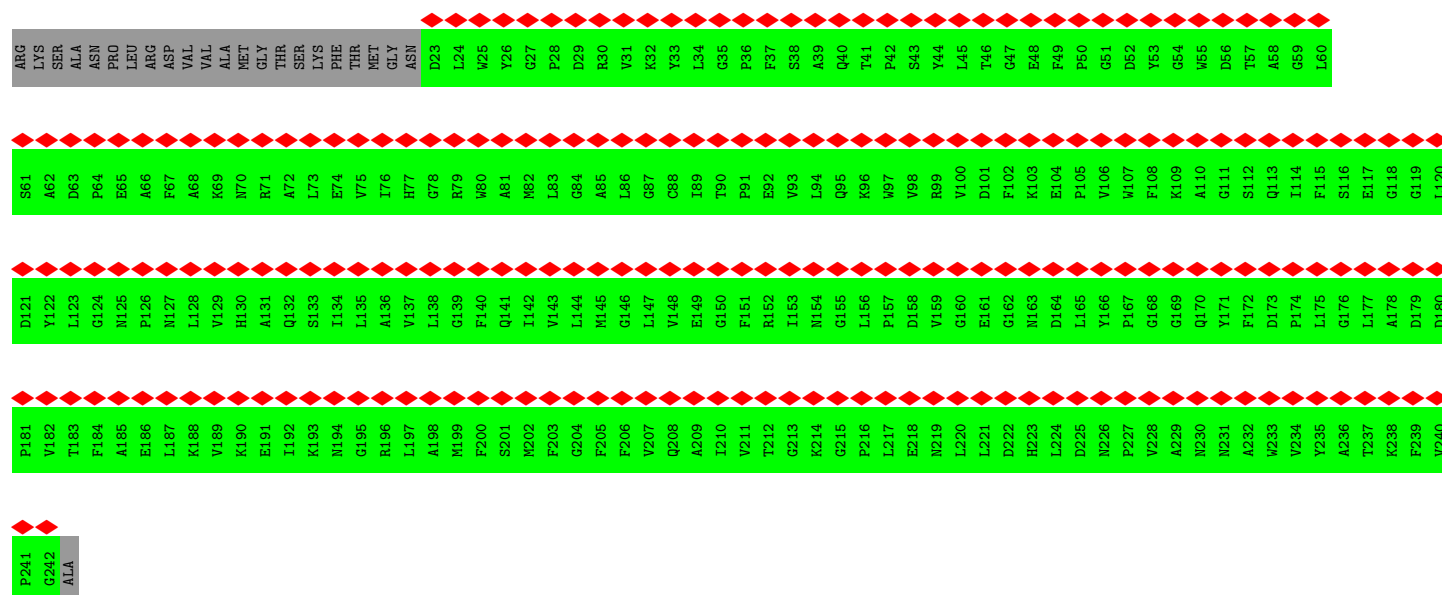


- Molecule 1: Chlorophyll a-b binding protein 8, chloroplastic

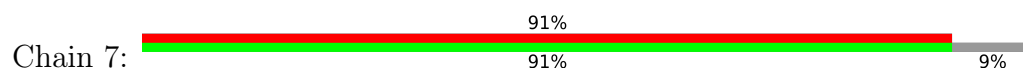


- Molecule 2: Chlorophyll a-b binding protein, chloroplastic

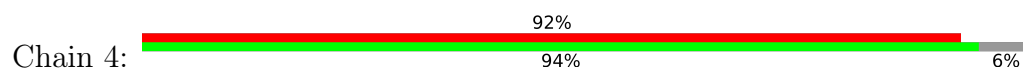


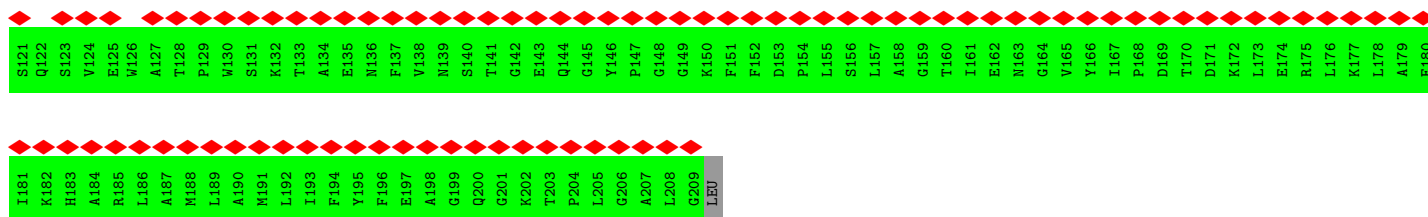


• Molecule 2: Chlorophyll a-b binding protein, chloroplastic

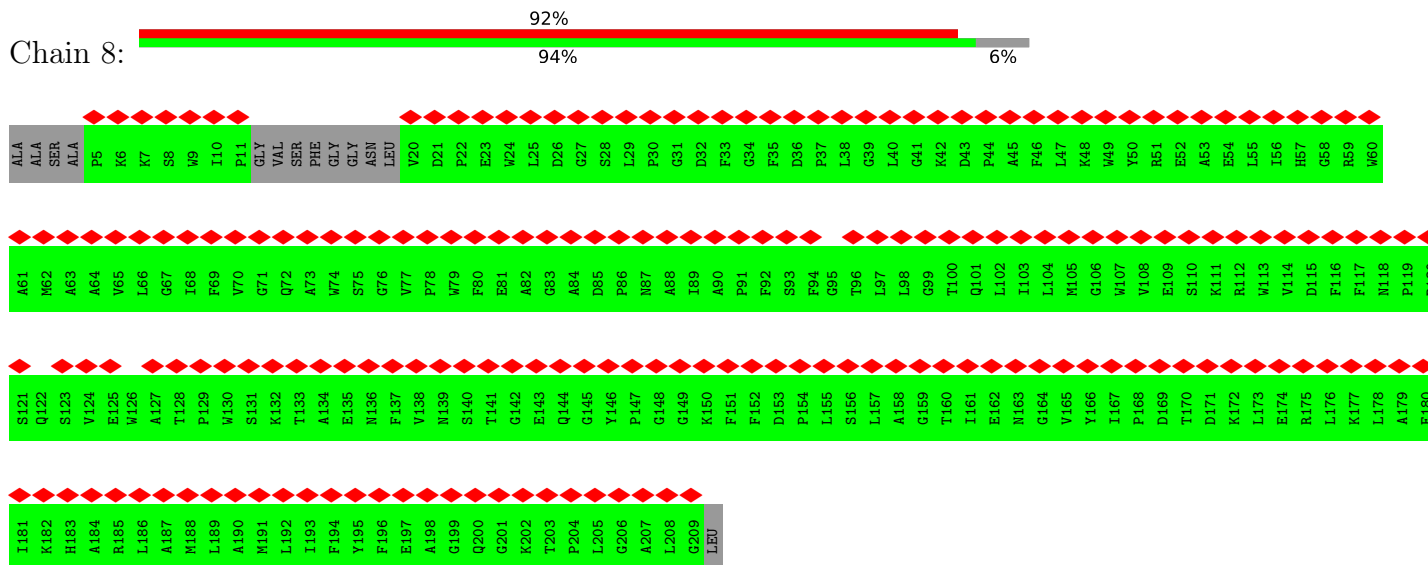


• Molecule 3: Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24

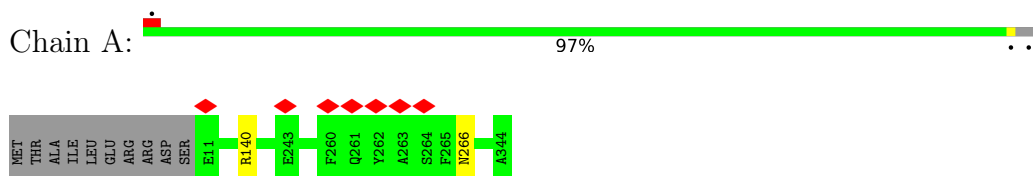




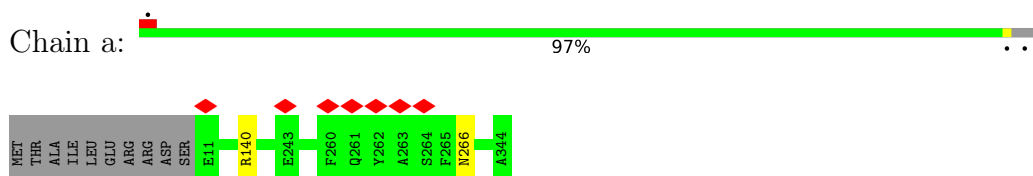
- Molecule 3: Light harvesting chlorophyll a/b-binding protein Lhcb6, CP24



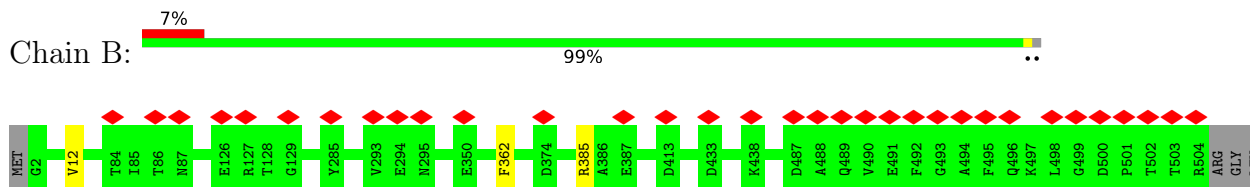
- Molecule 4: Photosystem II protein D1



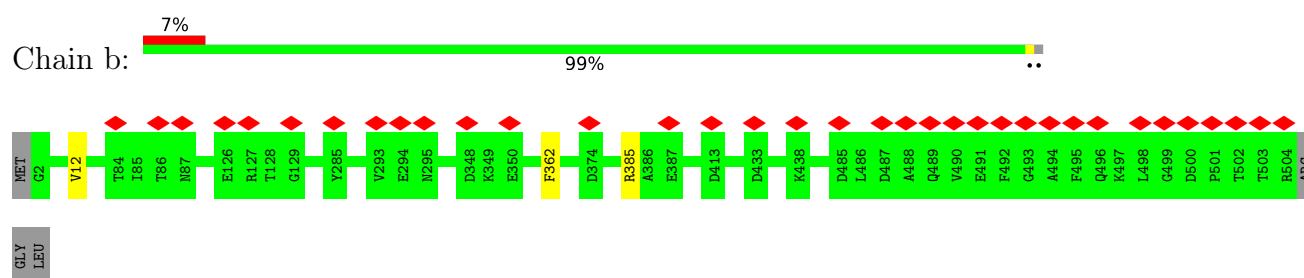
- Molecule 4: Photosystem II protein D1



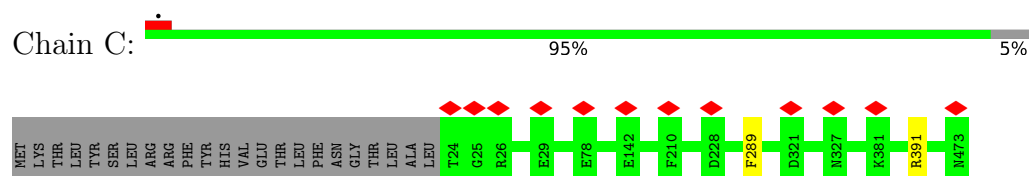
- Molecule 5: Photosystem II CP47 reaction center protein



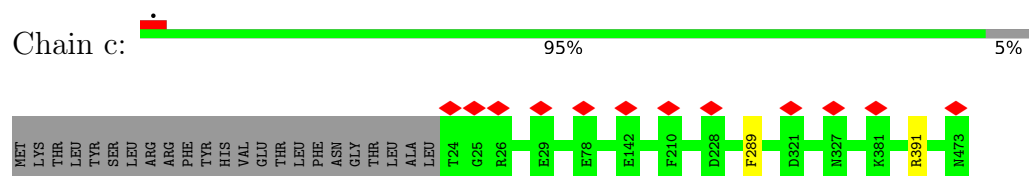
- Molecule 5: Photosystem II CP47 reaction center protein



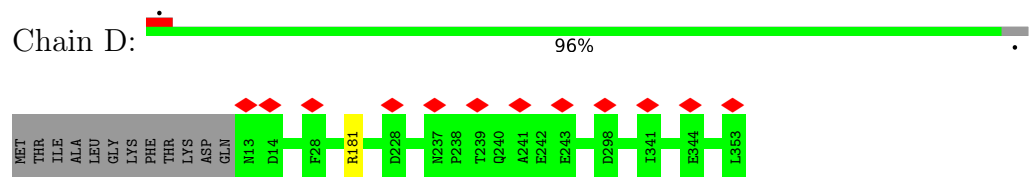
- Molecule 6: Photosystem II CP43 reaction center protein



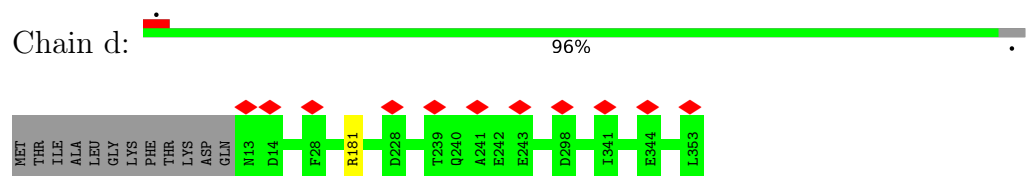
- Molecule 6: Photosystem II CP43 reaction center protein



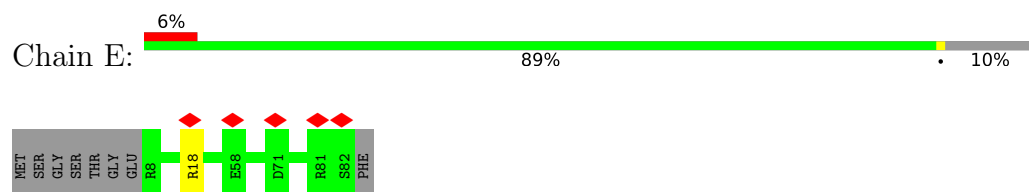
- Molecule 7: Photosystem II D2 protein



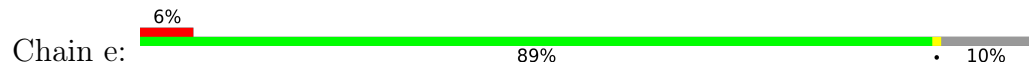
- Molecule 7: Photosystem II D2 protein

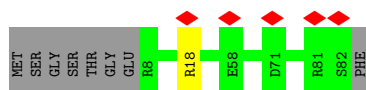


- Molecule 8: Cytochrome b559 subunit alpha

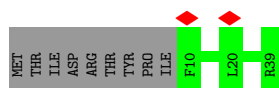
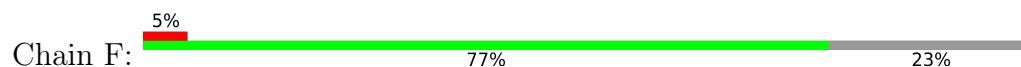


- Molecule 8: Cytochrome b559 subunit alpha

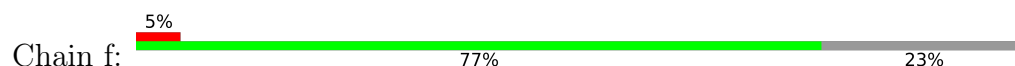




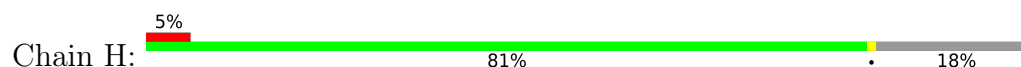
- Molecule 9: Cytochrome b559 subunit beta, PsbF



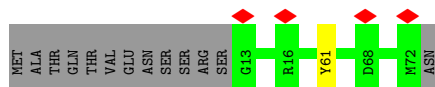
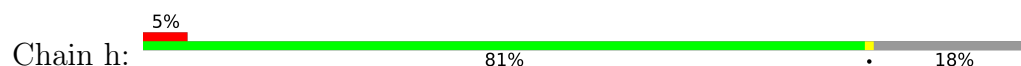
- Molecule 9: Cytochrome b559 subunit beta, PsbF



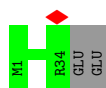
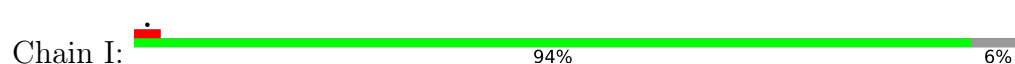
- Molecule 10: Photosystem II reaction center protein H



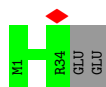
- Molecule 10: Photosystem II reaction center protein H



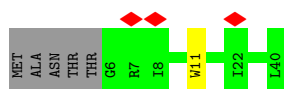
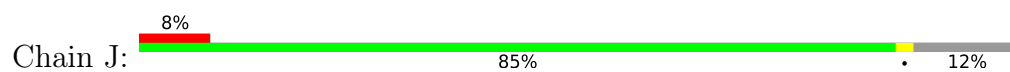
- Molecule 11: Photosystem II reaction center protein I, PsbI



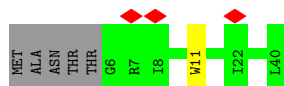
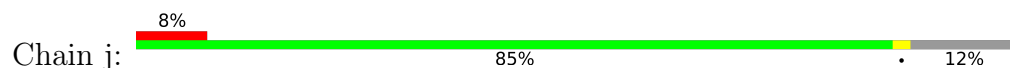
- Molecule 11: Photosystem II reaction center protein I, PsbI



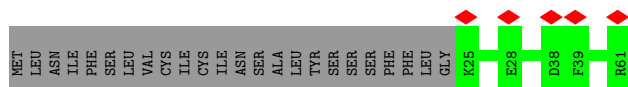
- Molecule 12: Photosystem II reaction center protein J



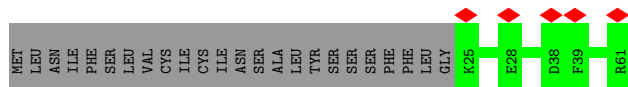
- Molecule 12: Photosystem II reaction center protein J



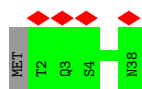
- Molecule 13: Photosystem II reaction center protein K



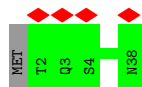
- Molecule 13: Photosystem II reaction center protein K



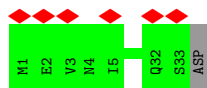
- Molecule 14: Photosystem II reaction center protein L



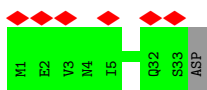
- Molecule 14: Photosystem II reaction center protein L



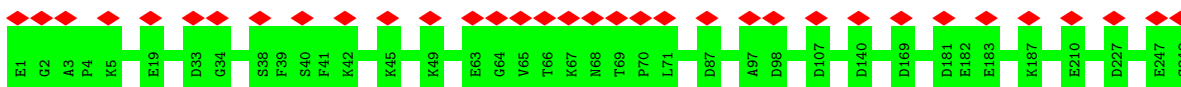
- Molecule 15: Photosystem II reaction center protein M



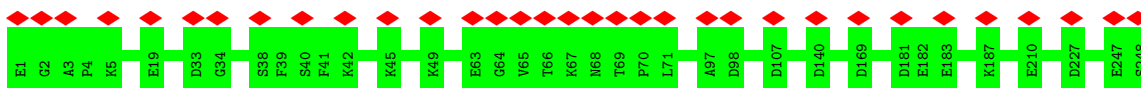
- Molecule 15: Photosystem II reaction center protein M



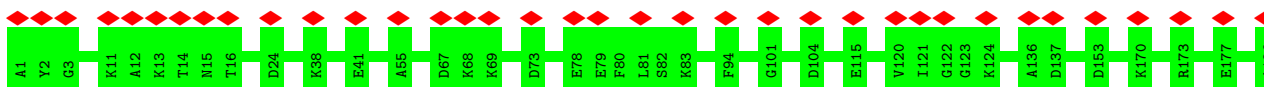
- Molecule 16: Oxygen-evolving enhancer protein 1, chloroplastic



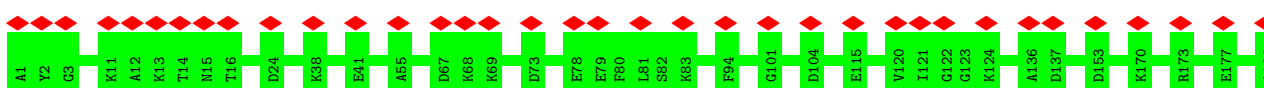
- Molecule 16: Oxygen-evolving enhancer protein 1, chloroplastic



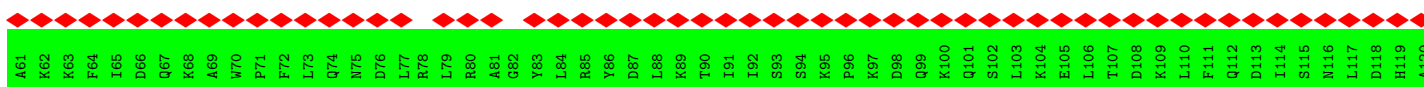
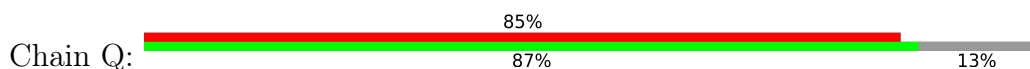
- Molecule 17: Oxygen-evolving enhancer protein 2, chloroplastic

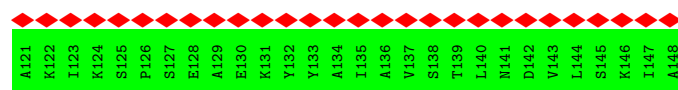


- Molecule 17: Oxygen-evolving enhancer protein 2, chloroplastic

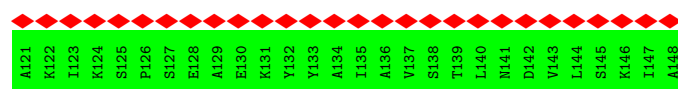
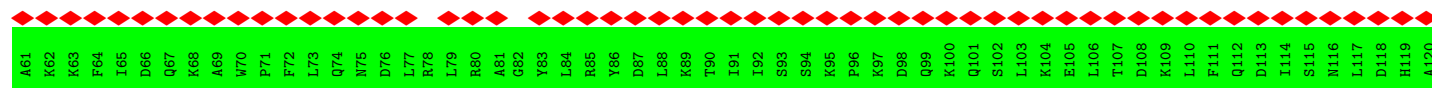
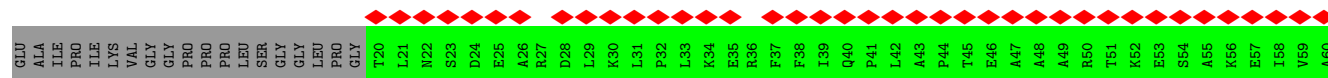
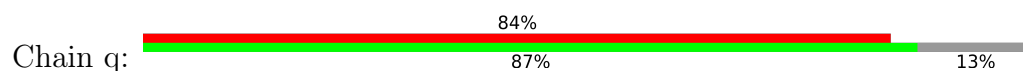


- Molecule 18: Oxygen-evolving enhancer protein 3

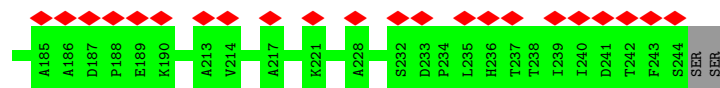
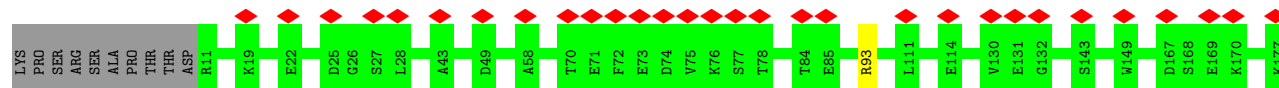




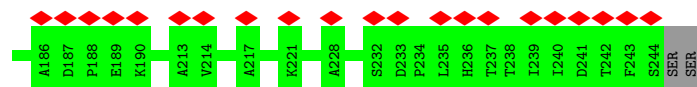
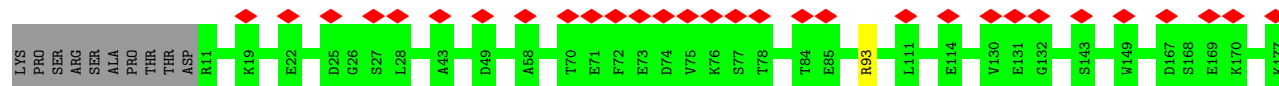
• Molecule 18: Oxygen-evolving enhancer protein 3



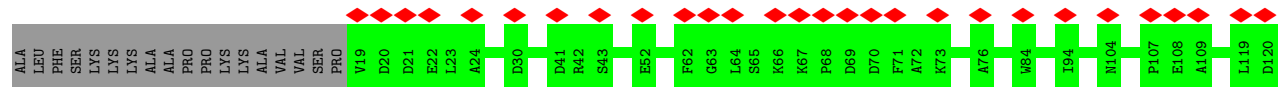
• Molecule 19: Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29

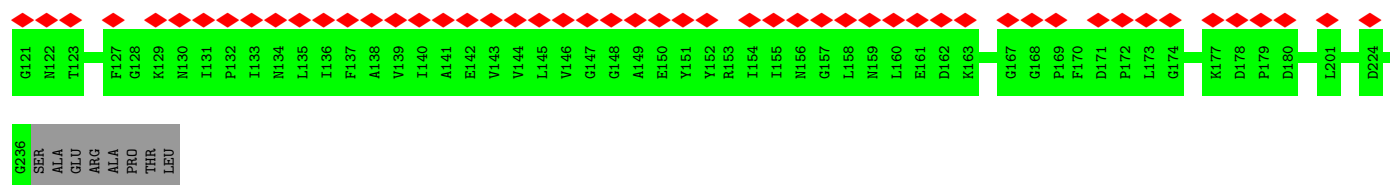


• Molecule 19: Light harvesting chlorophyll a/b-binding protein Lhcb4, CP29

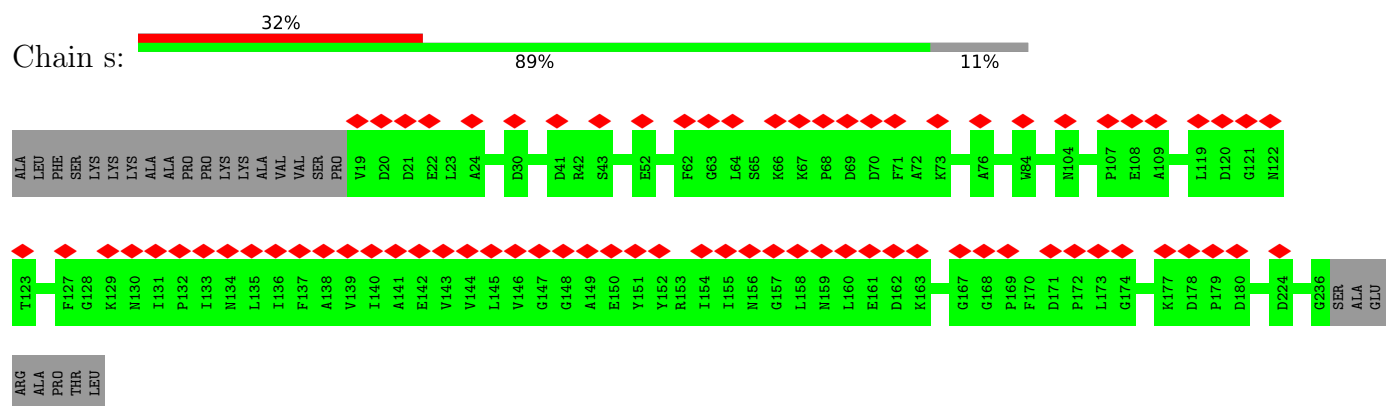


• Molecule 20: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26

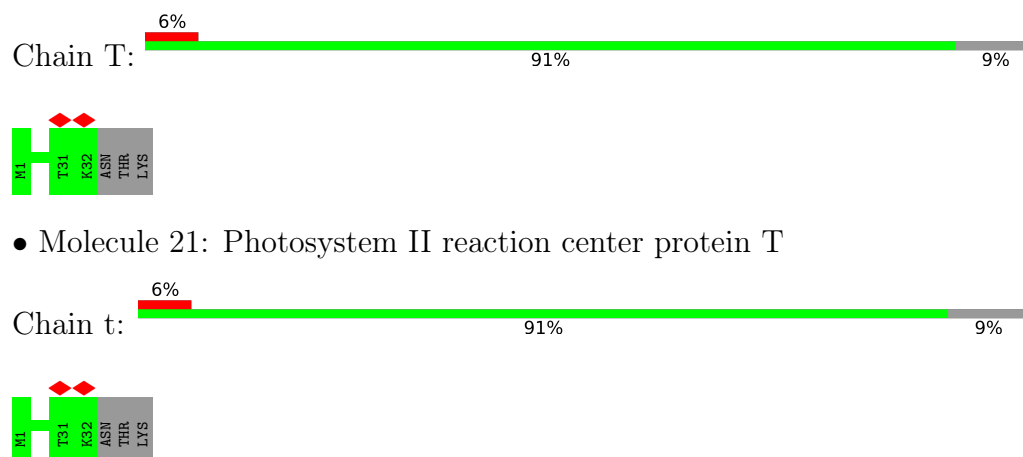




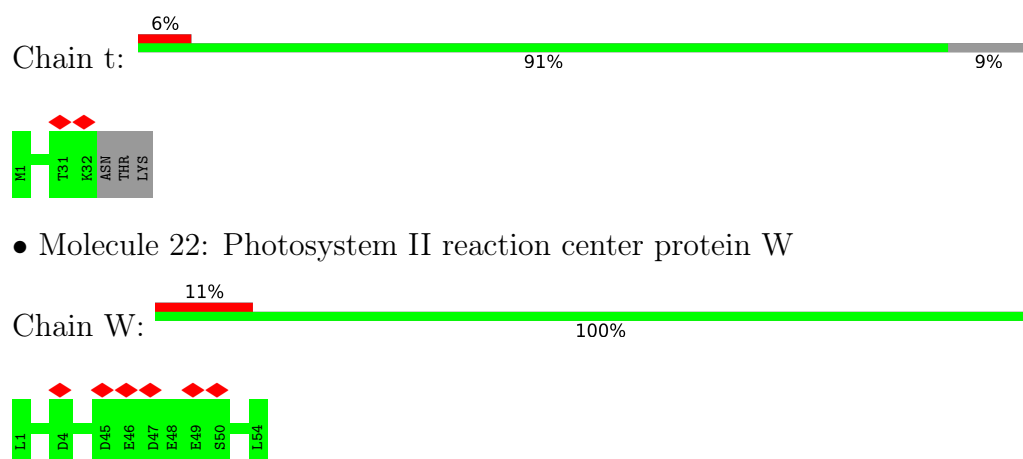
- Molecule 20: Light harvesting chlorophyll a/b-binding protein Lhcb5, CP26



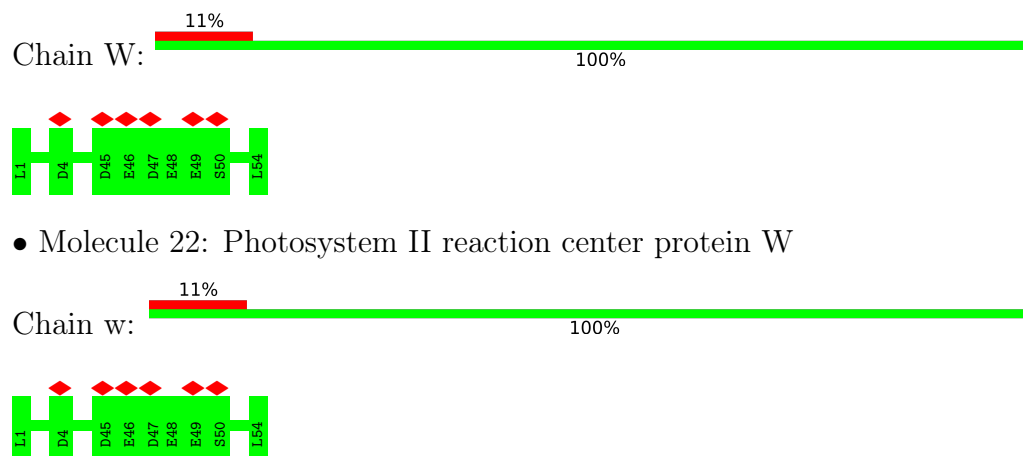
- Molecule 21: Photosystem II reaction center protein T



- Molecule 21: Photosystem II reaction center protein T

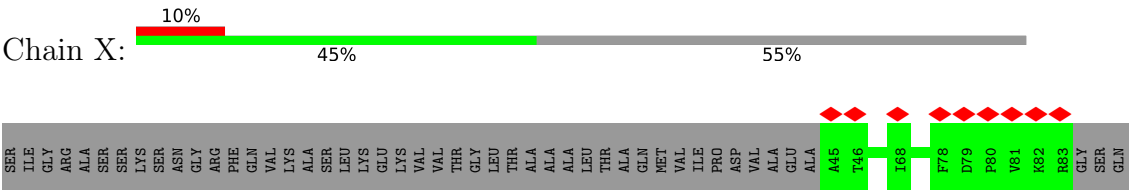


- Molecule 22: Photosystem II reaction center protein W

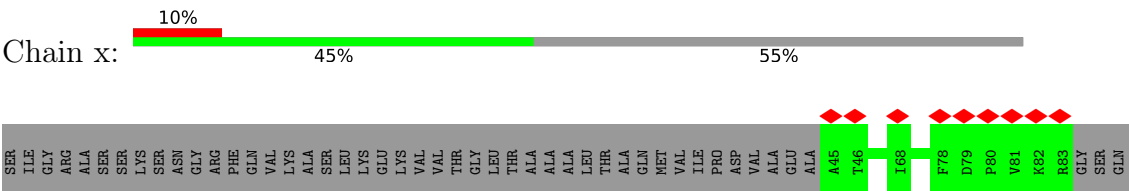


- Molecule 22: Photosystem II reaction center protein W

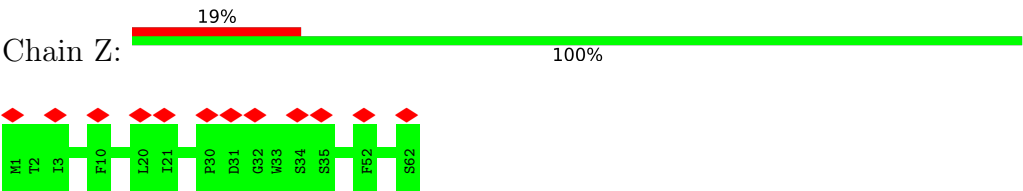
• Molecule 23: Photosystem II reaction center protein X



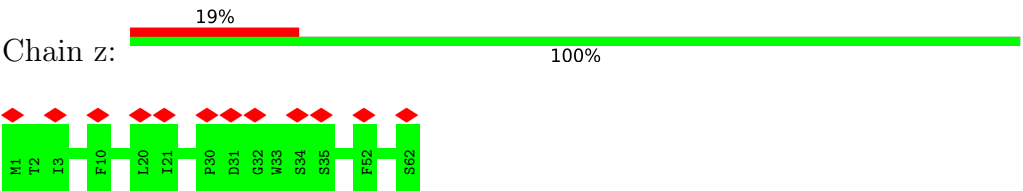
• Molecule 23: Photosystem II reaction center protein X



• Molecule 24: Photosystem II reaction center protein Z



• Molecule 24: 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	136521	Depositor
Resolution determination method	FSC 0.143 CUT-OFF	Depositor
CTF correction method	PHASE FLIPPING AND AMPLITUDE CORRECTION	Depositor
Microscope	FEI TITAN KRIOS	Depositor
Voltage (kV)	300	Depositor
Electron dose ($e^-/\text{\AA}^2$)	60	Depositor
Minimum defocus (nm)	Not provided	
Maximum defocus (nm)	Not provided	
Magnification	Not provided	
Image detector	GATAN K2 SUMMIT (4k x 4k)	Depositor
Maximum map value	168.730	Depositor
Minimum map value	-94.103	Depositor
Average map value	0.061	Depositor
Map value standard deviation	6.582	Depositor
Recommended contour level	17.5	Depositor
Map size (Å)	312.0, 312.0, 312.0	wwPDB
Map dimensions	300, 300, 300	wwPDB
Map angles (°)	90.0, 90.0, 90.0	wwPDB
Pixel spacing (Å)	1.04, 1.04, 1.04	Depositor

5 Model quality ⓘ

5.1 Standard geometry ⓘ

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

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

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
1	1	0.36	0/1720	0.50	0/2342
1	2	0.32	0/1716	0.51	1/2337 (0.0%)
1	5	0.37	0/1720	0.50	0/2342
1	6	0.33	0/1716	0.51	1/2337 (0.0%)
1	G	0.39	0/1720	0.52	0/2342
1	N	0.44	0/1720	0.56	0/2342
1	Y	0.43	0/1720	0.55	0/2342
1	g	0.39	0/1720	0.52	0/2342
1	n	0.45	0/1720	0.56	0/2342
1	y	0.43	0/1720	0.55	0/2342
2	3	0.37	0/1759	0.53	0/2396
2	7	0.37	0/1759	0.53	0/2396
3	4	0.34	0/1586	0.55	0/2158
3	8	0.34	0/1586	0.55	0/2158
4	A	0.54	0/2697	0.62	1/3677 (0.0%)
4	a	0.54	0/2697	0.62	1/3677 (0.0%)
5	B	0.54	0/4081	0.60	0/5556
5	b	0.54	0/4081	0.61	0/5556
6	C	0.58	0/3614	0.63	0/4922
6	c	0.58	0/3614	0.63	0/4922
7	D	0.47	0/2804	0.61	0/3823
7	d	0.48	0/2804	0.61	0/3823
8	E	0.47	0/630	0.52	0/857
8	e	0.48	0/630	0.52	0/857
9	F	0.60	0/248	0.64	0/335
9	f	0.60	0/248	0.64	0/335
10	H	0.50	0/461	0.56	0/626
10	h	0.50	0/461	0.56	0/626
11	I	0.52	0/286	0.68	0/386
11	i	0.52	0/286	0.68	0/386
12	J	0.58	1/262 (0.4%)	0.70	0/354

Mol	Chain	Bond lengths		Bond angles	
		RMSZ	# Z >5	RMSZ	# Z >5
12	j	0.58	1/262 (0.4%)	0.70	0/354
13	K	0.48	0/318	0.63	0/434
13	k	0.48	0/318	0.63	0/434
14	L	0.57	0/319	0.59	0/434
14	l	0.57	0/319	0.59	0/434
15	M	0.44	0/260	0.66	0/355
15	m	0.44	0/260	0.66	0/355
16	O	0.43	0/1906	0.60	0/2575
16	o	0.43	0/1906	0.60	0/2575
17	P	0.54	0/1464	0.63	0/1978
17	p	0.54	0/1464	0.63	0/1978
18	Q	0.29	0/1051	0.59	0/1414
18	q	0.29	0/1051	0.59	0/1414
19	R	0.50	0/1886	0.59	0/2569
19	r	0.50	0/1886	0.59	0/2569
20	S	0.43	0/1736	0.65	0/2359
20	s	0.43	0/1736	0.65	0/2359
21	T	0.46	0/269	0.51	0/365
21	t	0.46	0/269	0.51	0/365
22	W	0.55	0/429	0.63	0/581
22	w	0.55	0/429	0.63	0/581
23	X	0.33	0/279	0.48	0/380
23	x	0.33	0/279	0.48	0/380
24	Z	0.42	0/474	0.55	0/648
24	z	0.42	0/474	0.55	0/648
All	All	0.47	2/74830 (0.0%)	0.59	4/101774 (0.0%)

All (2) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
12	j	11	TRP	CB-CG	-5.25	1.40	1.50
12	J	11	TRP	CB-CG	-5.24	1.40	1.50

All (4) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
1	6	197	GLN	CA-CB-CG	5.70	125.94	113.40
1	2	197	GLN	CA-CB-CG	5.69	125.92	113.40
4	A	140	ARG	NE-CZ-NH1	-5.28	117.66	120.30
4	a	140	ARG	NE-CZ-NH1	-5.28	117.66	120.30

There are no chirality outliers.

There are no planarity outliers.

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	1	217/232 (94%)	209 (96%)	8 (4%)	0	100	100
1	2	216/232 (93%)	210 (97%)	5 (2%)	1 (0%)	29	54
1	5	217/232 (94%)	209 (96%)	8 (4%)	0	100	100
1	6	216/232 (93%)	210 (97%)	5 (2%)	1 (0%)	29	54
1	G	217/232 (94%)	213 (98%)	4 (2%)	0	100	100
1	N	217/232 (94%)	214 (99%)	3 (1%)	0	100	100
1	Y	217/232 (94%)	213 (98%)	4 (2%)	0	100	100
1	g	217/232 (94%)	213 (98%)	4 (2%)	0	100	100
1	n	217/232 (94%)	214 (99%)	3 (1%)	0	100	100
1	y	217/232 (94%)	213 (98%)	4 (2%)	0	100	100
2	3	218/243 (90%)	209 (96%)	9 (4%)	0	100	100
2	7	218/243 (90%)	209 (96%)	9 (4%)	0	100	100
3	4	193/210 (92%)	179 (93%)	14 (7%)	0	100	100
3	8	193/210 (92%)	179 (93%)	14 (7%)	0	100	100
4	A	332/344 (96%)	326 (98%)	6 (2%)	0	100	100
4	a	332/344 (96%)	326 (98%)	6 (2%)	0	100	100
5	B	501/507 (99%)	493 (98%)	8 (2%)	0	100	100
5	b	501/507 (99%)	493 (98%)	8 (2%)	0	100	100
6	C	448/473 (95%)	441 (98%)	7 (2%)	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
6	c	448/473 (95%)	442 (99%)	6 (1%)	0	100	100
7	D	339/353 (96%)	335 (99%)	4 (1%)	0	100	100
7	d	339/353 (96%)	335 (99%)	4 (1%)	0	100	100
8	E	73/83 (88%)	73 (100%)	0	0	100	100
8	e	73/83 (88%)	73 (100%)	0	0	100	100
9	F	28/39 (72%)	28 (100%)	0	0	100	100
9	f	28/39 (72%)	28 (100%)	0	0	100	100
10	H	58/73 (80%)	58 (100%)	0	0	100	100
10	h	58/73 (80%)	58 (100%)	0	0	100	100
11	I	32/36 (89%)	32 (100%)	0	0	100	100
11	i	32/36 (89%)	32 (100%)	0	0	100	100
12	J	33/40 (82%)	33 (100%)	0	0	100	100
12	j	33/40 (82%)	33 (100%)	0	0	100	100
13	K	35/61 (57%)	35 (100%)	0	0	100	100
13	k	35/61 (57%)	35 (100%)	0	0	100	100
14	L	35/38 (92%)	35 (100%)	0	0	100	100
14	l	35/38 (92%)	35 (100%)	0	0	100	100
15	M	31/34 (91%)	29 (94%)	2 (6%)	0	100	100
15	m	31/34 (91%)	29 (94%)	2 (6%)	0	100	100
16	O	246/248 (99%)	240 (98%)	6 (2%)	0	100	100
16	o	246/248 (99%)	240 (98%)	6 (2%)	0	100	100
17	P	184/186 (99%)	183 (100%)	1 (0%)	0	100	100
17	p	184/186 (99%)	183 (100%)	1 (0%)	0	100	100
18	Q	127/148 (86%)	125 (98%)	2 (2%)	0	100	100
18	q	127/148 (86%)	125 (98%)	2 (2%)	0	100	100
19	R	232/246 (94%)	228 (98%)	4 (2%)	0	100	100
19	r	232/246 (94%)	228 (98%)	4 (2%)	0	100	100
20	S	216/244 (88%)	209 (97%)	7 (3%)	0	100	100
20	s	216/244 (88%)	208 (96%)	8 (4%)	0	100	100
21	T	30/35 (86%)	30 (100%)	0	0	100	100
21	t	30/35 (86%)	30 (100%)	0	0	100	100

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Mol	Chain	Analysed	Favoured	Allowed	Outliers	Percentiles	
22	W	52/54 (96%)	52 (100%)	0	0	100	100
22	w	52/54 (96%)	52 (100%)	0	0	100	100
23	X	37/86 (43%)	36 (97%)	1 (3%)	0	100	100
23	x	37/86 (43%)	36 (97%)	1 (3%)	0	100	100
24	Z	60/62 (97%)	60 (100%)	0	0	100	100
24	z	60/62 (97%)	60 (100%)	0	0	100	100
All	All	9248/10006 (92%)	9056 (98%)	190 (2%)	2 (0%)	100	100

All (2) Ramachandran outliers are listed below:

Mol	Chain	Res	Type
1	2	119	VAL
1	6	119	VAL

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	1	171/182 (94%)	171 (100%)	0	100	100
1	2	171/182 (94%)	171 (100%)	0	100	100
1	5	171/182 (94%)	171 (100%)	0	100	100
1	6	171/182 (94%)	171 (100%)	0	100	100
1	G	171/182 (94%)	171 (100%)	0	100	100
1	N	171/182 (94%)	171 (100%)	0	100	100
1	Y	171/182 (94%)	170 (99%)	1 (1%)	86	95
1	g	171/182 (94%)	171 (100%)	0	100	100
1	n	171/182 (94%)	171 (100%)	0	100	100
1	y	171/182 (94%)	170 (99%)	1 (1%)	86	95
2	3	175/193 (91%)	175 (100%)	0	100	100
2	7	175/193 (91%)	175 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
3	4	154/162 (95%)	154 (100%)	0	100	100
3	8	154/162 (95%)	154 (100%)	0	100	100
4	A	270/279 (97%)	269 (100%)	1 (0%)	91	97
4	a	270/279 (97%)	269 (100%)	1 (0%)	91	97
5	B	400/403 (99%)	397 (99%)	3 (1%)	81	93
5	b	400/403 (99%)	397 (99%)	3 (1%)	81	93
6	C	352/373 (94%)	350 (99%)	2 (1%)	86	95
6	c	352/373 (94%)	350 (99%)	2 (1%)	86	95
7	D	275/285 (96%)	274 (100%)	1 (0%)	91	97
7	d	275/285 (96%)	274 (100%)	1 (0%)	91	97
8	E	67/73 (92%)	66 (98%)	1 (2%)	65	86
8	e	67/73 (92%)	66 (98%)	1 (2%)	65	86
9	F	25/34 (74%)	25 (100%)	0	100	100
9	f	25/34 (74%)	25 (100%)	0	100	100
10	H	49/61 (80%)	48 (98%)	1 (2%)	55	81
10	h	49/61 (80%)	48 (98%)	1 (2%)	55	81
11	I	31/33 (94%)	31 (100%)	0	100	100
11	i	31/33 (94%)	31 (100%)	0	100	100
12	J	26/30 (87%)	26 (100%)	0	100	100
12	j	26/30 (87%)	26 (100%)	0	100	100
13	K	32/54 (59%)	32 (100%)	0	100	100
13	k	32/54 (59%)	32 (100%)	0	100	100
14	L	35/36 (97%)	35 (100%)	0	100	100
14	l	35/36 (97%)	35 (100%)	0	100	100
15	M	29/30 (97%)	29 (100%)	0	100	100
15	m	29/30 (97%)	29 (100%)	0	100	100
16	O	204/204 (100%)	204 (100%)	0	100	100
16	o	204/204 (100%)	204 (100%)	0	100	100
17	P	150/150 (100%)	150 (100%)	0	100	100
17	p	150/150 (100%)	150 (100%)	0	100	100
18	Q	112/125 (90%)	112 (100%)	0	100	100

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Mol	Chain	Analysed	Rotameric	Outliers	Percentiles	
18	q	112/125 (90%)	112 (100%)	0	100	100
19	R	191/202 (95%)	190 (100%)	1 (0%)	88	96
19	r	191/202 (95%)	190 (100%)	1 (0%)	88	96
20	S	170/190 (90%)	170 (100%)	0	100	100
20	s	170/190 (90%)	170 (100%)	0	100	100
21	T	29/32 (91%)	29 (100%)	0	100	100
21	t	29/32 (91%)	29 (100%)	0	100	100
22	W	44/44 (100%)	44 (100%)	0	100	100
22	w	44/44 (100%)	44 (100%)	0	100	100
23	X	32/67 (48%)	32 (100%)	0	100	100
23	x	32/67 (48%)	32 (100%)	0	100	100
24	Z	54/54 (100%)	54 (100%)	0	100	100
24	z	54/54 (100%)	54 (100%)	0	100	100
All	All	7522/8048 (94%)	7500 (100%)	22 (0%)	92	98

All (22) residues with a non-rotameric sidechain are listed below:

Mol	Chain	Res	Type
4	A	266	ASN
5	B	12	VAL
5	B	362	PHE
5	B	385	ARG
6	C	289	PHE
6	C	391	ARG
7	D	181	ARG
8	E	18	ARG
10	H	61	TYR
19	R	93	ARG
1	Y	32	SER
4	a	266	ASN
5	b	12	VAL
5	b	362	PHE
5	b	385	ARG
6	c	289	PHE
6	c	391	ARG
7	d	181	ARG
8	e	18	ARG

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Mol	Chain	Res	Type
10	h	61	TYR
19	r	93	ARG
1	y	32	SER

Sometimes sidechains can be flipped to improve hydrogen bonding and reduce clashes. All (58) such sidechains are listed below:

Mol	Chain	Res	Type
1	1	61	ASN
1	2	61	ASN
1	2	88	ASN
2	3	95	GLN
2	3	113	GLN
2	3	219	ASN
4	A	234	ASN
4	A	266	ASN
4	A	303	ASN
5	B	216	HIS
5	B	332	ASN
5	B	343	HIS
5	B	496	GLN
6	C	28	GLN
6	C	313	GLN
6	C	332	GLN
7	D	84	ASN
7	D	143	ASN
7	D	221	ASN
7	D	351	ASN
9	F	38	GLN
16	O	74	GLN
17	P	112	ASN
18	Q	75	ASN
18	Q	99	GLN
19	R	47	GLN
19	R	56	ASN
19	R	236	HIS
1	Y	88	ASN
1	5	61	ASN
1	6	61	ASN
1	6	88	ASN
2	7	95	GLN
2	7	113	GLN
2	7	219	ASN

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Mol	Chain	Res	Type
4	a	234	ASN
4	a	266	ASN
4	a	303	ASN
5	b	216	HIS
5	b	332	ASN
5	b	343	HIS
5	b	496	GLN
6	c	28	GLN
6	c	313	GLN
6	c	332	GLN
7	d	84	ASN
7	d	143	ASN
7	d	221	ASN
7	d	351	ASN
9	f	38	GLN
16	o	74	GLN
17	p	112	ASN
18	q	75	ASN
18	q	99	GLN
19	r	47	GLN
19	r	56	ASN
19	r	236	HIS
1	y	88	ASN

5.3.3 RNA [i](#)

There are no RNA molecules in this entry.

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

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

5.5 Carbohydrates [i](#)

There are no monosaccharides in this entry.

5.6 Ligand geometry [i](#)

Of 490 ligands modelled in this entry, 6 are monoatomic - leaving 484 for Mogul analysis.

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

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# $ Z > 2$	Counts	RMSZ	# $ Z > 2$
25	CHL	R	608	42	61,69,74	1.90	10 (16%)	67,108,114	2.92	24 (35%)
26	CLA	r	613	19	60,68,73	1.59	8 (13%)	70,107,113	1.29	8 (11%)
28	XAT	4	622	-	39,47,47	0.93	1 (2%)	54,74,74	2.62	21 (38%)
26	CLA	s	603	20	45,53,73	1.78	10 (22%)	52,89,113	1.92	12 (23%)
26	CLA	g	610	1	64,72,73	1.50	6 (9%)	74,111,113	1.37	8 (10%)
37	LMG	D	411	-	46,46,55	0.92	3 (6%)	54,54,63	1.46	4 (7%)
26	CLA	y	613	1	65,73,73	1.49	9 (13%)	76,113,113	1.43	9 (11%)
26	CLA	5	613	1	55,63,73	1.65	9 (16%)	64,101,113	1.35	6 (9%)
26	CLA	y	614	1	48,56,73	1.67	10 (20%)	55,92,113	1.60	9 (16%)
30	LHG	R	2630	26	41,41,48	0.70	1 (2%)	44,47,54	1.27	6 (13%)
36	SQD	a	418	-	53,54,54	0.92	5 (9%)	62,65,65	1.67	14 (22%)
25	CHL	1	609	1	62,70,74	1.94	14 (22%)	68,109,114	2.72	20 (29%)
26	CLA	B	604	5	65,73,73	1.51	11 (16%)	76,113,113	1.46	10 (13%)
26	CLA	N	610	1	65,73,73	1.42	8 (12%)	76,113,113	1.42	10 (13%)
26	CLA	B	616	5	65,73,73	1.46	10 (15%)	76,113,113	1.45	12 (15%)
26	CLA	C	504	42	65,73,73	1.40	10 (15%)	76,113,113	1.68	8 (10%)
25	CHL	1	601	1	46,54,74	2.35	15 (32%)	49,90,114	3.07	21 (42%)
26	CLA	g	613	1	65,73,73	1.49	8 (12%)	76,113,113	1.35	7 (9%)
29	NEX	7	1623	-	38,46,46	0.87	1 (2%)	50,70,70	2.39	16 (32%)
30	LHG	d	409	-	48,48,48	0.75	1 (2%)	51,54,54	1.31	7 (13%)
26	CLA	B	612	5	65,73,73	1.50	8 (12%)	76,113,113	1.67	10 (13%)
30	LHG	b	2631	-	48,48,48	0.68	2 (4%)	51,54,54	1.22	6 (11%)
25	CHL	1	606	-	46,54,74	2.24	15 (32%)	49,90,114	3.08	20 (40%)
25	CHL	S	608	-	46,54,74	2.25	15 (32%)	49,90,114	3.15	16 (32%)
27	LUT	Y	1621	-	42,43,43	0.88	1 (2%)	51,60,60	1.69	13 (25%)
37	LMG	C	521	-	51,51,55	0.80	3 (5%)	59,59,63	1.38	6 (10%)
27	LUT	G	1621	-	42,43,43	0.89	1 (2%)	51,60,60	1.96	17 (33%)
25	CHL	G	605	1	46,54,74	2.27	15 (32%)	49,90,114	3.33	20 (40%)
26	CLA	4	611	30	45,53,73	1.81	8 (17%)	52,89,113	1.49	7 (13%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
27	LUT	N	1620	-	42,43,43	0.81	0	51,60,60	1.69	12 (23%)
25	CHL	N	609	1	66,74,74	1.88	14 (21%)	73,114,114	2.72	23 (31%)
26	CLA	Y	602	1	65,73,73	1.43	8 (12%)	76,113,113	1.53	10 (13%)
26	CLA	7	613	2	58,66,73	1.61	10 (17%)	67,104,113	1.42	8 (11%)
27	LUT	5	1621	-	42,43,43	0.90	2 (4%)	51,60,60	1.73	15 (29%)
26	CLA	B	609	5	65,73,73	1.40	8 (12%)	76,113,113	1.68	12 (15%)
26	CLA	n	611	30	60,68,73	1.55	7 (11%)	70,107,113	1.45	7 (10%)
25	CHL	3	609	2	61,69,74	2.02	14 (22%)	67,108,114	2.61	21 (31%)
31	BCR	c	515	-	41,41,41	0.93	2 (4%)	56,56,56	2.01	16 (28%)
27	LUT	g	1621	-	42,43,43	0.89	1 (2%)	51,60,60	1.95	17 (33%)
26	CLA	G	604	42	50,58,73	1.78	10 (20%)	58,95,113	1.71	10 (17%)
28	XAT	r	622	-	39,47,47	0.97	1 (2%)	54,74,74	2.77	21 (38%)
28	XAT	g	1622	-	39,47,47	0.98	2 (5%)	54,74,74	2.91	22 (40%)
26	CLA	n	612	1	60,68,73	1.55	7 (11%)	70,107,113	1.43	8 (11%)
26	CLA	b	606	5	65,73,73	1.54	12 (18%)	76,113,113	1.67	11 (14%)
26	CLA	5	611	30	45,53,73	1.79	9 (20%)	52,89,113	1.42	6 (11%)
26	CLA	3	603	2	55,63,73	1.56	11 (20%)	64,101,113	1.56	10 (15%)
25	CHL	Y	601	1	66,74,74	1.84	13 (19%)	73,114,114	2.86	22 (30%)
26	CLA	g	611	30	60,68,73	1.61	7 (11%)	70,107,113	1.60	7 (10%)
26	CLA	Y	614	1	48,56,73	1.67	10 (20%)	55,92,113	1.60	9 (16%)
41	HEM	f	101	9,8	41,50,50	1.46	4 (9%)	45,82,82	1.37	7 (15%)
26	CLA	Y	612	1	60,68,73	1.57	9 (15%)	70,107,113	1.42	7 (10%)
25	CHL	6	606	-	46,54,74	2.27	15 (32%)	49,90,114	3.09	17 (34%)
26	CLA	3	604	-	45,53,73	1.81	9 (20%)	52,89,113	1.51	6 (11%)
26	CLA	Y	613	1	65,73,73	1.48	9 (13%)	76,113,113	1.43	9 (11%)
26	CLA	5	614	1	45,53,73	1.79	7 (15%)	52,89,113	1.47	8 (15%)
25	CHL	y	606	42	50,58,74	2.04	13 (26%)	52,94,114	3.18	19 (36%)
26	CLA	b	609	5	65,73,73	1.40	8 (12%)	76,113,113	1.69	12 (15%)
26	CLA	5	612	1	45,53,73	1.84	10 (22%)	52,89,113	1.50	9 (17%)
26	CLA	B	614	5	65,73,73	1.43	9 (13%)	76,113,113	1.45	7 (9%)
26	CLA	r	612	19	49,57,73	1.74	7 (14%)	55,93,113	1.61	7 (12%)
27	LUT	8	620	-	42,43,43	0.80	0	51,60,60	1.87	18 (35%)
26	CLA	S	610	20	55,63,73	1.63	8 (14%)	64,101,113	1.58	10 (15%)
26	CLA	S	603	20	45,53,73	1.77	10 (22%)	52,89,113	1.92	12 (23%)
26	CLA	1	610	1	56,64,73	1.61	9 (16%)	65,102,113	1.25	6 (9%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	3	605	2	46,54,74	2.29	15 (32%)	49,90,114	3.13	21 (42%)
28	XAT	G	1622	-	39,47,47	0.98	2 (5%)	54,74,74	2.91	23 (42%)
25	CHL	Y	609	1	66,74,74	1.86	14 (21%)	73,114,114	2.72	22 (30%)
25	CHL	2	605	1	46,54,74	2.30	16 (34%)	49,90,114	3.15	19 (38%)
26	CLA	1	604	-	50,58,73	1.74	9 (18%)	58,95,113	1.52	9 (15%)
26	CLA	r	609	19	58,66,73	1.62	8 (13%)	67,104,113	1.54	7 (10%)
26	CLA	B	615	5	65,73,73	1.40	10 (15%)	76,113,113	1.46	10 (13%)
25	CHL	5	607	-	63,71,74	1.89	13 (20%)	69,110,114	2.87	20 (28%)
25	CHL	7	605	2	46,54,74	2.29	15 (32%)	49,90,114	3.13	21 (42%)
30	LHG	r	2630	26	41,41,48	0.70	1 (2%)	44,47,54	1.27	6 (13%)
26	CLA	Y	604	42	50,58,73	1.73	10 (20%)	58,95,113	1.77	8 (13%)
27	LUT	s	1621	-	42,43,43	0.85	1 (2%)	51,60,60	1.78	17 (33%)
26	CLA	r	601	19	49,57,73	1.64	5 (10%)	55,93,113	1.92	11 (20%)
26	CLA	4	603	3	45,53,73	1.80	9 (20%)	52,89,113	1.60	8 (15%)
26	CLA	S	612	20	49,57,73	1.64	7 (14%)	55,93,113	1.68	6 (10%)
30	LHG	G	2630	26	48,48,48	0.66	1 (2%)	51,54,54	1.28	6 (11%)
26	CLA	B	608	42	65,73,73	1.53	10 (15%)	76,113,113	1.68	11 (14%)
35	PHO	a	408	-	51,69,69	1.13	6 (11%)	47,99,99	1.46	10 (21%)
26	CLA	A	410	4	60,68,73	1.48	10 (16%)	70,107,113	1.63	9 (12%)
25	CHL	3	608	-	46,54,74	2.20	15 (32%)	49,90,114	3.28	18 (36%)
26	CLA	A	407	42	50,58,73	1.61	10 (20%)	58,95,113	1.68	10 (17%)
26	CLA	b	607	5	65,73,73	1.50	11 (16%)	76,113,113	1.60	13 (17%)
25	CHL	n	605	1	48,56,74	2.20	14 (29%)	51,92,114	3.24	20 (39%)
26	CLA	G	603	1	65,73,73	1.52	11 (16%)	76,113,113	1.58	13 (17%)
26	CLA	s	611	30	56,64,73	1.55	9 (16%)	65,102,113	1.48	7 (10%)
27	LUT	G	1620	-	42,43,43	0.76	0	51,60,60	1.64	12 (23%)
36	SQD	A	412	-	49,50,54	0.96	6 (12%)	58,61,65	1.74	11 (18%)
30	LHG	c	523	-	48,48,48	0.66	1 (2%)	51,54,54	1.20	5 (9%)
26	CLA	C	513	6	65,73,73	1.39	7 (10%)	76,113,113	1.60	14 (18%)
25	CHL	5	601	1	46,54,74	2.34	15 (32%)	49,90,114	3.07	21 (42%)
26	CLA	g	603	1	65,73,73	1.52	11 (16%)	76,113,113	1.58	13 (17%)
26	CLA	b	615	5	65,73,73	1.40	10 (15%)	76,113,113	1.46	10 (13%)
25	CHL	G	608	42	66,74,74	1.84	16 (24%)	73,114,114	2.73	21 (28%)
29	NEX	G	1623	-	38,46,46	1.00	2 (5%)	50,70,70	2.39	14 (28%)
26	CLA	S	609	20	45,53,73	1.82	6 (13%)	52,89,113	1.41	9 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	n	607	42	66,74,74	1.80	13 (19%)	73,114,114	2.84	20 (27%)
28	XAT	Y	1622	-	39,47,47	1.08	4 (10%)	54,74,74	3.00	21 (38%)
30	LHG	8	2630	26	20,20,48	0.91	0	23,26,54	1.29	2 (8%)
25	CHL	N	606	42	50,58,74	2.16	15 (30%)	52,94,114	3.03	21 (40%)
27	LUT	2	1621	-	42,43,43	0.84	1 (2%)	51,60,60	1.68	15 (29%)
37	LMG	b	2633	-	55,55,55	0.78	3 (5%)	63,63,63	1.32	7 (11%)
26	CLA	c	509	6	65,73,73	1.45	11 (16%)	76,113,113	1.73	11 (14%)
25	CHL	5	608	-	46,54,74	2.17	14 (30%)	49,90,114	3.26	14 (28%)
25	CHL	Y	607	42	66,74,74	1.80	13 (19%)	73,114,114	2.72	21 (28%)
30	LHG	g	2630	26	48,48,48	0.66	1 (2%)	51,54,54	1.28	6 (11%)
27	LUT	1	1621	-	42,43,43	0.90	2 (4%)	51,60,60	1.73	15 (29%)
30	LHG	c	522	-	48,48,48	0.69	1 (2%)	51,54,54	1.26	6 (11%)
29	NEX	n	1623	-	38,46,46	0.90	1 (2%)	50,70,70	2.36	15 (30%)
31	BCR	b	619	-	41,41,41	0.80	0	56,56,56	1.81	17 (30%)
26	CLA	c	508	6	65,73,73	1.47	11 (16%)	76,113,113	1.84	12 (15%)
25	CHL	6	601	1	46,54,74	2.26	13 (28%)	49,90,114	3.22	22 (44%)
26	CLA	2	611	30	45,53,73	1.79	7 (15%)	52,89,113	1.53	7 (13%)
26	CLA	8	603	3	45,53,73	1.80	9 (20%)	52,89,113	1.60	8 (15%)
26	CLA	5	610	1	56,64,73	1.61	9 (16%)	65,102,113	1.25	6 (9%)
28	XAT	n	1622	-	39,47,47	0.93	0	54,74,74	3.00	24 (44%)
26	CLA	a	405	4	65,73,73	1.49	10 (15%)	76,113,113	1.67	12 (15%)
26	CLA	A	406	42	65,73,73	1.42	8 (12%)	76,113,113	1.76	16 (21%)
26	CLA	c	504	42	65,73,73	1.40	10 (15%)	76,113,113	1.67	8 (10%)
26	CLA	R	613	19	60,68,73	1.59	7 (11%)	70,107,113	1.28	8 (11%)
27	LUT	s	1620	-	42,43,43	0.78	0	51,60,60	1.76	12 (23%)
26	CLA	2	614	1	45,53,73	1.82	6 (13%)	52,89,113	1.45	7 (13%)
35	PHO	A	408	-	51,69,69	1.13	6 (11%)	47,99,99	1.46	11 (23%)
26	CLA	4	604	-	45,53,73	1.81	8 (17%)	52,89,113	1.45	7 (13%)
26	CLA	g	602	1	65,73,73	1.45	8 (12%)	76,113,113	1.58	11 (14%)
30	LHG	N	2630	26	48,48,48	0.66	1 (2%)	51,54,54	1.30	6 (11%)
25	CHL	Y	608	42	66,74,74	1.80	13 (19%)	73,114,114	2.74	23 (31%)
25	CHL	S	607	42	58,66,74	1.93	12 (20%)	63,104,114	2.86	20 (31%)
31	BCR	8	623	-	41,41,41	0.74	0	56,56,56	2.31	17 (30%)
26	CLA	y	612	1	60,68,73	1.57	9 (15%)	70,107,113	1.42	8 (11%)
26	CLA	a	407	42	50,58,73	1.61	10 (20%)	58,95,113	1.67	10 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	3	607	-	53,61,74	2.24	16 (30%)	57,98,114	2.89	23 (40%)
26	CLA	g	604	42	50,58,73	1.78	10 (20%)	58,95,113	1.71	10 (17%)
26	CLA	5	603	1	55,63,73	1.57	11 (20%)	64,101,113	1.57	9 (14%)
37	LMG	c	521	-	51,51,55	0.79	3 (5%)	59,59,63	1.37	6 (10%)
26	CLA	c	502	6	65,73,73	1.40	9 (13%)	76,113,113	1.70	8 (10%)
27	LUT	n	1620	-	42,43,43	0.80	0	51,60,60	1.69	12 (23%)
26	CLA	d	402	7	65,73,73	1.55	10 (15%)	76,113,113	1.71	10 (13%)
25	CHL	2	607	-	61,69,74	1.96	15 (24%)	67,108,114	2.73	21 (31%)
25	CHL	s	608	-	46,54,74	2.24	15 (32%)	49,90,114	3.15	16 (32%)
26	CLA	4	612	3	45,53,73	1.77	7 (15%)	52,89,113	1.50	9 (17%)
30	LHG	s	2630	26	48,48,48	0.74	1 (2%)	51,54,54	1.26	7 (13%)
26	CLA	3	611	30	55,63,73	1.66	10 (18%)	64,101,113	1.51	11 (17%)
25	CHL	g	605	1	46,54,74	2.27	15 (32%)	49,90,114	3.32	20 (40%)
31	BCR	C	516	-	41,41,41	0.74	0	56,56,56	1.98	17 (30%)
26	CLA	6	602	1	61,69,73	1.52	8 (13%)	71,108,113	1.34	8 (11%)
27	LUT	2	1620	-	42,43,43	0.81	0	51,60,60	1.81	15 (29%)
28	XAT	1	1622	-	39,47,47	0.90	0	54,74,74	2.77	22 (40%)
26	CLA	3	614	2	48,56,73	1.72	8 (16%)	55,92,113	1.28	7 (12%)
26	CLA	C	511	6	65,73,73	1.44	8 (12%)	76,113,113	1.56	9 (11%)
26	CLA	7	603	2	55,63,73	1.56	11 (20%)	64,101,113	1.57	10 (15%)
30	LHG	L	101	-	48,48,48	0.90	1 (2%)	51,54,54	1.31	6 (11%)
25	CHL	5	609	1	62,70,74	1.93	14 (22%)	68,109,114	2.72	20 (29%)
26	CLA	1	602	1	61,69,73	1.51	10 (16%)	71,108,113	1.27	8 (11%)
30	LHG	y	2630	26	48,48,48	0.79	2 (4%)	51,54,54	1.23	6 (11%)
26	CLA	R	616	19	45,53,73	1.83	7 (15%)	52,89,113	1.44	5 (9%)
26	CLA	D	403	7	65,73,73	1.42	7 (10%)	76,113,113	1.69	11 (14%)
26	CLA	7	610	2	60,68,73	1.58	9 (15%)	70,107,113	1.28	8 (11%)
26	CLA	6	614	1	45,53,73	1.82	6 (13%)	52,89,113	1.45	6 (11%)
26	CLA	Y	611	30	60,68,73	1.58	9 (15%)	70,107,113	1.53	9 (12%)
26	CLA	c	505	6	65,73,73	1.43	10 (15%)	76,113,113	1.75	11 (14%)
26	CLA	n	604	42	50,58,73	1.79	10 (20%)	58,95,113	1.75	9 (15%)
31	BCR	4	623	-	41,41,41	0.74	0	56,56,56	2.31	17 (30%)
26	CLA	c	512	6	65,73,73	1.42	10 (15%)	76,113,113	1.51	7 (9%)
36	SQD	b	623	-	41,42,54	1.09	5 (12%)	50,53,65	1.77	10 (20%)
26	CLA	b	616	5	65,73,73	1.46	10 (15%)	76,113,113	1.45	12 (15%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	LMG	Z	101	-	51,51,55	0.84	1 (1%)	59,59,63	1.32	5 (8%)
26	CLA	s	613	20	55,63,73	1.56	7 (12%)	64,101,113	1.55	7 (10%)
30	LHG	D	408	-	45,45,48	0.77	1 (2%)	48,51,54	1.28	5 (10%)
39	DGD	c	519	-	63,63,67	1.11	5 (7%)	77,77,81	1.47	12 (15%)
26	CLA	r	604	42	48,56,73	1.64	8 (16%)	55,92,113	1.77	10 (18%)
26	CLA	R	612	19	49,57,73	1.74	7 (14%)	55,93,113	1.61	7 (12%)
26	CLA	8	602	3	45,53,73	1.75	9 (20%)	52,89,113	1.59	7 (13%)
26	CLA	b	614	5	65,73,73	1.43	10 (15%)	76,113,113	1.45	7 (9%)
26	CLA	1	614	1	45,53,73	1.79	7 (15%)	52,89,113	1.47	7 (13%)
26	CLA	1	612	1	45,53,73	1.84	10 (22%)	52,89,113	1.50	9 (17%)
31	BCR	A	411	-	41,41,41	0.79	0	56,56,56	1.78	13 (23%)
29	NEX	2	1623	-	38,46,46	0.93	1 (2%)	50,70,70	2.39	15 (30%)
25	CHL	g	608	42	66,74,74	1.84	16 (24%)	73,114,114	2.73	21 (28%)
26	CLA	C	507	42	65,73,73	1.47	12 (18%)	76,113,113	1.74	11 (14%)
25	CHL	4	607	-	46,54,74	2.31	15 (32%)	49,90,114	3.04	18 (36%)
26	CLA	R	602	19	60,68,73	1.49	6 (10%)	70,107,113	1.64	9 (12%)
26	CLA	g	614	1	48,56,73	1.74	6 (12%)	55,92,113	1.48	7 (12%)
25	CHL	G	601	1	66,74,74	1.82	12 (18%)	73,114,114	2.90	24 (32%)
26	CLA	g	612	1	60,68,73	1.55	7 (11%)	70,107,113	1.35	8 (11%)
31	BCR	c	516	-	41,41,41	0.73	0	56,56,56	1.98	17 (30%)
26	CLA	a	406	42	65,73,73	1.42	8 (12%)	76,113,113	1.76	16 (21%)
30	LHG	b	2630	-	46,46,48	0.66	1 (2%)	49,52,54	1.28	6 (12%)
26	CLA	2	613	1	45,53,73	1.82	9 (20%)	52,89,113	1.43	7 (13%)
26	CLA	1	603	1	55,63,73	1.57	11 (20%)	64,101,113	1.57	9 (14%)
26	CLA	2	603	1	55,63,73	1.63	10 (18%)	64,101,113	1.52	10 (15%)
25	CHL	6	609	1	61,69,74	1.98	14 (22%)	67,108,114	2.74	20 (29%)
26	CLA	C	503	6	65,73,73	1.48	9 (13%)	76,113,113	1.43	10 (13%)
26	CLA	G	613	1	65,73,73	1.49	8 (12%)	76,113,113	1.36	7 (9%)
26	CLA	R	603	19	60,68,73	1.45	9 (15%)	70,107,113	1.67	12 (17%)
39	DGD	C	520	-	61,61,67	1.17	8 (13%)	75,75,81	1.47	12 (16%)
37	LMG	a	413	-	48,48,55	0.79	0	56,56,63	1.31	6 (10%)
26	CLA	5	602	1	61,69,73	1.51	10 (16%)	71,108,113	1.28	8 (11%)
26	CLA	5	604	-	50,58,73	1.74	9 (18%)	58,95,113	1.52	9 (15%)
26	CLA	b	604	5	65,73,73	1.50	11 (16%)	76,113,113	1.46	10 (13%)
26	CLA	1	611	30	45,53,73	1.79	9 (20%)	52,89,113	1.41	6 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
39	DGD	c	520	-	61,61,67	1.17	8 (13%)	75,75,81	1.47	12 (16%)
25	CHL	2	606	-	46,54,74	2.26	15 (32%)	49,90,114	3.08	18 (36%)
25	CHL	R	606	42	66,74,74	1.87	14 (21%)	73,114,114	2.78	22 (30%)
30	LHG	B	2630	-	46,46,48	0.65	1 (2%)	49,52,54	1.28	6 (12%)
30	LHG	1	2630	26	40,40,48	0.72	1 (2%)	43,46,54	1.34	6 (13%)
26	CLA	c	510	6	65,73,73	1.44	7 (10%)	76,113,113	1.58	10 (13%)
27	LUT	r	620	-	42,43,43	0.87	2 (4%)	51,60,60	1.82	14 (27%)
25	CHL	6	607	-	61,69,74	1.95	15 (24%)	67,108,114	2.73	21 (31%)
27	LUT	4	620	-	42,43,43	0.80	0	51,60,60	1.87	18 (35%)
40	BCT	D	401	33	2,3,3	1.32	0	2,3,3	4.20	2 (100%)
26	CLA	S	611	30	56,64,73	1.55	9 (16%)	65,102,113	1.47	7 (10%)
26	CLA	A	405	4	65,73,73	1.49	10 (15%)	76,113,113	1.68	12 (15%)
25	CHL	n	608	42	66,74,74	1.82	13 (19%)	73,114,114	2.77	25 (34%)
25	CHL	5	606	-	46,54,74	2.24	15 (32%)	49,90,114	3.08	20 (40%)
26	CLA	N	613	1	60,68,73	1.49	8 (13%)	70,107,113	1.58	7 (10%)
26	CLA	N	603	1	65,73,73	1.54	11 (16%)	76,113,113	1.61	15 (19%)
31	BCR	c	514	-	41,41,41	0.90	2 (4%)	56,56,56	1.74	13 (23%)
25	CHL	S	606	42	46,54,74	2.27	15 (32%)	49,90,114	3.37	19 (38%)
26	CLA	B	605	5	65,73,73	1.54	11 (16%)	76,113,113	2.03	24 (31%)
26	CLA	N	604	42	50,58,73	1.79	10 (20%)	58,95,113	1.74	9 (15%)
26	CLA	s	612	20	49,57,73	1.64	7 (14%)	55,93,113	1.68	6 (10%)
37	LMG	A	413	-	48,48,55	0.79	0	56,56,63	1.31	6 (10%)
30	LHG	C	522	-	48,48,48	0.69	1 (2%)	51,54,54	1.26	6 (11%)
26	CLA	C	509	6	65,73,73	1.45	11 (16%)	76,113,113	1.73	11 (14%)
25	CHL	r	608	42	61,69,74	1.90	10 (16%)	67,108,114	2.91	23 (34%)
30	LHG	n	2630	26	48,48,48	0.66	1 (2%)	51,54,54	1.30	6 (11%)
40	BCT	d	401	33	2,3,3	1.32	0	2,3,3	4.19	2 (100%)
26	CLA	R	610	19	65,73,73	1.47	9 (13%)	76,113,113	1.38	11 (14%)
37	LMG	a	415	-	40,40,55	0.86	0	48,48,63	1.29	5 (10%)
31	BCR	a	411	-	41,41,41	0.79	0	56,56,56	1.78	13 (23%)
26	CLA	s	609	20	45,53,73	1.81	6 (13%)	52,89,113	1.41	9 (17%)
38	PL9	a	414	-	13,13,55	0.87	0	17,17,69	1.68	4 (23%)
25	CHL	N	601	1	66,74,74	1.84	14 (21%)	73,114,114	2.82	23 (31%)
25	CHL	s	607	42	58,66,74	1.93	12 (20%)	63,104,114	2.86	20 (31%)
25	CHL	g	607	42	66,74,74	1.88	13 (19%)	73,114,114	2.66	22 (30%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	Y	605	1	48,56,74	2.15	14 (29%)	51,92,114	3.33	17 (33%)
26	CLA	8	612	3	45,53,73	1.78	7 (15%)	52,89,113	1.51	9 (17%)
25	CHL	G	606	42	50,58,74	2.21	15 (30%)	52,94,114	3.06	22 (42%)
26	CLA	2	612	1	45,53,73	1.85	7 (15%)	52,89,113	1.50	8 (15%)
29	NEX	g	1623	-	38,46,46	1.00	3 (7%)	50,70,70	2.39	14 (28%)
25	CHL	s	606	42	46,54,74	2.27	15 (32%)	49,90,114	3.37	19 (38%)
26	CLA	b	605	5	65,73,73	1.55	11 (16%)	76,113,113	2.03	24 (31%)
26	CLA	y	604	42	50,58,73	1.73	10 (20%)	58,95,113	1.77	8 (13%)
25	CHL	8	607	-	46,54,74	2.31	15 (32%)	49,90,114	3.05	18 (36%)
28	XAT	8	622	-	39,47,47	0.93	1 (2%)	54,74,74	2.62	21 (38%)
26	CLA	c	501	6	65,73,73	1.48	9 (13%)	76,113,113	1.37	10 (13%)
25	CHL	n	606	42	50,58,74	2.16	15 (30%)	52,94,114	3.04	21 (40%)
25	CHL	y	609	1	66,74,74	1.86	14 (21%)	73,114,114	2.72	22 (30%)
37	LMG	B	2633	-	55,55,55	0.78	3 (5%)	63,63,63	1.32	7 (11%)
26	CLA	r	611	30	49,57,73	1.65	8 (16%)	55,93,113	1.74	12 (21%)
25	CHL	8	606	-	46,54,74	2.29	15 (32%)	49,90,114	3.19	22 (44%)
28	XAT	5	1622	-	39,47,47	0.90	0	54,74,74	2.77	22 (40%)
39	DGD	B	626	-	60,60,67	1.04	3 (5%)	74,74,81	1.39	12 (16%)
26	CLA	6	613	1	45,53,73	1.82	9 (20%)	52,89,113	1.43	7 (13%)
31	BCR	C	515	-	41,41,41	0.93	2 (4%)	56,56,56	2.01	16 (28%)
26	CLA	C	506	6	65,73,73	1.45	10 (15%)	76,113,113	1.58	11 (14%)
26	CLA	R	609	19	58,66,73	1.62	8 (13%)	67,104,113	1.54	7 (10%)
26	CLA	S	602	20	61,69,73	1.51	8 (13%)	71,108,113	1.46	11 (15%)
25	CHL	y	601	1	66,74,74	1.84	13 (19%)	73,114,114	2.86	22 (30%)
25	CHL	4	609	3	46,54,74	2.31	15 (32%)	49,90,114	3.07	17 (34%)
25	CHL	8	609	3	46,54,74	2.31	15 (32%)	49,90,114	3.08	17 (34%)
26	CLA	B	610	5	65,73,73	1.41	9 (13%)	76,113,113	1.60	9 (11%)
26	CLA	C	502	6	65,73,73	1.40	9 (13%)	76,113,113	1.70	9 (11%)
30	LHG	c	2630	-	48,48,48	0.66	1 (2%)	51,54,54	1.31	7 (13%)
30	LHG	C	523	-	48,48,48	0.66	1 (2%)	51,54,54	1.20	5 (9%)
25	CHL	8	601	3	44,53,74	2.43	16 (36%)	46,89,114	3.02	16 (34%)
39	DGD	b	626	-	60,60,67	1.05	3 (5%)	74,74,81	1.39	12 (16%)
25	CHL	r	607	42	56,64,74	2.01	12 (21%)	61,102,114	3.09	21 (34%)
37	LMG	d	411	-	46,46,55	0.92	3 (6%)	54,54,63	1.45	4 (7%)
26	CLA	b	610	5	65,73,73	1.41	9 (13%)	76,113,113	1.59	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
37	LMG	A	415	-	40,40,55	0.86	0	48,48,63	1.28	5 (10%)
30	LHG	C	2630	-	48,48,48	0.66	1 (2%)	51,54,54	1.31	7 (13%)
25	CHL	G	609	1	61,69,74	1.93	14 (22%)	67,108,114	2.78	22 (32%)
25	CHL	1	605	1	46,54,74	2.25	15 (32%)	49,90,114	3.22	21 (42%)
25	CHL	S	601	20	46,54,74	2.28	13 (28%)	49,90,114	3.13	20 (40%)
26	CLA	r	603	19	60,68,73	1.45	9 (15%)	70,107,113	1.66	12 (17%)
26	CLA	c	513	6	65,73,73	1.39	7 (10%)	76,113,113	1.60	14 (18%)
39	DGD	h	102	-	63,63,67	1.08	7 (11%)	77,77,81	1.41	11 (14%)
27	LUT	N	1621	-	42,43,43	0.89	2 (4%)	51,60,60	1.83	14 (27%)
26	CLA	b	608	42	65,73,73	1.53	10 (15%)	76,113,113	1.69	11 (14%)
29	NEX	Y	1623	-	38,46,46	0.94	2 (5%)	50,70,70	2.59	18 (36%)
27	LUT	3	1621	-	42,43,43	0.85	1 (2%)	51,60,60	1.60	11 (21%)
26	CLA	B	602	42	65,73,73	1.50	9 (13%)	76,113,113	1.41	7 (9%)
25	CHL	n	609	1	66,74,74	1.88	14 (21%)	73,114,114	2.72	23 (31%)
32	OEX	A	401	4,6	0,15,15	-	-	-	-	-
30	LHG	3	2630	26	46,46,48	0.70	1 (2%)	49,52,54	1.24	5 (10%)
28	XAT	N	1622	-	39,47,47	0.92	0	54,74,74	3.00	24 (44%)
25	CHL	1	607	-	63,71,74	1.89	13 (20%)	69,110,114	2.87	20 (28%)
26	CLA	b	612	5	65,73,73	1.50	8 (12%)	76,113,113	1.66	9 (11%)
25	CHL	y	608	42	66,74,74	1.80	13 (19%)	73,114,114	2.74	23 (31%)
26	CLA	b	613	5	65,73,73	1.47	9 (13%)	76,113,113	1.85	13 (17%)
26	CLA	N	611	30	60,68,73	1.54	7 (11%)	70,107,113	1.45	7 (10%)
25	CHL	n	601	1	66,74,74	1.85	14 (21%)	73,114,114	2.82	23 (31%)
30	LHG	Y	2630	26	48,48,48	0.79	2 (4%)	51,54,54	1.23	6 (11%)
31	BCR	H	101	-	41,41,41	0.78	0	56,56,56	1.90	10 (17%)
26	CLA	n	613	1	60,68,73	1.49	8 (13%)	70,107,113	1.58	7 (10%)
26	CLA	n	603	1	65,73,73	1.55	10 (15%)	76,113,113	1.61	15 (19%)
26	CLA	3	610	2	60,68,73	1.57	9 (15%)	70,107,113	1.28	8 (11%)
41	HEM	F	101	9,8	41,50,50	1.46	4 (9%)	45,82,82	1.37	7 (15%)
26	CLA	Y	603	1	65,73,73	1.59	10 (15%)	76,113,113	1.56	13 (17%)
27	LUT	S	1620	-	42,43,43	0.79	0	51,60,60	1.76	12 (23%)
25	CHL	g	609	1	61,69,74	1.93	14 (22%)	67,108,114	2.78	22 (32%)
30	LHG	4	2630	26	20,20,48	0.91	1 (5%)	23,26,54	1.30	2 (8%)
26	CLA	C	505	6	65,73,73	1.43	10 (15%)	76,113,113	1.75	11 (14%)
38	PL9	d	405	-	55,55,55	1.83	12 (21%)	68,69,69	1.57	12 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LHG	6	2630	26	36,36,48	0.74	1 (2%)	39,42,54	1.27	4 (10%)
26	CLA	C	512	6	65,73,73	1.42	10 (15%)	76,113,113	1.51	8 (10%)
25	CHL	1	608	-	46,54,74	2.17	14 (30%)	49,90,114	3.27	14 (28%)
25	CHL	4	606	-	46,54,74	2.29	15 (32%)	49,90,114	3.18	23 (46%)
26	CLA	C	501	6	65,73,73	1.48	9 (13%)	76,113,113	1.37	10 (13%)
25	CHL	s	601	20	46,54,74	2.28	14 (30%)	49,90,114	3.12	20 (40%)
31	BCR	c	517	-	41,41,41	0.89	1 (2%)	56,56,56	2.09	11 (19%)
26	CLA	G	610	1	64,72,73	1.50	7 (10%)	74,111,113	1.37	8 (10%)
30	LHG	l	101	-	48,48,48	0.90	1 (2%)	51,54,54	1.31	7 (13%)
31	BCR	h	101	-	41,41,41	0.78	0	56,56,56	1.89	10 (17%)
26	CLA	G	602	1	65,73,73	1.45	8 (12%)	76,113,113	1.59	11 (14%)
31	BCR	B	620	-	41,41,41	0.79	0	56,56,56	1.99	16 (28%)
26	CLA	R	601	19	49,57,73	1.64	5 (10%)	55,93,113	1.92	11 (20%)
35	PHO	A	409	-	51,69,69	1.09	4 (7%)	47,99,99	1.36	7 (14%)
26	CLA	6	603	1	55,63,73	1.63	11 (20%)	64,101,113	1.53	10 (15%)
26	CLA	6	611	30	45,53,73	1.79	8 (17%)	52,89,113	1.52	7 (13%)
28	XAT	R	622	-	39,47,47	0.97	1 (2%)	54,74,74	2.76	21 (38%)
25	CHL	2	609	1	61,69,74	1.98	15 (24%)	67,108,114	2.74	20 (29%)
29	NEX	6	1623	-	38,46,46	0.93	1 (2%)	50,70,70	2.38	15 (30%)
27	LUT	3	1620	-	42,43,43	0.85	0	51,60,60	1.72	13 (25%)
29	NEX	R	623	-	38,46,46	1.05	3 (7%)	50,70,70	2.51	19 (38%)
25	CHL	6	605	1	46,54,74	2.29	16 (34%)	49,90,114	3.15	19 (38%)
26	CLA	R	611	30	49,57,73	1.65	8 (16%)	55,93,113	1.75	12 (21%)
25	CHL	y	605	1	48,56,74	2.15	14 (29%)	51,92,114	3.33	17 (33%)
26	CLA	3	602	2	60,68,73	1.55	9 (15%)	70,107,113	1.34	8 (11%)
29	NEX	3	1623	-	38,46,46	0.87	1 (2%)	50,70,70	2.40	16 (32%)
25	CHL	5	605	1	46,54,74	2.25	15 (32%)	49,90,114	3.21	21 (42%)
26	CLA	G	612	1	60,68,73	1.54	8 (13%)	70,107,113	1.35	8 (11%)
29	NEX	1	1623	-	38,46,46	0.99	2 (5%)	50,70,70	2.42	15 (30%)
25	CHL	2	601	1	46,54,74	2.26	13 (28%)	49,90,114	3.23	22 (44%)
35	PHO	a	409	-	51,69,69	1.09	4 (7%)	47,99,99	1.36	7 (14%)
28	XAT	3	1622	-	39,47,47	1.03	2 (5%)	54,74,74	2.85	24 (44%)
29	NEX	S	1623	-	38,46,46	0.91	2 (5%)	50,70,70	2.24	15 (30%)
26	CLA	B	606	5	65,73,73	1.54	12 (18%)	76,113,113	1.67	11 (14%)
26	CLA	B	611	42	65,73,73	1.45	10 (15%)	76,113,113	1.70	13 (17%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	y	607	42	66,74,74	1.80	13 (19%)	73,114,114	2.72	21 (28%)
27	LUT	7	1621	-	42,43,43	0.86	1 (2%)	51,60,60	1.60	11 (21%)
28	XAT	y	1622	-	39,47,47	1.08	3 (7%)	54,74,74	3.00	21 (38%)
26	CLA	Y	610	1	60,68,73	1.55	10 (16%)	70,107,113	1.28	8 (11%)
26	CLA	r	616	19	45,53,73	1.82	7 (15%)	52,89,113	1.44	5 (9%)
26	CLA	B	603	5	65,73,73	1.43	7 (10%)	76,113,113	1.51	8 (10%)
26	CLA	2	602	1	61,69,73	1.52	8 (13%)	71,108,113	1.34	8 (11%)
31	BCR	C	517	-	41,41,41	0.89	1 (2%)	56,56,56	2.08	11 (19%)
25	CHL	7	606	-	46,54,74	2.20	15 (32%)	49,90,114	3.15	19 (38%)
26	CLA	y	611	30	60,68,73	1.58	9 (15%)	70,107,113	1.53	9 (12%)
27	LUT	y	1620	-	42,43,43	0.88	1 (2%)	51,60,60	1.72	13 (25%)
26	CLA	B	613	5	65,73,73	1.48	9 (13%)	76,113,113	1.84	13 (17%)
26	CLA	C	510	6	65,73,73	1.44	7 (10%)	76,113,113	1.59	10 (13%)
30	LHG	B	2631	-	48,48,48	0.68	2 (4%)	51,54,54	1.22	6 (11%)
26	CLA	c	506	6	65,73,73	1.45	10 (15%)	76,113,113	1.58	10 (13%)
26	CLA	7	602	2	60,68,73	1.55	9 (15%)	70,107,113	1.34	8 (11%)
31	BCR	C	514	-	41,41,41	0.90	1 (2%)	56,56,56	1.75	13 (23%)
30	LHG	S	2630	26	48,48,48	0.73	1 (2%)	51,54,54	1.26	7 (13%)
27	LUT	n	1621	-	42,43,43	0.89	2 (4%)	51,60,60	1.83	14 (27%)
25	CHL	7	609	2	61,69,74	2.02	15 (24%)	67,108,114	2.61	21 (31%)
26	CLA	6	610	1	50,58,73	1.67	9 (18%)	58,95,113	1.37	9 (15%)
26	CLA	y	603	1	65,73,73	1.59	10 (15%)	76,113,113	1.56	13 (17%)
26	CLA	y	610	1	60,68,73	1.55	10 (16%)	70,107,113	1.28	8 (11%)
28	XAT	6	1622	-	39,47,47	0.91	1 (2%)	54,74,74	2.81	21 (38%)
26	CLA	s	604	42	50,58,73	1.65	7 (14%)	58,95,113	1.97	9 (15%)
32	OEX	a	401	4,6	0,15,15	-	-	-	-	-
25	CHL	g	606	42	50,58,74	2.20	15 (30%)	52,94,114	3.06	22 (42%)
25	CHL	r	614	19	42,50,74	2.33	14 (33%)	44,85,114	3.45	19 (43%)
26	CLA	N	602	1	65,73,73	1.44	8 (12%)	76,113,113	1.58	11 (14%)
26	CLA	n	602	1	65,73,73	1.44	8 (12%)	76,113,113	1.58	11 (14%)
31	BCR	d	404	-	41,41,41	0.74	0	56,56,56	1.84	12 (21%)
25	CHL	7	601	2	64,72,74	1.91	12 (18%)	70,111,114	2.88	23 (32%)
26	CLA	G	614	1	48,56,73	1.73	6 (12%)	55,92,113	1.48	7 (12%)
26	CLA	7	614	2	48,56,73	1.72	8 (16%)	55,92,113	1.28	7 (12%)
36	SQD	B	621	-	53,54,54	0.94	4 (7%)	62,65,65	1.64	13 (20%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
26	CLA	4	610	3	45,53,73	1.81	9 (20%)	52,89,113	1.30	6 (11%)
26	CLA	8	604	-	45,53,73	1.81	8 (17%)	52,89,113	1.44	7 (13%)
30	LHG	D	409	-	48,48,48	0.75	1 (2%)	51,54,54	1.31	7 (13%)
25	CHL	N	605	1	48,56,74	2.19	14 (29%)	51,92,114	3.24	20 (39%)
30	LHG	5	2630	26	40,40,48	0.72	1 (2%)	43,46,54	1.33	6 (13%)
27	LUT	6	1620	-	42,43,43	0.81	0	51,60,60	1.80	15 (29%)
26	CLA	c	507	42	65,73,73	1.48	12 (18%)	76,113,113	1.73	11 (14%)
26	CLA	s	614	20	49,57,73	1.63	6 (12%)	55,93,113	1.75	10 (18%)
38	PL9	A	414	-	13,13,55	0.87	0	17,17,69	1.68	4 (23%)
39	DGD	c	518	-	56,56,67	1.17	7 (12%)	70,70,81	1.56	12 (17%)
26	CLA	n	614	1	48,56,73	1.66	6 (12%)	55,92,113	1.69	8 (14%)
25	CHL	G	607	42	66,74,74	1.88	13 (19%)	73,114,114	2.66	23 (31%)
31	BCR	B	619	-	41,41,41	0.80	0	56,56,56	1.81	17 (30%)
26	CLA	2	604	-	45,53,73	1.81	8 (17%)	52,89,113	1.50	6 (11%)
26	CLA	b	617	5	65,73,73	1.45	9 (13%)	76,113,113	1.62	11 (14%)
25	CHL	4	601	3	44,53,74	2.42	16 (36%)	46,89,114	3.02	16 (34%)
36	SQD	a	412	-	49,50,54	0.96	6 (12%)	58,61,65	1.75	11 (18%)
26	CLA	C	508	6	65,73,73	1.47	11 (16%)	76,113,113	1.84	11 (14%)
27	LUT	1	1620	-	42,43,43	0.79	0	51,60,60	1.66	14 (27%)
25	CHL	N	608	42	66,74,74	1.82	13 (19%)	73,114,114	2.77	25 (34%)
25	CHL	6	608	-	46,54,74	2.23	15 (32%)	49,90,114	3.26	17 (34%)
26	CLA	7	604	-	45,53,73	1.81	9 (20%)	52,89,113	1.51	7 (13%)
29	NEX	y	1623	-	38,46,46	0.94	2 (5%)	50,70,70	2.59	18 (36%)
26	CLA	b	611	42	65,73,73	1.44	10 (15%)	76,113,113	1.69	13 (17%)
29	NEX	r	623	-	38,46,46	1.04	3 (7%)	50,70,70	2.51	19 (38%)
25	CHL	3	601	2	64,72,74	1.91	12 (18%)	70,111,114	2.89	23 (32%)
25	CHL	8	608	-	46,54,74	2.16	14 (30%)	49,90,114	3.32	18 (36%)
27	LUT	g	1620	-	42,43,43	0.77	0	51,60,60	1.63	12 (23%)
31	BCR	b	618	-	41,41,41	0.84	1 (2%)	56,56,56	1.85	14 (25%)
26	CLA	d	403	7	65,73,73	1.42	7 (10%)	76,113,113	1.69	11 (14%)
26	CLA	4	602	3	45,53,73	1.75	9 (20%)	52,89,113	1.58	7 (13%)
26	CLA	b	603	5	65,73,73	1.42	7 (10%)	76,113,113	1.51	8 (10%)
27	LUT	6	1621	-	42,43,43	0.84	1 (2%)	51,60,60	1.68	15 (29%)
25	CHL	r	606	42	66,74,74	1.87	14 (21%)	73,114,114	2.78	22 (30%)
31	BCR	D	404	-	41,41,41	0.75	0	56,56,56	1.83	12 (21%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
25	CHL	2	608	-	46,54,74	2.23	15 (32%)	49,90,114	3.26	17 (34%)
26	CLA	1	613	1	55,63,73	1.64	9 (16%)	64,101,113	1.34	6 (9%)
30	LHG	2	2630	26	36,36,48	0.74	1 (2%)	39,42,54	1.27	4 (10%)
36	SQD	A	418	-	53,54,54	0.92	5 (9%)	62,65,65	1.67	14 (22%)
27	LUT	S	1621	-	42,43,43	0.85	1 (2%)	51,60,60	1.78	17 (33%)
25	CHL	3	606	-	46,54,74	2.20	15 (32%)	49,90,114	3.15	19 (38%)
38	PL9	D	405	-	55,55,55	1.83	12 (21%)	68,69,69	1.57	12 (17%)
30	LHG	d	408	-	45,45,48	0.78	1 (2%)	48,51,54	1.28	5 (10%)
25	CHL	7	607	-	53,61,74	2.24	16 (30%)	57,98,114	2.88	23 (40%)
31	BCR	T	101	-	41,41,41	0.75	0	56,56,56	2.55	19 (33%)
26	CLA	8	611	30	45,53,73	1.81	8 (17%)	52,89,113	1.50	7 (13%)
26	CLA	s	610	20	55,63,73	1.63	8 (14%)	64,101,113	1.58	10 (15%)
37	LMG	B	622	-	51,51,55	0.83	1 (1%)	59,59,63	1.30	4 (6%)
37	LMG	z	101	-	51,51,55	0.84	1 (1%)	59,59,63	1.32	5 (8%)
29	NEX	N	1623	-	38,46,46	0.90	1 (2%)	50,70,70	2.36	15 (30%)
26	CLA	3	612	2	45,53,73	1.78	10 (22%)	52,89,113	1.51	10 (19%)
25	CHL	Y	606	42	50,58,74	2.04	13 (26%)	52,94,114	3.18	19 (36%)
30	LHG	d	410	-	42,42,48	0.68	1 (2%)	45,48,54	1.22	4 (8%)
26	CLA	D	402	7	65,73,73	1.55	10 (15%)	76,113,113	1.71	10 (13%)
27	LUT	Y	1620	-	42,43,43	0.87	1 (2%)	51,60,60	1.73	13 (25%)
26	CLA	S	613	20	55,63,73	1.56	7 (12%)	64,101,113	1.55	7 (10%)
26	CLA	n	610	1	65,73,73	1.43	8 (12%)	76,113,113	1.42	10 (13%)
26	CLA	c	511	6	65,73,73	1.45	8 (12%)	76,113,113	1.55	9 (11%)
31	BCR	t	101	-	41,41,41	0.76	0	56,56,56	2.55	19 (33%)
25	CHL	g	601	1	66,74,74	1.82	12 (18%)	73,114,114	2.90	24 (32%)
26	CLA	S	614	20	49,57,73	1.62	6 (12%)	55,93,113	1.76	10 (18%)
27	LUT	5	1620	-	42,43,43	0.80	0	51,60,60	1.66	15 (29%)
26	CLA	G	611	30	60,68,73	1.61	7 (11%)	70,107,113	1.60	7 (10%)
26	CLA	7	611	30	55,63,73	1.66	10 (18%)	64,101,113	1.51	11 (17%)
37	LMG	b	622	-	51,51,55	0.83	1 (1%)	59,59,63	1.30	4 (6%)
25	CHL	7	608	-	46,54,74	2.20	15 (32%)	49,90,114	3.28	19 (38%)
31	BCR	b	620	-	41,41,41	0.80	0	56,56,56	1.99	16 (28%)
25	CHL	R	614	19	42,50,74	2.32	14 (33%)	44,85,114	3.45	19 (43%)
26	CLA	B	607	5	65,73,73	1.50	11 (16%)	76,113,113	1.60	12 (15%)
26	CLA	c	503	6	65,73,73	1.49	9 (13%)	76,113,113	1.44	9 (11%)

Mol	Type	Chain	Res	Link	Bond lengths			Bond angles		
					Counts	RMSZ	# Z > 2	Counts	RMSZ	# Z > 2
30	LHG	7	2630	26	46,46,48	0.70	1 (2%)	49,52,54	1.25	5 (10%)
26	CLA	r	610	19	65,73,73	1.48	9 (13%)	76,113,113	1.38	11 (14%)
39	DGD	C	518	-	56,56,67	1.17	7 (12%)	70,70,81	1.56	13 (18%)
31	BCR	B	618	-	41,41,41	0.84	1 (2%)	56,56,56	1.85	14 (25%)
26	CLA	s	602	20	61,69,73	1.51	8 (13%)	71,108,113	1.46	11 (15%)
29	NEX	s	1623	-	38,46,46	0.90	2 (5%)	50,70,70	2.24	15 (30%)
26	CLA	r	602	19	60,68,73	1.50	7 (11%)	70,107,113	1.65	9 (12%)
36	SQD	B	623	-	41,42,54	1.10	5 (12%)	50,53,65	1.77	10 (20%)
26	CLA	R	604	42	48,56,73	1.64	8 (16%)	55,92,113	1.77	10 (18%)
25	CHL	R	607	42	56,64,74	2.01	13 (23%)	61,102,114	3.09	21 (34%)
26	CLA	7	612	2	45,53,73	1.77	10 (22%)	52,89,113	1.51	10 (19%)
39	DGD	C	519	-	63,63,67	1.11	5 (7%)	77,77,81	1.47	12 (15%)
26	CLA	N	614	1	48,56,73	1.66	6 (12%)	55,92,113	1.68	8 (14%)
26	CLA	N	612	1	60,68,73	1.55	7 (11%)	70,107,113	1.43	8 (11%)
27	LUT	7	1620	-	42,43,43	0.84	0	51,60,60	1.71	12 (23%)
26	CLA	y	602	1	65,73,73	1.43	8 (12%)	76,113,113	1.53	10 (13%)
36	SQD	b	621	-	53,54,54	0.94	4 (7%)	62,65,65	1.64	13 (20%)
26	CLA	S	604	42	50,58,73	1.64	7 (14%)	58,95,113	1.96	8 (13%)
28	XAT	7	1622	-	39,47,47	1.03	2 (5%)	54,74,74	2.85	24 (44%)
25	CHL	4	608	-	46,54,74	2.16	14 (30%)	49,90,114	3.30	18 (36%)
26	CLA	3	613	2	58,66,73	1.61	10 (17%)	67,104,113	1.42	8 (11%)
26	CLA	8	610	3	45,53,73	1.81	9 (20%)	52,89,113	1.30	6 (11%)
26	CLA	B	617	5	65,73,73	1.45	9 (13%)	76,113,113	1.62	11 (14%)
27	LUT	y	1621	-	42,43,43	0.88	1 (2%)	51,60,60	1.69	13 (25%)
28	XAT	2	1622	-	39,47,47	0.91	1 (2%)	54,74,74	2.82	21 (38%)
25	CHL	N	607	42	66,74,74	1.80	13 (19%)	73,114,114	2.84	20 (27%)
26	CLA	2	610	1	50,58,73	1.67	9 (18%)	58,95,113	1.37	9 (15%)
26	CLA	6	604	-	45,53,73	1.81	8 (17%)	52,89,113	1.50	6 (11%)
26	CLA	a	410	4	60,68,73	1.48	10 (16%)	70,107,113	1.64	9 (12%)
30	LHG	D	410	-	42,42,48	0.68	1 (2%)	45,48,54	1.22	4 (8%)
27	LUT	R	620	-	42,43,43	0.86	2 (4%)	51,60,60	1.82	14 (27%)
26	CLA	6	612	1	45,53,73	1.85	8 (17%)	52,89,113	1.50	8 (15%)
26	CLA	b	602	42	65,73,73	1.50	9 (13%)	76,113,113	1.41	7 (9%)
29	NEX	5	1623	-	38,46,46	0.98	2 (5%)	50,70,70	2.41	16 (32%)
39	DGD	H	102	-	63,63,67	1.08	7 (11%)	77,77,81	1.40	11 (14%)

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
25	CHL	R	608	42	4/4/19/26	17/33/131/137	-
26	CLA	r	613	19	1/1/14/20	10/31/109/115	-
28	XAT	4	622	-	-	2/31/93/93	0/4/4/4
26	CLA	s	603	20	1/1/11/20	5/13/91/115	-
26	CLA	g	610	1	1/1/14/20	13/36/114/115	-
37	LMG	D	411	-	-	15/41/61/70	0/1/1/1
26	CLA	y	613	1	1/1/15/20	10/37/115/115	-
26	CLA	5	613	1	-	8/25/103/115	-
26	CLA	y	614	1	1/1/11/20	3/17/95/115	-
30	LHG	R	2630	26	-	19/46/46/53	-
36	SQD	a	418	-	-	22/49/69/69	0/1/1/1
25	CHL	1	609	1	4/4/19/26	16/35/133/137	-
26	CLA	B	604	5	1/1/15/20	10/37/115/115	-
26	CLA	N	610	1	1/1/15/20	12/37/115/115	-
26	CLA	B	616	5	1/1/15/20	13/37/115/115	-
26	CLA	C	504	42	1/1/15/20	18/37/115/115	-
25	CHL	1	601	1	3/3/16/26	6/15/113/137	-
26	CLA	g	613	1	1/1/15/20	12/37/115/115	-
29	NEX	7	1623	-	-	4/27/83/83	0/3/3/3
30	LHG	d	409	-	-	27/53/53/53	-
26	CLA	B	612	5	1/1/15/20	13/37/115/115	-
30	LHG	b	2631	-	-	22/53/53/53	-
25	CHL	1	606	-	3/3/16/26	8/15/113/137	-
25	CHL	S	608	-	3/3/16/26	4/15/113/137	-
27	LUT	Y	1621	-	-	1/29/67/67	0/2/2/2
37	LMG	C	521	-	-	22/46/66/70	0/1/1/1
27	LUT	G	1621	-	-	3/29/67/67	0/2/2/2
25	CHL	G	605	1	3/3/16/26	9/15/113/137	-
26	CLA	4	611	30	1/1/11/20	4/13/91/115	-
27	LUT	N	1620	-	-	2/29/67/67	0/2/2/2
25	CHL	N	609	1	4/4/20/26	13/39/137/137	-
26	CLA	Y	602	1	1/1/15/20	10/37/115/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	7	613	2	1/1/13/20	9/29/107/115	-
27	LUT	5	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	n	611	30	1/1/14/20	4/31/109/115	-
26	CLA	B	609	5	-	9/37/115/115	-
25	CHL	3	609	2	4/4/19/26	13/33/131/137	-
31	BCR	c	515	-	-	6/29/63/63	0/2/2/2
27	LUT	g	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	G	604	42	1/1/12/20	5/19/97/115	-
28	XAT	r	622	-	-	3/31/93/93	0/4/4/4
28	XAT	g	1622	-	-	2/31/93/93	0/4/4/4
26	CLA	n	612	1	1/1/14/20	9/31/109/115	-
26	CLA	b	606	5	1/1/15/20	14/37/115/115	-
26	CLA	5	611	30	1/1/11/20	6/13/91/115	-
26	CLA	3	603	2	1/1/13/20	13/25/103/115	-
25	CHL	Y	601	1	4/4/20/26	16/39/137/137	-
26	CLA	g	611	30	1/1/14/20	11/31/109/115	-
26	CLA	Y	614	1	1/1/11/20	3/17/95/115	-
41	HEM	f	101	9,8	-	1/12/54/54	-
26	CLA	Y	612	1	1/1/14/20	15/31/109/115	-
25	CHL	6	606	-	3/3/16/26	6/15/113/137	-
26	CLA	3	604	-	1/1/11/20	9/13/91/115	-
26	CLA	Y	613	1	1/1/15/20	10/37/115/115	-
26	CLA	5	614	1	1/1/11/20	2/13/91/115	-
25	CHL	y	606	42	3/3/16/26	6/20/118/137	-
26	CLA	b	609	5	-	9/37/115/115	-
26	CLA	5	612	1	1/1/11/20	3/13/91/115	-
26	CLA	B	614	5	1/1/15/20	13/37/115/115	-
26	CLA	r	612	19	1/1/11/20	6/18/96/115	-
27	LUT	8	620	-	-	4/29/67/67	0/2/2/2
26	CLA	S	610	20	1/1/13/20	4/25/103/115	-
26	CLA	S	603	20	1/1/11/20	5/13/91/115	-
26	CLA	1	610	1	1/1/13/20	5/27/105/115	-
25	CHL	3	605	2	3/3/16/26	9/15/113/137	-
28	XAT	G	1622	-	-	2/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	Y	609	1	4/4/20/26	13/39/137/137	-
25	CHL	2	605	1	3/3/16/26	9/15/113/137	-
26	CLA	r	609	19	1/1/13/20	3/29/107/115	-
26	CLA	1	604	-	-	10/19/97/115	-
26	CLA	B	615	5	1/1/15/20	13/37/115/115	-
25	CHL	5	607	-	4/4/19/26	20/36/134/137	-
25	CHL	7	605	2	3/3/16/26	9/15/113/137	-
30	LHG	r	2630	26	-	19/46/46/53	-
26	CLA	Y	604	42	1/1/12/20	3/19/97/115	-
27	LUT	s	1621	-	-	2/29/67/67	0/2/2/2
26	CLA	r	601	19	1/1/11/20	14/18/96/115	-
26	CLA	4	603	3	1/1/11/20	4/13/91/115	-
26	CLA	S	612	20	1/1/11/20	5/18/96/115	-
30	LHG	G	2630	26	-	26/53/53/53	-
26	CLA	B	608	42	1/1/15/20	11/37/115/115	-
35	PHO	a	408	-	-	12/37/103/103	0/5/6/6
26	CLA	A	410	4	1/1/14/20	5/31/109/115	-
25	CHL	3	608	-	3/3/16/26	3/15/113/137	-
26	CLA	b	607	5	1/1/15/20	9/37/115/115	-
26	CLA	A	407	42	-	3/19/97/115	-
25	CHL	n	605	1	3/3/16/26	9/18/116/137	-
26	CLA	G	603	1	1/1/15/20	11/37/115/115	-
26	CLA	s	611	30	1/1/13/20	9/27/105/115	-
27	LUT	G	1620	-	-	2/29/67/67	0/2/2/2
36	SQD	A	412	-	-	13/45/65/69	0/1/1/1
30	LHG	c	523	-	-	21/53/53/53	-
26	CLA	C	513	6	-	10/37/115/115	-
25	CHL	5	601	1	3/3/16/26	6/15/113/137	-
26	CLA	g	603	1	1/1/15/20	11/37/115/115	-
26	CLA	b	615	5	1/1/15/20	12/37/115/115	-
25	CHL	G	608	42	4/4/20/26	15/39/137/137	-
29	NEX	G	1623	-	-	5/27/83/83	0/3/3/3
26	CLA	S	609	20	1/1/11/20	5/13/91/115	-
25	CHL	n	607	42	4/4/20/26	14/39/137/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
28	XAT	Y	1622	-	-	2/31/93/93	0/4/4/4
30	LHG	8	2630	26	-	8/23/23/53	-
25	CHL	N	606	42	3/3/16/26	6/20/118/137	-
27	LUT	2	1621	-	-	3/29/67/67	0/2/2/2
37	LMG	b	2633	-	-	24/50/70/70	0/1/1/1
26	CLA	c	509	6	1/1/15/20	8/37/115/115	-
25	CHL	5	608	-	3/3/16/26	7/15/113/137	-
25	CHL	Y	607	42	4/4/20/26	16/39/137/137	-
30	LHG	g	2630	26	-	26/53/53/53	-
27	LUT	1	1621	-	-	3/29/67/67	0/2/2/2
30	LHG	c	522	-	-	20/53/53/53	-
29	NEX	n	1623	-	-	4/27/83/83	0/3/3/3
31	BCR	b	619	-	-	2/29/63/63	0/2/2/2
26	CLA	c	508	6	1/1/15/20	11/37/115/115	-
25	CHL	6	601	1	3/3/16/26	6/15/113/137	-
26	CLA	2	611	30	-	3/13/91/115	-
26	CLA	8	603	3	1/1/11/20	4/13/91/115	-
26	CLA	5	610	1	1/1/13/20	5/27/105/115	-
28	XAT	n	1622	-	-	3/31/93/93	0/4/4/4
26	CLA	a	405	4	1/1/15/20	7/37/115/115	-
26	CLA	A	406	42	1/1/15/20	12/37/115/115	-
26	CLA	c	504	42	1/1/15/20	18/37/115/115	-
26	CLA	R	613	19	1/1/14/20	10/31/109/115	-
27	LUT	s	1620	-	-	2/29/67/67	0/2/2/2
26	CLA	2	614	1	1/1/11/20	5/13/91/115	-
35	PHO	A	408	-	-	12/37/103/103	0/5/6/6
26	CLA	4	604	-	-	8/13/91/115	-
26	CLA	g	602	1	1/1/15/20	12/37/115/115	-
30	LHG	N	2630	26	-	24/53/53/53	-
25	CHL	Y	608	42	4/4/20/26	15/39/137/137	-
25	CHL	S	607	42	4/4/18/26	19/30/128/137	-
31	BCR	8	623	-	-	9/29/63/63	0/2/2/2
26	CLA	y	612	1	1/1/14/20	15/31/109/115	-
26	CLA	a	407	42	-	3/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	3	607	-	3/3/17/26	8/24/122/137	-
26	CLA	g	604	42	1/1/12/20	5/19/97/115	-
26	CLA	5	603	1	1/1/13/20	12/25/103/115	-
37	LMG	c	521	-	-	22/46/66/70	0/1/1/1
26	CLA	c	502	6	1/1/15/20	20/37/115/115	-
27	LUT	n	1620	-	-	2/29/67/67	0/2/2/2
26	CLA	d	402	7	1/1/15/20	4/37/115/115	-
25	CHL	2	607	-	4/4/19/26	14/33/131/137	-
25	CHL	s	608	-	3/3/16/26	4/15/113/137	-
26	CLA	4	612	3	1/1/11/20	5/13/91/115	-
30	LHG	s	2630	26	-	27/53/53/53	-
26	CLA	3	611	30	1/1/13/20	7/25/103/115	-
25	CHL	g	605	1	3/3/16/26	9/15/113/137	-
31	BCR	C	516	-	-	7/29/63/63	0/2/2/2
26	CLA	6	602	1	1/1/14/20	12/33/111/115	-
27	LUT	2	1620	-	-	2/29/67/67	0/2/2/2
28	XAT	1	1622	-	-	2/31/93/93	0/4/4/4
26	CLA	3	614	2	1/1/11/20	9/17/95/115	-
26	CLA	C	511	6	1/1/15/20	14/37/115/115	-
26	CLA	7	603	2	1/1/13/20	13/25/103/115	-
30	LHG	L	101	-	-	20/53/53/53	-
25	CHL	5	609	1	4/4/19/26	16/35/133/137	-
26	CLA	1	602	1	1/1/14/20	12/33/111/115	-
30	LHG	y	2630	26	-	24/53/53/53	-
26	CLA	R	616	19	-	6/13/91/115	-
26	CLA	D	403	7	-	12/37/115/115	-
26	CLA	7	610	2	1/1/14/20	7/31/109/115	-
26	CLA	6	614	1	1/1/11/20	5/13/91/115	-
26	CLA	Y	611	30	1/1/14/20	8/31/109/115	-
26	CLA	c	505	6	1/1/15/20	17/37/115/115	-
26	CLA	n	604	42	1/1/12/20	5/19/97/115	-
31	BCR	4	623	-	-	9/29/63/63	0/2/2/2
26	CLA	c	512	6	1/1/15/20	11/37/115/115	-
36	SQD	b	623	-	-	17/37/57/69	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	b	616	5	1/1/15/20	13/37/115/115	-
37	LMG	Z	101	-	-	24/46/66/70	0/1/1/1
26	CLA	s	613	20	1/1/13/20	6/25/103/115	-
30	LHG	D	408	-	-	19/50/50/53	-
39	DGD	c	519	-	-	26/51/91/95	0/2/2/2
26	CLA	r	604	42	1/1/11/20	6/17/95/115	-
26	CLA	R	612	19	1/1/11/20	6/18/96/115	-
26	CLA	8	602	3	1/1/11/20	7/13/91/115	-
26	CLA	b	614	5	1/1/15/20	13/37/115/115	-
26	CLA	1	614	1	1/1/11/20	2/13/91/115	-
26	CLA	1	612	1	1/1/11/20	3/13/91/115	-
31	BCR	A	411	-	-	6/29/63/63	0/2/2/2
29	NEX	2	1623	-	-	7/27/83/83	0/3/3/3
25	CHL	g	608	42	4/4/20/26	15/39/137/137	-
26	CLA	C	507	42	1/1/15/20	23/37/115/115	-
25	CHL	4	607	-	3/3/16/26	8/15/113/137	-
26	CLA	R	602	19	1/1/14/20	8/31/109/115	-
26	CLA	g	614	1	1/1/11/20	3/17/95/115	-
25	CHL	G	601	1	4/4/20/26	16/39/137/137	-
26	CLA	g	612	1	1/1/14/20	11/31/109/115	-
31	BCR	c	516	-	-	7/29/63/63	0/2/2/2
26	CLA	a	406	42	1/1/15/20	12/37/115/115	-
30	LHG	b	2630	-	-	31/51/51/53	-
26	CLA	2	613	1	-	5/13/91/115	-
26	CLA	1	603	1	1/1/13/20	12/25/103/115	-
26	CLA	2	603	1	1/1/13/20	11/25/103/115	-
25	CHL	6	609	1	4/4/19/26	11/33/131/137	-
26	CLA	C	503	6	1/1/15/20	14/37/115/115	-
26	CLA	G	613	1	1/1/15/20	12/37/115/115	-
26	CLA	R	603	19	1/1/14/20	14/31/109/115	-
39	DGD	C	520	-	-	21/49/89/95	0/2/2/2
37	LMG	a	413	-	-	28/43/63/70	0/1/1/1
26	CLA	5	602	1	1/1/14/20	12/33/111/115	-
26	CLA	5	604	-	-	10/19/97/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	b	604	5	1/1/15/20	10/37/115/115	-
26	CLA	1	611	30	1/1/11/20	6/13/91/115	-
39	DGD	c	520	-	-	21/49/89/95	0/2/2/2
25	CHL	2	606	-	3/3/16/26	6/15/113/137	-
25	CHL	R	606	42	4/4/20/26	19/39/137/137	-
30	LHG	B	2630	-	-	31/51/51/53	-
30	LHG	1	2630	26	-	15/45/45/53	-
26	CLA	c	510	6	1/1/15/20	14/37/115/115	-
27	LUT	r	620	-	-	3/29/67/67	0/2/2/2
25	CHL	6	607	-	4/4/19/26	14/33/131/137	-
27	LUT	4	620	-	-	4/29/67/67	0/2/2/2
26	CLA	S	611	30	1/1/13/20	9/27/105/115	-
26	CLA	A	405	4	1/1/15/20	7/37/115/115	-
25	CHL	n	608	42	4/4/20/26	13/39/137/137	-
25	CHL	5	606	-	3/3/16/26	8/15/113/137	-
26	CLA	N	613	1	1/1/14/20	8/31/109/115	-
26	CLA	N	603	1	1/1/15/20	15/37/115/115	-
31	BCR	c	514	-	-	4/29/63/63	0/2/2/2
25	CHL	S	606	42	3/3/16/26	10/15/113/137	-
26	CLA	B	605	5	1/1/15/20	14/37/115/115	-
26	CLA	N	604	42	1/1/12/20	5/19/97/115	-
26	CLA	s	612	20	1/1/11/20	5/18/96/115	-
37	LMG	A	413	-	-	28/43/63/70	0/1/1/1
30	LHG	C	522	-	-	20/53/53/53	-
26	CLA	C	509	6	1/1/15/20	8/37/115/115	-
25	CHL	r	608	42	4/4/19/26	17/33/131/137	-
30	LHG	n	2630	26	-	24/53/53/53	-
26	CLA	R	610	19	1/1/15/20	13/37/115/115	-
37	LMG	a	415	-	-	14/35/55/70	0/1/1/1
31	BCR	a	411	-	-	6/29/63/63	0/2/2/2
26	CLA	s	609	20	1/1/11/20	5/13/91/115	-
38	PL9	a	414	-	-	1/5/18/73	0/1/1/1
25	CHL	N	601	1	4/4/20/26	16/39/137/137	-
25	CHL	s	607	42	4/4/18/26	19/30/128/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	g	607	42	4/4/20/26	16/39/137/137	-
25	CHL	Y	605	1	3/3/16/26	8/18/116/137	-
26	CLA	8	612	3	1/1/11/20	5/13/91/115	-
25	CHL	G	606	42	3/3/16/26	9/20/118/137	-
26	CLA	2	612	1	1/1/11/20	5/13/91/115	-
29	NEX	g	1623	-	-	5/27/83/83	0/3/3/3
25	CHL	s	606	42	3/3/16/26	10/15/113/137	-
26	CLA	b	605	5	1/1/15/20	14/37/115/115	-
26	CLA	y	604	42	1/1/12/20	3/19/97/115	-
25	CHL	8	607	-	3/3/16/26	8/15/113/137	-
28	XAT	8	622	-	-	2/31/93/93	0/4/4/4
26	CLA	c	501	6	1/1/15/20	17/37/115/115	-
25	CHL	n	606	42	3/3/16/26	6/20/118/137	-
25	CHL	y	609	1	4/4/20/26	13/39/137/137	-
37	LMG	B	2633	-	-	24/50/70/70	0/1/1/1
26	CLA	r	611	30	1/1/11/20	8/18/96/115	-
25	CHL	8	606	-	3/3/16/26	8/15/113/137	-
28	XAT	5	1622	-	-	2/31/93/93	0/4/4/4
39	DGD	B	626	-	-	24/48/88/95	0/2/2/2
26	CLA	6	613	1	-	5/13/91/115	-
31	BCR	C	515	-	-	6/29/63/63	0/2/2/2
26	CLA	C	506	6	1/1/15/20	22/37/115/115	-
26	CLA	R	609	19	1/1/13/20	3/29/107/115	-
26	CLA	S	602	20	1/1/14/20	14/33/111/115	-
25	CHL	y	601	1	4/4/20/26	16/39/137/137	-
25	CHL	4	609	3	3/3/16/26	4/15/113/137	-
25	CHL	8	609	3	3/3/16/26	4/15/113/137	-
26	CLA	B	610	5	-	11/37/115/115	-
26	CLA	C	502	6	1/1/15/20	20/37/115/115	-
30	LHG	c	2630	-	-	27/53/53/53	-
30	LHG	C	523	-	-	21/53/53/53	-
25	CHL	8	601	3	3/3/16/26	7/13/111/137	-
39	DGD	b	626	-	-	24/48/88/95	0/2/2/2
25	CHL	r	607	42	4/4/18/26	9/27/125/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
37	LMG	d	411	-	-	15/41/61/70	0/1/1/1
26	CLA	b	610	5	-	11/37/115/115	-
37	LMG	A	415	-	-	14/35/55/70	0/1/1/1
30	LHG	C	2630	-	-	27/53/53/53	-
25	CHL	G	609	1	4/4/19/26	10/33/131/137	-
25	CHL	1	605	1	3/3/16/26	8/15/113/137	-
25	CHL	S	601	20	3/3/16/26	7/15/113/137	-
26	CLA	r	603	19	1/1/14/20	14/31/109/115	-
26	CLA	c	513	6	-	10/37/115/115	-
39	DGD	h	102	-	-	21/51/91/95	0/2/2/2
27	LUT	N	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	b	608	42	1/1/15/20	11/37/115/115	-
29	NEX	Y	1623	-	-	6/27/83/83	0/3/3/3
27	LUT	3	1621	-	-	3/29/67/67	0/2/2/2
26	CLA	B	602	42	1/1/15/20	15/37/115/115	-
25	CHL	n	609	1	4/4/20/26	14/39/137/137	-
30	LHG	3	2630	26	-	24/51/51/53	-
28	XAT	N	1622	-	-	3/31/93/93	0/4/4/4
25	CHL	1	607	-	4/4/19/26	20/36/134/137	-
26	CLA	b	612	5	1/1/15/20	13/37/115/115	-
25	CHL	y	608	42	4/4/20/26	15/39/137/137	-
26	CLA	b	613	5	1/1/15/20	16/37/115/115	-
26	CLA	N	611	30	1/1/14/20	4/31/109/115	-
25	CHL	n	601	1	4/4/20/26	16/39/137/137	-
30	LHG	Y	2630	26	-	24/53/53/53	-
31	BCR	H	101	-	-	4/29/63/63	0/2/2/2
26	CLA	n	613	1	1/1/14/20	8/31/109/115	-
26	CLA	n	603	1	1/1/15/20	15/37/115/115	-
26	CLA	3	610	2	1/1/14/20	7/31/109/115	-
41	HEM	F	101	9,8	-	1/12/54/54	-
26	CLA	Y	603	1	1/1/15/20	13/37/115/115	-
27	LUT	S	1620	-	-	2/29/67/67	0/2/2/2
25	CHL	g	609	1	4/4/19/26	10/33/131/137	-
30	LHG	4	2630	26	-	8/23/23/53	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	C	505	6	1/1/15/20	17/37/115/115	-
38	PL9	d	405	-	-	10/53/73/73	0/1/1/1
30	LHG	6	2630	26	-	16/41/41/53	-
26	CLA	C	512	6	1/1/15/20	11/37/115/115	-
25	CHL	1	608	-	3/3/16/26	7/15/113/137	-
25	CHL	4	606	-	3/3/16/26	8/15/113/137	-
26	CLA	C	501	6	1/1/15/20	17/37/115/115	-
25	CHL	s	601	20	3/3/16/26	7/15/113/137	-
31	BCR	c	517	-	-	4/29/63/63	0/2/2/2
26	CLA	G	610	1	1/1/14/20	13/36/114/115	-
30	LHG	l	101	-	-	20/53/53/53	-
31	BCR	h	101	-	-	4/29/63/63	0/2/2/2
26	CLA	G	602	1	1/1/15/20	12/37/115/115	-
31	BCR	B	620	-	-	6/29/63/63	0/2/2/2
26	CLA	R	601	19	1/1/11/20	14/18/96/115	-
35	PHO	A	409	-	-	7/37/103/103	0/5/6/6
26	CLA	6	603	1	1/1/13/20	11/25/103/115	-
26	CLA	6	611	30	-	3/13/91/115	-
28	XAT	R	622	-	-	3/31/93/93	0/4/4/4
25	CHL	2	609	1	4/4/19/26	11/33/131/137	-
29	NEX	6	1623	-	-	7/27/83/83	0/3/3/3
27	LUT	3	1620	-	-	2/29/67/67	0/2/2/2
29	NEX	R	623	-	-	4/27/83/83	0/3/3/3
25	CHL	6	605	1	3/3/16/26	9/15/113/137	-
26	CLA	R	611	30	1/1/11/20	8/18/96/115	-
25	CHL	y	605	1	3/3/16/26	8/18/116/137	-
26	CLA	3	602	2	1/1/14/20	14/31/109/115	-
29	NEX	3	1623	-	-	4/27/83/83	0/3/3/3
25	CHL	5	605	1	3/3/16/26	8/15/113/137	-
26	CLA	G	612	1	1/1/14/20	11/31/109/115	-
29	NEX	1	1623	-	-	6/27/83/83	0/3/3/3
25	CHL	2	601	1	3/3/16/26	6/15/113/137	-
35	PHO	a	409	-	-	7/37/103/103	0/5/6/6
28	XAT	3	1622	-	-	2/31/93/93	0/4/4/4

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
29	NEX	S	1623	-	-	5/27/83/83	0/3/3/3
26	CLA	B	606	5	1/1/15/20	14/37/115/115	-
26	CLA	B	611	42	1/1/15/20	10/37/115/115	-
25	CHL	y	607	42	4/4/20/26	16/39/137/137	-
27	LUT	7	1621	-	-	3/29/67/67	0/2/2/2
28	XAT	y	1622	-	-	2/31/93/93	0/4/4/4
26	CLA	Y	610	1	1/1/14/20	7/31/109/115	-
26	CLA	r	616	19	-	6/13/91/115	-
26	CLA	B	603	5	1/1/15/20	9/37/115/115	-
26	CLA	2	602	1	1/1/14/20	12/33/111/115	-
31	BCR	C	517	-	-	4/29/63/63	0/2/2/2
25	CHL	7	606	-	3/3/16/26	9/15/113/137	-
26	CLA	y	611	30	1/1/14/20	8/31/109/115	-
27	LUT	y	1620	-	-	2/29/67/67	0/2/2/2
26	CLA	B	613	5	1/1/15/20	16/37/115/115	-
26	CLA	C	510	6	1/1/15/20	15/37/115/115	-
30	LHG	B	2631	-	-	23/53/53/53	-
26	CLA	c	506	6	1/1/15/20	22/37/115/115	-
26	CLA	7	602	2	1/1/14/20	14/31/109/115	-
31	BCR	C	514	-	-	4/29/63/63	0/2/2/2
30	LHG	S	2630	26	-	27/53/53/53	-
27	LUT	n	1621	-	-	3/29/67/67	0/2/2/2
25	CHL	7	609	2	4/4/19/26	13/33/131/137	-
26	CLA	6	610	1	1/1/12/20	4/19/97/115	-
26	CLA	y	603	1	1/1/15/20	13/37/115/115	-
26	CLA	y	610	1	1/1/14/20	7/31/109/115	-
28	XAT	6	1622	-	-	3/31/93/93	0/4/4/4
26	CLA	s	604	42	1/1/12/20	6/19/97/115	-
25	CHL	g	606	42	3/3/16/26	9/20/118/137	-
25	CHL	r	614	19	3/3/15/26	6/10/108/137	-
26	CLA	N	602	1	1/1/15/20	12/37/115/115	-
26	CLA	n	602	1	1/1/15/20	11/37/115/115	-
31	BCR	d	404	-	-	7/29/63/63	0/2/2/2
25	CHL	7	601	2	4/4/19/26	18/37/135/137	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	G	614	1	1/1/11/20	3/17/95/115	-
26	CLA	7	614	2	1/1/11/20	9/17/95/115	-
36	SQD	B	621	-	-	32/49/69/69	0/1/1/1
26	CLA	4	610	3	1/1/11/20	4/13/91/115	-
26	CLA	8	604	-	-	8/13/91/115	-
30	LHG	D	409	-	-	27/53/53/53	-
25	CHL	N	605	1	3/3/16/26	9/18/116/137	-
30	LHG	5	2630	26	-	15/45/45/53	-
27	LUT	6	1620	-	-	2/29/67/67	0/2/2/2
26	CLA	c	507	42	1/1/15/20	23/37/115/115	-
26	CLA	s	614	20	1/1/11/20	3/18/96/115	-
38	PL9	A	414	-	-	1/5/18/73	0/1/1/1
39	DGD	c	518	-	-	15/44/84/95	0/2/2/2
26	CLA	n	614	1	1/1/11/20	6/17/95/115	-
25	CHL	G	607	42	4/4/20/26	16/39/137/137	-
31	BCR	B	619	-	-	2/29/63/63	0/2/2/2
26	CLA	2	604	-	1/1/11/20	8/13/91/115	-
26	CLA	b	617	5	1/1/15/20	18/37/115/115	-
25	CHL	4	601	3	3/3/16/26	7/13/111/137	-
36	SQD	a	412	-	-	13/45/65/69	0/1/1/1
26	CLA	C	508	6	1/1/15/20	11/37/115/115	-
27	LUT	1	1620	-	-	2/29/67/67	0/2/2/2
25	CHL	N	608	42	4/4/20/26	13/39/137/137	-
25	CHL	6	608	-	3/3/16/26	7/15/113/137	-
26	CLA	7	604	-	1/1/11/20	9/13/91/115	-
29	NEX	y	1623	-	-	6/27/83/83	0/3/3/3
26	CLA	b	611	42	1/1/15/20	10/37/115/115	-
29	NEX	r	623	-	-	4/27/83/83	0/3/3/3
25	CHL	3	601	2	4/4/19/26	18/37/135/137	-
25	CHL	8	608	-	3/3/16/26	5/15/113/137	-
27	LUT	g	1620	-	-	2/29/67/67	0/2/2/2
31	BCR	b	618	-	-	2/29/63/63	0/2/2/2
26	CLA	d	403	7	-	12/37/115/115	-
26	CLA	4	602	3	1/1/11/20	7/13/91/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
26	CLA	b	603	5	1/1/15/20	9/37/115/115	-
27	LUT	6	1621	-	-	3/29/67/67	0/2/2/2
25	CHL	r	606	42	4/4/20/26	19/39/137/137	-
31	BCR	D	404	-	-	7/29/63/63	0/2/2/2
25	CHL	2	608	-	3/3/16/26	7/15/113/137	-
26	CLA	1	613	1	-	8/25/103/115	-
30	LHG	2	2630	26	-	16/41/41/53	-
36	SQD	A	418	-	-	22/49/69/69	0/1/1/1
27	LUT	S	1621	-	-	2/29/67/67	0/2/2/2
25	CHL	3	606	-	3/3/16/26	9/15/113/137	-
38	PL9	D	405	-	-	10/53/73/73	0/1/1/1
30	LHG	d	408	-	-	19/50/50/53	-
25	CHL	7	607	-	3/3/17/26	8/24/122/137	-
31	BCR	T	101	-	-	13/29/63/63	0/2/2/2
26	CLA	8	611	30	1/1/11/20	4/13/91/115	-
26	CLA	s	610	20	1/1/13/20	4/25/103/115	-
37	LMG	B	622	-	-	23/46/66/70	0/1/1/1
37	LMG	z	101	-	-	24/46/66/70	0/1/1/1
29	NEX	N	1623	-	-	4/27/83/83	0/3/3/3
26	CLA	3	612	2	1/1/11/20	8/13/91/115	-
25	CHL	Y	606	42	3/3/16/26	6/20/118/137	-
30	LHG	d	410	-	-	30/47/47/53	-
26	CLA	D	402	7	1/1/15/20	4/37/115/115	-
27	LUT	Y	1620	-	-	2/29/67/67	0/2/2/2
26	CLA	S	613	20	1/1/13/20	6/25/103/115	-
26	CLA	n	610	1	1/1/15/20	12/37/115/115	-
26	CLA	c	511	6	1/1/15/20	14/37/115/115	-
31	BCR	t	101	-	-	13/29/63/63	0/2/2/2
25	CHL	g	601	1	4/4/20/26	16/39/137/137	-
26	CLA	S	614	20	1/1/11/20	3/18/96/115	-
27	LUT	5	1620	-	-	2/29/67/67	0/2/2/2
26	CLA	G	611	30	1/1/14/20	11/31/109/115	-
26	CLA	7	611	30	1/1/13/20	7/25/103/115	-
37	LMG	b	622	-	-	23/46/66/70	0/1/1/1

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
25	CHL	7	608	-	3/3/16/26	3/15/113/137	-
31	BCR	b	620	-	-	6/29/63/63	0/2/2/2
25	CHL	R	614	19	3/3/15/26	6/10/108/137	-
26	CLA	B	607	5	1/1/15/20	9/37/115/115	-
26	CLA	c	503	6	1/1/15/20	14/37/115/115	-
30	LHG	7	2630	26	-	24/51/51/53	-
26	CLA	r	610	19	1/1/15/20	13/37/115/115	-
39	DGD	C	518	-	-	15/44/84/95	0/2/2/2
31	BCR	B	618	-	-	2/29/63/63	0/2/2/2
26	CLA	s	602	20	1/1/14/20	14/33/111/115	-
29	NEX	s	1623	-	-	5/27/83/83	0/3/3/3
26	CLA	r	602	19	1/1/14/20	8/31/109/115	-
36	SQD	B	623	-	-	17/37/57/69	0/1/1/1
26	CLA	R	604	42	1/1/11/20	6/17/95/115	-
25	CHL	R	607	42	4/4/18/26	9/27/125/137	-
26	CLA	7	612	2	1/1/11/20	8/13/91/115	-
39	DGD	C	519	-	-	26/51/91/95	0/2/2/2
26	CLA	N	614	1	1/1/11/20	6/17/95/115	-
26	CLA	N	612	1	1/1/14/20	9/31/109/115	-
27	LUT	7	1620	-	-	2/29/67/67	0/2/2/2
26	CLA	y	602	1	1/1/15/20	10/37/115/115	-
36	SQD	b	621	-	-	32/49/69/69	0/1/1/1
26	CLA	S	604	42	1/1/12/20	6/19/97/115	-
28	XAT	7	1622	-	-	2/31/93/93	0/4/4/4
25	CHL	4	608	-	3/3/16/26	5/15/113/137	-
26	CLA	3	613	2	1/1/13/20	9/29/107/115	-
26	CLA	8	610	3	1/1/11/20	4/13/91/115	-
26	CLA	B	617	5	1/1/15/20	18/37/115/115	-
27	LUT	y	1621	-	-	1/29/67/67	0/2/2/2
28	XAT	2	1622	-	-	3/31/93/93	0/4/4/4
25	CHL	N	607	42	4/4/20/26	14/39/137/137	-
26	CLA	2	610	1	1/1/12/20	4/19/97/115	-
26	CLA	6	604	-	1/1/11/20	8/13/91/115	-
26	CLA	a	410	4	1/1/14/20	5/31/109/115	-

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Mol	Type	Chain	Res	Link	Chirals	Torsions	Rings
30	LHG	D	410	-	-	29/47/47/53	-
27	LUT	R	620	-	-	4/29/67/67	0/2/2/2
26	CLA	6	612	1	1/1/11/20	5/13/91/115	-
26	CLA	b	602	42	1/1/15/20	15/37/115/115	-
29	NEX	5	1623	-	-	6/27/83/83	0/3/3/3
39	DGD	H	102	-	-	21/51/91/95	0/2/2/2

All (3567) bond length outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	2	612	CLA	C4B-NB	8.06	1.42	1.35
26	R	609	CLA	C4B-NB	8.04	1.42	1.35
26	6	612	CLA	C4B-NB	8.04	1.42	1.35
26	r	609	CLA	C4B-NB	8.04	1.42	1.35
26	R	612	CLA	C4B-NB	7.91	1.42	1.35
26	r	612	CLA	C4B-NB	7.91	1.42	1.35
26	Y	603	CLA	C4B-NB	7.76	1.42	1.35
26	G	611	CLA	C4B-NB	7.74	1.42	1.35
26	g	611	CLA	C4B-NB	7.74	1.42	1.35
26	y	603	CLA	C4B-NB	7.73	1.42	1.35
26	6	614	CLA	C4B-NB	7.67	1.42	1.35
26	2	613	CLA	C4B-NB	7.67	1.42	1.35
26	6	613	CLA	C4B-NB	7.67	1.42	1.35
26	R	613	CLA	C4B-NB	7.65	1.42	1.35
26	2	614	CLA	C4B-NB	7.62	1.42	1.35
26	r	613	CLA	C4B-NB	7.61	1.42	1.35
26	R	616	CLA	C4B-NB	7.60	1.42	1.35
26	Y	611	CLA	C4B-NB	7.59	1.42	1.35
26	y	611	CLA	C4B-NB	7.59	1.42	1.35
26	6	604	CLA	C4B-NB	7.56	1.41	1.35
26	N	604	CLA	C4B-NB	7.54	1.41	1.35
26	n	604	CLA	C4B-NB	7.54	1.41	1.35
26	2	611	CLA	C4B-NB	7.54	1.41	1.35
26	r	616	CLA	C4B-NB	7.53	1.41	1.35
26	6	611	CLA	C4B-NB	7.52	1.41	1.35
26	2	604	CLA	C4B-NB	7.52	1.41	1.35
26	1	612	CLA	C4B-NB	7.51	1.41	1.35
26	G	604	CLA	C4B-NB	7.49	1.41	1.35
26	g	604	CLA	C4B-NB	7.49	1.41	1.35
26	5	612	CLA	C4B-NB	7.49	1.41	1.35
26	4	611	CLA	C4B-NB	7.48	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S	609	CLA	C4B-NB	7.47	1.41	1.35
26	s	609	CLA	C4B-NB	7.47	1.41	1.35
26	5	613	CLA	C4B-NB	7.45	1.41	1.35
26	g	614	CLA	C4B-NB	7.44	1.41	1.35
26	1	613	CLA	C4B-NB	7.44	1.41	1.35
26	8	611	CLA	C4B-NB	7.44	1.41	1.35
26	N	612	CLA	C4B-NB	7.42	1.41	1.35
26	n	612	CLA	C4B-NB	7.42	1.41	1.35
26	N	611	CLA	C4B-NB	7.40	1.41	1.35
26	n	611	CLA	C4B-NB	7.40	1.41	1.35
26	3	604	CLA	C4B-NB	7.39	1.41	1.35
26	7	604	CLA	C4B-NB	7.39	1.41	1.35
26	G	610	CLA	C4B-NB	7.39	1.41	1.35
26	g	612	CLA	C4B-NB	7.39	1.41	1.35
26	4	603	CLA	C4B-NB	7.37	1.41	1.35
26	8	603	CLA	C4B-NB	7.37	1.41	1.35
26	G	614	CLA	C4B-NB	7.36	1.41	1.35
26	5	604	CLA	C4B-NB	7.35	1.41	1.35
26	1	604	CLA	C4B-NB	7.34	1.41	1.35
26	1	611	CLA	C4B-NB	7.34	1.41	1.35
26	5	611	CLA	C4B-NB	7.34	1.41	1.35
26	3	613	CLA	C4B-NB	7.33	1.41	1.35
26	7	613	CLA	C4B-NB	7.33	1.41	1.35
26	8	604	CLA	C4B-NB	7.32	1.41	1.35
26	g	610	CLA	C4B-NB	7.32	1.41	1.35
26	4	604	CLA	C4B-NB	7.31	1.41	1.35
26	G	612	CLA	C4B-NB	7.28	1.41	1.35
26	2	603	CLA	C4B-NB	7.27	1.41	1.35
26	6	603	CLA	C4B-NB	7.27	1.41	1.35
26	g	613	CLA	C4B-NB	7.26	1.41	1.35
26	R	601	CLA	C4B-NB	7.25	1.41	1.35
26	r	601	CLA	C4B-NB	7.25	1.41	1.35
26	1	614	CLA	C4B-NB	7.24	1.41	1.35
26	G	613	CLA	C4B-NB	7.24	1.41	1.35
26	4	612	CLA	C4B-NB	7.23	1.41	1.35
26	8	612	CLA	C4B-NB	7.23	1.41	1.35
26	5	614	CLA	C4B-NB	7.23	1.41	1.35
26	S	602	CLA	C4B-NB	7.18	1.41	1.35
26	7	614	CLA	C4B-NB	7.17	1.41	1.35
26	3	614	CLA	C4B-NB	7.16	1.41	1.35
26	s	602	CLA	C4B-NB	7.15	1.41	1.35
26	S	612	CLA	C4B-NB	7.15	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	s	612	CLA	C4B-NB	7.15	1.41	1.35
26	S	610	CLA	C4B-NB	7.15	1.41	1.35
26	7	610	CLA	C4B-NB	7.15	1.41	1.35
26	s	610	CLA	C4B-NB	7.15	1.41	1.35
26	g	603	CLA	C4B-NB	7.14	1.41	1.35
26	3	610	CLA	C4B-NB	7.11	1.41	1.35
26	2	610	CLA	C4B-NB	7.10	1.41	1.35
26	6	610	CLA	C4B-NB	7.09	1.41	1.35
26	s	613	CLA	C4B-NB	7.09	1.41	1.35
26	G	603	CLA	C4B-NB	7.08	1.41	1.35
26	7	611	CLA	C4B-NB	7.07	1.41	1.35
26	S	613	CLA	C4B-NB	7.06	1.41	1.35
26	Y	604	CLA	C4B-NB	7.06	1.41	1.35
26	y	604	CLA	C4B-NB	7.05	1.41	1.35
26	4	610	CLA	C4B-NB	7.05	1.41	1.35
26	3	611	CLA	C4B-NB	7.04	1.41	1.35
26	8	610	CLA	C4B-NB	7.02	1.41	1.35
26	Y	612	CLA	C4B-NB	7.02	1.41	1.35
26	s	603	CLA	C4B-NB	7.02	1.41	1.35
26	y	612	CLA	C4B-NB	7.02	1.41	1.35
26	s	614	CLA	C4B-NB	7.02	1.41	1.35
26	y	613	CLA	C4B-NB	7.00	1.41	1.35
26	1	603	CLA	C4B-NB	6.99	1.41	1.35
26	5	603	CLA	C4B-NB	6.99	1.41	1.35
26	N	614	CLA	C4B-NB	6.99	1.41	1.35
26	n	614	CLA	C4B-NB	6.98	1.41	1.35
26	3	612	CLA	C4B-NB	6.98	1.41	1.35
26	7	612	CLA	C4B-NB	6.98	1.41	1.35
26	N	613	CLA	C4B-NB	6.96	1.41	1.35
26	n	613	CLA	C4B-NB	6.96	1.41	1.35
26	2	602	CLA	C4B-NB	6.96	1.41	1.35
26	6	602	CLA	C4B-NB	6.96	1.41	1.35
26	8	602	CLA	C4B-NB	6.95	1.41	1.35
26	S	603	CLA	C4B-NB	6.94	1.41	1.35
26	C	501	CLA	C4B-NB	6.94	1.41	1.35
26	4	602	CLA	C4B-NB	6.92	1.41	1.35
26	S	614	CLA	C4B-NB	6.92	1.41	1.35
26	7	602	CLA	C4B-NB	6.91	1.41	1.35
26	c	501	CLA	C4B-NB	6.89	1.41	1.35
26	Y	613	CLA	C4B-NB	6.89	1.41	1.35
26	1	610	CLA	C4B-NB	6.89	1.41	1.35
26	5	610	CLA	C4B-NB	6.89	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	n	603	CLA	C4B-NB	6.88	1.41	1.35
38	D	405	PL9	C7-C3	-6.86	1.44	1.51
26	s	611	CLA	C4B-NB	6.84	1.41	1.35
26	3	602	CLA	C4B-NB	6.82	1.41	1.35
26	b	607	CLA	C4B-NB	6.82	1.41	1.35
38	d	405	PL9	C7-C3	-6.82	1.44	1.51
26	N	603	CLA	C4B-NB	6.81	1.41	1.35
26	B	602	CLA	C4B-NB	6.80	1.41	1.35
26	b	602	CLA	C4B-NB	6.80	1.41	1.35
26	B	609	CLA	C4B-NB	6.77	1.41	1.35
26	S	611	CLA	C4B-NB	6.77	1.41	1.35
26	B	607	CLA	C4B-NB	6.75	1.41	1.35
26	Y	610	CLA	C4B-NB	6.75	1.41	1.35
26	b	609	CLA	C4B-NB	6.75	1.41	1.35
26	R	602	CLA	C4B-NB	6.74	1.41	1.35
26	r	602	CLA	C4B-NB	6.74	1.41	1.35
26	y	610	CLA	C4B-NB	6.72	1.41	1.35
26	S	604	CLA	C4B-NB	6.69	1.41	1.35
26	b	616	CLA	C4B-NB	6.69	1.41	1.35
26	s	604	CLA	C4B-NB	6.69	1.41	1.35
26	B	616	CLA	C4B-NB	6.66	1.41	1.35
26	r	604	CLA	C4B-NB	6.65	1.41	1.35
26	n	610	CLA	C4B-NB	6.64	1.41	1.35
26	3	603	CLA	C4B-NB	6.63	1.41	1.35
26	R	604	CLA	C4B-NB	6.62	1.41	1.35
26	N	610	CLA	C4B-NB	6.61	1.41	1.35
26	r	610	CLA	C4B-NB	6.59	1.41	1.35
26	b	608	CLA	C4B-NB	6.58	1.41	1.35
26	7	603	CLA	C4B-NB	6.57	1.41	1.35
26	1	602	CLA	C4B-NB	6.56	1.41	1.35
26	5	602	CLA	C4B-NB	6.56	1.41	1.35
26	B	608	CLA	C4B-NB	6.56	1.41	1.35
26	Y	614	CLA	C4B-NB	6.55	1.41	1.35
26	y	614	CLA	C4B-NB	6.52	1.41	1.35
26	R	610	CLA	C4B-NB	6.49	1.41	1.35
26	D	402	CLA	C4B-NB	6.48	1.41	1.35
26	c	511	CLA	C4B-NB	6.48	1.41	1.35
26	d	402	CLA	C4B-NB	6.48	1.41	1.35
26	G	602	CLA	C4B-NB	6.45	1.41	1.35
26	g	602	CLA	C4B-NB	6.44	1.41	1.35
26	C	511	CLA	C4B-NB	6.43	1.40	1.35
26	N	602	CLA	C4B-NB	6.36	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	n	602	CLA	C4B-NB	6.36	1.40	1.35
26	C	510	CLA	C4B-NB	6.34	1.40	1.35
26	c	510	CLA	C4B-NB	6.34	1.40	1.35
26	C	513	CLA	C4B-NB	6.33	1.40	1.35
26	c	513	CLA	C4B-NB	6.33	1.40	1.35
26	B	612	CLA	C4B-NB	6.32	1.40	1.35
26	b	612	CLA	C4B-NB	6.32	1.40	1.35
26	C	503	CLA	C4B-NB	6.31	1.40	1.35
26	c	503	CLA	C4B-NB	6.31	1.40	1.35
26	D	403	CLA	C4B-NB	6.29	1.40	1.35
26	d	403	CLA	C4B-NB	6.29	1.40	1.35
26	r	611	CLA	C4B-NB	6.28	1.40	1.35
26	B	603	CLA	C4B-NB	6.25	1.40	1.35
26	C	512	CLA	C4B-NB	6.23	1.40	1.35
26	r	603	CLA	C4B-NB	6.22	1.40	1.35
26	R	611	CLA	C4B-NB	6.21	1.40	1.35
26	R	603	CLA	C4B-NB	6.21	1.40	1.35
26	c	512	CLA	C4B-NB	6.20	1.40	1.35
26	b	603	CLA	C4B-NB	6.17	1.40	1.35
26	b	604	CLA	C4B-NB	6.17	1.40	1.35
26	B	604	CLA	C4B-NB	6.16	1.40	1.35
26	B	606	CLA	C4B-NB	6.14	1.40	1.35
26	b	606	CLA	C4B-NB	6.14	1.40	1.35
26	C	504	CLA	C4B-NB	6.14	1.40	1.35
26	c	504	CLA	C4B-NB	6.14	1.40	1.35
26	C	506	CLA	C4B-NB	6.10	1.40	1.35
26	B	611	CLA	C4B-NB	6.09	1.40	1.35
26	b	611	CLA	C4B-NB	6.09	1.40	1.35
26	c	506	CLA	C4B-NB	6.04	1.40	1.35
26	B	615	CLA	C4B-NB	6.03	1.40	1.35
26	b	610	CLA	C4B-NB	6.01	1.40	1.35
26	b	615	CLA	C4B-NB	6.01	1.40	1.35
26	c	509	CLA	C4B-NB	5.98	1.40	1.35
26	B	610	CLA	C4B-NB	5.97	1.40	1.35
26	B	617	CLA	C4B-NB	5.96	1.40	1.35
26	b	617	CLA	C4B-NB	5.96	1.40	1.35
26	C	509	CLA	C4B-NB	5.94	1.40	1.35
26	B	613	CLA	C4B-NB	5.91	1.40	1.35
26	b	613	CLA	C4B-NB	5.91	1.40	1.35
26	Y	602	CLA	C4B-NB	5.86	1.40	1.35
26	y	602	CLA	C4B-NB	5.86	1.40	1.35
26	c	507	CLA	C4B-NB	5.85	1.40	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	505	CLA	C4B-NB	5.84	1.40	1.35
26	c	505	CLA	C4B-NB	5.84	1.40	1.35
26	C	507	CLA	C4B-NB	5.80	1.40	1.35
26	A	410	CLA	C4B-NB	5.79	1.40	1.35
26	a	410	CLA	C4B-NB	5.79	1.40	1.35
26	a	406	CLA	C4B-NB	5.79	1.40	1.35
26	A	406	CLA	C4B-NB	5.78	1.40	1.35
25	R	608	CHL	C3D-C4D	-5.73	1.31	1.44
26	C	508	CLA	C4B-NB	5.72	1.40	1.35
25	r	608	CHL	C3D-C4D	-5.71	1.31	1.44
25	Y	601	CHL	C3D-C4D	-5.71	1.31	1.44
25	y	601	CHL	C3D-C4D	-5.71	1.31	1.44
26	c	508	CLA	C4B-NB	5.70	1.40	1.35
25	y	608	CHL	C3D-C4D	-5.68	1.31	1.44
25	Y	608	CHL	C3D-C4D	-5.68	1.31	1.44
26	A	407	CLA	C4B-NB	5.67	1.40	1.35
26	a	407	CLA	C4B-NB	5.66	1.40	1.35
26	B	614	CLA	C4B-NB	5.63	1.40	1.35
26	b	614	CLA	C4B-NB	5.63	1.40	1.35
25	3	601	CHL	C3D-C4D	-5.48	1.31	1.44
25	7	601	CHL	C3D-C4D	-5.48	1.31	1.44
25	S	601	CHL	C3D-C4D	-5.47	1.31	1.44
25	s	601	CHL	C3D-C4D	-5.47	1.31	1.44
25	8	601	CHL	C3B-C2B	5.45	1.47	1.40
26	A	405	CLA	C4B-NB	5.44	1.40	1.35
26	a	405	CLA	C4B-NB	5.44	1.40	1.35
25	G	601	CHL	C3D-C4D	-5.44	1.31	1.44
25	g	601	CHL	C3D-C4D	-5.44	1.31	1.44
26	c	502	CLA	C4B-NB	5.43	1.40	1.35
25	y	606	CHL	C3D-C4D	-5.43	1.31	1.44
26	C	502	CLA	C4B-NB	5.42	1.40	1.35
25	g	608	CHL	C3D-C4D	-5.41	1.32	1.44
25	n	601	CHL	C3D-C4D	-5.41	1.32	1.44
25	G	608	CHL	C3D-C4D	-5.40	1.32	1.44
25	4	601	CHL	C3B-C2B	5.40	1.47	1.40
25	Y	606	CHL	C3D-C4D	-5.39	1.32	1.44
25	N	601	CHL	C3D-C4D	-5.38	1.32	1.44
25	1	601	CHL	C3D-C4D	-5.36	1.32	1.44
25	N	608	CHL	C3D-C4D	-5.34	1.32	1.44
25	n	608	CHL	C3D-C4D	-5.34	1.32	1.44
25	5	601	CHL	C3D-C4D	-5.33	1.32	1.44
25	6	601	CHL	C3D-C4D	-5.33	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	606	CHL	O2D-CGD	5.32	1.46	1.33
25	2	601	CHL	C3D-C4D	-5.31	1.32	1.44
25	g	606	CHL	O2D-CGD	5.28	1.46	1.33
26	b	605	CLA	C4B-NB	5.27	1.39	1.35
25	g	607	CHL	CHC-C1C	5.26	1.48	1.35
25	G	607	CHL	CHC-C1C	5.24	1.48	1.35
25	R	606	CHL	C3D-C4D	-5.23	1.32	1.44
25	r	606	CHL	C3D-C4D	-5.23	1.32	1.44
25	7	606	CHL	C3D-C4D	-5.22	1.32	1.44
26	B	605	CLA	C4B-NB	5.22	1.39	1.35
25	Y	609	CHL	C3D-C4D	-5.22	1.32	1.44
25	y	609	CHL	C3D-C4D	-5.21	1.32	1.44
25	Y	607	CHL	C3D-C4D	-5.20	1.32	1.44
25	G	605	CHL	CHC-C1C	5.20	1.48	1.35
25	S	608	CHL	C3D-C4D	-5.19	1.32	1.44
25	3	608	CHL	C3D-C4D	-5.19	1.32	1.44
25	g	605	CHL	CHC-C1C	5.19	1.48	1.35
25	3	606	CHL	C3D-C4D	-5.18	1.32	1.44
25	8	609	CHL	C3D-C4D	-5.17	1.32	1.44
25	1	608	CHL	C3D-C4D	-5.17	1.32	1.44
25	5	608	CHL	C3D-C4D	-5.17	1.32	1.44
25	y	607	CHL	C3D-C4D	-5.17	1.32	1.44
25	7	608	CHL	C3D-C4D	-5.17	1.32	1.44
25	s	608	CHL	C3D-C4D	-5.16	1.32	1.44
25	3	605	CHL	O2D-CGD	5.16	1.45	1.33
25	7	605	CHL	O2D-CGD	5.16	1.45	1.33
25	N	609	CHL	C3D-C4D	-5.16	1.32	1.44
25	n	609	CHL	C3D-C4D	-5.16	1.32	1.44
25	s	601	CHL	O2D-CGD	5.14	1.45	1.33
25	R	607	CHL	C3D-C4D	-5.14	1.32	1.44
25	r	607	CHL	C3D-C4D	-5.14	1.32	1.44
25	2	605	CHL	O2D-CGD	5.14	1.45	1.33
25	5	601	CHL	O2D-CGD	5.14	1.45	1.33
25	1	606	CHL	C3D-C4D	-5.14	1.32	1.44
25	4	609	CHL	C3D-C4D	-5.14	1.32	1.44
25	2	601	CHL	O2D-CGD	5.13	1.45	1.33
25	n	601	CHL	O2D-CGD	5.13	1.45	1.33
25	5	606	CHL	C3D-C4D	-5.13	1.32	1.44
25	S	601	CHL	O2D-CGD	5.13	1.45	1.33
25	Y	605	CHL	C3D-C4D	-5.13	1.32	1.44
25	1	609	CHL	C3D-C4D	-5.12	1.32	1.44
25	5	609	CHL	C3D-C4D	-5.12	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	608	CHL	C3D-C4D	-5.12	1.32	1.44
25	4	607	CHL	O2D-CGD	5.12	1.45	1.33
25	8	607	CHL	O2D-CGD	5.12	1.45	1.33
25	N	601	CHL	O2D-CGD	5.12	1.45	1.33
25	y	605	CHL	C3D-C4D	-5.12	1.32	1.44
25	6	605	CHL	O2D-CGD	5.11	1.45	1.33
25	1	601	CHL	O2D-CGD	5.11	1.45	1.33
25	G	607	CHL	C3D-C4D	-5.11	1.32	1.44
25	6	606	CHL	O2D-CGD	5.11	1.45	1.33
25	S	607	CHL	O2D-CGD	5.11	1.45	1.33
25	s	607	CHL	O2D-CGD	5.11	1.45	1.33
25	6	601	CHL	O2D-CGD	5.10	1.45	1.33
25	8	608	CHL	C3D-C4D	-5.10	1.32	1.44
25	2	606	CHL	O2D-CGD	5.10	1.45	1.33
25	r	607	CHL	O2D-CGD	5.10	1.45	1.33
25	3	609	CHL	C3D-C4D	-5.09	1.32	1.44
25	7	609	CHL	C3D-C4D	-5.09	1.32	1.44
25	4	606	CHL	C3D-C4D	-5.09	1.32	1.44
25	8	606	CHL	C3D-C4D	-5.09	1.32	1.44
25	g	607	CHL	C3D-C4D	-5.08	1.32	1.44
25	5	606	CHL	O2D-CGD	5.08	1.45	1.33
25	7	607	CHL	C3D-C4D	-5.08	1.32	1.44
25	R	607	CHL	O2D-CGD	5.08	1.45	1.33
25	1	606	CHL	O2D-CGD	5.08	1.45	1.33
25	2	608	CHL	C3D-C4D	-5.07	1.32	1.44
25	n	606	CHL	O2D-CGD	5.07	1.45	1.33
25	4	601	CHL	CHC-C1C	5.06	1.47	1.35
25	6	608	CHL	C3D-C4D	-5.06	1.32	1.44
25	3	607	CHL	C3D-C4D	-5.05	1.32	1.44
25	1	605	CHL	C3D-C4D	-5.05	1.32	1.44
25	5	605	CHL	C3D-C4D	-5.05	1.32	1.44
25	8	601	CHL	CHC-C1C	5.05	1.47	1.35
25	n	608	CHL	O2D-CGD	5.05	1.45	1.33
25	N	606	CHL	O2D-CGD	5.05	1.45	1.33
25	3	607	CHL	O2D-CGD	5.05	1.45	1.33
25	7	607	CHL	O2D-CGD	5.05	1.45	1.33
25	6	609	CHL	C3D-C4D	-5.04	1.32	1.44
25	3	606	CHL	O2D-CGD	5.04	1.45	1.33
25	6	606	CHL	C3D-C4D	-5.04	1.32	1.44
25	n	609	CHL	O2D-CGD	5.03	1.45	1.33
25	n	605	CHL	C3D-C4D	-5.03	1.32	1.44
25	N	605	CHL	C3D-C4D	-5.03	1.32	1.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	606	CHL	O2D-CGD	5.03	1.45	1.33
25	N	608	CHL	O2D-CGD	5.03	1.45	1.33
25	N	606	CHL	C3D-C4D	-5.02	1.32	1.44
25	n	606	CHL	C3D-C4D	-5.02	1.32	1.44
25	G	601	CHL	O2D-CGD	5.02	1.45	1.33
25	2	607	CHL	O2D-CGD	5.02	1.45	1.33
25	4	606	CHL	O2D-CGD	5.01	1.45	1.33
25	R	608	CHL	O2D-CGD	5.01	1.45	1.33
25	r	608	CHL	O2D-CGD	5.01	1.45	1.33
25	6	607	CHL	O2D-CGD	5.01	1.45	1.33
25	N	605	CHL	O2D-CGD	5.01	1.45	1.33
25	n	605	CHL	O2D-CGD	5.01	1.45	1.33
25	8	608	CHL	O2D-CGD	5.01	1.45	1.33
25	2	609	CHL	C3D-C4D	-5.01	1.32	1.44
25	g	601	CHL	O2D-CGD	5.00	1.45	1.33
25	N	609	CHL	O2D-CGD	5.00	1.45	1.33
25	s	606	CHL	O2D-CGD	5.00	1.45	1.33
25	6	605	CHL	C3B-C2B	5.00	1.47	1.40
25	4	608	CHL	CHC-C1C	5.00	1.47	1.35
25	8	606	CHL	O2D-CGD	5.00	1.45	1.33
25	2	606	CHL	C3D-C4D	-5.00	1.32	1.44
25	8	608	CHL	CHC-C1C	5.00	1.47	1.35
25	S	606	CHL	O2D-CGD	4.99	1.45	1.33
25	G	608	CHL	O2D-CGD	4.99	1.45	1.33
25	g	608	CHL	O2D-CGD	4.99	1.45	1.33
25	G	606	CHL	C3D-C4D	-4.99	1.32	1.44
25	4	608	CHL	O2D-CGD	4.99	1.45	1.33
25	g	606	CHL	C3D-C4D	-4.99	1.32	1.44
25	3	601	CHL	O2D-CGD	4.98	1.45	1.33
25	7	601	CHL	O2D-CGD	4.98	1.45	1.33
25	1	605	CHL	O2D-CGD	4.98	1.45	1.33
25	4	609	CHL	O2D-CGD	4.98	1.45	1.33
25	5	605	CHL	O2D-CGD	4.98	1.45	1.33
25	8	607	CHL	C3D-C4D	-4.97	1.33	1.44
25	2	605	CHL	C3B-C2B	4.97	1.47	1.40
25	s	606	CHL	CHC-C1C	4.97	1.47	1.35
25	N	607	CHL	C3D-C4D	-4.96	1.33	1.44
25	n	607	CHL	C3D-C4D	-4.96	1.33	1.44
25	4	607	CHL	C3D-C4D	-4.96	1.33	1.44
25	S	606	CHL	CHC-C1C	4.96	1.47	1.35
25	8	609	CHL	O2D-CGD	4.95	1.45	1.33
25	3	601	CHL	CHC-C1C	4.94	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	609	CHL	O2D-CGD	4.94	1.45	1.33
25	7	601	CHL	CHC-C1C	4.94	1.47	1.35
25	7	607	CHL	CHC-C1C	4.93	1.47	1.35
25	S	608	CHL	C3B-C2B	4.93	1.47	1.40
25	3	607	CHL	CHC-C1C	4.92	1.47	1.35
25	6	605	CHL	CHC-C1C	4.92	1.47	1.35
25	2	609	CHL	O2D-CGD	4.92	1.45	1.33
25	6	609	CHL	O2D-CGD	4.92	1.45	1.33
25	7	609	CHL	O2D-CGD	4.92	1.45	1.33
25	2	605	CHL	CHC-C1C	4.91	1.47	1.35
25	4	609	CHL	CHC-C1C	4.91	1.47	1.35
25	8	609	CHL	CHC-C1C	4.91	1.47	1.35
25	g	605	CHL	C3D-C4D	-4.91	1.33	1.44
25	Y	605	CHL	CHC-C1C	4.91	1.47	1.35
25	5	607	CHL	C3D-C4D	-4.90	1.33	1.44
25	r	606	CHL	CHC-C1C	4.90	1.47	1.35
25	s	608	CHL	C3B-C2B	4.90	1.47	1.40
25	R	606	CHL	CHC-C1C	4.89	1.47	1.35
25	G	605	CHL	C3D-C4D	-4.89	1.33	1.44
25	N	606	CHL	C3B-C2B	4.89	1.47	1.40
25	5	601	CHL	CHC-C1C	4.89	1.47	1.35
25	G	608	CHL	CHC-C1C	4.89	1.47	1.35
25	g	608	CHL	CHC-C1C	4.89	1.47	1.35
25	1	607	CHL	C3D-C4D	-4.88	1.33	1.44
25	1	601	CHL	CHC-C1C	4.88	1.47	1.35
25	1	607	CHL	O2D-CGD	4.88	1.45	1.33
25	2	607	CHL	CHC-C1C	4.87	1.47	1.35
25	y	605	CHL	CHC-C1C	4.87	1.47	1.35
25	R	614	CHL	C3D-C4D	-4.87	1.33	1.44
25	r	614	CHL	C3D-C4D	-4.87	1.33	1.44
25	S	608	CHL	CHC-C1C	4.87	1.47	1.35
25	s	608	CHL	CHC-C1C	4.87	1.47	1.35
25	n	606	CHL	C3B-C2B	4.87	1.47	1.40
25	3	608	CHL	CHC-C1C	4.86	1.47	1.35
25	Y	608	CHL	CHC-C1C	4.86	1.47	1.35
25	5	607	CHL	O2D-CGD	4.86	1.45	1.33
25	G	609	CHL	O2D-CGD	4.85	1.45	1.33
25	N	608	CHL	CHC-C1C	4.85	1.47	1.35
25	n	608	CHL	CHC-C1C	4.85	1.47	1.35
25	4	601	CHL	C2C-C3C	4.85	1.47	1.36
25	y	608	CHL	CHC-C1C	4.85	1.47	1.35
25	2	608	CHL	O2D-CGD	4.84	1.45	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	g	609	CHL	O2D-CGD	4.84	1.45	1.33
25	6	607	CHL	CHC-C1C	4.84	1.47	1.35
25	G	609	CHL	C3D-C4D	-4.84	1.33	1.44
25	g	609	CHL	C3D-C4D	-4.84	1.33	1.44
25	y	605	CHL	O2D-CGD	4.84	1.45	1.33
25	S	601	CHL	C2C-C3C	4.84	1.47	1.36
25	s	601	CHL	C2C-C3C	4.84	1.47	1.36
25	r	614	CHL	CHC-C1C	4.84	1.47	1.35
25	3	605	CHL	C3B-C2B	4.84	1.47	1.40
25	7	605	CHL	C3B-C2B	4.84	1.47	1.40
25	3	605	CHL	CHC-C1C	4.83	1.47	1.35
25	Y	606	CHL	O2D-CGD	4.83	1.45	1.33
25	y	606	CHL	O2D-CGD	4.83	1.45	1.33
25	3	607	CHL	O2A-CGA	4.83	1.47	1.33
25	7	607	CHL	O2A-CGA	4.83	1.47	1.33
25	Y	605	CHL	O2D-CGD	4.83	1.45	1.33
25	7	605	CHL	C3D-C4D	-4.83	1.33	1.44
25	7	608	CHL	CHC-C1C	4.83	1.47	1.35
25	5	605	CHL	CHC-C1C	4.83	1.47	1.35
25	8	601	CHL	C2C-C3C	4.83	1.47	1.36
25	R	614	CHL	CHC-C1C	4.83	1.47	1.35
25	1	608	CHL	O2D-CGD	4.83	1.45	1.33
25	5	608	CHL	O2D-CGD	4.83	1.45	1.33
25	3	605	CHL	C3D-C4D	-4.83	1.33	1.44
25	8	601	CHL	C3D-C4D	-4.83	1.33	1.44
25	7	605	CHL	CHC-C1C	4.82	1.47	1.35
25	1	605	CHL	CHC-C1C	4.82	1.47	1.35
25	6	608	CHL	O2D-CGD	4.82	1.45	1.33
25	6	607	CHL	C3D-C4D	-4.82	1.33	1.44
25	G	606	CHL	CHC-C1C	4.81	1.47	1.35
25	3	608	CHL	O2D-CGD	4.81	1.44	1.33
25	2	608	CHL	CHC-C1C	4.80	1.47	1.35
25	4	601	CHL	C3D-C4D	-4.80	1.33	1.44
25	s	606	CHL	C3D-C4D	-4.80	1.33	1.44
25	S	606	CHL	C3D-C4D	-4.80	1.33	1.44
25	7	608	CHL	O2D-CGD	4.80	1.44	1.33
25	1	607	CHL	CHC-C1C	4.80	1.47	1.35
25	5	607	CHL	CHC-C1C	4.80	1.47	1.35
25	r	606	CHL	O2D-CGD	4.80	1.44	1.33
25	G	607	CHL	O2D-CGD	4.79	1.44	1.33
25	g	606	CHL	CHC-C1C	4.79	1.47	1.35
25	S	601	CHL	CHC-C1C	4.79	1.47	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	609	CHL	O2D-CGD	4.79	1.44	1.33
25	4	607	CHL	CHC-C1C	4.78	1.47	1.35
25	s	601	CHL	CHC-C1C	4.78	1.47	1.35
25	G	605	CHL	O2D-CGD	4.78	1.44	1.33
25	R	608	CHL	CHC-C1C	4.78	1.47	1.35
25	8	607	CHL	CHC-C1C	4.78	1.47	1.35
25	r	608	CHL	CHC-C1C	4.78	1.47	1.35
25	2	607	CHL	C3D-C4D	-4.78	1.33	1.44
25	6	608	CHL	CHC-C1C	4.78	1.47	1.35
25	5	609	CHL	O2D-CGD	4.77	1.44	1.33
25	1	606	CHL	CHC-C1C	4.77	1.47	1.35
25	5	606	CHL	CHC-C1C	4.77	1.47	1.35
25	2	608	CHL	C3B-C2B	4.77	1.47	1.40
25	R	606	CHL	O2D-CGD	4.77	1.44	1.33
25	g	605	CHL	O2D-CGD	4.76	1.44	1.33
25	y	609	CHL	O2D-CGD	4.76	1.44	1.33
25	g	607	CHL	O2D-CGD	4.75	1.44	1.33
25	3	607	CHL	C2C-C3C	4.75	1.46	1.36
25	6	608	CHL	C3B-C2B	4.75	1.47	1.40
25	N	605	CHL	CHC-C1C	4.74	1.47	1.35
25	n	605	CHL	CHC-C1C	4.74	1.47	1.35
25	N	606	CHL	CHC-C1C	4.74	1.47	1.35
25	n	606	CHL	CHC-C1C	4.74	1.47	1.35
25	5	601	CHL	C3B-C2B	4.74	1.46	1.40
25	1	601	CHL	C3B-C2B	4.74	1.46	1.40
25	Y	609	CHL	O2D-CGD	4.73	1.44	1.33
25	7	607	CHL	C2C-C3C	4.73	1.46	1.36
25	6	609	CHL	CHC-C1C	4.73	1.47	1.35
25	S	607	CHL	C3D-C4D	-4.72	1.33	1.44
25	R	607	CHL	CHC-C1C	4.72	1.47	1.35
25	y	607	CHL	O2D-CGD	4.72	1.44	1.33
25	r	607	CHL	CHC-C1C	4.72	1.47	1.35
25	2	605	CHL	C3D-C4D	-4.71	1.33	1.44
25	6	605	CHL	C3D-C4D	-4.71	1.33	1.44
25	6	601	CHL	CHC-C1C	4.71	1.47	1.35
25	y	601	CHL	O2D-CGD	4.71	1.44	1.33
25	1	601	CHL	CHD-C1D	4.71	1.47	1.38
25	2	609	CHL	CHC-C1C	4.70	1.47	1.35
25	N	607	CHL	CHC-C1C	4.70	1.47	1.35
25	n	607	CHL	CHC-C1C	4.70	1.47	1.35
25	s	607	CHL	C3D-C4D	-4.69	1.33	1.44
25	y	608	CHL	O2D-CGD	4.69	1.44	1.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	601	CHL	O2D-CGD	4.69	1.44	1.33
25	R	614	CHL	O2D-CGD	4.69	1.44	1.33
25	r	614	CHL	O2D-CGD	4.69	1.44	1.33
25	4	601	CHL	O2D-CGD	4.69	1.45	1.30
25	8	601	CHL	O2D-CGD	4.69	1.45	1.30
25	Y	607	CHL	O2D-CGD	4.69	1.44	1.33
25	4	606	CHL	CHC-C1C	4.68	1.47	1.35
25	2	601	CHL	CHC-C1C	4.68	1.47	1.35
25	5	601	CHL	CHD-C1D	4.68	1.47	1.38
25	8	601	CHL	CHD-C1D	4.67	1.47	1.38
25	Y	608	CHL	O2D-CGD	4.67	1.44	1.33
25	7	609	CHL	CHD-C1D	4.67	1.47	1.38
25	N	607	CHL	O2D-CGD	4.66	1.44	1.33
25	n	607	CHL	O2D-CGD	4.66	1.44	1.33
25	3	609	CHL	CHC-C1C	4.66	1.46	1.35
25	5	608	CHL	CHC-C1C	4.66	1.46	1.35
25	3	609	CHL	CHD-C1D	4.65	1.47	1.38
25	8	606	CHL	CHC-C1C	4.65	1.46	1.35
25	1	605	CHL	C3B-C2B	4.64	1.46	1.40
25	1	608	CHL	CHC-C1C	4.64	1.46	1.35
25	4	601	CHL	CHD-C1D	4.63	1.47	1.38
25	3	607	CHL	CHD-C1D	4.63	1.47	1.38
25	7	609	CHL	CHC-C1C	4.63	1.46	1.35
25	r	614	CHL	C2C-C3C	4.63	1.46	1.36
25	5	605	CHL	C3B-C2B	4.63	1.46	1.40
25	r	606	CHL	C2C-C3C	4.62	1.46	1.36
25	s	608	CHL	O2D-CGD	4.62	1.44	1.33
25	7	609	CHL	C2C-C3C	4.62	1.46	1.36
25	6	606	CHL	C2C-C3C	4.62	1.46	1.36
25	3	608	CHL	C3B-C2B	4.62	1.46	1.40
25	S	608	CHL	O2D-CGD	4.62	1.44	1.33
25	R	614	CHL	C2C-C3C	4.62	1.46	1.36
25	3	609	CHL	C2C-C3C	4.61	1.46	1.36
25	G	606	CHL	C3B-C2B	4.60	1.46	1.40
25	g	606	CHL	C3B-C2B	4.60	1.46	1.40
25	2	605	CHL	C2C-C3C	4.59	1.46	1.36
25	6	605	CHL	C2C-C3C	4.59	1.46	1.36
25	7	607	CHL	CHD-C1D	4.59	1.47	1.38
25	2	606	CHL	C2C-C3C	4.59	1.46	1.36
25	7	608	CHL	C3B-C2B	4.59	1.46	1.40
25	6	609	CHL	C2C-C3C	4.58	1.46	1.36
25	3	606	CHL	CHC-C1C	4.58	1.46	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	R	606	CHL	C2C-C3C	4.58	1.46	1.36
25	2	609	CHL	C2C-C3C	4.57	1.46	1.36
25	4	606	CHL	C2C-C3C	4.57	1.46	1.36
25	8	609	CHL	CHD-C1D	4.57	1.47	1.38
25	g	609	CHL	C2C-C3C	4.57	1.46	1.36
25	3	607	CHL	C3B-C2B	4.57	1.46	1.40
25	S	608	CHL	C2C-C3C	4.57	1.46	1.36
25	s	608	CHL	C2C-C3C	4.57	1.46	1.36
25	7	606	CHL	CHC-C1C	4.56	1.46	1.35
25	G	609	CHL	C2C-C3C	4.56	1.46	1.36
25	n	605	CHL	O2A-CGA	4.55	1.46	1.33
25	N	605	CHL	O2A-CGA	4.54	1.46	1.33
25	y	606	CHL	C3B-C2B	4.54	1.46	1.40
25	N	606	CHL	C2C-C3C	4.54	1.46	1.36
25	n	606	CHL	C2C-C3C	4.54	1.46	1.36
25	8	606	CHL	C2C-C3C	4.54	1.46	1.36
25	4	609	CHL	CHD-C1D	4.53	1.47	1.38
25	2	606	CHL	CHC-C1C	4.53	1.46	1.35
25	6	606	CHL	CHC-C1C	4.53	1.46	1.35
25	6	608	CHL	O2A-CGA	4.53	1.46	1.30
25	7	607	CHL	C3B-C2B	4.53	1.46	1.40
25	2	608	CHL	O2A-CGA	4.53	1.46	1.30
25	Y	606	CHL	C3B-C2B	4.52	1.46	1.40
25	5	608	CHL	O2A-CGA	4.52	1.45	1.30
25	G	605	CHL	C3B-C2B	4.52	1.46	1.40
25	g	605	CHL	C3B-C2B	4.52	1.46	1.40
25	1	601	CHL	O2A-CGA	4.51	1.45	1.30
25	5	601	CHL	O2A-CGA	4.51	1.45	1.30
25	3	605	CHL	O2A-CGA	4.51	1.45	1.30
25	3	606	CHL	O2A-CGA	4.51	1.45	1.30
25	S	606	CHL	O2A-CGA	4.51	1.45	1.30
25	n	601	CHL	CHC-C1C	4.51	1.46	1.35
25	S	601	CHL	CHD-C1D	4.51	1.47	1.38
25	1	608	CHL	O2A-CGA	4.50	1.45	1.30
25	7	605	CHL	O2A-CGA	4.50	1.45	1.30
25	1	605	CHL	O2A-CGA	4.50	1.45	1.30
25	N	601	CHL	CHC-C1C	4.50	1.46	1.35
25	G	606	CHL	O2A-CGA	4.50	1.46	1.33
25	g	606	CHL	O2A-CGA	4.50	1.46	1.33
25	5	605	CHL	O2A-CGA	4.49	1.45	1.30
25	s	606	CHL	O2A-CGA	4.49	1.45	1.30
25	7	606	CHL	O2A-CGA	4.49	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	601	CHL	O2A-CGA	4.49	1.45	1.30
25	S	607	CHL	CHC-C1C	4.49	1.46	1.35
25	4	607	CHL	C2C-C3C	4.49	1.46	1.36
25	G	607	CHL	C2C-C3C	4.49	1.46	1.36
25	g	607	CHL	C2C-C3C	4.49	1.46	1.36
25	s	607	CHL	CHC-C1C	4.49	1.46	1.35
25	2	607	CHL	C3B-C2B	4.48	1.46	1.40
25	6	607	CHL	C3B-C2B	4.48	1.46	1.40
25	2	606	CHL	O2A-CGA	4.48	1.45	1.30
25	6	606	CHL	O2A-CGA	4.48	1.45	1.30
25	s	601	CHL	CHD-C1D	4.48	1.47	1.38
25	G	601	CHL	CHC-C1C	4.48	1.46	1.35
25	6	605	CHL	O2A-CGA	4.48	1.45	1.30
25	4	607	CHL	O2A-CGA	4.48	1.45	1.30
25	4	607	CHL	C3B-C2B	4.48	1.46	1.40
25	8	607	CHL	C3B-C2B	4.48	1.46	1.40
25	g	601	CHL	CHC-C1C	4.48	1.46	1.35
25	8	601	CHL	O2A-CGA	4.48	1.45	1.30
25	7	605	CHL	C2C-C3C	4.48	1.46	1.36
25	8	608	CHL	O2A-CGA	4.48	1.45	1.30
25	3	605	CHL	C2C-C3C	4.47	1.46	1.36
25	S	607	CHL	O2A-CGA	4.47	1.46	1.33
25	s	607	CHL	O2A-CGA	4.47	1.46	1.33
25	4	606	CHL	O2A-CGA	4.47	1.45	1.30
25	4	608	CHL	O2A-CGA	4.47	1.45	1.30
25	N	607	CHL	C3B-C2B	4.47	1.46	1.40
25	2	605	CHL	O2A-CGA	4.47	1.45	1.30
25	1	606	CHL	O2A-CGA	4.47	1.45	1.30
25	5	606	CHL	O2A-CGA	4.47	1.45	1.30
25	8	606	CHL	O2A-CGA	4.47	1.45	1.30
25	8	607	CHL	O2A-CGA	4.47	1.45	1.30
25	s	606	CHL	C3B-C2B	4.47	1.46	1.40
25	8	607	CHL	C2C-C3C	4.47	1.46	1.36
25	3	608	CHL	O2A-CGA	4.46	1.45	1.30
25	4	609	CHL	O2A-CGA	4.46	1.45	1.30
25	8	609	CHL	O2A-CGA	4.46	1.45	1.30
25	7	609	CHL	O2A-CGA	4.46	1.46	1.33
25	7	608	CHL	O2A-CGA	4.46	1.45	1.30
25	3	609	CHL	O2A-CGA	4.46	1.46	1.33
25	1	601	CHL	C2C-C3C	4.46	1.46	1.36
25	2	601	CHL	C3B-C2B	4.45	1.46	1.40
25	S	601	CHL	O2A-CGA	4.45	1.45	1.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	s	601	CHL	O2A-CGA	4.45	1.45	1.30
25	1	607	CHL	C2C-C3C	4.45	1.46	1.36
25	2	601	CHL	O2A-CGA	4.45	1.45	1.30
25	6	601	CHL	O2A-CGA	4.45	1.45	1.30
25	5	601	CHL	C2C-C3C	4.44	1.46	1.36
25	1	609	CHL	C2C-C3C	4.44	1.46	1.36
25	5	609	CHL	C2C-C3C	4.44	1.46	1.36
25	Y	606	CHL	O2A-CGA	4.44	1.46	1.33
25	y	606	CHL	O2A-CGA	4.44	1.46	1.33
25	g	605	CHL	O2A-CGA	4.44	1.45	1.30
25	8	607	CHL	CHD-C1D	4.43	1.47	1.38
25	n	607	CHL	C3B-C2B	4.43	1.46	1.40
25	G	605	CHL	O2A-CGA	4.43	1.45	1.30
25	5	607	CHL	C2C-C3C	4.43	1.46	1.36
25	G	606	CHL	C2C-C3C	4.43	1.46	1.36
25	g	606	CHL	C2C-C3C	4.43	1.46	1.36
25	S	608	CHL	O2A-CGA	4.42	1.45	1.30
25	g	608	CHL	C2C-C3C	4.42	1.46	1.36
25	6	609	CHL	C3B-C2B	4.42	1.46	1.40
25	S	606	CHL	C3B-C2B	4.42	1.46	1.40
25	2	609	CHL	C3B-C2B	4.42	1.46	1.40
25	4	606	CHL	C3B-C2B	4.42	1.46	1.40
25	Y	605	CHL	C3B-C2B	4.41	1.46	1.40
25	S	606	CHL	C2C-C3C	4.41	1.46	1.36
25	6	601	CHL	C3B-C2B	4.41	1.46	1.40
25	8	606	CHL	C3B-C2B	4.41	1.46	1.40
25	8	609	CHL	C2C-C3C	4.41	1.46	1.36
25	Y	609	CHL	C2C-C3C	4.41	1.46	1.36
25	G	608	CHL	C2C-C3C	4.41	1.46	1.36
25	N	605	CHL	C2C-C3C	4.41	1.46	1.36
25	n	605	CHL	C2C-C3C	4.41	1.46	1.36
25	s	608	CHL	O2A-CGA	4.41	1.45	1.30
25	4	609	CHL	C2C-C3C	4.40	1.46	1.36
25	y	609	CHL	C2C-C3C	4.40	1.46	1.36
26	a	406	CLA	C4D-ND	-4.40	1.31	1.37
25	1	609	CHL	CHC-C1C	4.40	1.46	1.35
25	s	606	CHL	C2C-C3C	4.40	1.46	1.36
25	Y	609	CHL	CHC-C1C	4.40	1.46	1.35
25	y	609	CHL	CHC-C1C	4.40	1.46	1.35
25	y	605	CHL	C3B-C2B	4.40	1.46	1.40
25	n	609	CHL	C2C-C3C	4.39	1.46	1.36
25	4	607	CHL	CHD-C1D	4.39	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	5	609	CHL	CHC-C1C	4.39	1.46	1.35
26	A	406	CLA	C4D-ND	-4.39	1.31	1.37
25	7	608	CHL	C2C-C3C	4.39	1.46	1.36
25	Y	605	CHL	O2A-CGA	4.38	1.46	1.33
25	y	605	CHL	O2A-CGA	4.38	1.46	1.33
25	2	608	CHL	C2C-C3C	4.38	1.46	1.36
25	n	606	CHL	O2A-CGA	4.38	1.46	1.33
25	N	609	CHL	C2C-C3C	4.38	1.46	1.36
25	3	608	CHL	C2C-C3C	4.37	1.46	1.36
25	2	607	CHL	C2C-C3C	4.37	1.46	1.36
25	N	606	CHL	O2A-CGA	4.37	1.46	1.33
25	3	606	CHL	C3B-C2B	4.36	1.46	1.40
25	7	606	CHL	C3B-C2B	4.36	1.46	1.40
25	y	605	CHL	C2C-C3C	4.36	1.46	1.36
25	6	608	CHL	C2C-C3C	4.36	1.46	1.36
25	1	608	CHL	C3B-C2B	4.36	1.46	1.40
25	5	608	CHL	C3B-C2B	4.36	1.46	1.40
25	R	614	CHL	C3B-C2B	4.35	1.46	1.40
25	r	614	CHL	C3B-C2B	4.35	1.46	1.40
25	n	609	CHL	CHC-C1C	4.35	1.46	1.35
26	c	503	CLA	C4D-ND	-4.35	1.31	1.37
25	2	606	CHL	C3B-C2B	4.35	1.46	1.40
25	N	609	CHL	CHC-C1C	4.34	1.46	1.35
25	R	608	CHL	C2C-C3C	4.34	1.46	1.36
25	Y	605	CHL	C2C-C3C	4.34	1.46	1.36
25	6	606	CHL	C3B-C2B	4.34	1.46	1.40
26	B	604	CLA	C4D-ND	-4.33	1.31	1.37
25	1	609	CHL	O2A-CGA	4.33	1.46	1.33
25	6	607	CHL	C2C-C3C	4.33	1.46	1.36
25	n	609	CHL	O2A-CGA	4.33	1.46	1.33
25	y	607	CHL	CHC-C1C	4.33	1.46	1.35
25	r	608	CHL	C2C-C3C	4.32	1.46	1.36
25	4	609	CHL	C3B-C2B	4.32	1.46	1.40
25	Y	607	CHL	CHC-C1C	4.32	1.46	1.35
26	C	503	CLA	C4D-ND	-4.32	1.31	1.37
26	b	604	CLA	C4D-ND	-4.31	1.31	1.37
25	1	606	CHL	C2C-C3C	4.31	1.46	1.36
25	5	606	CHL	C2C-C3C	4.31	1.46	1.36
25	4	608	CHL	C3B-C2B	4.31	1.46	1.40
25	5	609	CHL	O2A-CGA	4.31	1.45	1.33
25	g	609	CHL	O2A-CGA	4.31	1.45	1.33
25	G	605	CHL	C2C-C3C	4.31	1.46	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	609	CHL	C3B-C2B	4.31	1.46	1.40
25	N	609	CHL	O2A-CGA	4.30	1.45	1.33
26	C	502	CLA	C4D-ND	-4.30	1.31	1.37
26	c	502	CLA	C4D-ND	-4.30	1.31	1.37
25	G	606	CHL	CHD-C1D	4.30	1.46	1.38
25	G	609	CHL	O2A-CGA	4.28	1.45	1.33
25	g	606	CHL	CHD-C1D	4.28	1.46	1.38
25	8	608	CHL	C3B-C2B	4.27	1.46	1.40
25	g	605	CHL	C2C-C3C	4.27	1.45	1.36
25	R	607	CHL	O2A-CGA	4.27	1.45	1.33
25	r	606	CHL	CHD-C1D	4.27	1.46	1.38
25	g	609	CHL	CHC-C1C	4.27	1.45	1.35
25	R	607	CHL	C2C-C3C	4.27	1.45	1.36
25	r	607	CHL	O2A-CGA	4.26	1.45	1.33
26	C	508	CLA	C4D-ND	-4.26	1.31	1.37
25	n	609	CHL	CHD-C1D	4.25	1.46	1.38
25	r	607	CHL	C2C-C3C	4.25	1.45	1.36
25	N	607	CHL	O2A-CGA	4.25	1.45	1.33
25	n	607	CHL	O2A-CGA	4.25	1.45	1.33
25	R	606	CHL	CHD-C1D	4.25	1.46	1.38
25	n	605	CHL	C3B-C2B	4.25	1.46	1.40
25	G	609	CHL	CHC-C1C	4.25	1.45	1.35
25	G	609	CHL	CHD-C1D	4.25	1.46	1.38
26	c	508	CLA	C4D-ND	-4.24	1.31	1.37
25	n	601	CHL	C3B-C2B	4.24	1.46	1.40
25	2	607	CHL	O2A-CGA	4.24	1.45	1.33
25	g	609	CHL	CHD-C1D	4.24	1.46	1.38
25	Y	606	CHL	CHC-C1C	4.23	1.45	1.35
25	5	608	CHL	C2C-C3C	4.23	1.45	1.36
25	6	607	CHL	O2A-CGA	4.23	1.45	1.33
25	8	608	CHL	C2C-C3C	4.23	1.45	1.36
25	1	609	CHL	CHD-C1D	4.23	1.46	1.38
25	8	606	CHL	CHD-C1D	4.22	1.46	1.38
25	N	607	CHL	C2C-C3C	4.22	1.45	1.36
25	n	607	CHL	C2C-C3C	4.22	1.45	1.36
25	6	606	CHL	CHD-C1D	4.22	1.46	1.38
25	2	606	CHL	CHD-C1D	4.22	1.46	1.38
25	2	609	CHL	O2A-CGA	4.21	1.45	1.33
25	6	609	CHL	O2A-CGA	4.21	1.45	1.33
25	R	608	CHL	O2A-CGA	4.21	1.45	1.33
25	r	608	CHL	O2A-CGA	4.21	1.45	1.33
25	N	609	CHL	CHD-C1D	4.21	1.46	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	601	CHL	CHD-C1D	4.21	1.46	1.38
25	1	608	CHL	C2C-C3C	4.21	1.45	1.36
25	Y	609	CHL	O2A-CGA	4.20	1.45	1.33
25	y	609	CHL	O2A-CGA	4.20	1.45	1.33
25	2	607	CHL	CHD-C1D	4.20	1.46	1.38
25	2	601	CHL	C2C-C3C	4.20	1.45	1.36
25	N	605	CHL	C3B-C2B	4.20	1.46	1.40
25	y	606	CHL	CHC-C1C	4.20	1.45	1.35
25	6	601	CHL	C2C-C3C	4.20	1.45	1.36
26	B	610	CLA	C4D-ND	-4.20	1.31	1.37
26	b	610	CLA	C4D-ND	-4.20	1.31	1.37
26	Y	604	CLA	CMB-C2B	-4.20	1.42	1.51
26	y	604	CLA	CMB-C2B	-4.20	1.42	1.51
25	6	601	CHL	CHD-C1D	4.20	1.46	1.38
25	5	605	CHL	C2C-C3C	4.20	1.45	1.36
25	5	609	CHL	C3B-C2B	4.20	1.46	1.40
25	4	608	CHL	C2C-C3C	4.20	1.45	1.36
25	4	606	CHL	CHD-C1D	4.20	1.46	1.38
25	1	605	CHL	C2C-C3C	4.19	1.45	1.36
25	y	601	CHL	CHC-C1C	4.19	1.45	1.35
25	N	601	CHL	C3B-C2B	4.19	1.46	1.40
25	R	606	CHL	O2A-CGA	4.19	1.45	1.33
25	Y	601	CHL	CHC-C1C	4.19	1.45	1.35
25	Y	601	CHL	CHD-C1D	4.18	1.46	1.38
25	y	601	CHL	CHD-C1D	4.18	1.46	1.38
25	r	606	CHL	O2A-CGA	4.18	1.45	1.33
25	G	608	CHL	C3B-C2B	4.18	1.46	1.40
26	A	405	CLA	C4D-ND	-4.18	1.32	1.37
26	a	405	CLA	C4D-ND	-4.18	1.32	1.37
26	a	407	CLA	C4D-ND	-4.18	1.32	1.37
25	5	609	CHL	CHD-C1D	4.17	1.46	1.38
25	3	609	CHL	C3B-C2B	4.17	1.46	1.40
25	1	601	CHL	CHD-C4C	4.17	1.48	1.39
25	5	601	CHL	CHD-C4C	4.17	1.48	1.39
25	1	609	CHL	C3B-C2B	4.17	1.46	1.40
25	1	605	CHL	CHD-C1D	4.17	1.46	1.38
25	5	605	CHL	CHD-C1D	4.17	1.46	1.38
25	N	601	CHL	O2A-CGA	4.17	1.45	1.33
25	y	607	CHL	C2C-C3C	4.17	1.45	1.36
25	G	605	CHL	CHD-C1D	4.17	1.46	1.38
25	g	605	CHL	CHD-C1D	4.17	1.46	1.38
25	Y	607	CHL	C2C-C3C	4.16	1.45	1.36

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	601	CHL	O2A-CGA	4.16	1.45	1.33
25	6	607	CHL	CHD-C1D	4.16	1.46	1.38
26	A	407	CLA	C4D-ND	-4.16	1.32	1.37
25	G	608	CHL	O2A-CGA	4.16	1.45	1.33
25	3	601	CHL	O2A-CGA	4.15	1.45	1.33
25	7	601	CHL	C3B-C2B	4.15	1.46	1.40
25	g	608	CHL	C3B-C2B	4.14	1.46	1.40
25	7	609	CHL	C3B-C2B	4.14	1.46	1.40
25	3	601	CHL	C3B-C2B	4.14	1.46	1.40
25	5	606	CHL	CHD-C1D	4.14	1.46	1.38
25	g	608	CHL	O2A-CGA	4.13	1.45	1.33
25	y	601	CHL	O2A-CGA	4.13	1.45	1.33
25	Y	601	CHL	O2A-CGA	4.12	1.45	1.33
30	l	101	LHG	O7-C5	-4.12	1.36	1.46
25	1	607	CHL	O2A-CGA	4.12	1.45	1.33
26	c	507	CLA	C4D-ND	-4.12	1.32	1.37
25	G	607	CHL	O2A-CGA	4.12	1.45	1.33
25	g	607	CHL	O2A-CGA	4.12	1.45	1.33
25	7	601	CHL	O2A-CGA	4.12	1.45	1.33
25	7	606	CHL	CHD-C1D	4.12	1.46	1.38
25	g	609	CHL	C3B-C2B	4.11	1.46	1.40
26	S	609	CLA	C1D-ND	4.11	1.42	1.37
25	N	606	CHL	CHD-C1D	4.11	1.46	1.38
25	n	606	CHL	CHD-C1D	4.11	1.46	1.38
25	y	609	CHL	CHD-C1D	4.11	1.46	1.38
26	b	606	CLA	C4D-ND	-4.11	1.32	1.37
25	5	607	CHL	O2A-CGA	4.11	1.45	1.33
25	2	609	CHL	CHD-C1D	4.11	1.46	1.38
25	6	609	CHL	CHD-C1D	4.11	1.46	1.38
25	1	606	CHL	CHD-C1D	4.11	1.46	1.38
26	s	609	CLA	C1D-ND	4.11	1.42	1.37
25	3	605	CHL	CHD-C1D	4.11	1.46	1.38
25	7	605	CHL	CHD-C1D	4.11	1.46	1.38
25	3	606	CHL	CHD-C1D	4.10	1.46	1.38
25	G	609	CHL	C3B-C2B	4.10	1.46	1.40
26	N	604	CLA	CMB-C2B	-4.10	1.43	1.51
25	2	605	CHL	CHD-C1D	4.10	1.46	1.38
25	Y	609	CHL	CHD-C1D	4.10	1.46	1.38
25	6	605	CHL	CHD-C1D	4.10	1.46	1.38
25	N	608	CHL	C2C-C3C	4.09	1.45	1.36
30	L	101	LHG	O7-C5	-4.09	1.36	1.46
26	B	606	CLA	C4D-ND	-4.08	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	D	405	PL9	C3-C4	-4.08	1.42	1.49
38	d	405	PL9	C3-C4	-4.08	1.42	1.49
25	G	601	CHL	C3B-C2B	4.07	1.46	1.40
25	r	607	CHL	C3B-C2B	4.07	1.46	1.40
25	3	601	CHL	C2C-C3C	4.06	1.45	1.36
26	C	507	CLA	C4D-ND	-4.06	1.32	1.37
25	7	601	CHL	C2C-C3C	4.06	1.45	1.36
26	D	402	CLA	C4D-ND	-4.06	1.32	1.37
25	Y	608	CHL	C3B-C2B	4.06	1.46	1.40
25	n	608	CHL	C2C-C3C	4.06	1.45	1.36
25	Y	601	CHL	CHD-C4C	4.06	1.48	1.39
25	y	601	CHL	CHD-C4C	4.06	1.48	1.39
26	n	604	CLA	CMB-C2B	-4.06	1.43	1.51
25	G	601	CHL	C2C-C3C	4.05	1.45	1.36
25	g	601	CHL	C2C-C3C	4.05	1.45	1.36
25	g	601	CHL	C3B-C2B	4.05	1.46	1.40
26	A	410	CLA	C4D-ND	-4.05	1.32	1.37
25	4	601	CHL	CHD-C4C	4.05	1.48	1.39
25	r	614	CHL	CHD-C1D	4.05	1.46	1.38
25	R	606	CHL	C3B-C2B	4.05	1.46	1.40
25	r	606	CHL	C3B-C2B	4.05	1.46	1.40
26	b	603	CLA	C4D-ND	-4.04	1.32	1.37
25	R	607	CHL	C3B-C2B	4.04	1.46	1.40
25	l	607	CHL	CHD-C1D	4.04	1.46	1.38
25	5	607	CHL	CHD-C1D	4.04	1.46	1.38
26	R	602	CLA	C4D-ND	-4.04	1.32	1.37
25	8	601	CHL	CHD-C4C	4.03	1.48	1.39
25	n	608	CHL	C3B-C2B	4.03	1.46	1.40
26	d	402	CLA	C4D-ND	-4.03	1.32	1.37
26	G	604	CLA	CMB-C2B	-4.03	1.43	1.51
26	g	604	CLA	CMB-C2B	-4.03	1.43	1.51
25	N	608	CHL	C3B-C2B	4.02	1.46	1.40
25	y	608	CHL	C3B-C2B	4.02	1.46	1.40
25	l	606	CHL	C3B-C2B	4.02	1.45	1.40
26	a	410	CLA	C4D-ND	-4.02	1.32	1.37
26	r	602	CLA	C4D-ND	-4.02	1.32	1.37
26	C	504	CLA	C4D-ND	-4.02	1.32	1.37
25	R	614	CHL	CHD-C1D	4.02	1.46	1.38
25	S	607	CHL	C3B-C2B	4.01	1.45	1.40
25	s	607	CHL	C3B-C2B	4.01	1.45	1.40
26	Y	613	CLA	C4D-ND	-4.00	1.32	1.37
26	y	613	CLA	C4D-ND	-4.00	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	A	405	CLA	CMC-C2C	-4.00	1.42	1.50
26	a	405	CLA	CMC-C2C	-4.00	1.42	1.50
25	r	614	CHL	C3A-C2A	-4.00	1.50	1.54
25	n	608	CHL	O2A-CGA	4.00	1.45	1.33
25	R	614	CHL	OBD-CAD	4.00	1.29	1.22
25	r	614	CHL	OBD-CAD	4.00	1.29	1.22
25	5	606	CHL	C3B-C2B	3.99	1.45	1.40
26	B	603	CLA	C4D-ND	-3.99	1.32	1.37
26	b	617	CLA	C4D-ND	-3.98	1.32	1.37
25	3	607	CHL	CHD-C4C	3.98	1.48	1.39
25	g	601	CHL	O2A-CGA	3.98	1.45	1.33
25	4	607	CHL	CHD-C4C	3.98	1.48	1.39
25	G	601	CHL	O2A-CGA	3.98	1.45	1.33
25	N	608	CHL	O2A-CGA	3.98	1.45	1.33
25	2	601	CHL	CHD-C4C	3.98	1.48	1.39
26	d	403	CLA	C4D-ND	-3.98	1.32	1.37
26	B	617	CLA	C4D-ND	-3.97	1.32	1.37
25	7	607	CHL	CHD-C4C	3.97	1.48	1.39
26	B	608	CLA	C4D-ND	-3.97	1.32	1.37
25	Y	609	CHL	C3B-C2B	3.97	1.45	1.40
25	y	609	CHL	C3B-C2B	3.97	1.45	1.40
25	6	601	CHL	CHD-C4C	3.97	1.48	1.39
25	Y	606	CHL	C2C-C3C	3.97	1.45	1.36
25	R	614	CHL	C3A-C2A	-3.96	1.50	1.54
26	b	608	CLA	C4D-ND	-3.96	1.32	1.37
25	G	607	CHL	CHD-C1D	3.96	1.46	1.38
25	g	607	CHL	CHD-C1D	3.96	1.46	1.38
25	y	606	CHL	C2C-C3C	3.96	1.45	1.36
26	C	506	CLA	C4D-ND	-3.96	1.32	1.37
26	c	506	CLA	C4D-ND	-3.96	1.32	1.37
25	8	607	CHL	CHD-C4C	3.96	1.48	1.39
26	c	504	CLA	C4D-ND	-3.96	1.32	1.37
26	G	614	CLA	C1D-ND	3.95	1.42	1.37
25	Y	608	CHL	O2A-CGA	3.95	1.44	1.33
25	y	608	CHL	O2A-CGA	3.95	1.44	1.33
25	S	601	CHL	C3B-C2B	3.95	1.45	1.40
25	s	601	CHL	C3B-C2B	3.95	1.45	1.40
26	g	610	CLA	C1D-ND	3.95	1.42	1.37
25	Y	608	CHL	C2C-C3C	3.95	1.45	1.36
25	3	601	CHL	CHD-C1D	3.95	1.46	1.38
25	7	601	CHL	CHD-C1D	3.95	1.46	1.38
25	3	609	CHL	CHD-C4C	3.95	1.48	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	7	609	CHL	CHD-C4C	3.95	1.48	1.39
25	y	608	CHL	C2C-C3C	3.93	1.45	1.36
25	N	601	CHL	CHD-C1D	3.93	1.46	1.38
25	n	601	CHL	CHD-C1D	3.93	1.46	1.38
26	B	605	CLA	CMD-C2D	-3.93	1.42	1.50
26	D	403	CLA	C4D-ND	-3.93	1.32	1.37
25	S	606	CHL	CHD-C1D	3.92	1.46	1.38
25	S	607	CHL	C2C-C3C	3.92	1.45	1.36
25	y	601	CHL	C2C-C3C	3.92	1.45	1.36
38	D	405	PL9	C7-C8	-3.92	1.45	1.50
26	Y	602	CLA	C4D-ND	-3.92	1.32	1.37
25	Y	601	CHL	C2C-C3C	3.92	1.45	1.36
26	B	611	CLA	C4D-ND	-3.92	1.32	1.37
25	N	601	CHL	C2C-C3C	3.91	1.45	1.36
26	g	614	CLA	C1D-ND	3.91	1.42	1.37
25	4	609	CHL	CHD-C4C	3.91	1.48	1.39
25	n	601	CHL	C2C-C3C	3.91	1.45	1.36
41	F	101	HEM	C3C-CAC	3.91	1.55	1.47
41	f	101	HEM	C3C-CAC	3.91	1.55	1.47
25	s	606	CHL	CHD-C1D	3.91	1.46	1.38
25	3	601	CHL	CHD-C4C	3.91	1.48	1.39
25	7	601	CHL	CHD-C4C	3.91	1.48	1.39
26	b	605	CLA	CMD-C2D	-3.91	1.42	1.50
26	G	610	CLA	C1D-ND	3.91	1.42	1.37
25	g	605	CHL	OBD-CAD	3.91	1.29	1.22
26	y	602	CLA	C4D-ND	-3.90	1.32	1.37
26	y	612	CLA	C4D-ND	-3.90	1.32	1.37
25	6	608	CHL	CHD-C1D	3.90	1.46	1.38
25	8	609	CHL	CHD-C4C	3.89	1.48	1.39
25	s	607	CHL	C2C-C3C	3.89	1.45	1.36
26	B	605	CLA	C4D-ND	-3.89	1.32	1.37
26	b	605	CLA	C4D-ND	-3.89	1.32	1.37
25	2	608	CHL	CHD-C1D	3.89	1.45	1.38
26	B	612	CLA	C4D-ND	-3.88	1.32	1.37
26	b	611	CLA	C4D-ND	-3.88	1.32	1.37
25	S	601	CHL	CHD-C4C	3.88	1.48	1.39
25	s	601	CHL	CHD-C4C	3.88	1.48	1.39
25	N	605	CHL	OBD-CAD	3.88	1.29	1.22
25	n	605	CHL	OBD-CAD	3.88	1.29	1.22
26	B	614	CLA	C4D-ND	-3.87	1.32	1.37
26	Y	612	CLA	C4D-ND	-3.87	1.32	1.37
26	b	614	CLA	C4D-ND	-3.87	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	S	607	CHL	CHD-C1D	3.87	1.45	1.38
25	s	607	CHL	CHD-C1D	3.87	1.45	1.38
26	C	510	CLA	C4D-ND	-3.87	1.32	1.37
26	c	510	CLA	C4D-ND	-3.87	1.32	1.37
25	n	605	CHL	CHD-C1D	3.87	1.45	1.38
25	N	605	CHL	CHD-C1D	3.87	1.45	1.38
26	R	611	CLA	C4D-ND	-3.87	1.32	1.37
26	r	611	CLA	C4D-ND	-3.87	1.32	1.37
38	d	405	PL9	C7-C8	-3.86	1.45	1.50
25	G	605	CHL	OBD-CAD	3.86	1.29	1.22
26	b	612	CLA	C4D-ND	-3.86	1.32	1.37
26	N	612	CLA	C1D-ND	3.86	1.42	1.37
26	n	612	CLA	C1D-ND	3.86	1.42	1.37
25	Y	607	CHL	O2A-CGA	3.85	1.44	1.33
25	y	607	CHL	O2A-CGA	3.85	1.44	1.33
25	s	608	CHL	CHD-C1D	3.84	1.45	1.38
25	1	607	CHL	C3B-C2B	3.83	1.45	1.40
25	5	607	CHL	C3B-C2B	3.83	1.45	1.40
25	G	607	CHL	C3B-C2B	3.82	1.45	1.40
25	g	607	CHL	C3B-C2B	3.82	1.45	1.40
26	G	602	CLA	C4D-ND	-3.82	1.32	1.37
26	g	602	CLA	C4D-ND	-3.82	1.32	1.37
25	G	601	CHL	CHD-C4C	3.82	1.47	1.39
25	7	606	CHL	C2C-C3C	3.82	1.45	1.36
25	4	606	CHL	CHD-C4C	3.81	1.47	1.39
26	c	505	CLA	C4D-ND	-3.81	1.32	1.37
25	R	608	CHL	CHD-C1D	3.81	1.45	1.38
25	r	608	CHL	CHD-C1D	3.81	1.45	1.38
25	8	606	CHL	CHD-C4C	3.81	1.47	1.39
25	S	608	CHL	CHD-C1D	3.81	1.45	1.38
26	C	505	CLA	C4D-ND	-3.80	1.32	1.37
25	g	601	CHL	CHD-C4C	3.80	1.47	1.39
25	3	606	CHL	C2C-C3C	3.78	1.44	1.36
25	5	609	CHL	CHD-C4C	3.78	1.47	1.39
25	n	608	CHL	CHD-C1D	3.77	1.45	1.38
41	F	101	HEM	C3C-C2C	-3.77	1.35	1.40
25	R	608	CHL	C3B-C2B	3.77	1.45	1.40
25	r	608	CHL	C3B-C2B	3.77	1.45	1.40
26	4	611	CLA	C1D-ND	3.76	1.42	1.37
25	g	601	CHL	CHD-C1D	3.76	1.45	1.38
26	b	613	CLA	CMD-C2D	-3.76	1.42	1.50
26	B	613	CLA	CMD-C2D	-3.76	1.42	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
38	d	405	PL9	C6-C1	-3.76	1.41	1.48
25	1	609	CHL	CHD-C4C	3.76	1.47	1.39
25	G	601	CHL	CHD-C1D	3.76	1.45	1.38
25	N	608	CHL	CHD-C1D	3.76	1.45	1.38
25	N	601	CHL	CHD-C4C	3.75	1.47	1.39
25	n	601	CHL	CHD-C4C	3.75	1.47	1.39
26	8	611	CLA	C1D-ND	3.75	1.42	1.37
25	g	606	CHL	CHD-C4C	3.75	1.47	1.39
26	N	602	CLA	C4D-ND	-3.75	1.32	1.37
26	n	602	CLA	C4D-ND	-3.75	1.32	1.37
26	4	603	CLA	C1D-ND	3.74	1.42	1.37
25	G	606	CHL	CHD-C4C	3.74	1.47	1.39
25	2	607	CHL	CHD-C4C	3.74	1.47	1.39
25	6	607	CHL	CHD-C4C	3.74	1.47	1.39
26	5	612	CLA	C1D-ND	3.74	1.42	1.37
25	G	608	CHL	CHD-C1D	3.74	1.45	1.38
25	6	609	CHL	CHD-C4C	3.73	1.47	1.39
26	B	604	CLA	CMB-C2B	-3.73	1.43	1.51
26	b	604	CLA	CMB-C2B	-3.73	1.43	1.51
26	y	603	CLA	C4D-ND	-3.73	1.32	1.37
41	f	101	HEM	C3C-C2C	-3.73	1.35	1.40
38	D	405	PL9	C6-C1	-3.73	1.41	1.48
26	4	610	CLA	C4D-ND	-3.73	1.32	1.37
26	8	610	CLA	C4D-ND	-3.73	1.32	1.37
26	b	607	CLA	C4D-ND	-3.73	1.32	1.37
25	Y	607	CHL	C3B-C2B	3.72	1.45	1.40
25	y	607	CHL	C3B-C2B	3.72	1.45	1.40
25	g	608	CHL	CHD-C1D	3.72	1.45	1.38
26	2	612	CLA	C1D-ND	3.72	1.42	1.37
25	Y	608	CHL	CHD-C1D	3.72	1.45	1.38
26	Y	603	CLA	C4D-ND	-3.71	1.32	1.37
26	1	612	CLA	C1D-ND	3.71	1.42	1.37
26	8	603	CLA	C1D-ND	3.71	1.42	1.37
25	G	606	CHL	OBD-CAD	3.71	1.28	1.22
25	g	606	CHL	OBD-CAD	3.71	1.28	1.22
26	c	508	CLA	CMB-C2B	-3.71	1.43	1.51
26	2	614	CLA	C1D-ND	3.71	1.42	1.37
26	B	602	CLA	C4D-ND	-3.71	1.32	1.37
26	C	513	CLA	C4D-ND	-3.71	1.32	1.37
26	b	602	CLA	C4D-ND	-3.71	1.32	1.37
25	G	609	CHL	CHD-C4C	3.70	1.47	1.39
25	g	609	CHL	CHD-C4C	3.70	1.47	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	y	614	CLA	C4D-ND	-3.70	1.32	1.37
25	2	609	CHL	CHD-C4C	3.70	1.47	1.39
26	c	513	CLA	C4D-ND	-3.70	1.32	1.37
26	n	614	CLA	C1D-ND	3.70	1.42	1.37
26	s	603	CLA	C1D-ND	3.70	1.42	1.37
26	c	506	CLA	CMB-C2B	-3.70	1.44	1.51
25	r	607	CHL	OBD-CAD	3.69	1.28	1.22
26	C	508	CLA	CMB-C2B	-3.69	1.44	1.51
25	y	608	CHL	CHD-C1D	3.68	1.45	1.38
26	G	612	CLA	C1D-ND	3.68	1.42	1.37
26	g	612	CLA	C1D-ND	3.68	1.42	1.37
26	C	511	CLA	C4D-ND	-3.68	1.32	1.37
26	C	506	CLA	CMB-C2B	-3.68	1.44	1.51
25	R	607	CHL	OBD-CAD	3.68	1.28	1.22
26	B	607	CLA	C4D-ND	-3.68	1.32	1.37
26	6	612	CLA	C1D-ND	3.68	1.42	1.37
26	Y	614	CLA	C4D-ND	-3.68	1.32	1.37
25	R	607	CHL	CHD-C1D	3.67	1.45	1.38
25	3	605	CHL	CHD-C4C	3.67	1.47	1.39
25	7	605	CHL	CHD-C4C	3.67	1.47	1.39
25	5	607	CHL	CHD-C4C	3.67	1.47	1.39
26	S	603	CLA	C1D-ND	3.67	1.42	1.37
25	1	607	CHL	CHD-C4C	3.67	1.47	1.39
26	N	614	CLA	C1D-ND	3.67	1.42	1.37
26	6	614	CLA	C1D-ND	3.66	1.42	1.37
26	B	605	CLA	CMB-C2B	-3.66	1.44	1.51
25	Y	601	CHL	C3B-C2B	3.66	1.45	1.40
25	y	601	CHL	C3B-C2B	3.66	1.45	1.40
26	1	614	CLA	C1D-ND	3.66	1.42	1.37
26	b	605	CLA	CMB-C2B	-3.66	1.44	1.51
25	1	608	CHL	CHD-C1D	3.65	1.45	1.38
25	6	606	CHL	CHD-C4C	3.65	1.47	1.39
25	2	609	CHL	OBD-CAD	3.65	1.28	1.22
25	6	609	CHL	OBD-CAD	3.65	1.28	1.22
26	R	610	CLA	C4D-ND	-3.65	1.32	1.37
26	r	610	CLA	C4D-ND	-3.65	1.32	1.37
26	G	613	CLA	C4D-ND	-3.64	1.32	1.37
26	g	613	CLA	C4D-ND	-3.64	1.32	1.37
26	c	511	CLA	C4D-ND	-3.64	1.32	1.37
25	r	607	CHL	CHD-C1D	3.64	1.45	1.38
25	2	606	CHL	CHD-C4C	3.64	1.47	1.39
26	B	612	CLA	CMC-C2C	-3.64	1.43	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	612	CLA	CMC-C2C	-3.64	1.43	1.50
25	2	605	CHL	CHD-C4C	3.63	1.47	1.39
26	c	501	CLA	C4D-ND	-3.63	1.32	1.37
26	C	501	CLA	C4D-ND	-3.63	1.32	1.37
26	y	610	CLA	C4D-ND	-3.63	1.32	1.37
26	R	609	CLA	C1D-ND	3.63	1.42	1.37
25	6	605	CHL	CHD-C4C	3.62	1.47	1.39
26	R	616	CLA	C1D-ND	3.62	1.42	1.37
26	r	616	CLA	C1D-ND	3.62	1.42	1.37
26	5	614	CLA	C1D-ND	3.61	1.42	1.37
25	2	605	CHL	OBD-CAD	3.61	1.28	1.22
26	Y	610	CLA	C4D-ND	-3.61	1.32	1.37
25	5	608	CHL	CHD-C1D	3.61	1.45	1.38
25	4	601	CHL	OBD-CAD	3.60	1.28	1.22
25	6	606	CHL	OBD-CAD	3.60	1.28	1.22
26	8	610	CLA	C1D-ND	3.60	1.42	1.37
25	R	614	CHL	CHD-C4C	3.60	1.47	1.39
25	8	601	CHL	OBD-CAD	3.60	1.28	1.22
25	G	607	CHL	CHD-C4C	3.60	1.47	1.39
25	3	605	CHL	OBD-CAD	3.60	1.28	1.22
25	G	605	CHL	CHD-C4C	3.60	1.47	1.39
25	g	605	CHL	CHD-C4C	3.60	1.47	1.39
25	S	607	CHL	OBD-CAD	3.60	1.28	1.22
25	N	609	CHL	CHD-C4C	3.60	1.47	1.39
25	n	609	CHL	CHD-C4C	3.60	1.47	1.39
25	Y	609	CHL	CHD-C4C	3.59	1.47	1.39
25	S	606	CHL	OBD-CAD	3.59	1.28	1.22
25	s	606	CHL	OBD-CAD	3.59	1.28	1.22
25	N	609	CHL	C3B-C2B	3.59	1.45	1.40
25	s	607	CHL	OBD-CAD	3.59	1.28	1.22
26	G	611	CLA	CMB-C2B	-3.59	1.44	1.51
25	g	607	CHL	CHD-C4C	3.59	1.47	1.39
26	R	604	CLA	C4D-ND	-3.59	1.32	1.37
25	y	609	CHL	CHD-C4C	3.58	1.47	1.39
25	r	614	CHL	CHD-C4C	3.58	1.47	1.39
26	C	509	CLA	C4D-ND	-3.57	1.32	1.37
26	b	609	CLA	C4D-ND	-3.57	1.32	1.37
26	S	610	CLA	C1D-ND	3.57	1.42	1.37
39	B	626	DGD	O2G-C2G	-3.57	1.37	1.46
39	b	626	DGD	O2G-C2G	-3.57	1.37	1.46
26	c	509	CLA	C4D-ND	-3.57	1.32	1.37
25	4	606	CHL	OBD-CAD	3.57	1.28	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	606	CHL	OBD-CAD	3.57	1.28	1.22
25	4	607	CHL	OBD-CAD	3.57	1.28	1.22
26	r	609	CLA	C1D-ND	3.57	1.42	1.37
25	n	609	CHL	C3B-C2B	3.57	1.45	1.40
26	s	610	CLA	C1D-ND	3.56	1.42	1.37
25	6	605	CHL	OBD-CAD	3.56	1.28	1.22
26	3	604	CLA	C1D-ND	3.56	1.42	1.37
25	2	606	CHL	OBD-CAD	3.56	1.28	1.22
26	8	612	CLA	C1D-ND	3.56	1.42	1.37
25	s	607	CHL	CHD-C4C	3.56	1.47	1.39
26	C	512	CLA	C4D-ND	-3.56	1.32	1.37
26	c	512	CLA	C4D-ND	-3.56	1.32	1.37
26	g	611	CLA	CMB-C2B	-3.56	1.44	1.51
25	5	605	CHL	CHD-C4C	3.55	1.47	1.39
26	r	604	CLA	C4D-ND	-3.55	1.32	1.37
25	7	607	CHL	OBD-CAD	3.55	1.28	1.22
25	G	607	CHL	OBD-CAD	3.55	1.28	1.22
25	8	607	CHL	OBD-CAD	3.55	1.28	1.22
26	B	613	CLA	C4D-ND	-3.55	1.32	1.37
26	7	613	CLA	C4D-ND	-3.55	1.32	1.37
26	7	604	CLA	C1D-ND	3.55	1.42	1.37
26	r	611	CLA	C1D-ND	3.55	1.42	1.37
25	1	605	CHL	CHD-C4C	3.54	1.47	1.39
26	3	613	CLA	C4D-ND	-3.54	1.32	1.37
25	G	608	CHL	CHD-C4C	3.54	1.47	1.39
26	n	604	CLA	C4D-ND	-3.54	1.32	1.37
25	1	606	CHL	CHD-C4C	3.54	1.47	1.39
25	5	606	CHL	CHD-C4C	3.54	1.47	1.39
25	7	605	CHL	OBD-CAD	3.54	1.28	1.22
26	B	609	CLA	C4D-ND	-3.54	1.32	1.37
25	g	607	CHL	OBD-CAD	3.54	1.28	1.22
26	7	611	CLA	C4D-ND	-3.54	1.32	1.37
26	3	611	CLA	C4D-ND	-3.54	1.32	1.37
25	g	608	CHL	CHD-C4C	3.53	1.47	1.39
26	B	608	CLA	CMB-C2B	-3.53	1.44	1.51
26	4	610	CLA	C1D-ND	3.53	1.42	1.37
26	N	604	CLA	C4D-ND	-3.53	1.32	1.37
26	d	402	CLA	CMD-C2D	-3.53	1.43	1.50
26	n	611	CLA	C1D-ND	3.53	1.42	1.37
25	n	606	CHL	CHD-C4C	3.53	1.47	1.39
25	3	608	CHL	CHD-C1D	3.53	1.45	1.38
25	7	608	CHL	CHD-C1D	3.53	1.45	1.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	507	CLA	C1D-ND	3.52	1.42	1.37
26	c	507	CLA	C1D-ND	3.52	1.42	1.37
26	G	603	CLA	C4D-ND	-3.52	1.32	1.37
26	g	603	CLA	C4D-ND	-3.52	1.32	1.37
26	n	603	CLA	C4D-ND	-3.52	1.32	1.37
26	y	604	CLA	C4D-ND	-3.52	1.32	1.37
25	3	607	CHL	OBD-CAD	3.52	1.28	1.22
26	3	610	CLA	C1D-ND	3.52	1.42	1.37
26	7	610	CLA	C1D-ND	3.52	1.42	1.37
26	4	604	CLA	C1D-ND	3.52	1.42	1.37
26	Y	604	CLA	C4D-ND	-3.52	1.32	1.37
26	b	608	CLA	CMB-C2B	-3.52	1.44	1.51
26	R	612	CLA	C1D-ND	3.52	1.42	1.37
25	S	607	CHL	CHD-C4C	3.51	1.47	1.39
25	7	606	CHL	CHD-C4C	3.51	1.47	1.39
26	1	613	CLA	C4D-ND	-3.51	1.32	1.37
26	5	613	CLA	C4D-ND	-3.51	1.32	1.37
25	2	607	CHL	OBD-CAD	3.51	1.28	1.22
26	D	402	CLA	CMD-C2D	-3.51	1.43	1.50
25	3	609	CHL	OBD-CAD	3.51	1.28	1.22
25	7	609	CHL	OBD-CAD	3.51	1.28	1.22
25	N	606	CHL	CHD-C4C	3.51	1.47	1.39
26	2	602	CLA	C4D-ND	-3.51	1.32	1.37
26	R	611	CLA	C1D-ND	3.50	1.42	1.37
26	4	612	CLA	C1D-ND	3.50	1.42	1.37
25	3	606	CHL	CHD-C4C	3.50	1.47	1.39
26	N	603	CLA	C4D-ND	-3.50	1.32	1.37
26	6	602	CLA	C4D-ND	-3.50	1.32	1.37
25	R	606	CHL	CHD-C4C	3.49	1.47	1.39
25	r	606	CHL	CHD-C4C	3.49	1.47	1.39
25	N	607	CHL	CHD-C1D	3.49	1.45	1.38
26	4	604	CLA	C4D-ND	-3.49	1.32	1.37
26	8	604	CLA	C4D-ND	-3.49	1.32	1.37
26	C	505	CLA	CMD-C2D	-3.48	1.43	1.50
26	B	617	CLA	CMC-C2C	-3.48	1.43	1.50
26	b	617	CLA	CMC-C2C	-3.48	1.43	1.50
26	c	505	CLA	CMD-C2D	-3.48	1.43	1.50
26	y	611	CLA	C4D-ND	-3.47	1.32	1.37
26	8	604	CLA	C1D-ND	3.47	1.42	1.37
26	3	602	CLA	C1D-ND	3.47	1.42	1.37
25	s	606	CHL	CHD-C4C	3.47	1.47	1.39
26	R	612	CLA	C4D-ND	-3.47	1.32	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	r	612	CLA	C4D-ND	-3.47	1.32	1.37
26	R	613	CLA	C1D-ND	3.47	1.42	1.37
26	r	613	CLA	C1D-ND	3.47	1.42	1.37
25	2	608	CHL	CHD-C4C	3.47	1.47	1.39
25	6	607	CHL	OBD-CAD	3.46	1.28	1.22
26	N	611	CLA	C1D-ND	3.46	1.42	1.37
26	b	613	CLA	C4D-ND	-3.46	1.32	1.37
26	5	604	CLA	C4D-ND	-3.46	1.32	1.37
26	s	604	CLA	C4D-ND	-3.46	1.32	1.37
26	3	602	CLA	C4D-ND	-3.46	1.32	1.37
26	7	614	CLA	C4D-ND	-3.46	1.32	1.37
25	6	608	CHL	CHD-C4C	3.46	1.47	1.39
25	5	607	CHL	OBD-CAD	3.46	1.28	1.22
26	B	606	CLA	C1D-ND	3.46	1.42	1.37
26	b	606	CLA	C1D-ND	3.46	1.42	1.37
25	y	607	CHL	CHD-C1D	3.46	1.45	1.38
26	4	602	CLA	C1D-ND	3.46	1.42	1.37
26	8	602	CLA	C1D-ND	3.46	1.42	1.37
25	1	605	CHL	OBD-CAD	3.46	1.28	1.22
25	n	607	CHL	CHD-C1D	3.45	1.45	1.38
26	6	611	CLA	C1D-ND	3.45	1.42	1.37
25	1	607	CHL	OBD-CAD	3.45	1.28	1.22
25	S	606	CHL	CHD-C4C	3.45	1.47	1.39
25	Y	607	CHL	CHD-C1D	3.45	1.45	1.38
25	r	606	CHL	OBD-CAD	3.45	1.28	1.22
26	7	602	CLA	C1D-ND	3.44	1.42	1.37
26	r	612	CLA	C1D-ND	3.44	1.42	1.37
30	d	409	LHG	O7-C5	-3.44	1.38	1.46
26	2	604	CLA	C1D-ND	3.44	1.42	1.37
25	5	605	CHL	OBD-CAD	3.44	1.28	1.22
26	3	613	CLA	C1D-ND	3.44	1.42	1.37
26	7	613	CLA	C1D-ND	3.44	1.42	1.37
25	7	608	CHL	CHD-C4C	3.44	1.47	1.39
26	Y	611	CLA	C4D-ND	-3.44	1.33	1.37
25	Y	605	CHL	CHD-C1D	3.44	1.45	1.38
25	y	605	CHL	CHD-C1D	3.44	1.45	1.38
26	S	610	CLA	C4D-ND	-3.43	1.33	1.37
26	s	610	CLA	C4D-ND	-3.43	1.33	1.37
30	D	409	LHG	O7-C5	-3.43	1.38	1.46
25	3	608	CHL	CHD-C4C	3.43	1.47	1.39
26	3	612	CLA	C4D-ND	-3.43	1.33	1.37
26	S	604	CLA	C4D-ND	-3.43	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	608	CHL	CHD-C1D	3.43	1.45	1.38
25	8	608	CHL	CHD-C1D	3.43	1.45	1.38
26	g	611	CLA	C1D-ND	3.43	1.42	1.37
26	1	602	CLA	C4D-ND	-3.42	1.33	1.37
26	5	602	CLA	C4D-ND	-3.42	1.33	1.37
26	7	602	CLA	C4D-ND	-3.42	1.33	1.37
26	b	602	CLA	C1D-ND	3.42	1.42	1.37
26	7	614	CLA	C1D-ND	3.42	1.42	1.37
26	3	614	CLA	C4D-ND	-3.42	1.33	1.37
26	1	604	CLA	C4D-ND	-3.42	1.33	1.37
25	1	606	CHL	OBD-CAD	3.42	1.28	1.22
25	5	606	CHL	OBD-CAD	3.42	1.28	1.22
26	5	604	CLA	CMB-C2B	-3.41	1.44	1.51
25	R	606	CHL	OBD-CAD	3.41	1.28	1.22
26	5	611	CLA	C1D-ND	3.41	1.42	1.37
26	6	604	CLA	C1D-ND	3.41	1.42	1.37
25	N	607	CHL	OBD-CAD	3.41	1.28	1.22
25	n	607	CHL	OBD-CAD	3.41	1.28	1.22
26	1	604	CLA	CMB-C2B	-3.40	1.44	1.51
26	6	610	CLA	C1D-ND	3.40	1.42	1.37
26	S	614	CLA	C4D-ND	-3.40	1.33	1.37
26	s	614	CLA	C4D-ND	-3.40	1.33	1.37
26	b	615	CLA	C4D-ND	-3.40	1.33	1.37
26	7	612	CLA	C4D-ND	-3.40	1.33	1.37
39	c	520	DGD	O5D-C6D	-3.40	1.37	1.43
26	1	611	CLA	C1D-ND	3.39	1.42	1.37
25	g	609	CHL	OBD-CAD	3.39	1.28	1.22
26	B	612	CLA	CMB-C2B	-3.39	1.44	1.51
26	b	612	CLA	CMB-C2B	-3.39	1.44	1.51
26	2	611	CLA	C1D-ND	3.38	1.41	1.37
26	B	602	CLA	C1D-ND	3.38	1.41	1.37
26	D	402	CLA	CMB-C2B	-3.38	1.44	1.51
26	d	402	CLA	CMB-C2B	-3.38	1.44	1.51
25	n	609	CHL	OBD-CAD	3.38	1.28	1.22
25	n	608	CHL	CHD-C4C	3.38	1.46	1.39
25	1	609	CHL	OBD-CAD	3.38	1.28	1.22
25	5	609	CHL	OBD-CAD	3.38	1.28	1.22
26	3	614	CLA	C1D-ND	3.38	1.41	1.37
25	G	609	CHL	OBD-CAD	3.38	1.28	1.22
25	N	608	CHL	CHD-C4C	3.38	1.46	1.39
26	B	615	CLA	C4D-ND	-3.37	1.33	1.37
26	G	611	CLA	C1D-ND	3.37	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	5	613	CLA	C1D-ND	3.37	1.41	1.37
39	C	520	DGD	O5D-C6D	-3.37	1.37	1.43
25	8	609	CHL	OBD-CAD	3.37	1.28	1.22
26	B	616	CLA	C4D-ND	-3.36	1.33	1.37
26	b	616	CLA	C4D-ND	-3.36	1.33	1.37
26	n	613	CLA	C4D-ND	-3.36	1.33	1.37
26	G	604	CLA	C4D-ND	-3.36	1.33	1.37
25	N	609	CHL	OBD-CAD	3.35	1.28	1.22
26	1	611	CLA	C4D-ND	-3.35	1.33	1.37
26	5	611	CLA	C4D-ND	-3.35	1.33	1.37
26	3	611	CLA	CMB-C2B	-3.34	1.44	1.51
26	7	611	CLA	CMB-C2B	-3.34	1.44	1.51
26	3	604	CLA	C4D-ND	-3.34	1.33	1.37
26	1	613	CLA	C1D-ND	3.34	1.41	1.37
26	N	613	CLA	C4D-ND	-3.34	1.33	1.37
25	1	601	CHL	OBD-CAD	3.34	1.28	1.22
25	4	609	CHL	OBD-CAD	3.33	1.28	1.22
26	s	604	CLA	C1D-ND	3.33	1.41	1.37
30	d	408	LHG	O7-C5	-3.33	1.38	1.46
25	S	608	CHL	OBD-CAD	3.33	1.28	1.22
25	s	608	CHL	OBD-CAD	3.33	1.28	1.22
25	8	608	CHL	CHD-C4C	3.33	1.46	1.39
26	S	609	CLA	C4D-ND	-3.33	1.33	1.37
26	s	611	CLA	C4D-ND	-3.32	1.33	1.37
25	Y	608	CHL	CHD-C4C	3.32	1.46	1.39
26	S	602	CLA	C4D-ND	-3.32	1.33	1.37
26	R	613	CLA	C4D-ND	-3.32	1.33	1.37
26	r	613	CLA	C4D-ND	-3.32	1.33	1.37
25	y	608	CHL	CHD-C4C	3.31	1.46	1.39
26	2	610	CLA	C1D-ND	3.31	1.41	1.37
26	s	602	CLA	C4D-ND	-3.31	1.33	1.37
26	S	604	CLA	C1D-ND	3.30	1.41	1.37
25	r	607	CHL	CHD-C4C	3.30	1.46	1.39
26	7	604	CLA	C4D-ND	-3.30	1.33	1.37
25	5	608	CHL	CHD-C4C	3.30	1.46	1.39
26	R	609	CLA	C4D-ND	-3.30	1.33	1.37
30	D	408	LHG	O7-C5	-3.30	1.38	1.46
26	s	609	CLA	C4D-ND	-3.30	1.33	1.37
25	4	608	CHL	CHD-C4C	3.30	1.46	1.39
25	n	605	CHL	CHD-C4C	3.30	1.46	1.39
25	R	607	CHL	CHD-C4C	3.30	1.46	1.39
26	n	603	CLA	C3B-C2B	-3.29	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	607	CHL	OBD-CAD	3.29	1.28	1.22
26	g	604	CLA	C4D-ND	-3.29	1.33	1.37
26	N	603	CLA	C3B-C2B	-3.29	1.35	1.40
26	S	611	CLA	C4D-ND	-3.29	1.33	1.37
25	y	605	CHL	OBD-CAD	3.29	1.28	1.22
26	Y	603	CLA	C3B-C2B	-3.28	1.35	1.40
26	N	610	CLA	C4D-ND	-3.28	1.33	1.37
26	n	610	CLA	C4D-ND	-3.28	1.33	1.37
25	5	601	CHL	OBD-CAD	3.28	1.28	1.22
25	1	608	CHL	CHD-C4C	3.28	1.46	1.39
26	a	407	CLA	C1D-ND	3.28	1.41	1.37
26	2	602	CLA	C1D-ND	3.28	1.41	1.37
26	6	602	CLA	C1D-ND	3.28	1.41	1.37
25	S	608	CHL	CHD-C4C	3.28	1.46	1.39
25	s	608	CHL	CHD-C4C	3.28	1.46	1.39
26	2	611	CLA	C4D-ND	-3.28	1.33	1.37
26	6	611	CLA	C4D-ND	-3.28	1.33	1.37
25	N	605	CHL	CHD-C4C	3.27	1.46	1.39
38	D	405	PL9	C52-C5	-3.27	1.43	1.50
38	d	405	PL9	C52-C5	-3.27	1.43	1.50
26	S	612	CLA	C1D-ND	3.27	1.41	1.37
26	r	609	CLA	C4D-ND	-3.27	1.33	1.37
25	Y	605	CHL	OBD-CAD	3.27	1.28	1.22
25	Y	607	CHL	OBD-CAD	3.27	1.28	1.22
26	4	602	CLA	C4D-ND	-3.26	1.33	1.37
26	8	602	CLA	C4D-ND	-3.26	1.33	1.37
26	A	407	CLA	C1D-ND	3.26	1.41	1.37
26	G	604	CLA	C1D-ND	3.26	1.41	1.37
26	g	604	CLA	C1D-ND	3.26	1.41	1.37
26	S	603	CLA	C4D-ND	-3.26	1.33	1.37
26	s	612	CLA	C1D-ND	3.25	1.41	1.37
26	n	603	CLA	C1D-ND	3.25	1.41	1.37
26	n	610	CLA	C1D-ND	3.25	1.41	1.37
26	6	613	CLA	C4D-ND	-3.24	1.33	1.37
26	s	603	CLA	C4D-ND	-3.24	1.33	1.37
26	y	603	CLA	C3B-C2B	-3.24	1.35	1.40
26	2	603	CLA	C1D-ND	3.24	1.41	1.37
26	6	603	CLA	C1D-ND	3.24	1.41	1.37
26	N	603	CLA	C1D-ND	3.23	1.41	1.37
26	2	613	CLA	C4D-ND	-3.23	1.33	1.37
26	3	611	CLA	C3B-C2B	-3.22	1.35	1.40
26	7	611	CLA	C3B-C2B	-3.22	1.35	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
36	b	623	SQD	O48-C23	3.22	1.42	1.33
26	1	610	CLA	C4D-ND	-3.21	1.33	1.37
26	1	614	CLA	C4D-ND	-3.21	1.33	1.37
26	4	611	CLA	C4D-ND	-3.21	1.33	1.37
36	B	623	SQD	O48-C23	3.21	1.42	1.33
41	F	101	HEM	CAB-C3B	3.21	1.56	1.47
26	2	610	CLA	C4D-ND	-3.21	1.33	1.37
26	5	614	CLA	C4D-ND	-3.21	1.33	1.37
26	6	610	CLA	C4D-ND	-3.21	1.33	1.37
26	s	613	CLA	C1D-ND	3.20	1.41	1.37
41	f	101	HEM	CAB-C3B	3.20	1.56	1.47
26	C	501	CLA	C1D-ND	3.20	1.41	1.37
26	S	613	CLA	C1D-ND	3.20	1.41	1.37
26	7	611	CLA	C1D-ND	3.20	1.41	1.37
26	Y	602	CLA	C1D-ND	3.19	1.41	1.37
26	y	602	CLA	C1D-ND	3.19	1.41	1.37
26	G	611	CLA	CHC-C1C	3.19	1.43	1.35
26	g	611	CLA	CHC-C1C	3.19	1.43	1.35
26	g	602	CLA	C1D-ND	3.19	1.41	1.37
26	S	614	CLA	C1D-ND	3.19	1.41	1.37
26	s	614	CLA	C1D-ND	3.19	1.41	1.37
26	7	610	CLA	C4D-ND	-3.19	1.33	1.37
38	D	405	PL9	C53-C6	-3.18	1.44	1.50
38	d	405	PL9	C53-C6	-3.18	1.44	1.50
26	5	610	CLA	C4D-ND	-3.18	1.33	1.37
26	N	611	CLA	C4D-ND	-3.18	1.33	1.37
26	R	601	CLA	C4D-ND	-3.18	1.33	1.37
26	N	610	CLA	C1D-ND	3.18	1.41	1.37
26	r	601	CLA	C4D-ND	-3.17	1.33	1.37
26	8	611	CLA	C4D-ND	-3.17	1.33	1.37
25	3	607	CHL	MG-NA	-3.17	1.98	2.06
29	1	1623	NEX	C7-C8	-3.17	1.26	1.32
26	N	602	CLA	C1D-ND	3.17	1.41	1.37
26	S	613	CLA	C4D-ND	-3.17	1.33	1.37
26	A	406	CLA	C1D-ND	3.17	1.41	1.37
26	a	406	CLA	C1D-ND	3.17	1.41	1.37
26	c	501	CLA	C1D-ND	3.17	1.41	1.37
26	B	603	CLA	C1D-ND	3.16	1.41	1.37
26	s	602	CLA	CHC-C1C	3.16	1.43	1.35
26	S	602	CLA	CHC-C1C	3.16	1.43	1.35
26	3	611	CLA	C1D-ND	3.16	1.41	1.37
26	b	603	CLA	C1D-ND	3.16	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	n	606	CHL	OBD-CAD	3.15	1.27	1.22
26	3	610	CLA	C4D-ND	-3.15	1.33	1.37
26	s	613	CLA	C4D-ND	-3.15	1.33	1.37
26	G	602	CLA	C1D-ND	3.15	1.41	1.37
25	Y	609	CHL	OBD-CAD	3.15	1.27	1.22
26	r	610	CLA	C1D-ND	3.15	1.41	1.37
26	5	603	CLA	C4D-ND	-3.15	1.33	1.37
25	7	606	CHL	OBD-CAD	3.15	1.27	1.22
26	S	611	CLA	C1D-ND	3.15	1.41	1.37
26	s	611	CLA	C1D-ND	3.15	1.41	1.37
26	8	612	CLA	C4D-ND	-3.15	1.33	1.37
25	y	609	CHL	OBD-CAD	3.14	1.27	1.22
26	6	614	CLA	C4D-ND	-3.14	1.33	1.37
26	1	603	CLA	C4D-ND	-3.13	1.33	1.37
29	5	1623	NEX	C7-C8	-3.13	1.26	1.32
25	7	607	CHL	MG-NA	-3.13	1.98	2.06
26	B	605	CLA	MG-ND	-3.13	1.99	2.05
26	b	605	CLA	MG-ND	-3.13	1.99	2.05
26	n	611	CLA	C4D-ND	-3.13	1.33	1.37
26	4	612	CLA	C4D-ND	-3.13	1.33	1.37
26	2	603	CLA	C4D-ND	-3.12	1.33	1.37
26	6	603	CLA	C4D-ND	-3.12	1.33	1.37
26	2	614	CLA	C4D-ND	-3.12	1.33	1.37
26	1	610	CLA	C1D-ND	3.12	1.41	1.37
26	5	610	CLA	C1D-ND	3.12	1.41	1.37
25	N	606	CHL	OBD-CAD	3.12	1.27	1.22
26	Y	612	CLA	C1D-ND	3.12	1.41	1.37
26	y	612	CLA	C1D-ND	3.12	1.41	1.37
26	3	603	CLA	C4D-ND	-3.12	1.33	1.37
25	3	606	CHL	OBD-CAD	3.12	1.27	1.22
29	R	623	NEX	C7-C8	-3.12	1.26	1.32
29	r	623	NEX	C7-C8	-3.12	1.26	1.32
26	C	502	CLA	CMB-C2B	-3.12	1.45	1.51
26	c	502	CLA	CMB-C2B	-3.12	1.45	1.51
26	g	613	CLA	CHC-C1C	3.12	1.43	1.35
26	R	610	CLA	C1D-ND	3.12	1.41	1.37
26	7	603	CLA	C4D-ND	-3.12	1.33	1.37
26	4	603	CLA	C4D-ND	-3.11	1.33	1.37
26	r	603	CLA	C4D-ND	-3.11	1.33	1.37
26	a	405	CLA	CMD-C2D	-3.10	1.44	1.50
26	n	602	CLA	C1D-ND	3.10	1.41	1.37
25	2	601	CHL	OBD-CAD	3.10	1.27	1.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	6	601	CHL	OBD-CAD	3.10	1.27	1.22
25	7	601	CHL	OBD-CAD	3.10	1.27	1.22
26	G	613	CLA	CHC-C1C	3.10	1.42	1.35
26	G	611	CLA	C4D-ND	-3.10	1.33	1.37
26	g	611	CLA	C4D-ND	-3.10	1.33	1.37
25	y	606	CHL	CHD-C1D	3.10	1.44	1.38
25	3	601	CHL	OBD-CAD	3.10	1.27	1.22
26	S	612	CLA	C4D-ND	-3.09	1.33	1.37
36	B	621	SQD	O47-C7	3.09	1.43	1.34
26	R	603	CLA	C4D-ND	-3.09	1.33	1.37
26	C	509	CLA	CMB-C2B	-3.09	1.45	1.51
26	c	509	CLA	CMB-C2B	-3.09	1.45	1.51
26	6	613	CLA	C1D-ND	3.09	1.41	1.37
26	8	603	CLA	C4D-ND	-3.09	1.33	1.37
26	B	607	CLA	CMC-C2C	-3.09	1.44	1.50
26	Y	603	CLA	C1D-ND	3.09	1.41	1.37
26	A	405	CLA	CMD-C2D	-3.08	1.44	1.50
26	c	508	CLA	C1D-ND	3.08	1.41	1.37
36	B	623	SQD	O47-C7	3.08	1.43	1.34
26	b	607	CLA	CMC-C2C	-3.08	1.44	1.50
26	s	612	CLA	C4D-ND	-3.08	1.33	1.37
26	2	613	CLA	C1D-ND	3.08	1.41	1.37
25	y	605	CHL	CHD-C4C	3.07	1.46	1.39
36	b	621	SQD	O47-C7	3.07	1.43	1.34
26	R	604	CLA	C1D-ND	3.07	1.41	1.37
26	r	604	CLA	C1D-ND	3.07	1.41	1.37
36	b	623	SQD	O47-C7	3.07	1.43	1.34
25	Y	606	CHL	CHD-C1D	3.07	1.44	1.38
26	y	614	CLA	C1D-ND	3.06	1.41	1.37
26	y	603	CLA	C1D-ND	3.06	1.41	1.37
26	5	602	CLA	C1D-ND	3.06	1.41	1.37
26	r	616	CLA	C4D-ND	-3.06	1.33	1.37
26	y	604	CLA	C1D-ND	3.06	1.41	1.37
25	Y	605	CHL	CHD-C4C	3.06	1.46	1.39
26	G	614	CLA	C4D-ND	-3.06	1.33	1.37
29	y	1623	NEX	C7-C8	-3.06	1.26	1.32
26	G	613	CLA	C1D-ND	3.06	1.41	1.37
25	1	608	CHL	OBD-CAD	3.05	1.27	1.22
25	5	608	CHL	OBD-CAD	3.05	1.27	1.22
26	r	602	CLA	CHC-C1C	3.05	1.42	1.35
26	g	613	CLA	C1D-ND	3.05	1.41	1.37
26	R	602	CLA	C1D-ND	3.05	1.41	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	r	602	CLA	C1D-ND	3.05	1.41	1.37
26	r	601	CLA	C1D-ND	3.05	1.41	1.37
39	c	518	DGD	O1G-C1G	-3.04	1.38	1.45
25	Y	601	CHL	MG-NA	-3.04	1.99	2.06
25	y	601	CHL	MG-NA	-3.04	1.99	2.06
26	l	604	CLA	C1D-ND	3.04	1.41	1.37
26	c	511	CLA	C1D-ND	3.04	1.41	1.37
26	5	610	CLA	C3B-C2B	-3.04	1.36	1.40
26	B	606	CLA	CMC-C2C	-3.04	1.44	1.50
26	b	606	CLA	CMC-C2C	-3.04	1.44	1.50
26	R	601	CLA	C1D-ND	3.04	1.41	1.37
26	G	603	CLA	C1D-ND	3.04	1.41	1.37
25	2	608	CHL	OBD-CAD	3.03	1.27	1.22
25	6	608	CHL	OBD-CAD	3.03	1.27	1.22
26	C	511	CLA	C1D-ND	3.03	1.41	1.37
26	g	603	CLA	C1D-ND	3.03	1.41	1.37
26	r	612	CLA	CHC-C1C	3.03	1.42	1.35
26	g	614	CLA	C4D-ND	-3.03	1.33	1.37
26	N	614	CLA	C4D-ND	-3.03	1.33	1.37
26	5	604	CLA	C1D-ND	3.03	1.41	1.37
39	C	518	DGD	O1G-C1G	-3.03	1.38	1.45
26	Y	614	CLA	C1D-ND	3.03	1.41	1.37
26	s	604	CLA	CMB-C2B	-3.02	1.45	1.51
26	l	610	CLA	C3B-C2B	-3.02	1.36	1.40
26	B	613	CLA	CMB-C2B	-3.02	1.45	1.51
29	6	1623	NEX	C7-C8	-3.02	1.26	1.32
26	R	616	CLA	C4D-ND	-3.02	1.33	1.37
26	S	604	CLA	CMB-C2B	-3.02	1.45	1.51
26	Y	604	CLA	C1D-ND	3.02	1.41	1.37
26	n	614	CLA	C4D-ND	-3.02	1.33	1.37
29	Y	1623	NEX	C7-C8	-3.02	1.26	1.32
26	5	612	CLA	C3B-C2B	-3.02	1.36	1.40
26	b	613	CLA	CMB-C2B	-3.02	1.45	1.51
26	G	603	CLA	C3B-C2B	-3.02	1.36	1.40
26	g	603	CLA	C3B-C2B	-3.02	1.36	1.40
26	r	610	CLA	C3B-C2B	-3.02	1.36	1.40
26	R	602	CLA	CHC-C1C	3.02	1.42	1.35
26	l	602	CLA	C1D-ND	3.02	1.41	1.37
26	C	508	CLA	C1D-ND	3.02	1.41	1.37
26	2	604	CLA	C4D-ND	-3.01	1.33	1.37
26	B	616	CLA	C3B-C2B	-3.01	1.36	1.40
26	R	610	CLA	C3B-C2B	-3.01	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	505	CLA	MG-ND	-3.01	1.99	2.05
26	7	603	CLA	C1D-ND	3.01	1.41	1.37
26	R	612	CLA	CHC-C1C	3.01	1.42	1.35
39	c	520	DGD	O2G-C2G	-3.01	1.39	1.46
26	b	607	CLA	C1D-ND	3.01	1.41	1.37
29	2	1623	NEX	C7-C8	-3.01	1.27	1.32
26	R	610	CLA	CHC-C1C	3.00	1.42	1.35
26	r	616	CLA	CMB-C2B	-3.00	1.45	1.51
35	A	409	PHO	CAC-C3C	-3.00	1.46	1.52
35	a	409	PHO	CAC-C3C	-3.00	1.46	1.52
26	B	614	CLA	CMB-C2B	-3.00	1.45	1.51
26	n	613	CLA	C1D-ND	2.99	1.41	1.37
26	b	616	CLA	C3B-C2B	-2.99	1.36	1.40
26	C	505	CLA	MG-ND	-2.99	1.99	2.05
26	r	610	CLA	CHC-C1C	2.99	1.42	1.35
26	3	603	CLA	C1D-ND	2.99	1.41	1.37
26	6	604	CLA	C4D-ND	-2.98	1.33	1.37
26	n	604	CLA	C1D-ND	2.98	1.41	1.37
26	3	612	CLA	C1D-ND	2.98	1.41	1.37
26	3	610	CLA	CHC-C1C	2.98	1.42	1.35
26	D	403	CLA	C1D-ND	2.98	1.41	1.37
26	d	403	CLA	C1D-ND	2.98	1.41	1.37
26	1	612	CLA	C3B-C2B	-2.98	1.36	1.40
39	C	520	DGD	O2G-C2G	-2.98	1.39	1.46
26	S	610	CLA	CHC-C1C	2.98	1.42	1.35
26	7	612	CLA	C1D-ND	2.97	1.41	1.37
26	s	610	CLA	CHC-C1C	2.97	1.42	1.35
26	1	603	CLA	C1D-ND	2.97	1.41	1.37
26	5	603	CLA	C1D-ND	2.97	1.41	1.37
26	B	607	CLA	C1D-ND	2.97	1.41	1.37
25	S	601	CHL	OBD-CAD	2.97	1.27	1.22
25	s	601	CHL	OBD-CAD	2.97	1.27	1.22
26	B	606	CLA	CMB-C2B	-2.96	1.45	1.51
26	b	606	CLA	CMB-C2B	-2.96	1.45	1.51
26	B	617	CLA	C1D-ND	2.96	1.41	1.37
25	R	608	CHL	CHD-C4C	2.96	1.46	1.39
26	7	610	CLA	CHC-C1C	2.96	1.42	1.35
25	r	608	CHL	CHD-C4C	2.96	1.46	1.39
26	N	604	CLA	C1D-ND	2.96	1.41	1.37
26	b	617	CLA	C1D-ND	2.96	1.41	1.37
26	b	614	CLA	CMB-C2B	-2.95	1.45	1.51
25	R	614	CHL	C1D-C2D	2.95	1.51	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	r	614	CHL	C1D-C2D	2.95	1.51	1.45
26	R	616	CLA	CMB-C2B	-2.95	1.45	1.51
26	C	509	CLA	CMD-C2D	-2.95	1.44	1.50
26	c	509	CLA	CMD-C2D	-2.95	1.44	1.50
25	Y	607	CHL	CHD-C4C	2.95	1.46	1.39
25	y	607	CHL	CHD-C4C	2.95	1.46	1.39
36	A	418	SQD	O47-C7	2.95	1.42	1.34
36	a	418	SQD	O47-C7	2.95	1.42	1.34
26	B	615	CLA	CMD-C2D	-2.95	1.44	1.50
26	b	615	CLA	CMD-C2D	-2.95	1.44	1.50
39	C	519	DGD	O1G-C1G	-2.95	1.38	1.45
39	c	519	DGD	O1G-C1G	-2.95	1.38	1.45
26	4	602	CLA	CHC-C1C	2.95	1.42	1.35
26	8	602	CLA	CHC-C1C	2.95	1.42	1.35
26	Y	610	CLA	C1D-ND	2.95	1.41	1.37
26	b	613	CLA	MG-ND	-2.95	1.99	2.05
25	n	607	CHL	CHD-C4C	2.94	1.46	1.39
37	D	411	LMG	O8-C9	-2.94	1.38	1.45
26	Y	610	CLA	CHC-C1C	2.94	1.42	1.35
26	8	610	CLA	CHC-C1C	2.94	1.42	1.35
25	N	607	CHL	CHD-C4C	2.94	1.45	1.39
26	4	610	CLA	CHC-C1C	2.94	1.42	1.35
26	B	613	CLA	MG-ND	-2.93	2.00	2.05
26	N	613	CLA	C1D-ND	2.93	1.41	1.37
25	g	601	CHL	MG-NA	-2.93	1.99	2.06
26	7	604	CLA	CHC-C1C	2.93	1.42	1.35
26	G	614	CLA	CHC-C1C	2.93	1.42	1.35
26	g	614	CLA	CHC-C1C	2.93	1.42	1.35
26	2	614	CLA	CHC-C1C	2.93	1.42	1.35
26	6	614	CLA	CHC-C1C	2.93	1.42	1.35
26	y	610	CLA	CHC-C1C	2.93	1.42	1.35
26	y	610	CLA	C1D-ND	2.92	1.41	1.37
25	4	609	CHL	C1D-C2D	2.92	1.51	1.45
25	8	607	CHL	C1D-C2D	2.92	1.51	1.45
26	6	604	CLA	CMB-C2B	-2.92	1.45	1.51
26	3	604	CLA	CHC-C1C	2.92	1.42	1.35
26	1	602	CLA	CHC-C1C	2.92	1.42	1.35
26	c	503	CLA	CHC-C1C	2.92	1.42	1.35
25	2	601	CHL	C1D-C2D	2.91	1.51	1.45
26	B	603	CLA	CHC-C1C	2.91	1.42	1.35
26	b	608	CLA	C1D-ND	2.91	1.41	1.37
29	n	1623	NEX	C7-C8	-2.91	1.27	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	C	520	DGD	O1G-C1G	-2.91	1.38	1.45
39	c	520	DGD	O1G-C1G	-2.91	1.38	1.45
26	B	615	CLA	CHC-C1C	2.91	1.42	1.35
26	b	615	CLA	CHC-C1C	2.91	1.42	1.35
25	4	607	CHL	C1D-C2D	2.91	1.51	1.45
26	1	604	CLA	C3B-C2B	-2.91	1.36	1.40
26	5	604	CLA	C3B-C2B	-2.91	1.36	1.40
26	2	604	CLA	CMB-C2B	-2.91	1.45	1.51
26	C	503	CLA	CHC-C1C	2.91	1.42	1.35
25	8	609	CHL	C1D-C2D	2.91	1.51	1.45
26	5	602	CLA	CHC-C1C	2.90	1.42	1.35
37	d	411	LMG	O8-C9	-2.90	1.38	1.45
25	6	601	CHL	C1D-C2D	2.90	1.51	1.45
26	B	617	CLA	CHC-C1C	2.90	1.42	1.35
26	b	617	CLA	CHC-C1C	2.90	1.42	1.35
26	G	612	CLA	C4D-ND	-2.90	1.33	1.37
26	g	612	CLA	C4D-ND	-2.90	1.33	1.37
26	y	610	CLA	C3B-C2B	-2.90	1.36	1.40
25	G	601	CHL	MG-NA	-2.90	1.99	2.06
26	N	611	CLA	CHC-C1C	2.89	1.42	1.35
26	n	611	CLA	CHC-C1C	2.89	1.42	1.35
26	Y	610	CLA	C3B-C2B	-2.89	1.36	1.40
30	C	522	LHG	O7-C5	-2.89	1.39	1.46
30	c	522	LHG	O7-C5	-2.89	1.39	1.46
26	C	512	CLA	CMB-C2B	-2.89	1.45	1.51
26	c	512	CLA	CMB-C2B	-2.89	1.45	1.51
26	C	501	CLA	C3B-C2B	-2.89	1.36	1.40
26	c	501	CLA	C3B-C2B	-2.89	1.36	1.40
29	N	1623	NEX	C7-C8	-2.89	1.27	1.32
26	y	603	CLA	CMB-C2B	-2.89	1.45	1.51
26	C	504	CLA	CMB-C2B	-2.89	1.45	1.51
26	y	603	CLA	CHC-C1C	2.89	1.42	1.35
25	1	601	CHL	C1D-C2D	2.89	1.51	1.45
25	5	601	CHL	C1D-C2D	2.89	1.51	1.45
26	b	603	CLA	CHC-C1C	2.89	1.42	1.35
26	B	604	CLA	CMD-C2D	-2.88	1.44	1.50
26	Y	603	CLA	CMB-C2B	-2.88	1.45	1.51
26	Y	603	CLA	CHC-C1C	2.88	1.42	1.35
26	b	604	CLA	CMD-C2D	-2.88	1.44	1.50
36	A	418	SQD	O48-C23	2.88	1.41	1.33
26	N	602	CLA	CHC-C1C	2.88	1.42	1.35
26	n	602	CLA	CHC-C1C	2.88	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	604	CLA	MG-ND	-2.88	2.00	2.05
26	c	503	CLA	C1D-ND	2.88	1.41	1.37
26	B	603	CLA	CMB-C2B	-2.88	1.45	1.51
26	b	603	CLA	CMB-C2B	-2.88	1.45	1.51
26	2	612	CLA	C4D-ND	-2.88	1.33	1.37
26	6	612	CLA	C4D-ND	-2.88	1.33	1.37
26	B	608	CLA	C1D-ND	2.88	1.41	1.37
26	C	513	CLA	C1D-ND	2.87	1.41	1.37
26	c	513	CLA	C1D-ND	2.87	1.41	1.37
26	c	507	CLA	CMB-C2B	-2.87	1.45	1.51
26	B	613	CLA	CHC-C1C	2.87	1.42	1.35
26	R	603	CLA	C1D-ND	2.87	1.41	1.37
39	c	518	DGD	O2G-C2G	-2.87	1.39	1.46
26	B	602	CLA	CHC-C1C	2.87	1.42	1.35
25	Y	601	CHL	C1D-C2D	2.87	1.51	1.45
26	B	604	CLA	MG-ND	-2.87	2.00	2.05
26	2	611	CLA	CHC-C1C	2.87	1.42	1.35
26	6	611	CLA	CHC-C1C	2.87	1.42	1.35
26	5	614	CLA	CHC-C1C	2.87	1.42	1.35
26	6	610	CLA	CHC-C1C	2.87	1.42	1.35
26	s	610	CLA	CMB-C2B	-2.87	1.45	1.51
36	a	418	SQD	O48-C23	2.87	1.41	1.33
25	4	601	CHL	C1D-C2D	2.86	1.51	1.45
26	D	402	CLA	CHC-C1C	2.86	1.42	1.35
26	d	402	CLA	CHC-C1C	2.86	1.42	1.35
25	y	601	CHL	C1D-C2D	2.86	1.51	1.45
26	2	610	CLA	CHC-C1C	2.86	1.42	1.35
26	N	603	CLA	CMD-C2D	-2.86	1.44	1.50
26	y	602	CLA	CHC-C1C	2.86	1.42	1.35
26	n	603	CLA	CMD-C2D	-2.86	1.44	1.50
25	S	608	CHL	MG-NA	-2.86	1.99	2.06
26	1	614	CLA	CHC-C1C	2.86	1.42	1.35
26	b	605	CLA	CMA-C3A	-2.86	1.47	1.53
26	S	610	CLA	CMB-C2B	-2.86	1.45	1.51
26	b	613	CLA	CHC-C1C	2.86	1.42	1.35
25	8	601	CHL	C1D-C2D	2.85	1.51	1.45
26	c	507	CLA	CMC-C2C	-2.85	1.44	1.50
25	N	601	CHL	C1D-C2D	2.85	1.51	1.45
25	n	601	CHL	C1D-C2D	2.85	1.51	1.45
26	g	602	CLA	CHC-C1C	2.85	1.42	1.35
26	c	504	CLA	CMB-C2B	-2.85	1.45	1.51
26	b	602	CLA	CHC-C1C	2.85	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	602	CLA	CHC-C1C	2.85	1.42	1.35
26	B	605	CLA	CMA-C3A	-2.85	1.47	1.53
26	r	603	CLA	C1D-ND	2.84	1.41	1.37
26	G	612	CLA	CHC-C1C	2.84	1.42	1.35
26	g	612	CLA	CHC-C1C	2.84	1.42	1.35
39	C	518	DGD	O2G-C2G	-2.84	1.39	1.46
26	7	602	CLA	CHC-C1C	2.84	1.42	1.35
26	Y	611	CLA	CMD-C2D	-2.84	1.44	1.50
26	y	611	CLA	CMD-C2D	-2.84	1.44	1.50
26	n	603	CLA	CMB-C2B	-2.84	1.45	1.51
26	G	610	CLA	C4D-ND	-2.84	1.33	1.37
26	2	613	CLA	CHC-C1C	2.84	1.42	1.35
25	s	608	CHL	MG-NA	-2.84	1.99	2.06
26	4	604	CLA	CMB-C2B	-2.83	1.45	1.51
26	8	604	CLA	CMB-C2B	-2.83	1.45	1.51
26	C	507	CLA	CMC-C2C	-2.83	1.44	1.50
26	3	602	CLA	CHC-C1C	2.83	1.42	1.35
26	C	507	CLA	CMB-C2B	-2.83	1.45	1.51
25	g	605	CHL	C1D-C2D	2.83	1.50	1.45
30	S	2630	LHG	O7-C5	-2.83	1.39	1.46
30	s	2630	LHG	O7-C5	-2.83	1.39	1.46
25	N	601	CHL	OBD-CAD	2.83	1.27	1.22
26	1	610	CLA	CMB-C2B	-2.83	1.45	1.51
26	5	610	CLA	CMB-C2B	-2.83	1.45	1.51
25	G	608	CHL	OBD-CAD	2.83	1.27	1.22
25	n	601	CHL	OBD-CAD	2.83	1.27	1.22
26	Y	611	CLA	C1D-ND	2.83	1.41	1.37
26	Y	602	CLA	CHC-C1C	2.83	1.42	1.35
26	3	610	CLA	CMB-C2B	-2.83	1.45	1.51
26	7	610	CLA	CMB-C2B	-2.83	1.45	1.51
26	C	511	CLA	CHC-C1C	2.83	1.42	1.35
26	Y	611	CLA	CHC-C1C	2.83	1.42	1.35
26	y	611	CLA	CHC-C1C	2.83	1.42	1.35
26	N	614	CLA	CHC-C1C	2.83	1.42	1.35
26	6	613	CLA	CHC-C1C	2.83	1.42	1.35
26	c	511	CLA	CHC-C1C	2.82	1.42	1.35
26	B	604	CLA	C3B-C2B	-2.82	1.36	1.40
26	S	612	CLA	CHC-C1C	2.82	1.42	1.35
26	s	612	CLA	CHC-C1C	2.82	1.42	1.35
26	B	615	CLA	CMB-C2B	-2.82	1.45	1.51
26	C	503	CLA	C1D-ND	2.82	1.41	1.37
26	n	612	CLA	C4D-ND	-2.82	1.33	1.37

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	610	CLA	CHC-C1C	2.82	1.42	1.35
26	3	604	CLA	CMB-C2B	-2.82	1.45	1.51
26	n	614	CLA	CHC-C1C	2.82	1.42	1.35
26	8	603	CLA	CHC-C1C	2.82	1.42	1.35
26	g	610	CLA	CHC-C1C	2.82	1.42	1.35
25	g	608	CHL	OBD-CAD	2.82	1.27	1.22
26	G	603	CLA	CHC-C1C	2.82	1.42	1.35
26	g	603	CLA	CHC-C1C	2.82	1.42	1.35
26	C	505	CLA	CMB-C2B	-2.82	1.45	1.51
26	b	615	CLA	CMB-C2B	-2.82	1.45	1.51
26	c	505	CLA	CMB-C2B	-2.82	1.45	1.51
26	C	510	CLA	CMD-C2D	-2.82	1.44	1.50
26	R	604	CLA	CHC-C1C	2.82	1.42	1.35
26	r	604	CLA	CHC-C1C	2.82	1.42	1.35
26	1	610	CLA	CHC-C1C	2.82	1.42	1.35
26	Y	614	CLA	CHC-C1C	2.81	1.42	1.35
26	y	614	CLA	CHC-C1C	2.81	1.42	1.35
26	N	603	CLA	CMB-C2B	-2.81	1.45	1.51
26	C	510	CLA	CHC-C1C	2.81	1.42	1.35
26	c	510	CLA	CHC-C1C	2.81	1.42	1.35
26	7	604	CLA	CMB-C2B	-2.81	1.45	1.51
26	c	501	CLA	CHC-C1C	2.81	1.42	1.35
25	3	607	CHL	C1D-C2D	2.81	1.50	1.45
25	R	606	CHL	C1D-C2D	2.81	1.50	1.45
26	c	510	CLA	CMD-C2D	-2.81	1.44	1.50
26	A	405	CLA	CMB-C2B	-2.81	1.45	1.51
25	4	609	CHL	MG-NA	-2.81	1.99	2.06
25	8	609	CHL	MG-NA	-2.81	1.99	2.06
26	C	501	CLA	CHC-C1C	2.81	1.42	1.35
25	7	609	CHL	MG-NA	-2.81	1.99	2.06
25	1	607	CHL	C1D-C2D	2.81	1.50	1.45
26	5	610	CLA	CHC-C1C	2.81	1.42	1.35
25	7	607	CHL	C1D-C2D	2.80	1.50	1.45
26	a	405	CLA	CMB-C2B	-2.80	1.45	1.51
26	A	410	CLA	CMB-C2B	-2.80	1.45	1.51
26	1	610	CLA	C3B-CAB	-2.80	1.42	1.47
25	1	607	CHL	MG-NA	-2.80	1.99	2.06
25	5	607	CHL	MG-NA	-2.80	1.99	2.06
26	4	611	CLA	CHC-C1C	2.80	1.42	1.35
26	g	610	CLA	C4D-ND	-2.80	1.33	1.37
36	b	621	SQD	O48-C23	2.80	1.41	1.33
26	S	604	CLA	CHC-C1C	2.80	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	609	CHL	MG-NA	-2.80	1.99	2.06
26	8	611	CLA	CHC-C1C	2.80	1.42	1.35
26	4	603	CLA	CHC-C1C	2.79	1.42	1.35
26	a	410	CLA	CMB-C2B	-2.79	1.45	1.51
25	G	605	CHL	C1D-C2D	2.79	1.50	1.45
26	Y	612	CLA	C3B-C2B	-2.79	1.36	1.40
36	B	621	SQD	O48-C23	2.79	1.41	1.33
26	y	611	CLA	C1D-ND	2.79	1.41	1.37
26	Y	612	CLA	CHC-C1C	2.79	1.42	1.35
25	3	601	CHL	C1D-C2D	2.79	1.50	1.45
25	y	601	CHL	OBD-CAD	2.79	1.27	1.22
25	5	607	CHL	C1D-C2D	2.79	1.50	1.45
25	r	606	CHL	C1D-C2D	2.79	1.50	1.45
26	R	604	CLA	CMB-C2B	-2.79	1.45	1.51
26	r	604	CLA	CMB-C2B	-2.79	1.45	1.51
26	N	612	CLA	CHC-C1C	2.79	1.42	1.35
26	n	612	CLA	CHC-C1C	2.79	1.42	1.35
26	N	612	CLA	C4D-ND	-2.79	1.33	1.37
26	5	610	CLA	C3B-CAB	-2.79	1.42	1.47
25	4	601	CHL	C3D-C2D	2.79	1.46	1.39
26	6	603	CLA	CHC-C1C	2.78	1.42	1.35
26	b	608	CLA	CMC-C2C	-2.78	1.44	1.50
26	4	612	CLA	CHC-C1C	2.78	1.42	1.35
26	8	612	CLA	CHC-C1C	2.78	1.42	1.35
26	N	603	CLA	CHC-C1C	2.78	1.42	1.35
26	n	603	CLA	CHC-C1C	2.78	1.42	1.35
26	s	604	CLA	CHC-C1C	2.78	1.42	1.35
26	b	604	CLA	C3B-C2B	-2.78	1.36	1.40
26	B	608	CLA	CMC-C2C	-2.78	1.44	1.50
26	2	602	CLA	CHC-C1C	2.78	1.42	1.35
25	Y	601	CHL	OBD-CAD	2.78	1.27	1.22
25	4	601	CHL	MG-NA	-2.78	1.99	2.06
25	8	601	CHL	MG-NA	-2.78	1.99	2.06
25	s	606	CHL	C1D-C2D	2.78	1.50	1.45
25	S	606	CHL	C1D-C2D	2.78	1.50	1.45
35	A	409	PHO	CMD-C2D	-2.78	1.44	1.51
35	a	409	PHO	CMD-C2D	-2.78	1.44	1.51
26	6	602	CLA	CHC-C1C	2.78	1.42	1.35
26	y	612	CLA	CHC-C1C	2.78	1.42	1.35
25	R	607	CHL	MG-NA	-2.78	1.99	2.06
26	b	616	CLA	CMB-C2B	-2.78	1.45	1.51
26	B	616	CLA	CMB-C2B	-2.78	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R	610	CLA	CMB-C2B	-2.78	1.45	1.51
26	r	610	CLA	CMB-C2B	-2.78	1.45	1.51
26	Y	610	CLA	CMB-C2B	-2.78	1.45	1.51
26	y	610	CLA	CMB-C2B	-2.78	1.45	1.51
26	B	602	CLA	CMB-C2B	-2.77	1.45	1.51
25	y	607	CHL	MG-NA	-2.77	1.99	2.06
26	6	604	CLA	CHC-C1C	2.77	1.42	1.35
26	y	612	CLA	C3B-C2B	-2.77	1.36	1.40
26	c	506	CLA	C1D-ND	2.77	1.41	1.37
26	r	609	CLA	CHC-C1C	2.77	1.42	1.35
26	B	609	CLA	CHC-C1C	2.77	1.42	1.35
26	b	609	CLA	CHC-C1C	2.77	1.42	1.35
26	R	601	CLA	CHC-C1C	2.77	1.42	1.35
26	r	601	CLA	CHC-C1C	2.77	1.42	1.35
26	N	604	CLA	CHC-C1C	2.77	1.42	1.35
26	R	609	CLA	CHC-C1C	2.77	1.42	1.35
26	S	609	CLA	CHC-C1C	2.77	1.42	1.35
26	n	604	CLA	CHC-C1C	2.77	1.42	1.35
26	y	611	CLA	C3B-C2B	-2.77	1.36	1.40
26	2	604	CLA	CHC-C1C	2.77	1.42	1.35
26	D	403	CLA	CHC-C1C	2.77	1.42	1.35
26	d	403	CLA	CHC-C1C	2.77	1.42	1.35
25	Y	607	CHL	MG-NA	-2.77	1.99	2.06
26	Y	611	CLA	C3B-C2B	-2.77	1.36	1.40
26	b	602	CLA	CMB-C2B	-2.76	1.45	1.51
25	3	609	CHL	C1D-C2D	2.76	1.50	1.45
25	7	609	CHL	C1D-C2D	2.76	1.50	1.45
26	B	607	CLA	CMD-C2D	-2.76	1.44	1.50
26	b	607	CLA	CMD-C2D	-2.76	1.44	1.50
25	7	601	CHL	C1D-C2D	2.76	1.50	1.45
25	8	601	CHL	C3D-C2D	2.76	1.46	1.39
26	5	611	CLA	CHC-C1C	2.76	1.42	1.35
25	r	607	CHL	MG-NA	-2.76	1.99	2.06
26	1	611	CLA	CHC-C1C	2.76	1.42	1.35
26	s	609	CLA	CHC-C1C	2.76	1.42	1.35
25	4	607	CHL	MG-NA	-2.76	1.99	2.06
26	G	602	CLA	CMC-C2C	-2.76	1.45	1.50
26	g	602	CLA	CMC-C2C	-2.76	1.45	1.50
26	B	616	CLA	C1D-ND	2.76	1.41	1.37
26	B	609	CLA	CMD-C2D	-2.76	1.45	1.50
26	b	609	CLA	CMD-C2D	-2.76	1.45	1.50
25	8	607	CHL	MG-NA	-2.76	1.99	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	n	604	CLA	C3B-C2B	-2.76	1.36	1.40
26	D	402	CLA	CMC-C2C	-2.76	1.45	1.50
26	d	402	CLA	CMC-C2C	-2.76	1.45	1.50
26	b	616	CLA	C1D-ND	2.76	1.41	1.37
26	S	613	CLA	CHC-C1C	2.76	1.42	1.35
26	s	613	CLA	CHC-C1C	2.76	1.42	1.35
26	6	603	CLA	CMB-C2B	-2.76	1.45	1.51
26	1	604	CLA	CHC-C1C	2.75	1.42	1.35
26	R	613	CLA	CMB-C2B	-2.75	1.45	1.51
26	r	613	CLA	CMB-C2B	-2.75	1.45	1.51
25	N	608	CHL	OBD-CAD	2.75	1.27	1.22
25	n	608	CHL	OBD-CAD	2.75	1.27	1.22
25	7	605	CHL	C1D-C2D	2.75	1.50	1.45
30	Y	2630	LHG	O7-C5	-2.75	1.39	1.46
30	y	2630	LHG	O7-C5	-2.75	1.39	1.46
26	2	603	CLA	CHC-C1C	2.75	1.42	1.35
26	g	604	CLA	CHC-C1C	2.75	1.42	1.35
26	2	603	CLA	CMB-C2B	-2.75	1.45	1.51
25	4	606	CHL	MG-NA	-2.75	1.99	2.06
26	C	508	CLA	CMC-C2C	-2.75	1.45	1.50
26	B	610	CLA	CMB-C2B	-2.75	1.45	1.51
26	3	610	CLA	C3B-C2B	-2.75	1.36	1.40
26	7	610	CLA	C3B-C2B	-2.75	1.36	1.40
26	c	508	CLA	CMC-C2C	-2.75	1.45	1.50
39	H	102	DGD	O5D-C6D	-2.75	1.38	1.43
39	h	102	DGD	O5D-C6D	-2.75	1.38	1.43
26	s	614	CLA	CHC-C1C	2.74	1.42	1.35
26	b	608	CLA	C3B-C2B	-2.74	1.36	1.40
26	a	407	CLA	CMB-C2B	-2.74	1.45	1.51
26	C	509	CLA	CHC-C1C	2.74	1.42	1.35
26	c	509	CLA	CHC-C1C	2.74	1.42	1.35
26	r	613	CLA	CHC-C1C	2.74	1.42	1.35
26	S	614	CLA	CHC-C1C	2.74	1.42	1.35
26	B	609	CLA	CMB-C2B	-2.74	1.45	1.51
26	C	506	CLA	C1D-ND	2.74	1.41	1.37
36	A	412	SQD	O48-C23	2.74	1.41	1.33
36	a	412	SQD	O48-C23	2.74	1.41	1.33
26	C	512	CLA	CHC-C1C	2.74	1.42	1.35
26	R	613	CLA	CHC-C1C	2.73	1.42	1.35
26	a	410	CLA	CHC-C1C	2.73	1.42	1.35
25	n	601	CHL	MG-NA	-2.73	1.99	2.06
26	5	604	CLA	CHC-C1C	2.73	1.42	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	614	CLA	C1D-ND	2.73	1.41	1.37
26	b	614	CLA	C1D-ND	2.73	1.41	1.37
25	8	606	CHL	MG-NA	-2.73	1.99	2.06
26	5	612	CLA	C4D-ND	-2.73	1.33	1.37
25	Y	606	CHL	CHD-C4C	2.73	1.45	1.39
25	3	605	CHL	C1D-C2D	2.72	1.50	1.45
25	N	609	CHL	C1B-NB	-2.72	1.32	1.35
25	n	609	CHL	C1B-NB	-2.72	1.32	1.35
26	7	612	CLA	C3B-C2B	-2.72	1.36	1.40
26	B	608	CLA	C3B-C2B	-2.72	1.36	1.40
26	G	604	CLA	CHC-C1C	2.72	1.41	1.35
26	A	407	CLA	CMB-C2B	-2.71	1.46	1.51
25	N	601	CHL	MG-NA	-2.71	1.99	2.06
26	b	610	CLA	CMB-C2B	-2.71	1.46	1.51
26	N	604	CLA	C3B-C2B	-2.71	1.36	1.40
26	B	611	CLA	CMB-C2B	-2.71	1.46	1.51
26	y	611	CLA	CMB-C2B	-2.71	1.46	1.51
25	4	608	CHL	MG-NA	-2.71	1.99	2.06
25	8	608	CHL	MG-NA	-2.71	1.99	2.06
26	B	602	CLA	C3B-C2B	-2.71	1.36	1.40
26	b	602	CLA	C3B-C2B	-2.71	1.36	1.40
25	y	606	CHL	CHD-C4C	2.71	1.45	1.39
26	5	613	CLA	CHC-C1C	2.70	1.41	1.35
39	C	518	DGD	O3E-C3E	-2.70	1.36	1.43
26	C	509	CLA	C1D-ND	2.70	1.41	1.37
26	c	509	CLA	C1D-ND	2.70	1.41	1.37
26	1	612	CLA	C4D-ND	-2.70	1.34	1.37
25	g	601	CHL	C1D-C2D	2.70	1.50	1.45
26	C	503	CLA	CMB-C2B	-2.70	1.46	1.51
26	c	503	CLA	CMB-C2B	-2.70	1.46	1.51
26	c	512	CLA	CHC-C1C	2.70	1.41	1.35
26	b	609	CLA	CMB-C2B	-2.70	1.46	1.51
26	s	602	CLA	CMB-C2B	-2.70	1.46	1.51
39	c	518	DGD	O3E-C3E	-2.70	1.36	1.43
39	H	102	DGD	O3G-C3G	-2.70	1.38	1.43
39	h	102	DGD	O3G-C3G	-2.70	1.38	1.43
26	A	410	CLA	CHC-C1C	2.70	1.41	1.35
26	S	611	CLA	CHC-C1C	2.70	1.41	1.35
25	4	608	CHL	OBD-CAD	2.69	1.27	1.22
25	2	605	CHL	C1D-C2D	2.69	1.50	1.45
25	6	605	CHL	C1D-C2D	2.69	1.50	1.45
25	G	601	CHL	C1D-C2D	2.69	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	b	611	CLA	CMB-C2B	-2.69	1.46	1.51
26	1	613	CLA	CHC-C1C	2.69	1.41	1.35
26	B	607	CLA	CMB-C2B	-2.69	1.46	1.51
26	Y	611	CLA	CMB-C2B	-2.69	1.46	1.51
26	b	607	CLA	CMB-C2B	-2.69	1.46	1.51
26	3	612	CLA	CMB-C2B	-2.69	1.46	1.51
26	B	606	CLA	CMD-C2D	-2.69	1.45	1.50
26	b	606	CLA	CMD-C2D	-2.69	1.45	1.50
37	D	411	LMG	O1-C7	-2.69	1.38	1.43
37	d	411	LMG	O1-C7	-2.69	1.38	1.43
25	8	608	CHL	OBD-CAD	2.69	1.27	1.22
26	1	612	CLA	CHC-C1C	2.68	1.41	1.35
26	5	612	CLA	CHC-C1C	2.68	1.41	1.35
25	2	605	CHL	MG-NA	-2.68	1.99	2.06
25	6	605	CHL	MG-NA	-2.68	1.99	2.06
26	S	602	CLA	CMB-C2B	-2.68	1.46	1.51
26	Y	602	CLA	CMC-C2C	-2.68	1.45	1.50
26	y	602	CLA	CMC-C2C	-2.68	1.45	1.50
26	N	610	CLA	CHC-C1C	2.68	1.41	1.35
26	n	610	CLA	CHC-C1C	2.68	1.41	1.35
26	4	604	CLA	CHC-C1C	2.68	1.41	1.35
26	8	604	CLA	CHC-C1C	2.68	1.41	1.35
26	s	611	CLA	CHC-C1C	2.68	1.41	1.35
26	7	612	CLA	CMB-C2B	-2.68	1.46	1.51
25	7	608	CHL	OBD-CAD	2.68	1.27	1.22
26	3	614	CLA	CHC-C1C	2.68	1.41	1.35
26	3	613	CLA	CHC-C1C	2.68	1.41	1.35
26	N	613	CLA	CHC-C1C	2.68	1.41	1.35
26	n	613	CLA	CHC-C1C	2.68	1.41	1.35
25	G	605	CHL	C3D-C2D	2.67	1.46	1.39
25	g	605	CHL	C3D-C2D	2.67	1.46	1.39
26	C	513	CLA	CHC-C1C	2.67	1.41	1.35
26	3	612	CLA	C3B-C2B	-2.67	1.36	1.40
26	r	603	CLA	CMB-C2B	-2.67	1.46	1.51
26	B	606	CLA	CHC-C1C	2.67	1.41	1.35
26	b	606	CLA	CHC-C1C	2.67	1.41	1.35
26	Y	613	CLA	CHC-C1C	2.67	1.41	1.35
26	y	613	CLA	CHC-C1C	2.67	1.41	1.35
29	G	1623	NEX	O4-C5	-2.67	1.38	1.43
29	g	1623	NEX	O4-C5	-2.67	1.38	1.43
25	4	606	CHL	C1D-C2D	2.67	1.50	1.45
25	8	606	CHL	C1D-C2D	2.67	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	513	CLA	CHC-C1C	2.67	1.41	1.35
26	b	608	CLA	C4B-CHC	-2.67	1.33	1.41
25	5	609	CHL	MG-NA	-2.67	1.99	2.06
26	a	406	CLA	CMB-C2B	-2.66	1.46	1.51
26	B	608	CLA	C4B-CHC	-2.66	1.33	1.41
25	3	608	CHL	OBD-CAD	2.66	1.27	1.22
26	Y	613	CLA	CMD-C2D	-2.66	1.45	1.50
26	y	613	CLA	CMD-C2D	-2.66	1.45	1.50
26	c	512	CLA	CMD-C2D	-2.66	1.45	1.50
26	6	612	CLA	CHC-C1C	2.66	1.41	1.35
26	R	603	CLA	CMB-C2B	-2.66	1.46	1.51
26	Y	613	CLA	C1D-ND	2.66	1.41	1.37
26	y	613	CLA	C1D-ND	2.66	1.41	1.37
26	r	603	CLA	CHC-C1C	2.66	1.41	1.35
25	1	609	CHL	MG-NA	-2.65	2.00	2.06
25	G	606	CHL	C1D-C2D	2.65	1.50	1.45
25	g	606	CHL	C1D-C2D	2.65	1.50	1.45
26	4	603	CLA	CMB-C2B	-2.65	1.46	1.51
26	Y	602	CLA	CMB-C2B	-2.65	1.46	1.51
26	y	602	CLA	CMB-C2B	-2.65	1.46	1.51
26	7	613	CLA	CHC-C1C	2.65	1.41	1.35
26	3	613	CLA	C3B-C2B	-2.65	1.36	1.40
26	7	613	CLA	C3B-C2B	-2.65	1.36	1.40
26	7	613	CLA	CMB-C2B	-2.65	1.46	1.51
26	R	603	CLA	CHC-C1C	2.65	1.41	1.35
26	B	611	CLA	CMC-C2C	-2.65	1.45	1.50
26	Y	610	CLA	CMD-C2D	-2.65	1.45	1.50
26	y	610	CLA	CMD-C2D	-2.65	1.45	1.50
25	3	607	CHL	C3D-C2D	2.65	1.46	1.39
25	7	607	CHL	C3D-C2D	2.65	1.46	1.39
25	G	605	CHL	C4B-CHC	2.65	1.48	1.41
26	A	405	CLA	CHC-C1C	2.65	1.41	1.35
26	a	405	CLA	CHC-C1C	2.65	1.41	1.35
26	7	614	CLA	CHC-C1C	2.65	1.41	1.35
25	2	605	CHL	C3D-C2D	2.64	1.46	1.39
25	6	605	CHL	C3D-C2D	2.64	1.46	1.39
26	A	406	CLA	CMB-C2B	-2.64	1.46	1.51
26	G	602	CLA	CMB-C2B	-2.64	1.46	1.51
25	5	609	CHL	C1D-C2D	2.64	1.50	1.45
26	3	613	CLA	CMB-C2B	-2.64	1.46	1.51
26	B	605	CLA	C1D-ND	2.64	1.41	1.37
25	2	609	CHL	MG-NA	-2.64	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	g	602	CLA	CMB-C2B	-2.64	1.46	1.51
25	S	607	CHL	MG-NA	-2.64	2.00	2.06
25	s	607	CHL	MG-NA	-2.64	2.00	2.06
26	b	604	CLA	CHC-C1C	2.64	1.41	1.35
26	2	612	CLA	CHC-C1C	2.63	1.41	1.35
26	6	610	CLA	CMB-C2B	-2.63	1.46	1.51
26	2	610	CLA	CMB-C2B	-2.63	1.46	1.51
26	y	610	CLA	CMC-C2C	-2.63	1.45	1.50
26	Y	614	CLA	CMB-C2B	-2.63	1.46	1.51
25	s	601	CHL	C1D-C2D	2.63	1.50	1.45
25	7	605	CHL	C3D-C2D	2.63	1.46	1.39
25	1	609	CHL	C1D-C2D	2.63	1.50	1.45
26	b	608	CLA	CMD-C2D	-2.63	1.45	1.50
25	6	609	CHL	MG-NA	-2.63	2.00	2.06
26	B	615	CLA	C1D-ND	2.63	1.41	1.37
26	b	615	CLA	C1D-ND	2.63	1.41	1.37
25	g	605	CHL	C4B-CHC	2.63	1.48	1.41
26	B	604	CLA	CHC-C1C	2.63	1.41	1.35
36	A	412	SQD	O47-C7	2.62	1.41	1.34
26	3	603	CLA	C3B-C2B	-2.62	1.36	1.40
26	C	512	CLA	CMD-C2D	-2.62	1.45	1.50
26	g	610	CLA	CMB-C2B	-2.62	1.46	1.51
25	S	601	CHL	C1D-C2D	2.62	1.50	1.45
26	S	603	CLA	CHC-C1C	2.62	1.41	1.35
26	s	603	CLA	CHC-C1C	2.62	1.41	1.35
36	a	412	SQD	O47-C7	2.62	1.41	1.34
26	Y	612	CLA	CMD-C2D	-2.62	1.45	1.50
26	y	612	CLA	CMD-C2D	-2.62	1.45	1.50
25	3	605	CHL	C3D-C2D	2.62	1.46	1.39
26	Y	610	CLA	CMC-C2C	-2.62	1.45	1.50
26	8	603	CLA	CMB-C2B	-2.61	1.46	1.51
26	b	611	CLA	CMC-C2C	-2.61	1.45	1.50
26	7	603	CLA	C3B-C2B	-2.61	1.36	1.40
26	8	610	CLA	CMB-C2B	-2.61	1.46	1.51
26	y	614	CLA	CMB-C2B	-2.61	1.46	1.51
26	3	602	CLA	CMC-C2C	-2.61	1.45	1.50
26	7	602	CLA	CMC-C2C	-2.61	1.45	1.50
25	n	605	CHL	MG-NA	-2.61	2.00	2.06
26	3	614	CLA	C3B-C2B	-2.61	1.36	1.40
26	b	605	CLA	C1D-ND	2.61	1.41	1.37
26	B	611	CLA	CHC-C1C	2.61	1.41	1.35
29	S	1623	NEX	C7-C8	-2.61	1.27	1.32

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
29	s	1623	NEX	C7-C8	-2.61	1.27	1.32
26	4	610	CLA	CMB-C2B	-2.61	1.46	1.51
26	R	616	CLA	CHC-C1C	2.60	1.41	1.35
26	3	602	CLA	CMB-C2B	-2.60	1.46	1.51
26	7	602	CLA	CMB-C2B	-2.60	1.46	1.51
25	y	606	CHL	OBD-CAD	2.60	1.27	1.22
26	3	614	CLA	CMB-C2B	-2.60	1.46	1.51
26	7	614	CLA	CMB-C2B	-2.60	1.46	1.51
26	7	614	CLA	C3B-C2B	-2.60	1.36	1.40
25	g	609	CHL	C1D-C2D	2.60	1.50	1.45
25	N	605	CHL	MG-NA	-2.60	2.00	2.06
27	N	1621	LUT	C22-C21	-2.60	1.51	1.54
26	c	506	CLA	MG-ND	-2.60	2.00	2.05
25	Y	606	CHL	OBD-CAD	2.60	1.27	1.22
25	5	605	CHL	C1D-C2D	2.60	1.50	1.45
25	R	614	CHL	MG-NA	-2.60	2.00	2.06
25	r	614	CHL	MG-NA	-2.60	2.00	2.06
25	y	608	CHL	MG-NA	-2.60	2.00	2.06
26	N	610	CLA	CMB-C2B	-2.59	1.46	1.51
26	Y	613	CLA	CMB-C2B	-2.59	1.46	1.51
26	n	610	CLA	CMB-C2B	-2.59	1.46	1.51
26	y	613	CLA	CMB-C2B	-2.59	1.46	1.51
25	G	607	CHL	MG-NA	-2.59	2.00	2.06
25	g	607	CHL	MG-NA	-2.59	2.00	2.06
25	G	601	CHL	OBD-CAD	2.59	1.26	1.22
25	g	601	CHL	OBD-CAD	2.59	1.26	1.22
39	H	102	DGD	O4D-C4D	-2.59	1.36	1.43
39	h	102	DGD	O4D-C4D	-2.59	1.36	1.43
25	7	609	CHL	C3D-C2D	2.59	1.46	1.39
25	3	609	CHL	C3D-C2D	2.59	1.46	1.39
26	3	603	CLA	CMB-C2B	-2.59	1.46	1.51
26	7	603	CLA	CMB-C2B	-2.59	1.46	1.51
26	S	613	CLA	CMB-C2B	-2.59	1.46	1.51
26	s	613	CLA	CMB-C2B	-2.59	1.46	1.51
26	B	614	CLA	CHC-C1C	2.59	1.41	1.35
26	b	614	CLA	CHC-C1C	2.59	1.41	1.35
25	2	607	CHL	MG-NA	-2.59	2.00	2.06
26	Y	612	CLA	CMB-C2B	-2.59	1.46	1.51
26	y	612	CLA	CMB-C2B	-2.59	1.46	1.51
26	B	608	CLA	CMD-C2D	-2.59	1.45	1.50
25	S	606	CHL	C4B-CHC	2.59	1.48	1.41
25	s	606	CHL	C4B-CHC	2.59	1.48	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	511	CLA	CMB-C2B	-2.59	1.46	1.51
26	G	610	CLA	CMB-C2B	-2.59	1.46	1.51
26	5	613	CLA	CMB-C2B	-2.59	1.46	1.51
26	B	612	CLA	CHC-C1C	2.58	1.41	1.35
26	b	612	CLA	CHC-C1C	2.58	1.41	1.35
35	a	408	PHO	CMB-C2B	-2.58	1.45	1.51
25	n	609	CHL	MG-NA	-2.58	2.00	2.06
26	2	602	CLA	CMB-C2B	-2.58	1.46	1.51
26	b	611	CLA	CHC-C1C	2.58	1.41	1.35
25	6	607	CHL	MG-NA	-2.58	2.00	2.06
25	G	609	CHL	C1D-C2D	2.58	1.50	1.45
25	4	609	CHL	C3D-C2D	2.58	1.46	1.39
25	8	609	CHL	C3D-C2D	2.58	1.46	1.39
26	C	501	CLA	CMB-C2B	-2.58	1.46	1.51
26	C	511	CLA	CMB-C2B	-2.58	1.46	1.51
26	r	616	CLA	CHC-C1C	2.58	1.41	1.35
26	C	506	CLA	MG-ND	-2.58	2.00	2.05
26	A	407	CLA	CHC-C1C	2.58	1.41	1.35
26	g	604	CLA	C3B-C2B	-2.58	1.36	1.40
25	Y	608	CHL	MG-NA	-2.58	2.00	2.06
35	A	409	PHO	CMC-C2C	-2.58	1.45	1.51
25	Y	605	CHL	MG-NA	-2.57	2.00	2.06
25	y	605	CHL	MG-NA	-2.57	2.00	2.06
26	5	602	CLA	C3B-C2B	-2.57	1.36	1.40
25	7	601	CHL	MG-NA	-2.57	2.00	2.06
26	G	604	CLA	C3B-C2B	-2.57	1.36	1.40
25	Y	609	CHL	C1D-C2D	2.57	1.50	1.45
26	1	603	CLA	CMB-C2B	-2.57	1.46	1.51
26	5	603	CLA	CMB-C2B	-2.57	1.46	1.51
26	6	602	CLA	CMB-C2B	-2.57	1.46	1.51
25	N	609	CHL	MG-NA	-2.57	2.00	2.06
38	d	405	PL9	C11-C9	-2.56	1.46	1.51
25	6	607	CHL	C1D-C2D	2.56	1.50	1.45
26	1	612	CLA	CMB-C2B	-2.56	1.46	1.51
26	5	612	CLA	CMB-C2B	-2.56	1.46	1.51
26	Y	614	CLA	CMD-C2D	-2.56	1.45	1.50
26	y	614	CLA	CMD-C2D	-2.56	1.45	1.50
25	8	606	CHL	C3D-C2D	2.56	1.46	1.39
26	A	405	CLA	C1D-ND	2.56	1.40	1.37
26	a	405	CLA	C1D-ND	2.56	1.40	1.37
35	A	408	PHO	CMB-C2B	-2.56	1.45	1.51
26	a	407	CLA	CHC-C1C	2.56	1.41	1.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	g	1621	LUT	C22-C21	-2.56	1.51	1.54
25	1	605	CHL	C1D-C2D	2.56	1.50	1.45
25	y	609	CHL	C1D-C2D	2.56	1.50	1.45
25	2	608	CHL	C1D-C2D	2.56	1.50	1.45
25	6	608	CHL	C1D-C2D	2.56	1.50	1.45
26	1	603	CLA	CHC-C1C	2.56	1.41	1.35
26	5	603	CLA	CHC-C1C	2.56	1.41	1.35
39	h	102	DGD	O1G-C1G	-2.56	1.39	1.45
26	c	510	CLA	C1D-ND	2.55	1.40	1.37
26	d	403	CLA	CMB-C2B	-2.55	1.46	1.51
35	a	409	PHO	CMC-C2C	-2.55	1.45	1.51
25	N	607	CHL	MG-NA	-2.55	2.00	2.06
26	C	511	CLA	CMD-C2D	-2.55	1.45	1.50
26	c	511	CLA	CMD-C2D	-2.55	1.45	1.50
26	1	613	CLA	CMB-C2B	-2.55	1.46	1.51
25	N	609	CHL	C3D-C2D	2.55	1.46	1.39
25	3	601	CHL	MG-NA	-2.55	2.00	2.06
25	2	607	CHL	C1D-C2D	2.55	1.50	1.45
26	N	602	CLA	CMB-C2B	-2.55	1.46	1.51
26	n	602	CLA	CMB-C2B	-2.55	1.46	1.51
25	7	605	CHL	MG-NA	-2.55	2.00	2.06
26	3	612	CLA	CHC-C1C	2.55	1.41	1.35
26	g	611	CLA	C3B-C2B	-2.54	1.36	1.40
26	B	602	CLA	CMC-C2C	-2.54	1.45	1.50
26	b	602	CLA	CMC-C2C	-2.54	1.45	1.50
26	c	501	CLA	CMD-C2D	-2.54	1.45	1.50
26	B	611	CLA	C1D-ND	2.54	1.40	1.37
26	b	611	CLA	C1D-ND	2.54	1.40	1.37
27	y	1620	LUT	C30-C29	-2.54	1.32	1.35
26	r	610	CLA	CMC-C2C	-2.54	1.45	1.50
26	1	602	CLA	C3B-C2B	-2.54	1.36	1.40
25	n	607	CHL	MG-NA	-2.54	2.00	2.06
25	4	607	CHL	C3D-C2D	2.54	1.46	1.39
26	4	610	CLA	C3B-C2B	-2.54	1.36	1.40
26	2	613	CLA	CMB-C2B	-2.54	1.46	1.51
26	6	613	CLA	CMB-C2B	-2.54	1.46	1.51
39	h	102	DGD	O2G-C2G	-2.54	1.40	1.46
25	4	606	CHL	C3D-C2D	2.54	1.46	1.39
26	c	501	CLA	CMB-C2B	-2.54	1.46	1.51
25	6	609	CHL	C3D-C2D	2.54	1.46	1.39
26	C	501	CLA	CMD-C2D	-2.54	1.45	1.50
25	n	609	CHL	C3D-C2D	2.54	1.46	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	7	602	CLA	C3B-C2B	-2.54	1.36	1.40
26	5	611	CLA	CMB-C2B	-2.53	1.46	1.51
26	1	611	CLA	CMB-C2B	-2.53	1.46	1.51
27	n	1621	LUT	C22-C21	-2.53	1.51	1.54
26	1	614	CLA	CMB-C2B	-2.53	1.46	1.51
26	5	614	CLA	CMB-C2B	-2.53	1.46	1.51
26	b	614	CLA	CMD-C2D	-2.53	1.45	1.50
30	1	2630	LHG	O7-C5	-2.53	1.40	1.46
25	3	605	CHL	MG-NA	-2.53	2.00	2.06
26	8	604	CLA	C3B-C2B	-2.53	1.36	1.40
26	C	502	CLA	MG-ND	-2.53	2.00	2.05
25	s	601	CHL	MG-NA	-2.53	2.00	2.06
39	H	102	DGD	O1G-C1G	-2.53	1.39	1.45
27	G	1621	LUT	C22-C21	-2.53	1.51	1.54
38	D	405	PL9	C11-C9	-2.53	1.46	1.51
26	D	403	CLA	CMB-C2B	-2.53	1.46	1.51
26	R	610	CLA	CMC-C2C	-2.53	1.45	1.50
26	3	611	CLA	CMD-C2D	-2.53	1.45	1.50
26	7	611	CLA	CMD-C2D	-2.53	1.45	1.50
26	s	602	CLA	CMD-C2D	-2.53	1.45	1.50
25	S	607	CHL	C1D-C2D	2.53	1.50	1.45
39	c	519	DGD	O2G-C2G	-2.53	1.40	1.46
30	5	2630	LHG	O7-C5	-2.52	1.40	1.46
26	N	611	CLA	CMB-C2B	-2.52	1.46	1.51
26	n	611	CLA	CMB-C2B	-2.52	1.46	1.51
39	C	519	DGD	O2G-C2G	-2.52	1.40	1.46
26	R	602	CLA	CMB-C2B	-2.52	1.46	1.51
26	r	602	CLA	CMB-C2B	-2.52	1.46	1.51
39	H	102	DGD	O2G-C2G	-2.52	1.40	1.46
26	6	614	CLA	CMB-C2B	-2.52	1.46	1.51
26	s	602	CLA	C1D-ND	2.52	1.40	1.37
25	8	607	CHL	C3D-C2D	2.52	1.46	1.39
26	C	510	CLA	C1D-ND	2.52	1.40	1.37
26	S	611	CLA	CMB-C2B	-2.52	1.46	1.51
26	s	611	CLA	CMB-C2B	-2.52	1.46	1.51
26	A	410	CLA	CMD-C2D	-2.52	1.45	1.50
26	B	615	CLA	CMC-C2C	-2.52	1.45	1.50
26	Y	603	CLA	CMD-C2D	-2.52	1.45	1.50
25	2	606	CHL	C1D-C2D	2.52	1.50	1.45
25	6	606	CHL	C1D-C2D	2.52	1.50	1.45
25	s	607	CHL	C1D-C2D	2.52	1.50	1.45
26	3	602	CLA	C3B-C2B	-2.52	1.36	1.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	614	CLA	CMD-C2D	-2.52	1.45	1.50
26	B	616	CLA	CHC-C1C	2.52	1.41	1.35
26	8	610	CLA	C3B-C2B	-2.51	1.36	1.40
35	A	408	PHO	CAC-C3C	-2.51	1.47	1.52
26	G	611	CLA	C3B-C2B	-2.51	1.36	1.40
26	6	612	CLA	CMB-C2B	-2.51	1.46	1.51
26	Y	604	CLA	CHC-C1C	2.51	1.41	1.35
26	y	604	CLA	CHC-C1C	2.51	1.41	1.35
25	S	601	CHL	MG-NA	-2.51	2.00	2.06
26	B	613	CLA	CMA-C3A	-2.51	1.47	1.53
25	S	606	CHL	C3D-C2D	2.51	1.46	1.39
25	s	606	CHL	C3D-C2D	2.51	1.46	1.39
26	S	602	CLA	CMD-C2D	-2.51	1.45	1.50
26	7	612	CLA	CHC-C1C	2.51	1.41	1.35
25	G	608	CHL	C1D-C2D	2.51	1.50	1.45
25	Y	605	CHL	C3D-C2D	2.51	1.46	1.39
26	B	612	CLA	C1D-ND	2.51	1.40	1.37
26	g	603	CLA	CMB-C2B	-2.51	1.46	1.51
26	G	611	CLA	CMD-C2D	-2.51	1.45	1.50
26	B	610	CLA	CHC-C1C	2.51	1.41	1.35
26	4	612	CLA	CMB-C2B	-2.51	1.46	1.51
26	y	603	CLA	CMD-C2D	-2.51	1.45	1.50
27	Y	1621	LUT	C22-C21	-2.51	1.51	1.54
26	G	603	CLA	CMB-C2B	-2.51	1.46	1.51
26	2	613	CLA	CMD-C2D	-2.51	1.45	1.50
26	6	613	CLA	CMD-C2D	-2.51	1.45	1.50
26	b	613	CLA	CMC-C2C	-2.51	1.45	1.50
25	2	609	CHL	C3D-C2D	2.51	1.46	1.39
26	G	613	CLA	CMB-C2B	-2.50	1.46	1.51
26	g	613	CLA	CMB-C2B	-2.50	1.46	1.51
26	C	504	CLA	C1D-ND	2.50	1.40	1.37
25	Y	608	CHL	OBD-CAD	2.50	1.26	1.22
26	C	508	CLA	C4B-CHC	-2.50	1.34	1.41
26	c	508	CLA	C4B-CHC	-2.50	1.34	1.41
26	2	612	CLA	CMB-C2B	-2.50	1.46	1.51
26	R	611	CLA	CMB-C2B	-2.50	1.46	1.51
26	3	612	CLA	CMD-C2D	-2.50	1.45	1.50
26	7	612	CLA	CMD-C2D	-2.50	1.45	1.50
25	6	601	CHL	MG-NA	-2.50	2.00	2.06
25	1	605	CHL	C3D-C2D	2.50	1.45	1.39
25	5	605	CHL	C3D-C2D	2.50	1.45	1.39
26	S	603	CLA	CMD-C2D	-2.50	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	1	601	CHL	MG-NA	-2.50	2.00	2.06
25	5	601	CHL	MG-NA	-2.50	2.00	2.06
25	Y	609	CHL	C3D-C2D	2.50	1.45	1.39
25	y	609	CHL	C3D-C2D	2.50	1.45	1.39
26	a	410	CLA	CMD-C2D	-2.50	1.45	1.50
25	N	609	CHL	C1D-C2D	2.50	1.50	1.45
25	n	609	CHL	C1D-C2D	2.50	1.50	1.45
26	1	602	CLA	C3B-CAB	-2.50	1.42	1.47
26	b	616	CLA	CHC-C1C	2.50	1.41	1.35
25	g	608	CHL	C1D-C2D	2.50	1.50	1.45
26	1	602	CLA	CMB-C2B	-2.50	1.46	1.51
26	5	602	CLA	CMB-C2B	-2.50	1.46	1.51
26	S	602	CLA	C1D-ND	2.50	1.40	1.37
26	s	603	CLA	CMD-C2D	-2.50	1.45	1.50
25	y	605	CHL	C3D-C2D	2.49	1.45	1.39
26	N	602	CLA	CMD-C2D	-2.49	1.45	1.50
26	2	614	CLA	CMB-C2B	-2.49	1.46	1.51
27	y	1621	LUT	C22-C21	-2.49	1.51	1.54
25	n	606	CHL	C3D-C2D	2.49	1.45	1.39
25	1	608	CHL	MG-NA	-2.49	2.00	2.06
26	b	613	CLA	CMA-C3A	-2.49	1.47	1.53
35	a	408	PHO	CAC-C3C	-2.49	1.47	1.52
26	c	502	CLA	MG-ND	-2.49	2.00	2.05
25	y	608	CHL	OBD-CAD	2.49	1.26	1.22
25	1	606	CHL	MG-NA	-2.49	2.00	2.06
25	r	614	CHL	C3D-C2D	2.49	1.45	1.39
26	y	604	CLA	MG-ND	-2.49	2.00	2.05
26	A	410	CLA	C1D-ND	2.48	1.40	1.37
26	a	410	CLA	C1D-ND	2.48	1.40	1.37
25	2	607	CHL	C3D-C2D	2.48	1.45	1.39
25	6	607	CHL	C3D-C2D	2.48	1.45	1.39
26	B	613	CLA	CMC-C2C	-2.48	1.45	1.50
25	R	614	CHL	C3D-C2D	2.48	1.45	1.39
26	g	611	CLA	CMD-C2D	-2.48	1.45	1.50
26	n	602	CLA	CMD-C2D	-2.48	1.45	1.50
26	R	611	CLA	C3B-C2B	-2.48	1.36	1.40
26	r	611	CLA	C3B-C2B	-2.48	1.36	1.40
26	b	612	CLA	C1D-ND	2.48	1.40	1.37
26	B	610	CLA	CMD-C2D	-2.48	1.45	1.50
25	N	606	CHL	C3D-C2D	2.48	1.45	1.39
26	c	509	CLA	MG-ND	-2.48	2.00	2.05
25	5	606	CHL	MG-NA	-2.48	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	4	602	CLA	CMB-C2B	-2.48	1.46	1.51
27	Y	1620	LUT	C30-C29	-2.47	1.32	1.35
26	b	610	CLA	CHC-C1C	2.47	1.41	1.35
26	b	615	CLA	CMC-C2C	-2.47	1.45	1.50
25	5	608	CHL	MG-NA	-2.47	2.00	2.06
26	C	509	CLA	MG-ND	-2.47	2.00	2.05
26	8	612	CLA	CMB-C2B	-2.47	1.46	1.51
26	B	603	CLA	CMD-C2D	-2.47	1.45	1.50
26	b	603	CLA	CMD-C2D	-2.47	1.45	1.50
25	Y	609	CHL	MG-NA	-2.47	2.00	2.06
25	y	609	CHL	MG-NA	-2.47	2.00	2.06
26	r	611	CLA	CMB-C2B	-2.47	1.46	1.51
26	N	602	CLA	CMC-C2C	-2.47	1.45	1.50
26	g	603	CLA	CMD-C2D	-2.47	1.45	1.50
26	n	602	CLA	CMC-C2C	-2.47	1.45	1.50
26	c	503	CLA	CMD-C2D	-2.47	1.45	1.50
26	C	513	CLA	CMC-C2C	-2.46	1.45	1.50
26	r	613	CLA	CMD-C2D	-2.46	1.45	1.50
26	8	602	CLA	CMB-C2B	-2.46	1.46	1.51
26	2	610	CLA	C3B-C2B	-2.46	1.36	1.40
26	6	610	CLA	C3B-C2B	-2.46	1.36	1.40
26	C	503	CLA	CMD-C2D	-2.46	1.45	1.50
25	2	601	CHL	MG-NA	-2.46	2.00	2.06
26	G	603	CLA	CMD-C2D	-2.46	1.45	1.50
26	4	604	CLA	C3B-C2B	-2.46	1.37	1.40
37	B	622	LMG	O7-C8	-2.46	1.40	1.46
26	5	602	CLA	C3B-CAB	-2.46	1.42	1.47
26	3	603	CLA	CHC-C1C	2.46	1.41	1.35
26	C	512	CLA	MG-ND	-2.46	2.00	2.05
26	c	512	CLA	MG-ND	-2.46	2.00	2.05
37	b	622	LMG	O7-C8	-2.46	1.40	1.46
26	Y	604	CLA	MG-ND	-2.46	2.00	2.05
26	c	513	CLA	CMC-C2C	-2.46	1.45	1.50
26	S	609	CLA	CMB-C2B	-2.46	1.46	1.51
26	c	504	CLA	C1D-ND	2.45	1.40	1.37
26	6	611	CLA	CMB-C2B	-2.45	1.46	1.51
26	5	613	CLA	CMD-C2D	-2.45	1.45	1.50
26	a	410	CLA	MG-ND	-2.45	2.00	2.05
25	n	605	CHL	C3D-C2D	2.45	1.45	1.39
26	7	603	CLA	CHC-C1C	2.44	1.41	1.35
25	G	606	CHL	C3D-C2D	2.44	1.45	1.39
25	g	606	CHL	C3D-C2D	2.44	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	S	603	CLA	CMB-C2B	-2.44	1.46	1.51
26	a	406	CLA	CHC-C1C	2.44	1.41	1.35
26	2	602	CLA	CMC-C2C	-2.44	1.45	1.50
26	2	602	CLA	CMD-C2D	-2.44	1.45	1.50
26	6	602	CLA	CMD-C2D	-2.44	1.45	1.50
26	c	507	CLA	C3B-C2B	-2.44	1.37	1.40
25	n	608	CHL	MG-NA	-2.44	2.00	2.06
28	Y	1622	XAT	C10-C9	-2.44	1.32	1.35
28	y	1622	XAT	C10-C9	-2.44	1.32	1.35
25	6	609	CHL	C1B-CHB	2.44	1.47	1.41
26	C	502	CLA	C4B-CHC	-2.44	1.34	1.41
26	4	611	CLA	CMB-C2B	-2.44	1.46	1.51
26	8	611	CLA	CMB-C2B	-2.44	1.46	1.51
30	3	2630	LHG	O7-C5	-2.44	1.40	1.46
25	g	609	CHL	MG-NA	-2.44	2.00	2.06
26	R	612	CLA	CMB-C2B	-2.44	1.46	1.51
26	b	610	CLA	CMD-C2D	-2.44	1.45	1.50
26	6	602	CLA	CMC-C2C	-2.44	1.45	1.50
25	G	605	CHL	MG-NA	-2.44	2.00	2.06
26	2	611	CLA	CMB-C2B	-2.44	1.46	1.51
25	5	605	CHL	MG-NA	-2.43	2.00	2.06
26	N	604	CLA	CMD-C2D	-2.43	1.45	1.50
26	R	609	CLA	CMB-C2B	-2.43	1.46	1.51
26	B	607	CLA	C3B-C2B	-2.43	1.37	1.40
26	1	602	CLA	CMC-C2C	-2.43	1.45	1.50
26	5	602	CLA	CMC-C2C	-2.43	1.45	1.50
30	G	2630	LHG	O7-C5	-2.43	1.40	1.46
30	g	2630	LHG	O7-C5	-2.43	1.40	1.46
39	C	520	DGD	O3G-C3G	-2.43	1.39	1.43
39	c	520	DGD	O3G-C3G	-2.43	1.39	1.43
39	C	519	DGD	O5D-C6D	-2.43	1.39	1.43
39	c	519	DGD	O5D-C6D	-2.43	1.39	1.43
25	2	609	CHL	C1B-CHB	2.43	1.47	1.41
26	N	612	CLA	CMB-C2B	-2.43	1.46	1.51
26	n	612	CLA	CMB-C2B	-2.43	1.46	1.51
25	N	605	CHL	C3D-C2D	2.43	1.45	1.39
26	6	612	CLA	C3B-C2B	-2.43	1.37	1.40
26	b	607	CLA	C3B-C2B	-2.43	1.37	1.40
26	2	604	CLA	C3B-C2B	-2.43	1.37	1.40
26	6	604	CLA	C3B-C2B	-2.43	1.37	1.40
26	2	603	CLA	CMD-C2D	-2.43	1.45	1.50
25	S	607	CHL	C3D-C2D	2.43	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	s	607	CHL	C3D-C2D	2.43	1.45	1.39
25	l	605	CHL	MG-NA	-2.43	2.00	2.06
26	r	611	CLA	MG-ND	-2.43	2.01	2.05
35	A	408	PHO	CMC-C2C	-2.42	1.45	1.51
35	a	408	PHO	CMC-C2C	-2.42	1.45	1.51
26	2	612	CLA	C3B-C2B	-2.42	1.37	1.40
26	A	406	CLA	CHC-C1C	2.42	1.41	1.35
26	r	612	CLA	CMB-C2B	-2.42	1.46	1.51
26	b	610	CLA	C1D-ND	2.42	1.40	1.37
26	s	609	CLA	CMB-C2B	-2.42	1.46	1.51
25	N	608	CHL	MG-NA	-2.42	2.00	2.06
26	G	612	CLA	CMB-C2B	-2.42	1.46	1.51
26	g	612	CLA	CMB-C2B	-2.42	1.46	1.51
26	R	613	CLA	CMD-C2D	-2.42	1.45	1.50
26	B	602	CLA	CMD-C2D	-2.42	1.45	1.50
26	6	603	CLA	C3B-C2B	-2.42	1.37	1.40
26	Y	602	CLA	CMD-C2D	-2.42	1.45	1.50
26	y	602	CLA	CMD-C2D	-2.42	1.45	1.50
26	1	613	CLA	CMD-C2D	-2.42	1.45	1.50
25	2	606	CHL	C4C-C3C	2.42	1.49	1.45
26	B	610	CLA	C1D-ND	2.42	1.40	1.37
26	R	611	CLA	MG-ND	-2.42	2.01	2.05
26	s	602	CLA	CMC-C2C	-2.42	1.45	1.50
26	S	602	CLA	CMC-C2C	-2.42	1.45	1.50
26	s	603	CLA	CMB-C2B	-2.42	1.46	1.51
25	8	607	CHL	C1B-CHB	2.42	1.47	1.41
26	3	612	CLA	CMC-C2C	-2.42	1.45	1.50
35	a	408	PHO	C3B-C2B	-2.41	1.37	1.40
26	n	604	CLA	CMD-C2D	-2.41	1.45	1.50
26	c	502	CLA	C4B-CHC	-2.41	1.34	1.41
26	A	410	CLA	MG-ND	-2.41	2.01	2.05
26	a	410	CLA	C3B-C2B	-2.41	1.37	1.40
26	g	613	CLA	CMD-C2D	-2.41	1.45	1.50
26	r	609	CLA	CMB-C2B	-2.41	1.46	1.51
26	G	613	CLA	CMD-C2D	-2.41	1.45	1.50
30	B	2630	LHG	O7-C5	-2.41	1.40	1.46
30	b	2630	LHG	O7-C5	-2.41	1.40	1.46
26	C	508	CLA	CHC-C1C	2.41	1.41	1.35
26	c	508	CLA	CHC-C1C	2.41	1.41	1.35
25	7	608	CHL	MG-NA	-2.41	2.00	2.06
39	C	519	DGD	O6D-C5D	-2.41	1.38	1.44
25	G	607	CHL	C1D-C2D	2.41	1.50	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
31	c	515	BCR	C21-C22	-2.41	1.32	1.35
26	2	603	CLA	C3B-C2B	-2.41	1.37	1.40
25	6	606	CHL	C3D-C2D	2.41	1.45	1.39
26	C	507	CLA	C3B-C2B	-2.41	1.37	1.40
25	3	608	CHL	MG-NA	-2.41	2.00	2.06
26	R	609	CLA	C3B-C2B	-2.41	1.37	1.40
26	r	609	CLA	C3B-C2B	-2.41	1.37	1.40
26	3	614	CLA	CMD-C2D	-2.41	1.45	1.50
26	7	612	CLA	CMC-C2C	-2.41	1.45	1.50
26	G	604	CLA	CMD-C2D	-2.40	1.45	1.50
25	S	606	CHL	C1B-CHB	2.40	1.47	1.41
25	s	606	CHL	C1B-CHB	2.40	1.47	1.41
25	8	607	CHL	C4C-C3C	2.40	1.49	1.45
35	A	408	PHO	C3B-C2B	-2.40	1.37	1.40
25	g	605	CHL	MG-NA	-2.40	2.00	2.06
25	2	606	CHL	C3D-C2D	2.40	1.45	1.39
30	7	2630	LHG	O7-C5	-2.40	1.40	1.46
25	g	607	CHL	C1D-C2D	2.40	1.50	1.45
35	A	408	PHO	CMD-C2D	-2.40	1.45	1.51
25	6	608	CHL	MG-NA	-2.40	2.00	2.06
31	b	618	BCR	C21-C22	-2.40	1.32	1.35
39	c	519	DGD	O6D-C5D	-2.40	1.38	1.44
31	C	515	BCR	C21-C22	-2.40	1.32	1.35
26	B	614	CLA	MG-ND	-2.40	2.01	2.05
26	C	506	CLA	CHC-C1C	2.40	1.41	1.35
26	R	603	CLA	MG-ND	-2.40	2.01	2.05
26	r	603	CLA	MG-ND	-2.40	2.01	2.05
26	b	614	CLA	MG-ND	-2.39	2.01	2.05
26	b	602	CLA	CMD-C2D	-2.39	1.45	1.50
25	G	609	CHL	MG-NA	-2.39	2.00	2.06
26	C	505	CLA	C1D-ND	2.39	1.40	1.37
26	c	505	CLA	C1D-ND	2.39	1.40	1.37
26	b	616	CLA	CMD-C2D	-2.39	1.45	1.50
26	b	605	CLA	CMC-C2C	-2.39	1.45	1.50
26	A	410	CLA	C3B-C2B	-2.39	1.37	1.40
26	C	504	CLA	CHC-C1C	2.39	1.41	1.35
31	B	618	BCR	C21-C22	-2.39	1.32	1.35
26	7	611	CLA	CHC-C1C	2.39	1.41	1.35
29	r	623	NEX	C30-C29	-2.39	1.32	1.35
25	2	609	CHL	C1D-C2D	2.39	1.50	1.45
25	4	607	CHL	C1B-CHB	2.39	1.47	1.41
26	6	603	CLA	CMD-C2D	-2.39	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	B	616	CLA	CMD-C2D	-2.39	1.45	1.50
30	B	2631	LHG	O7-C5	-2.39	1.40	1.46
26	c	504	CLA	CHC-C1C	2.38	1.41	1.35
25	g	609	CHL	C4C-C3C	2.38	1.49	1.45
26	N	602	CLA	MG-ND	-2.38	2.01	2.05
26	n	602	CLA	MG-ND	-2.38	2.01	2.05
26	N	614	CLA	CMB-C2B	-2.38	1.46	1.51
25	Y	606	CHL	MG-NA	-2.38	2.00	2.06
25	2	608	CHL	MG-NA	-2.38	2.00	2.06
26	3	611	CLA	CHC-C1C	2.38	1.41	1.35
26	b	617	CLA	CMB-C2B	-2.38	1.46	1.51
26	c	504	CLA	CMD-C2D	-2.38	1.45	1.50
30	n	2630	LHG	O7-C5	-2.38	1.40	1.46
26	c	503	CLA	MG-ND	-2.38	2.01	2.05
25	G	609	CHL	C3D-C2D	2.38	1.45	1.39
26	B	602	CLA	C3B-CAB	-2.38	1.43	1.47
26	b	602	CLA	C3B-CAB	-2.38	1.43	1.47
29	R	623	NEX	C30-C29	-2.37	1.32	1.35
39	C	518	DGD	O5D-C6D	-2.37	1.39	1.43
28	y	1622	XAT	C34-C33	-2.37	1.32	1.35
26	7	614	CLA	CMD-C2D	-2.37	1.45	1.50
26	7	603	CLA	MG-ND	-2.37	2.01	2.05
26	S	612	CLA	CMD-C2D	-2.37	1.45	1.50
26	g	604	CLA	CMD-C2D	-2.37	1.45	1.50
26	s	612	CLA	CMD-C2D	-2.37	1.45	1.50
30	C	2630	LHG	O7-C5	-2.37	1.40	1.46
26	C	513	CLA	CMB-C2B	-2.37	1.46	1.51
26	B	605	CLA	CMC-C2C	-2.37	1.45	1.50
28	Y	1622	XAT	C34-C33	-2.37	1.32	1.35
25	G	609	CHL	C4C-C3C	2.37	1.49	1.45
25	y	606	CHL	MG-NA	-2.37	2.00	2.06
30	N	2630	LHG	O7-C5	-2.37	1.40	1.46
25	6	609	CHL	C1D-C2D	2.37	1.50	1.45
35	a	408	PHO	CMD-C2D	-2.37	1.45	1.51
25	6	606	CHL	C4C-C3C	2.37	1.49	1.45
26	c	506	CLA	CHC-C1C	2.37	1.41	1.35
26	C	503	CLA	MG-ND	-2.37	2.01	2.05
25	1	606	CHL	C3D-C2D	2.37	1.45	1.39
25	5	606	CHL	C3D-C2D	2.37	1.45	1.39
26	n	614	CLA	CMB-C2B	-2.37	1.46	1.51
25	6	607	CHL	C4C-C3C	2.37	1.49	1.45
25	g	609	CHL	C3D-C2D	2.37	1.45	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	C	509	CLA	CMA-C3A	-2.37	1.48	1.53
26	c	509	CLA	CMA-C3A	-2.37	1.48	1.53
26	R	603	CLA	CMD-C2D	-2.37	1.45	1.50
26	c	502	CLA	C1D-ND	2.37	1.40	1.37
26	5	604	CLA	CMD-C2D	-2.37	1.45	1.50
26	B	605	CLA	CHC-C1C	2.37	1.41	1.35
26	b	605	CLA	CHC-C1C	2.37	1.41	1.35
25	n	606	CHL	C1D-C2D	2.36	1.50	1.45
25	4	607	CHL	C4C-C3C	2.36	1.49	1.45
26	c	513	CLA	CMB-C2B	-2.36	1.46	1.51
26	C	504	CLA	CMD-C2D	-2.36	1.45	1.50
30	R	2630	LHG	O7-C5	-2.36	1.40	1.46
39	c	518	DGD	O5D-C6D	-2.36	1.39	1.43
26	r	603	CLA	CMD-C2D	-2.36	1.45	1.50
26	B	610	CLA	CMC-C2C	-2.36	1.45	1.50
26	b	610	CLA	CMC-C2C	-2.36	1.45	1.50
25	R	606	CHL	C3D-C2D	2.36	1.45	1.39
25	G	607	CHL	C3D-C2D	2.36	1.45	1.39
25	g	607	CHL	C3D-C2D	2.36	1.45	1.39
26	B	606	CLA	C3B-C2B	-2.36	1.37	1.40
26	b	606	CLA	C3B-C2B	-2.36	1.37	1.40
37	Z	101	LMG	C7-C8	2.36	1.57	1.50
37	z	101	LMG	C7-C8	2.36	1.57	1.50
26	b	611	CLA	CMD-C2D	-2.36	1.45	1.50
26	n	603	CLA	CMC-C2C	-2.36	1.45	1.50
30	r	2630	LHG	O7-C5	-2.36	1.40	1.46
26	c	505	CLA	C4B-CHC	-2.35	1.34	1.41
25	7	608	CHL	C1D-C2D	2.35	1.50	1.45
26	N	613	CLA	CMB-C2B	-2.35	1.46	1.51
26	n	613	CLA	CMB-C2B	-2.35	1.46	1.51
26	b	611	CLA	C3B-C2B	-2.35	1.37	1.40
30	b	2631	LHG	O7-C5	-2.35	1.40	1.46
30	c	2630	LHG	O7-C5	-2.35	1.40	1.46
26	N	604	CLA	MG-ND	-2.35	2.01	2.05
26	n	604	CLA	MG-ND	-2.35	2.01	2.05
26	1	604	CLA	CMD-C2D	-2.35	1.45	1.50
26	B	611	CLA	CMD-C2D	-2.35	1.45	1.50
26	G	613	CLA	C3B-C2B	-2.35	1.37	1.40
25	4	608	CHL	C1D-C2D	2.35	1.50	1.45
25	3	608	CHL	C1D-C2D	2.35	1.50	1.45
26	3	603	CLA	MG-ND	-2.35	2.01	2.05
26	g	614	CLA	CMB-C2B	-2.35	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	2	607	CHL	C4C-C3C	2.35	1.49	1.45
26	C	505	CLA	C4B-CHC	-2.35	1.34	1.41
26	N	603	CLA	CMC-C2C	-2.35	1.45	1.50
26	b	604	CLA	CMC-C2C	-2.35	1.45	1.50
25	N	606	CHL	C1D-C2D	2.35	1.50	1.45
25	g	606	CHL	MG-NA	-2.34	2.00	2.06
25	r	606	CHL	C3D-C2D	2.34	1.45	1.39
26	B	604	CLA	CMC-C2C	-2.34	1.45	1.50
26	C	510	CLA	CMB-C2B	-2.34	1.46	1.51
26	c	510	CLA	CMB-C2B	-2.34	1.46	1.51
25	1	601	CHL	C4C-C3C	2.34	1.49	1.45
25	5	601	CHL	C4C-C3C	2.34	1.49	1.45
26	2	613	CLA	MG-ND	-2.34	2.01	2.05
25	3	605	CHL	C4B-CHC	2.34	1.47	1.41
25	7	605	CHL	C4B-CHC	2.34	1.47	1.41
26	3	604	CLA	C3B-C2B	-2.34	1.37	1.40
25	G	606	CHL	MG-NA	-2.34	2.00	2.06
26	7	611	CLA	C4B-CHC	-2.34	1.34	1.41
26	B	617	CLA	CMB-C2B	-2.34	1.46	1.51
26	B	616	CLA	CMC-C2C	-2.34	1.45	1.50
26	b	616	CLA	CMC-C2C	-2.34	1.45	1.50
27	6	1621	LUT	C22-C21	-2.34	1.51	1.54
26	c	502	CLA	CMD-C2D	-2.34	1.45	1.50
26	C	506	CLA	CMC-C2C	-2.34	1.45	1.50
26	c	507	CLA	CAC-C3C	-2.33	1.45	1.51
25	1	609	CHL	C3D-C2D	2.33	1.45	1.39
25	5	609	CHL	C3D-C2D	2.33	1.45	1.39
26	3	610	CLA	C3B-CAB	-2.33	1.43	1.47
26	c	506	CLA	CMC-C2C	-2.33	1.45	1.50
26	C	502	CLA	C1D-ND	2.33	1.40	1.37
26	C	507	CLA	CHC-C1C	2.33	1.40	1.35
26	Y	604	CLA	CMD-C2D	-2.33	1.45	1.50
26	y	604	CLA	CMD-C2D	-2.33	1.45	1.50
25	N	607	CHL	C3D-C2D	2.33	1.45	1.39
25	2	605	CHL	C4B-CHC	2.33	1.47	1.41
26	S	604	CLA	CMD-C2D	-2.33	1.45	1.50
25	g	608	CHL	MG-NA	-2.33	2.00	2.06
26	C	502	CLA	CMD-C2D	-2.33	1.45	1.50
26	R	610	CLA	CMD-C2D	-2.33	1.45	1.50
26	r	610	CLA	CMD-C2D	-2.33	1.45	1.50
25	4	601	CHL	C4B-CHC	2.33	1.47	1.41
25	8	601	CHL	C4B-CHC	2.33	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	n	603	CLA	MG-ND	-2.33	2.01	2.05
27	2	1621	LUT	C22-C21	-2.33	1.51	1.54
26	7	604	CLA	C3B-C2B	-2.32	1.37	1.40
25	3	606	CHL	C3D-C2D	2.32	1.45	1.39
25	7	606	CHL	C3D-C2D	2.32	1.45	1.39
25	3	606	CHL	MG-NA	-2.32	2.00	2.06
25	Y	605	CHL	C4B-CHC	2.32	1.47	1.41
25	y	605	CHL	C4B-CHC	2.32	1.47	1.41
26	6	613	CLA	MG-ND	-2.32	2.01	2.05
25	G	608	CHL	MG-NA	-2.32	2.00	2.06
26	s	614	CLA	CMD-C2D	-2.32	1.45	1.50
26	a	406	CLA	C4B-CHC	-2.32	1.34	1.41
26	S	614	CLA	CMB-C2B	-2.32	1.46	1.51
26	s	614	CLA	CMB-C2B	-2.32	1.46	1.51
26	B	615	CLA	C3B-C2B	-2.32	1.37	1.40
26	G	602	CLA	CMD-C2D	-2.32	1.45	1.50
26	g	602	CLA	CMD-C2D	-2.32	1.45	1.50
26	Y	611	CLA	CMC-C2C	-2.32	1.45	1.50
26	y	611	CLA	CMC-C2C	-2.32	1.45	1.50
26	s	604	CLA	CMD-C2D	-2.32	1.45	1.50
39	b	626	DGD	O3G-C3G	-2.32	1.39	1.43
26	S	614	CLA	CMD-C2D	-2.31	1.45	1.50
25	8	608	CHL	C1D-C2D	2.31	1.49	1.45
26	B	610	CLA	MG-ND	-2.31	2.01	2.05
26	y	614	CLA	MG-ND	-2.31	2.01	2.05
25	1	607	CHL	C3D-C2D	2.31	1.45	1.39
25	5	607	CHL	C3D-C2D	2.31	1.45	1.39
25	5	608	CHL	C1D-C2D	2.31	1.49	1.45
26	B	616	CLA	C4B-CHC	-2.31	1.34	1.41
26	4	610	CLA	CMD-C2D	-2.31	1.45	1.50
35	A	408	PHO	C1C-NC	-2.31	1.31	1.38
35	a	408	PHO	C1C-NC	-2.31	1.31	1.38
26	b	608	CLA	MG-ND	-2.31	2.01	2.05
31	C	517	BCR	C21-C22	-2.31	1.32	1.35
25	n	607	CHL	C3D-C2D	2.31	1.45	1.39
26	8	610	CLA	CMD-C2D	-2.31	1.45	1.50
25	6	605	CHL	C4B-CHC	2.31	1.47	1.41
26	G	614	CLA	CMB-C2B	-2.31	1.46	1.51
36	a	412	SQD	O2-C2	-2.31	1.37	1.43
26	N	603	CLA	MG-ND	-2.31	2.01	2.05
26	A	406	CLA	CMD-C2D	-2.31	1.45	1.50
26	a	406	CLA	CMD-C2D	-2.31	1.45	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	4	609	CHL	C4C-C3C	2.31	1.49	1.45
26	7	610	CLA	C3B-CAB	-2.31	1.43	1.47
26	b	616	CLA	C4B-CHC	-2.31	1.34	1.41
25	8	609	CHL	C4C-C3C	2.31	1.49	1.45
26	c	507	CLA	CHC-C1C	2.31	1.40	1.35
26	3	611	CLA	C4B-CHC	-2.31	1.34	1.41
26	S	610	CLA	C3B-CAB	-2.31	1.43	1.47
26	s	610	CLA	C3B-CAB	-2.31	1.43	1.47
26	b	615	CLA	C3B-C2B	-2.30	1.37	1.40
25	3	609	CHL	C4C-C3C	2.30	1.49	1.45
25	s	601	CHL	C4C-C3C	2.30	1.49	1.45
26	C	507	CLA	CAC-C3C	-2.30	1.45	1.51
26	R	604	CLA	CMD-C2D	-2.30	1.45	1.50
26	r	604	CLA	CMD-C2D	-2.30	1.45	1.50
25	3	607	CHL	C4C-C3C	2.30	1.49	1.45
26	B	608	CLA	MG-ND	-2.30	2.01	2.05
26	D	402	CLA	C3B-C2B	-2.30	1.37	1.40
26	g	613	CLA	C3B-C2B	-2.30	1.37	1.40
25	S	606	CHL	MG-NA	-2.30	2.00	2.06
25	s	606	CHL	MG-NA	-2.30	2.00	2.06
26	S	610	CLA	C3B-C2B	-2.30	1.37	1.40
26	s	610	CLA	C3B-C2B	-2.30	1.37	1.40
26	N	613	CLA	CMD-C2D	-2.30	1.45	1.50
26	n	613	CLA	CMD-C2D	-2.30	1.45	1.50
25	R	607	CHL	C1D-C2D	2.30	1.49	1.45
25	r	607	CHL	C1D-C2D	2.30	1.49	1.45
25	7	606	CHL	C1D-C2D	2.30	1.49	1.45
25	7	601	CHL	C4B-CHC	2.29	1.47	1.41
25	s	608	CHL	C1B-CHB	2.29	1.47	1.41
36	A	412	SQD	O2-C2	-2.29	1.37	1.43
26	7	610	CLA	CMC-C2C	-2.29	1.45	1.50
25	7	607	CHL	C4C-C3C	2.29	1.49	1.45
26	5	613	CLA	MG-ND	-2.29	2.01	2.05
26	Y	614	CLA	MG-ND	-2.29	2.01	2.05
26	c	512	CLA	C1D-ND	2.29	1.40	1.37
26	A	406	CLA	C4B-CHC	-2.29	1.34	1.41
26	A	410	CLA	C3B-CAB	-2.29	1.43	1.47
26	a	410	CLA	C3B-CAB	-2.29	1.43	1.47
25	1	606	CHL	C1D-C2D	2.29	1.49	1.45
26	d	402	CLA	C3B-C2B	-2.29	1.37	1.40
25	7	609	CHL	C4C-C3C	2.29	1.49	1.45
25	7	606	CHL	MG-NA	-2.29	2.00	2.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	y	604	CLA	C3B-C2B	-2.29	1.37	1.40
25	1	608	CHL	C1D-C2D	2.29	1.49	1.45
25	R	606	CHL	MG-NA	-2.29	2.00	2.06
26	3	603	CLA	CMD-C2D	-2.29	1.46	1.50
26	B	611	CLA	C3B-C2B	-2.29	1.37	1.40
25	2	606	CHL	MG-NA	-2.29	2.00	2.06
26	n	614	CLA	CMD-C2D	-2.29	1.46	1.50
25	S	601	CHL	C4C-C3C	2.29	1.49	1.45
25	4	601	CHL	C1B-CHB	2.29	1.47	1.41
25	8	601	CHL	C1B-CHB	2.29	1.47	1.41
25	6	606	CHL	MG-NA	-2.29	2.00	2.06
25	S	608	CHL	C1B-CHB	2.29	1.47	1.41
31	c	517	BCR	C21-C22	-2.28	1.32	1.35
26	1	613	CLA	MG-ND	-2.28	2.01	2.05
39	B	626	DGD	O3G-C3G	-2.28	1.39	1.43
26	y	613	CLA	MG-ND	-2.28	2.01	2.05
25	Y	605	CHL	C1D-C2D	2.28	1.49	1.45
25	2	608	CHL	C4B-CHC	2.28	1.47	1.41
26	c	507	CLA	C4B-CHC	-2.28	1.34	1.41
26	7	603	CLA	CMD-C2D	-2.28	1.46	1.50
26	R	612	CLA	C3B-C2B	-2.28	1.37	1.40
26	r	612	CLA	C3B-C2B	-2.28	1.37	1.40
26	7	611	CLA	MG-ND	-2.28	2.01	2.05
25	r	606	CHL	MG-NA	-2.28	2.00	2.06
26	1	612	CLA	CMD-C2D	-2.28	1.46	1.50
26	5	612	CLA	CMD-C2D	-2.28	1.46	1.50
25	3	606	CHL	C1D-C2D	2.28	1.49	1.45
26	6	604	CLA	CMD-C2D	-2.28	1.46	1.50
26	A	406	CLA	CAC-C3C	-2.28	1.45	1.51
26	b	610	CLA	MG-ND	-2.28	2.01	2.05
26	g	602	CLA	MG-ND	-2.28	2.01	2.05
26	c	507	CLA	CMD-C2D	-2.28	1.46	1.50
38	D	405	PL9	C16-C14	-2.28	1.46	1.51
38	d	405	PL9	C16-C14	-2.28	1.46	1.51
26	y	602	CLA	MG-ND	-2.27	2.01	2.05
26	C	507	CLA	C4B-CHC	-2.27	1.34	1.41
26	5	603	CLA	C3B-C2B	-2.27	1.37	1.40
26	a	405	CLA	C1C-NC	-2.27	1.34	1.37
25	3	601	CHL	C4B-CHC	2.27	1.47	1.41
25	2	608	CHL	C1B-CHB	2.27	1.47	1.41
25	6	608	CHL	C1B-CHB	2.27	1.47	1.41
26	6	603	CLA	MG-ND	-2.27	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	1	602	CLA	CMD-C2D	-2.27	1.46	1.50
26	2	604	CLA	CMD-C2D	-2.27	1.46	1.50
26	5	602	CLA	CMD-C2D	-2.27	1.46	1.50
35	A	409	PHO	C1C-NC	-2.27	1.31	1.38
25	1	601	CHL	C3D-C2D	2.27	1.45	1.39
26	B	607	CLA	CHC-C1C	2.27	1.40	1.35
25	6	608	CHL	C4B-CHC	2.27	1.47	1.41
26	b	607	CLA	CHC-C1C	2.27	1.40	1.35
26	3	611	CLA	MG-ND	-2.27	2.01	2.05
25	5	601	CHL	C3D-C2D	2.27	1.45	1.39
26	C	505	CLA	CMC-C2C	-2.27	1.46	1.50
25	4	608	CHL	C1B-CHB	2.27	1.47	1.41
25	8	608	CHL	C1B-CHB	2.27	1.47	1.41
25	y	605	CHL	C1D-C2D	2.27	1.49	1.45
25	4	608	CHL	C3D-C2D	2.27	1.45	1.39
25	8	608	CHL	C3D-C2D	2.27	1.45	1.39
26	R	601	CLA	CMB-C2B	-2.27	1.46	1.51
26	7	610	CLA	CMD-C2D	-2.27	1.46	1.50
26	S	613	CLA	CMD-C2D	-2.26	1.46	1.50
25	8	608	CHL	C4B-CHC	2.26	1.47	1.41
26	b	617	CLA	CMD-C2D	-2.26	1.46	1.50
25	N	609	CHL	C4C-C3C	2.26	1.48	1.45
26	B	614	CLA	CMC-C2C	-2.26	1.46	1.50
26	r	601	CLA	CMB-C2B	-2.26	1.46	1.51
25	5	606	CHL	C1D-C2D	2.26	1.49	1.45
35	a	409	PHO	C1C-NC	-2.26	1.31	1.38
26	G	614	CLA	CMD-C2D	-2.26	1.46	1.50
26	2	614	CLA	CMD-C2D	-2.26	1.46	1.50
26	G	602	CLA	MG-ND	-2.26	2.01	2.05
26	Y	602	CLA	MG-ND	-2.26	2.01	2.05
26	c	505	CLA	CMC-C2C	-2.26	1.46	1.50
26	g	614	CLA	CMD-C2D	-2.26	1.46	1.50
25	y	607	CHL	C1C-NC	-2.26	1.34	1.37
26	a	406	CLA	CAC-C3C	-2.26	1.45	1.51
26	D	403	CLA	CMD-C2D	-2.26	1.46	1.50
25	Y	607	CHL	C1C-NC	-2.26	1.34	1.37
26	b	611	CLA	MG-ND	-2.26	2.01	2.05
26	R	616	CLA	CMD-C2D	-2.26	1.46	1.50
26	r	616	CLA	CMD-C2D	-2.26	1.46	1.50
26	y	614	CLA	C3B-C2B	-2.25	1.37	1.40
26	N	614	CLA	CMD-C2D	-2.25	1.46	1.50
26	G	603	CLA	CAC-C3C	-2.25	1.45	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	N	606	CHL	C1B-CHB	2.25	1.47	1.41
26	s	613	CLA	CMD-C2D	-2.25	1.46	1.50
26	B	612	CLA	CMD-C2D	-2.25	1.46	1.50
26	b	612	CLA	CMD-C2D	-2.25	1.46	1.50
25	4	608	CHL	C4B-CHC	2.25	1.47	1.41
26	Y	603	CLA	MG-ND	-2.25	2.01	2.05
26	y	603	CLA	MG-ND	-2.25	2.01	2.05
25	r	607	CHL	C3D-C2D	2.25	1.45	1.39
26	g	603	CLA	CAC-C3C	-2.25	1.45	1.51
38	D	405	PL9	C31-C29	-2.25	1.46	1.51
38	d	405	PL9	C31-C29	-2.25	1.46	1.51
26	3	610	CLA	CMC-C2C	-2.25	1.46	1.50
26	3	613	CLA	CMD-C2D	-2.25	1.46	1.50
26	7	613	CLA	CMD-C2D	-2.25	1.46	1.50
26	2	611	CLA	C3B-C2B	-2.25	1.37	1.40
26	Y	604	CLA	C3B-C2B	-2.25	1.37	1.40
26	6	611	CLA	C3B-C2B	-2.25	1.37	1.40
36	b	623	SQD	O2-C2	-2.25	1.37	1.43
26	2	603	CLA	MG-ND	-2.25	2.01	2.05
25	2	605	CHL	C1B-CHB	2.25	1.47	1.41
25	6	605	CHL	C1B-CHB	2.25	1.47	1.41
26	4	603	CLA	MG-ND	-2.25	2.01	2.05
26	A	407	CLA	C3B-C2B	-2.25	1.37	1.40
25	N	608	CHL	C1D-C2D	2.25	1.49	1.45
25	n	608	CHL	C1D-C2D	2.25	1.49	1.45
26	1	603	CLA	MG-ND	-2.25	2.01	2.05
26	5	603	CLA	MG-ND	-2.25	2.01	2.05
26	C	505	CLA	CHC-C1C	2.25	1.40	1.35
26	b	605	CLA	C3B-C2B	-2.24	1.37	1.40
26	5	603	CLA	CMD-C2D	-2.24	1.46	1.50
25	R	607	CHL	C3D-C2D	2.24	1.45	1.39
26	b	604	CLA	C1D-ND	2.24	1.40	1.37
26	7	603	CLA	C4B-CHC	-2.24	1.34	1.41
26	B	617	CLA	CMD-C2D	-2.24	1.46	1.50
26	5	614	CLA	CMD-C2D	-2.24	1.46	1.50
26	C	507	CLA	CMD-C2D	-2.24	1.46	1.50
25	n	609	CHL	C4C-C3C	2.24	1.48	1.45
26	B	611	CLA	MG-ND	-2.24	2.01	2.05
26	Y	613	CLA	MG-ND	-2.24	2.01	2.05
26	A	407	CLA	CMD-C2D	-2.24	1.46	1.50
25	n	606	CHL	C1B-CHB	2.24	1.47	1.41
26	3	613	CLA	CMC-C2C	-2.24	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	505	CLA	CHC-C1C	2.24	1.40	1.35
26	3	610	CLA	CMD-C2D	-2.24	1.46	1.50
25	1	608	CHL	C1B-CHB	2.24	1.47	1.41
25	5	608	CHL	C1B-CHB	2.24	1.47	1.41
25	3	608	CHL	C3D-C2D	2.24	1.45	1.39
26	B	610	CLA	C4B-CHC	-2.24	1.34	1.41
26	b	610	CLA	C4B-CHC	-2.24	1.34	1.41
26	3	603	CLA	C4B-CHC	-2.23	1.34	1.41
26	6	614	CLA	CMD-C2D	-2.23	1.46	1.50
25	g	606	CHL	C4B-CHC	2.23	1.47	1.41
26	C	512	CLA	C1D-ND	2.23	1.40	1.37
25	G	606	CHL	C4B-CHC	2.23	1.47	1.41
25	2	608	CHL	C3D-C2D	2.23	1.45	1.39
25	S	601	CHL	C3D-C2D	2.23	1.45	1.39
25	6	608	CHL	C3D-C2D	2.23	1.45	1.39
25	s	601	CHL	C3D-C2D	2.23	1.45	1.39
26	B	603	CLA	CMC-C2C	-2.23	1.46	1.50
26	A	405	CLA	C1C-NC	-2.23	1.34	1.37
26	c	513	CLA	CMD-C2D	-2.23	1.46	1.50
36	B	623	SQD	O2-C2	-2.23	1.37	1.43
26	1	603	CLA	C3B-C2B	-2.23	1.37	1.40
26	7	613	CLA	CMC-C2C	-2.23	1.46	1.50
26	r	609	CLA	CMD-C2D	-2.23	1.46	1.50
26	b	614	CLA	CMC-C2C	-2.23	1.46	1.50
25	N	601	CHL	C4C-C3C	2.23	1.48	1.45
25	7	608	CHL	C3D-C2D	2.23	1.45	1.39
26	B	612	CLA	C4B-CHC	-2.22	1.34	1.41
26	1	610	CLA	CMD-C2D	-2.22	1.46	1.50
25	5	608	CHL	C4B-CHC	2.22	1.47	1.41
26	C	504	CLA	C4B-CHC	-2.22	1.34	1.41
26	4	610	CLA	CMC-C2C	-2.22	1.46	1.50
26	8	610	CLA	CMC-C2C	-2.22	1.46	1.50
26	N	604	CLA	CMC-C2C	-2.22	1.46	1.50
26	N	611	CLA	CMD-C2D	-2.22	1.46	1.50
26	n	611	CLA	CMD-C2D	-2.22	1.46	1.50
30	b	2631	LHG	P-O6	2.22	1.68	1.59
26	5	610	CLA	CMD-C2D	-2.22	1.46	1.50
25	G	607	CHL	C4B-CHC	2.22	1.47	1.41
25	g	607	CHL	C4B-CHC	2.22	1.47	1.41
25	Y	606	CHL	C1D-ND	-2.22	1.35	1.37
26	c	512	CLA	C3B-C2B	-2.22	1.37	1.40
26	1	614	CLA	CMD-C2D	-2.22	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	c	508	CLA	CMD-C2D	-2.22	1.46	1.50
25	1	608	CHL	C4B-CHC	2.22	1.47	1.41
25	y	606	CHL	C1D-ND	-2.22	1.35	1.37
26	8	603	CLA	MG-ND	-2.22	2.01	2.05
30	B	2631	LHG	P-O6	2.22	1.68	1.59
26	d	403	CLA	CMD-C2D	-2.22	1.46	1.50
26	8	612	CLA	C3B-C2B	-2.22	1.37	1.40
26	a	407	CLA	CMD-C2D	-2.22	1.46	1.50
26	B	607	CLA	C4B-CHC	-2.22	1.34	1.41
26	b	607	CLA	C4B-CHC	-2.22	1.34	1.41
26	B	604	CLA	C1D-ND	2.21	1.40	1.37
36	B	623	SQD	O4-C4	-2.21	1.37	1.43
25	G	606	CHL	C4C-C3C	2.21	1.48	1.45
25	g	606	CHL	C4C-C3C	2.21	1.48	1.45
26	4	612	CLA	C3B-C2B	-2.21	1.37	1.40
26	b	612	CLA	C4B-CHC	-2.21	1.34	1.41
26	S	612	CLA	CMC-C2C	-2.21	1.46	1.50
26	s	612	CLA	CMC-C2C	-2.21	1.46	1.50
25	R	614	CHL	C1B-CHB	2.21	1.47	1.41
26	Y	610	CLA	C3B-CAB	-2.21	1.43	1.47
26	y	610	CLA	C3B-CAB	-2.21	1.43	1.47
26	C	508	CLA	CMD-C2D	-2.21	1.46	1.50
26	D	402	CLA	CMA-C3A	-2.21	1.48	1.53
26	d	402	CLA	CMA-C3A	-2.21	1.48	1.53
26	Y	613	CLA	C3B-C2B	-2.21	1.37	1.40
26	y	613	CLA	C3B-C2B	-2.21	1.37	1.40
25	3	605	CHL	C1B-CHB	2.21	1.47	1.41
26	5	611	CLA	C3B-C2B	-2.21	1.37	1.40
26	Y	603	CLA	CMC-C2C	-2.21	1.46	1.50
26	n	604	CLA	CMC-C2C	-2.21	1.46	1.50
26	y	603	CLA	CMC-C2C	-2.21	1.46	1.50
26	S	611	CLA	CMD-C2D	-2.21	1.46	1.50
39	C	520	DGD	O2E-C2E	-2.21	1.37	1.43
39	c	520	DGD	O2E-C2E	-2.21	1.37	1.43
26	s	611	CLA	CMD-C2D	-2.21	1.46	1.50
26	A	407	CLA	C4B-CHC	-2.21	1.34	1.41
26	a	407	CLA	C4B-CHC	-2.21	1.34	1.41
26	Y	612	CLA	CMC-C2C	-2.21	1.46	1.50
26	s	611	CLA	CMC-C2C	-2.21	1.46	1.50
26	B	606	CLA	C3B-CAB	-2.20	1.43	1.47
26	1	603	CLA	CMD-C2D	-2.20	1.46	1.50
26	A	410	CLA	CMC-C2C	-2.20	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	a	410	CLA	CMC-C2C	-2.20	1.46	1.50
25	r	614	CHL	C1B-CHB	2.20	1.47	1.41
26	c	504	CLA	C4B-CHC	-2.20	1.34	1.41
26	B	607	CLA	MG-ND	-2.20	2.01	2.05
26	b	607	CLA	MG-ND	-2.20	2.01	2.05
26	Y	614	CLA	C3B-C2B	-2.20	1.37	1.40
25	n	601	CHL	C4C-C3C	2.20	1.48	1.45
26	N	612	CLA	CMD-C2D	-2.20	1.46	1.50
26	n	612	CLA	CMD-C2D	-2.20	1.46	1.50
26	3	602	CLA	C3B-CAB	-2.20	1.43	1.47
26	7	602	CLA	C3B-CAB	-2.20	1.43	1.47
25	7	605	CHL	C1B-CHB	2.20	1.47	1.41
26	y	612	CLA	CMC-C2C	-2.20	1.46	1.50
26	a	407	CLA	C3B-C2B	-2.20	1.37	1.40
36	b	623	SQD	O4-C4	-2.20	1.37	1.43
25	N	601	CHL	C4B-CHC	2.20	1.47	1.41
25	n	601	CHL	C4B-CHC	2.20	1.47	1.41
39	c	520	DGD	O4D-C4D	-2.20	1.37	1.43
26	C	512	CLA	C3B-C2B	-2.20	1.37	1.40
26	R	612	CLA	CMD-C2D	-2.20	1.46	1.50
26	7	613	CLA	MG-ND	-2.20	2.01	2.05
31	C	514	BCR	C21-C22	-2.20	1.32	1.35
39	C	520	DGD	O4D-C4D	-2.20	1.37	1.43
29	r	623	NEX	O24-C25	-2.19	1.43	1.46
39	C	520	DGD	O3D-C3D	-2.19	1.37	1.43
39	c	520	DGD	O3D-C3D	-2.19	1.37	1.43
26	b	603	CLA	CMC-C2C	-2.19	1.46	1.50
26	C	511	CLA	CMC-C2C	-2.19	1.46	1.50
26	c	511	CLA	CMC-C2C	-2.19	1.46	1.50
30	D	410	LHG	O7-C5	-2.19	1.41	1.46
25	Y	609	CHL	C1B-NB	-2.19	1.33	1.35
25	y	609	CHL	C1B-NB	-2.19	1.33	1.35
26	r	612	CLA	CMD-C2D	-2.19	1.46	1.50
26	B	605	CLA	C3B-C2B	-2.19	1.37	1.40
26	b	606	CLA	C3B-CAB	-2.19	1.43	1.47
26	b	605	CLA	C4B-CHC	-2.19	1.34	1.41
26	S	611	CLA	CMC-C2C	-2.19	1.46	1.50
26	c	504	CLA	MG-ND	-2.19	2.01	2.05
26	1	612	CLA	C4B-CHC	-2.19	1.34	1.41
26	5	612	CLA	C4B-CHC	-2.19	1.34	1.41
25	R	606	CHL	C4B-CHC	2.19	1.47	1.41
25	r	606	CHL	C4B-CHC	2.19	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R	609	CLA	CMD-C2D	-2.19	1.46	1.50
26	N	610	CLA	CMD-C2D	-2.19	1.46	1.50
26	n	610	CLA	CMD-C2D	-2.19	1.46	1.50
29	R	623	NEX	O24-C25	-2.18	1.43	1.46
25	n	606	CHL	C4B-CHC	2.18	1.47	1.41
26	C	513	CLA	CMD-C2D	-2.18	1.46	1.50
26	5	602	CLA	MG-ND	-2.18	2.01	2.05
26	5	603	CLA	C4B-CHC	-2.18	1.34	1.41
25	4	606	CHL	C4C-C3C	2.18	1.48	1.45
25	8	606	CHL	C4C-C3C	2.18	1.48	1.45
26	S	602	CLA	MG-ND	-2.18	2.01	2.05
26	s	602	CLA	MG-ND	-2.18	2.01	2.05
25	7	606	CHL	C4B-CHC	2.18	1.47	1.41
30	d	410	LHG	O7-C5	-2.18	1.41	1.46
26	1	614	CLA	C3B-C2B	-2.18	1.37	1.40
26	5	614	CLA	C3B-C2B	-2.18	1.37	1.40
25	3	606	CHL	C4B-CHC	2.17	1.47	1.41
26	S	612	CLA	CMB-C2B	-2.17	1.47	1.51
36	A	418	SQD	O2-C2	-2.17	1.37	1.43
26	c	503	CLA	CMC-C2C	-2.17	1.46	1.50
25	1	601	CHL	C4B-CHC	2.17	1.47	1.41
25	5	601	CHL	C4B-CHC	2.17	1.47	1.41
26	C	504	CLA	MG-ND	-2.17	2.01	2.05
26	g	604	CLA	MG-ND	-2.17	2.01	2.05
26	1	603	CLA	C4B-CHC	-2.17	1.35	1.41
26	B	608	CLA	CHC-C1C	2.17	1.40	1.35
26	1	610	CLA	CMC-C2C	-2.17	1.46	1.50
25	N	606	CHL	C4B-CHC	2.17	1.47	1.41
26	B	613	CLA	C3B-CAB	-2.17	1.43	1.47
25	4	606	CHL	C4B-CHC	2.17	1.47	1.41
39	C	519	DGD	O4E-C4E	-2.17	1.37	1.43
26	R	611	CLA	CHC-C1C	2.17	1.40	1.35
25	N	608	CHL	C4B-CHC	2.17	1.47	1.41
26	B	604	CLA	C4B-CHC	-2.17	1.35	1.41
38	D	405	PL9	C46-C44	-2.17	1.46	1.51
38	d	405	PL9	C46-C44	-2.17	1.46	1.51
25	g	608	CHL	C4C-C3C	2.17	1.48	1.45
26	b	608	CLA	CHC-C1C	2.17	1.40	1.35
26	1	611	CLA	C3B-C2B	-2.17	1.37	1.40
26	S	609	CLA	C3B-C2B	-2.17	1.37	1.40
26	s	609	CLA	C3B-C2B	-2.17	1.37	1.40
25	n	605	CHL	C4C-C3C	2.17	1.48	1.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	8	606	CHL	C4B-CHC	2.17	1.47	1.41
25	8	601	CHL	C4C-C3C	2.17	1.48	1.45
26	C	503	CLA	CMC-C2C	-2.17	1.46	1.50
26	N	613	CLA	CMC-C2C	-2.17	1.46	1.50
26	N	603	CLA	CAC-C3C	-2.17	1.45	1.51
26	n	603	CLA	CAC-C3C	-2.17	1.45	1.51
39	c	519	DGD	O4E-C4E	-2.17	1.37	1.43
25	N	606	CHL	MG-NA	-2.17	2.01	2.06
25	n	606	CHL	MG-NA	-2.17	2.01	2.06
26	C	504	CLA	CMC-C2C	-2.17	1.46	1.50
26	1	613	CLA	C3B-C2B	-2.17	1.37	1.40
25	3	605	CHL	C4C-C3C	2.17	1.48	1.45
26	n	613	CLA	CMC-C2C	-2.17	1.46	1.50
28	3	1622	XAT	C34-C33	-2.17	1.32	1.35
28	7	1622	XAT	C34-C33	-2.17	1.32	1.35
26	R	616	CLA	C3B-C2B	-2.16	1.37	1.40
27	R	620	LUT	C30-C29	-2.16	1.32	1.35
27	r	620	LUT	C30-C29	-2.16	1.32	1.35
25	2	609	CHL	C4C-C3C	2.16	1.48	1.45
25	6	609	CHL	C4C-C3C	2.16	1.48	1.45
26	8	603	CLA	CMD-C2D	-2.16	1.46	1.50
25	7	605	CHL	C4C-C3C	2.16	1.48	1.45
25	g	605	CHL	C1B-CHB	2.16	1.47	1.41
25	n	608	CHL	C4B-CHC	2.16	1.47	1.41
26	n	613	CLA	MG-ND	-2.16	2.01	2.05
26	3	613	CLA	MG-ND	-2.16	2.01	2.05
25	1	605	CHL	C4B-CHC	2.16	1.47	1.41
26	B	605	CLA	C4B-CHC	-2.16	1.35	1.41
26	s	603	CLA	C3B-C2B	-2.16	1.37	1.40
25	g	609	CHL	C1B-NB	-2.16	1.33	1.35
26	5	610	CLA	CMC-C2C	-2.16	1.46	1.50
25	G	605	CHL	C1B-CHB	2.16	1.47	1.41
26	B	609	CLA	MG-ND	-2.16	2.01	2.05
26	b	609	CLA	MG-ND	-2.16	2.01	2.05
26	c	504	CLA	CMC-C2C	-2.16	1.46	1.50
25	N	605	CHL	C4C-C3C	2.16	1.48	1.45
26	R	613	CLA	C3B-C2B	-2.16	1.37	1.40
26	r	613	CLA	C3B-C2B	-2.16	1.37	1.40
25	N	606	CHL	C4C-C3C	2.16	1.48	1.45
26	B	611	CLA	C3B-CAB	-2.16	1.43	1.47
26	y	604	CLA	CMC-C2C	-2.16	1.46	1.50
25	2	606	CHL	C4B-CHC	2.16	1.47	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	3	607	CHL	C4B-CHC	2.16	1.47	1.41
26	R	602	CLA	CMD-C2D	-2.16	1.46	1.50
26	r	602	CLA	CMD-C2D	-2.16	1.46	1.50
25	5	605	CHL	C4B-CHC	2.16	1.47	1.41
26	1	611	CLA	CMD-C2D	-2.16	1.46	1.50
26	5	611	CLA	CMD-C2D	-2.16	1.46	1.50
31	c	514	BCR	C21-C22	-2.16	1.32	1.35
31	C	515	BCR	C10-C9	-2.15	1.32	1.35
26	s	612	CLA	CMB-C2B	-2.15	1.47	1.51
26	4	603	CLA	C3B-C2B	-2.15	1.37	1.40
26	8	603	CLA	C3B-C2B	-2.15	1.37	1.40
26	C	501	CLA	CMC-C2C	-2.15	1.46	1.50
25	7	607	CHL	C4B-CHC	2.15	1.47	1.41
36	A	412	SQD	O4-C4	-2.15	1.37	1.43
36	a	412	SQD	O4-C4	-2.15	1.37	1.43
26	B	606	CLA	MG-ND	-2.15	2.01	2.05
26	4	603	CLA	CMD-C2D	-2.15	1.46	1.50
26	b	615	CLA	C3B-CAB	-2.15	1.43	1.47
26	c	504	CLA	CAC-C3C	-2.15	1.45	1.51
26	G	604	CLA	MG-ND	-2.15	2.01	2.05
26	4	610	CLA	C3B-CAB	-2.15	1.43	1.47
26	8	610	CLA	C3B-CAB	-2.15	1.43	1.47
25	4	606	CHL	C1B-CHB	2.15	1.47	1.41
25	7	609	CHL	C1B-CHB	2.15	1.47	1.41
25	8	606	CHL	C1B-CHB	2.15	1.47	1.41
26	S	604	CLA	MG-ND	-2.15	2.01	2.05
26	C	506	CLA	C4B-CHC	-2.15	1.35	1.41
26	c	506	CLA	C4B-CHC	-2.15	1.35	1.41
26	c	511	CLA	CMA-C3A	-2.15	1.48	1.53
39	B	626	DGD	O1G-C1G	-2.15	1.40	1.45
39	b	626	DGD	O1G-C1G	-2.15	1.40	1.45
25	3	606	CHL	C4C-C3C	2.15	1.48	1.45
25	7	606	CHL	C4C-C3C	2.15	1.48	1.45
25	s	608	CHL	C1C-NC	-2.15	1.34	1.37
26	b	606	CLA	MG-ND	-2.15	2.01	2.05
26	r	611	CLA	CHC-C1C	2.15	1.40	1.35
25	n	606	CHL	C4C-C3C	2.15	1.48	1.45
26	b	604	CLA	C4B-CHC	-2.15	1.35	1.41
26	b	611	CLA	C3B-CAB	-2.15	1.43	1.47
25	S	608	CHL	C1D-C2D	2.15	1.49	1.45
25	s	608	CHL	C1D-C2D	2.15	1.49	1.45
26	s	604	CLA	MG-ND	-2.14	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	Y	607	CHL	C3D-C2D	2.14	1.45	1.39
26	b	613	CLA	C3B-CAB	-2.14	1.43	1.47
37	B	2633	LMG	C3-C2	2.14	1.57	1.52
37	b	2633	LMG	C3-C2	2.14	1.57	1.52
39	H	102	DGD	O2D-C2D	-2.14	1.37	1.43
39	h	102	DGD	O2D-C2D	-2.14	1.37	1.43
25	y	607	CHL	C3D-C2D	2.14	1.45	1.39
26	B	615	CLA	C3B-CAB	-2.14	1.43	1.47
26	c	506	CLA	CMD-C2D	-2.14	1.46	1.50
26	c	509	CLA	C3B-CAB	-2.14	1.43	1.47
25	N	607	CHL	C1C-NC	-2.14	1.34	1.37
26	1	604	CLA	MG-ND	-2.14	2.01	2.05
27	S	1621	LUT	C30-C29	-2.14	1.32	1.35
25	N	605	CHL	C1D-C2D	2.14	1.49	1.45
25	n	605	CHL	C1D-C2D	2.14	1.49	1.45
25	6	606	CHL	C4B-CHC	2.14	1.46	1.41
25	7	608	CHL	C1B-CHB	2.14	1.46	1.41
25	n	607	CHL	C1C-NC	-2.14	1.34	1.37
26	B	606	CLA	C4B-CHC	-2.14	1.35	1.41
26	b	606	CLA	C4B-CHC	-2.14	1.35	1.41
37	D	411	LMG	O7-C8	-2.14	1.41	1.46
37	d	411	LMG	O7-C8	-2.14	1.41	1.46
36	a	418	SQD	O2-C2	-2.14	1.37	1.43
25	3	609	CHL	C1B-CHB	2.14	1.46	1.41
26	4	602	CLA	CMD-C2D	-2.14	1.46	1.50
26	8	602	CLA	CMD-C2D	-2.14	1.46	1.50
26	C	507	CLA	C3B-CAB	-2.14	1.43	1.47
28	3	1622	XAT	O4-C5	-2.14	1.43	1.46
28	7	1622	XAT	O4-C5	-2.14	1.43	1.46
26	Y	613	CLA	CMC-C2C	-2.14	1.46	1.50
26	6	613	CLA	C3B-C2B	-2.14	1.37	1.40
25	y	608	CHL	C1D-C2D	2.14	1.49	1.45
26	3	602	CLA	CMD-C2D	-2.14	1.46	1.50
26	Y	604	CLA	CMC-C2C	-2.14	1.46	1.50
26	7	602	CLA	CMD-C2D	-2.14	1.46	1.50
39	H	102	DGD	O2E-C2E	-2.14	1.37	1.43
39	h	102	DGD	O2E-C2E	-2.14	1.37	1.43
26	1	602	CLA	MG-ND	-2.14	2.01	2.05
36	A	418	SQD	O3-C3	-2.13	1.37	1.43
36	a	418	SQD	O3-C3	-2.13	1.37	1.43
26	r	616	CLA	C3B-C2B	-2.13	1.37	1.40
38	d	405	PL9	C36-C34	-2.13	1.46	1.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	G	609	CHL	C1B-NB	-2.13	1.33	1.35
26	y	613	CLA	CMC-C2C	-2.13	1.46	1.50
36	A	412	SQD	O47-C45	-2.13	1.41	1.46
25	Y	605	CHL	C1B-CHB	2.13	1.46	1.41
25	y	605	CHL	C1B-CHB	2.13	1.46	1.41
26	4	602	CLA	CMC-C2C	-2.13	1.46	1.50
27	s	1621	LUT	C30-C29	-2.13	1.33	1.35
31	c	515	BCR	C10-C9	-2.13	1.33	1.35
26	6	612	CLA	CMD-C2D	-2.13	1.46	1.50
25	Y	608	CHL	C3D-C2D	2.13	1.44	1.39
25	y	608	CHL	C3D-C2D	2.13	1.44	1.39
26	N	613	CLA	MG-ND	-2.13	2.01	2.05
26	Y	604	CLA	C4B-CHC	-2.13	1.35	1.41
26	c	501	CLA	CMC-C2C	-2.13	1.46	1.50
26	C	512	CLA	CMC-C2C	-2.13	1.46	1.50
26	c	512	CLA	CMC-C2C	-2.13	1.46	1.50
25	S	608	CHL	C1C-NC	-2.13	1.34	1.37
26	s	611	CLA	MG-ND	-2.13	2.01	2.05
26	C	502	CLA	CHC-C1C	2.13	1.40	1.35
26	c	502	CLA	CHC-C1C	2.13	1.40	1.35
26	C	506	CLA	CMD-C2D	-2.13	1.46	1.50
26	2	612	CLA	CMD-C2D	-2.13	1.46	1.50
26	C	504	CLA	CAC-C3C	-2.13	1.45	1.51
25	Y	608	CHL	C1D-C2D	2.13	1.49	1.45
27	7	1621	LUT	C22-C21	-2.12	1.52	1.54
26	5	604	CLA	MG-ND	-2.12	2.01	2.05
25	Y	608	CHL	C1C-NC	-2.12	1.34	1.37
26	S	613	CLA	CMC-C2C	-2.12	1.46	1.50
26	S	611	CLA	MG-ND	-2.12	2.01	2.05
25	4	601	CHL	C4C-C3C	2.12	1.48	1.45
25	G	608	CHL	C4C-C3C	2.12	1.48	1.45
26	B	606	CLA	CMA-C3A	-2.12	1.48	1.53
26	c	507	CLA	C3B-CAB	-2.12	1.43	1.47
26	R	611	CLA	CMD-C2D	-2.12	1.46	1.50
26	r	611	CLA	CMD-C2D	-2.12	1.46	1.50
26	8	602	CLA	CMC-C2C	-2.12	1.46	1.50
25	7	607	CHL	C4D-CHA	2.12	1.45	1.38
26	s	613	CLA	CMC-C2C	-2.12	1.46	1.50
26	C	509	CLA	C3B-CAB	-2.12	1.43	1.47
26	N	611	CLA	C3B-C2B	-2.12	1.37	1.40
26	n	611	CLA	C3B-C2B	-2.12	1.37	1.40
26	C	511	CLA	CMA-C3A	-2.12	1.48	1.53

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	s	611	CLA	C3B-CAB	-2.11	1.43	1.47
26	G	603	CLA	CMC-C2C	-2.11	1.46	1.50
26	g	603	CLA	CMC-C2C	-2.11	1.46	1.50
38	D	405	PL9	C36-C34	-2.11	1.46	1.51
27	1	1621	LUT	C22-C21	-2.11	1.52	1.54
25	3	608	CHL	C1B-CHB	2.11	1.46	1.41
26	C	508	CLA	MG-ND	-2.11	2.01	2.05
37	C	521	LMG	O1-C7	-2.11	1.39	1.43
26	y	604	CLA	C4B-CHC	-2.11	1.35	1.41
25	4	609	CHL	C1B-CHB	2.11	1.46	1.41
25	8	609	CHL	C1B-CHB	2.11	1.46	1.41
25	8	609	CHL	C4B-CHC	2.11	1.46	1.41
25	S	608	CHL	C3D-C2D	2.11	1.44	1.39
26	8	604	CLA	CMD-C2D	-2.11	1.46	1.50
36	a	412	SQD	O47-C45	-2.11	1.41	1.46
26	8	603	CLA	CMC-C2C	-2.11	1.46	1.50
26	y	603	CLA	CAC-C3C	-2.11	1.45	1.51
26	B	615	CLA	MG-ND	-2.11	2.01	2.05
26	b	615	CLA	MG-ND	-2.11	2.01	2.05
26	N	610	CLA	CMC-C2C	-2.11	1.46	1.50
25	1	601	CHL	C1B-CHB	2.11	1.46	1.41
25	y	608	CHL	C1C-NC	-2.11	1.34	1.37
28	4	622	XAT	O4-C5	-2.11	1.43	1.46
26	1	613	CLA	CMC-C2C	-2.11	1.46	1.50
30	y	2630	LHG	O8-C6	-2.11	1.40	1.45
25	g	608	CHL	C4B-CHC	2.11	1.46	1.41
26	C	509	CLA	C4B-CHC	-2.11	1.35	1.41
26	c	509	CLA	C4B-CHC	-2.11	1.35	1.41
26	g	610	CLA	CMD-C2D	-2.11	1.46	1.50
26	N	612	CLA	CMC-C2C	-2.10	1.46	1.50
26	5	613	CLA	CMC-C2C	-2.10	1.46	1.50
28	8	622	XAT	O4-C5	-2.10	1.43	1.46
27	3	1621	LUT	C22-C21	-2.10	1.52	1.54
25	1	606	CHL	C1B-CHB	2.10	1.46	1.41
26	6	613	CLA	CMC-C2C	-2.10	1.46	1.50
27	1	1621	LUT	C1-C6	-2.10	1.50	1.53
28	G	1622	XAT	O4-C5	-2.10	1.43	1.46
25	2	601	CHL	C3D-C2D	2.10	1.44	1.39
25	6	601	CHL	C3D-C2D	2.10	1.44	1.39
25	2	601	CHL	C4B-CHC	2.10	1.46	1.41
25	3	607	CHL	C4D-CHA	2.10	1.45	1.38
25	5	608	CHL	C3D-C2D	2.10	1.44	1.39

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	Y	603	CLA	CAC-C3C	-2.10	1.45	1.51
26	c	508	CLA	MG-ND	-2.10	2.01	2.05
37	C	521	LMG	C4-C5	2.10	1.57	1.53
26	2	611	CLA	CMD-C2D	-2.10	1.46	1.50
26	6	611	CLA	CMD-C2D	-2.10	1.46	1.50
26	7	604	CLA	CMC-C2C	-2.10	1.46	1.50
26	3	612	CLA	MG-ND	-2.10	2.01	2.05
26	7	612	CLA	MG-ND	-2.10	2.01	2.05
26	c	505	CLA	C3B-C2B	-2.10	1.37	1.40
36	B	621	SQD	O2-C2	-2.10	1.38	1.43
26	g	603	CLA	MG-ND	-2.10	2.01	2.05
26	s	603	CLA	MG-ND	-2.10	2.01	2.05
26	5	613	CLA	C3B-C2B	-2.10	1.37	1.40
26	a	405	CLA	MG-ND	-2.09	2.01	2.05
26	3	604	CLA	CMC-C2C	-2.09	1.46	1.50
26	2	613	CLA	CMC-C2C	-2.09	1.46	1.50
25	2	606	CHL	C1B-CHB	2.09	1.46	1.41
25	G	608	CHL	C4B-CHC	2.09	1.46	1.41
25	5	601	CHL	C1B-CHB	2.09	1.46	1.41
25	6	606	CHL	C1B-CHB	2.09	1.46	1.41
26	4	612	CLA	CMD-C2D	-2.09	1.46	1.50
26	8	612	CLA	CMD-C2D	-2.09	1.46	1.50
26	n	610	CLA	CMC-C2C	-2.09	1.46	1.50
26	3	603	CLA	CAC-C3C	-2.09	1.45	1.51
26	C	508	CLA	C1C-NC	-2.09	1.34	1.37
25	3	608	CHL	C4B-CHC	2.09	1.46	1.41
25	7	608	CHL	C4B-CHC	2.09	1.46	1.41
26	A	407	CLA	C3B-CAB	-2.09	1.43	1.47
25	4	601	CHL	C4D-CHA	2.09	1.45	1.38
25	8	601	CHL	C4D-CHA	2.09	1.45	1.38
26	3	612	CLA	C4B-CHC	-2.09	1.35	1.41
26	2	613	CLA	C3B-C2B	-2.09	1.37	1.40
26	C	508	CLA	C3B-C2B	-2.09	1.37	1.40
25	3	607	CHL	C1B-CHB	2.09	1.46	1.41
25	7	607	CHL	C1B-CHB	2.09	1.46	1.41
36	b	621	SQD	O2-C2	-2.09	1.38	1.43
37	c	521	LMG	C4-C5	2.09	1.57	1.53
26	r	604	CLA	MG-ND	-2.09	2.01	2.05
26	y	612	CLA	MG-ND	-2.09	2.01	2.05
29	1	1623	NEX	O24-C25	-2.09	1.43	1.46
29	5	1623	NEX	O24-C25	-2.09	1.43	1.46
26	a	407	CLA	C3B-CAB	-2.09	1.43	1.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
27	5	1621	LUT	C22-C21	-2.09	1.52	1.54
25	5	605	CHL	C1B-CHB	2.09	1.46	1.41
26	b	606	CLA	CMA-C3A	-2.09	1.48	1.53
25	1	608	CHL	C3D-C2D	2.09	1.44	1.39
26	3	614	CLA	CMC-C2C	-2.09	1.46	1.50
37	B	2633	LMG	C7-C8	2.09	1.57	1.50
26	C	505	CLA	C3B-C2B	-2.08	1.37	1.40
26	S	611	CLA	C3B-CAB	-2.08	1.43	1.47
30	Y	2630	LHG	O8-C6	-2.08	1.40	1.45
26	7	614	CLA	CMC-C2C	-2.08	1.46	1.50
26	A	405	CLA	MG-ND	-2.08	2.01	2.05
26	C	507	CLA	MG-ND	-2.08	2.01	2.05
26	S	603	CLA	C3B-CAB	-2.08	1.43	1.47
39	C	520	DGD	O3E-C3E	-2.08	1.38	1.43
28	R	622	XAT	O4-C5	-2.08	1.43	1.46
28	r	622	XAT	O4-C5	-2.08	1.43	1.46
25	N	601	CHL	C3D-C2D	2.08	1.44	1.39
26	1	604	CLA	CMC-C2C	-2.08	1.46	1.50
26	5	604	CLA	CMC-C2C	-2.08	1.46	1.50
25	1	607	CHL	C4C-C3C	2.08	1.48	1.45
25	5	607	CHL	C4C-C3C	2.08	1.48	1.45
26	S	603	CLA	C3B-C2B	-2.08	1.37	1.40
26	4	604	CLA	CMD-C2D	-2.08	1.46	1.50
25	1	606	CHL	C4C-C3C	2.08	1.48	1.45
25	5	606	CHL	C4C-C3C	2.08	1.48	1.45
26	S	603	CLA	MG-ND	-2.08	2.01	2.05
26	G	610	CLA	CMD-C2D	-2.08	1.46	1.50
26	4	603	CLA	CMC-C2C	-2.08	1.46	1.50
25	5	606	CHL	C1B-CHB	2.08	1.46	1.41
25	r	614	CHL	C4C-C3C	2.08	1.48	1.45
25	4	609	CHL	C4B-CHC	2.08	1.46	1.41
26	7	603	CLA	CAC-C3C	-2.08	1.45	1.51
26	D	402	CLA	MG-ND	-2.08	2.01	2.05
26	G	603	CLA	MG-ND	-2.08	2.01	2.05
26	d	402	CLA	MG-ND	-2.08	2.01	2.05
26	n	612	CLA	CMC-C2C	-2.08	1.46	1.50
25	R	608	CHL	C4B-CHC	2.08	1.46	1.41
25	r	608	CHL	C4B-CHC	2.08	1.46	1.41
26	y	614	CLA	C3B-CAB	-2.08	1.43	1.47
25	4	607	CHL	C4B-CHC	2.08	1.46	1.41
25	8	607	CHL	C4B-CHC	2.08	1.46	1.41
39	c	520	DGD	O3E-C3E	-2.08	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
25	y	606	CHL	C1B-CHB	2.08	1.46	1.41
38	D	405	PL9	C26-C24	-2.08	1.47	1.51
38	d	405	PL9	C26-C24	-2.08	1.47	1.51
26	C	509	CLA	CMC-C2C	-2.07	1.46	1.50
26	c	509	CLA	CMC-C2C	-2.07	1.46	1.50
37	b	2633	LMG	C7-C8	2.07	1.57	1.50
25	s	608	CHL	C3D-C2D	2.07	1.44	1.39
25	N	605	CHL	C4B-CHC	2.07	1.46	1.41
26	b	604	CLA	C3B-CAB	-2.07	1.43	1.47
26	G	612	CLA	CMD-C2D	-2.07	1.46	1.50
26	g	612	CLA	CMD-C2D	-2.07	1.46	1.50
25	1	605	CHL	C1B-CHB	2.07	1.46	1.41
26	Y	614	CLA	C3B-CAB	-2.07	1.43	1.47
25	6	601	CHL	C4B-CHC	2.07	1.46	1.41
25	s	608	CHL	C4B-CHC	2.07	1.46	1.41
37	c	521	LMG	O1-C7	-2.07	1.40	1.43
25	1	609	CHL	C1B-CHB	2.07	1.46	1.41
29	7	1623	NEX	O24-C25	-2.07	1.43	1.46
26	S	603	CLA	C4B-CHC	-2.07	1.35	1.41
26	s	603	CLA	C4B-CHC	-2.07	1.35	1.41
26	c	508	CLA	C3B-C2B	-2.07	1.37	1.40
25	g	608	CHL	C1B-CHB	2.07	1.46	1.41
26	6	602	CLA	MG-ND	-2.07	2.01	2.05
26	3	603	CLA	C3B-CAB	-2.07	1.43	1.47
26	7	603	CLA	C3B-CAB	-2.07	1.43	1.47
25	5	609	CHL	C1B-CHB	2.07	1.46	1.41
26	1	603	CLA	CMC-C2C	-2.07	1.46	1.50
28	g	1622	XAT	O4-C5	-2.07	1.43	1.46
25	n	601	CHL	C3D-C2D	2.07	1.44	1.39
26	c	507	CLA	MG-ND	-2.07	2.01	2.05
26	7	612	CLA	C4B-CHC	-2.07	1.35	1.41
26	s	603	CLA	C3B-CAB	-2.07	1.43	1.47
26	y	614	CLA	CMC-C2C	-2.07	1.46	1.50
25	1	606	CHL	C4B-CHC	2.06	1.46	1.41
25	3	606	CHL	C1B-CHB	2.06	1.46	1.41
26	s	610	CLA	CMD-C2D	-2.06	1.46	1.50
26	B	609	CLA	CMC-C2C	-2.06	1.46	1.50
26	B	617	CLA	C1C-NC	-2.06	1.34	1.37
26	b	617	CLA	C1C-NC	-2.06	1.34	1.37
25	n	605	CHL	C4B-CHC	2.06	1.46	1.41
26	Y	612	CLA	MG-ND	-2.06	2.01	2.05
29	3	1623	NEX	O24-C25	-2.06	1.43	1.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
30	C	523	LHG	P-O6	2.06	1.67	1.59
30	c	523	LHG	P-O6	2.06	1.67	1.59
26	G	613	CLA	MG-ND	-2.06	2.01	2.05
26	g	613	CLA	MG-ND	-2.06	2.01	2.05
37	b	2633	LMG	O2-C2	-2.06	1.38	1.43
26	B	614	CLA	C4B-CHC	-2.06	1.35	1.41
26	4	611	CLA	CMD-C2D	-2.06	1.46	1.50
26	C	502	CLA	CAC-C3C	-2.06	1.45	1.51
25	2	605	CHL	C2C-C1C	2.06	1.49	1.44
26	n	604	CLA	C4B-CHC	-2.06	1.35	1.41
36	B	621	SQD	O3-C3	-2.06	1.38	1.43
26	D	402	CLA	C3B-CAB	-2.06	1.43	1.47
26	1	611	CLA	MG-ND	-2.06	2.01	2.05
26	5	611	CLA	MG-ND	-2.06	2.01	2.05
26	a	407	CLA	CAC-C3C	-2.06	1.45	1.51
41	F	101	HEM	CMB-C2B	2.06	1.55	1.50
41	f	101	HEM	CMB-C2B	2.06	1.55	1.50
25	Y	606	CHL	C1B-CHB	2.06	1.46	1.41
26	y	611	CLA	MG-ND	-2.06	2.01	2.05
26	c	503	CLA	C3B-C2B	-2.06	1.37	1.40
27	5	1621	LUT	C1-C6	-2.06	1.50	1.53
26	b	614	CLA	C4B-CHC	-2.06	1.35	1.41
25	5	606	CHL	C4B-CHC	2.06	1.46	1.41
36	A	418	SQD	O4-C4	-2.06	1.38	1.43
36	a	418	SQD	O4-C4	-2.06	1.38	1.43
25	r	606	CHL	C1B-CHB	2.06	1.46	1.41
26	Y	611	CLA	MG-ND	-2.06	2.01	2.05
26	1	603	CLA	CAC-C3C	-2.06	1.45	1.51
39	c	518	DGD	O3G-C1D	-2.06	1.36	1.40
25	G	608	CHL	C1B-CHB	2.06	1.46	1.41
26	C	503	CLA	C3B-C2B	-2.06	1.37	1.40
26	C	512	CLA	C3B-CAB	-2.06	1.43	1.47
26	c	512	CLA	C3B-CAB	-2.06	1.43	1.47
25	R	606	CHL	C1B-CHB	2.06	1.46	1.41
25	S	608	CHL	C4B-CHC	2.06	1.46	1.41
26	R	604	CLA	MG-ND	-2.06	2.01	2.05
29	Y	1623	NEX	O24-C25	-2.06	1.43	1.46
29	y	1623	NEX	O24-C25	-2.06	1.43	1.46
26	3	604	CLA	CMD-C2D	-2.05	1.46	1.50
26	7	604	CLA	CMD-C2D	-2.05	1.46	1.50
27	r	620	LUT	C22-C21	-2.05	1.52	1.54
26	2	602	CLA	MG-ND	-2.05	2.01	2.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	8	611	CLA	C3B-C2B	-2.05	1.37	1.40
26	1	612	CLA	CMC-C2C	-2.05	1.46	1.50
26	8	611	CLA	CMD-C2D	-2.05	1.46	1.50
25	G	608	CHL	C3D-C2D	2.05	1.44	1.39
36	B	623	SQD	O3-C3	-2.05	1.38	1.43
36	b	623	SQD	O3-C3	-2.05	1.38	1.43
26	4	611	CLA	MG-ND	-2.05	2.01	2.05
26	4	602	CLA	C3B-CAB	-2.05	1.43	1.47
26	R	603	CLA	C4B-CHC	-2.05	1.35	1.41
26	r	603	CLA	C4B-CHC	-2.05	1.35	1.41
26	1	612	CLA	MG-ND	-2.05	2.01	2.05
39	c	518	DGD	O3G-C3G	-2.05	1.40	1.43
26	N	604	CLA	C4B-CHC	-2.05	1.35	1.41
26	Y	614	CLA	CMC-C2C	-2.05	1.46	1.50
25	7	606	CHL	C1B-CHB	2.05	1.46	1.41
26	g	604	CLA	C4B-CHC	-2.05	1.35	1.41
25	y	606	CHL	C1B-NB	-2.05	1.33	1.35
25	y	607	CHL	C4B-NB	-2.05	1.33	1.35
26	C	501	CLA	C3B-CAB	-2.05	1.43	1.47
26	c	501	CLA	C3B-CAB	-2.05	1.43	1.47
26	S	610	CLA	CMD-C2D	-2.04	1.46	1.50
25	g	608	CHL	C2C-C1C	2.04	1.49	1.44
26	A	407	CLA	CAC-C3C	-2.04	1.45	1.51
26	c	502	CLA	CAC-C3C	-2.04	1.45	1.51
26	d	402	CLA	C3B-CAB	-2.04	1.43	1.47
26	6	610	CLA	CMD-C2D	-2.04	1.46	1.50
25	6	605	CHL	C2C-C1C	2.04	1.48	1.44
26	r	604	CLA	CMC-C2C	-2.04	1.46	1.50
27	N	1621	LUT	C10-C9	-2.04	1.33	1.35
27	n	1621	LUT	C10-C9	-2.04	1.33	1.35
25	7	608	CHL	C2C-C1C	2.04	1.48	1.44
29	g	1623	NEX	C7-C8	-2.04	1.28	1.32
26	G	612	CLA	C3B-C2B	-2.04	1.37	1.40
26	R	604	CLA	CMC-C2C	-2.04	1.46	1.50
26	C	510	CLA	MG-ND	-2.04	2.01	2.05
26	c	510	CLA	MG-ND	-2.04	2.01	2.05
36	A	412	SQD	O3-C3	-2.04	1.38	1.43
36	a	412	SQD	O3-C3	-2.04	1.38	1.43
26	a	405	CLA	C4B-CHC	-2.04	1.35	1.41
28	y	1622	XAT	O4-C5	-2.04	1.43	1.46
26	Y	610	CLA	MG-ND	-2.04	2.01	2.05
26	D	403	CLA	C4B-CHC	-2.04	1.35	1.41

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	N	603	CLA	C3B-CAB	-2.04	1.43	1.47
26	c	508	CLA	C1C-NC	-2.04	1.34	1.37
26	4	602	CLA	C3B-C2B	-2.04	1.37	1.40
26	8	602	CLA	C3B-C2B	-2.04	1.37	1.40
39	C	518	DGD	O3G-C1D	-2.04	1.36	1.40
25	Y	606	CHL	C1B-NB	-2.04	1.33	1.35
26	A	405	CLA	C4B-CHC	-2.04	1.35	1.41
26	8	611	CLA	MG-ND	-2.04	2.01	2.05
25	y	609	CHL	C4C-C3C	2.04	1.48	1.45
26	B	617	CLA	MG-ND	-2.04	2.01	2.05
26	5	612	CLA	MG-ND	-2.04	2.01	2.05
26	2	610	CLA	CMD-C2D	-2.04	1.46	1.50
26	4	604	CLA	CMC-C2C	-2.04	1.46	1.50
26	5	603	CLA	CMC-C2C	-2.04	1.46	1.50
26	8	604	CLA	CMC-C2C	-2.04	1.46	1.50
25	3	608	CHL	C2C-C1C	2.04	1.48	1.44
25	6	608	CHL	C2C-C1C	2.04	1.48	1.44
25	Y	601	CHL	C4C-C3C	2.04	1.48	1.45
25	2	607	CHL	C4B-CHC	2.03	1.46	1.41
25	6	607	CHL	C4B-CHC	2.03	1.46	1.41
26	d	403	CLA	C4B-CHC	-2.03	1.35	1.41
26	B	609	CLA	C1D-ND	2.03	1.40	1.37
26	b	609	CLA	C1D-ND	2.03	1.40	1.37
26	8	602	CLA	C3B-CAB	-2.03	1.43	1.47
25	G	601	CHL	C4B-CHC	2.03	1.46	1.41
25	N	608	CHL	C3D-C2D	2.03	1.44	1.39
25	S	606	CHL	C4C-C3C	2.03	1.48	1.45
25	s	606	CHL	C4C-C3C	2.03	1.48	1.45
26	6	611	CLA	MG-ND	-2.03	2.01	2.05
26	N	610	CLA	C3B-CAB	-2.03	1.43	1.47
26	6	610	CLA	C3B-CAB	-2.03	1.43	1.47
26	5	603	CLA	CAC-C3C	-2.03	1.45	1.51
25	5	605	CHL	C4C-C3C	2.03	1.48	1.45
26	3	613	CLA	C3B-CAB	-2.03	1.43	1.47
25	R	607	CHL	C1C-NC	-2.03	1.34	1.37
26	r	609	CLA	CMC-C2C	-2.03	1.46	1.50
26	B	604	CLA	C3B-CAB	-2.03	1.43	1.47
26	7	613	CLA	C3B-CAB	-2.03	1.43	1.47
25	g	608	CHL	C3D-C2D	2.03	1.44	1.39
26	6	610	CLA	CMC-C2C	-2.03	1.46	1.50
26	b	609	CLA	CMC-C2C	-2.03	1.46	1.50
36	b	621	SQD	O3-C3	-2.03	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	G	604	CLA	C4B-CHC	-2.03	1.35	1.41
26	3	611	CLA	C3B-CAB	-2.03	1.43	1.47
29	S	1623	NEX	O24-C25	-2.03	1.43	1.46
29	s	1623	NEX	O24-C25	-2.03	1.43	1.46
28	G	1622	XAT	C10-C9	-2.03	1.33	1.35
28	g	1622	XAT	C10-C9	-2.03	1.33	1.35
26	5	611	CLA	CMC-C2C	-2.02	1.46	1.50
25	G	608	CHL	C2C-C1C	2.02	1.48	1.44
26	3	604	CLA	C3B-CAB	-2.02	1.43	1.47
26	7	604	CLA	C3B-CAB	-2.02	1.43	1.47
25	G	606	CHL	C1B-CHB	2.02	1.46	1.41
25	g	606	CHL	C1B-CHB	2.02	1.46	1.41
26	b	607	CLA	CMA-C3A	-2.02	1.48	1.53
26	4	611	CLA	C3B-C2B	-2.02	1.37	1.40
26	y	610	CLA	MG-ND	-2.02	2.01	2.05
25	R	614	CHL	C4C-C3C	2.02	1.48	1.45
25	y	601	CHL	C4C-C3C	2.02	1.48	1.45
25	n	608	CHL	C3D-C2D	2.02	1.44	1.39
37	B	2633	LMG	O2-C2	-2.02	1.38	1.43
39	C	518	DGD	O3G-C3G	-2.02	1.40	1.43
26	2	603	CLA	CAC-C3C	-2.02	1.45	1.51
26	6	603	CLA	CAC-C3C	-2.02	1.45	1.51
26	5	612	CLA	CMC-C2C	-2.02	1.46	1.50
26	C	506	CLA	C3B-C2B	-2.02	1.37	1.40
26	c	506	CLA	C3B-C2B	-2.02	1.37	1.40
26	G	610	CLA	C3B-C2B	-2.02	1.37	1.40
29	g	1623	NEX	O24-C25	-2.02	1.43	1.46
25	1	605	CHL	C4C-C3C	2.02	1.48	1.45
25	2	605	CHL	C4C-C3C	2.02	1.48	1.45
25	6	605	CHL	C4C-C3C	2.02	1.48	1.45
29	G	1623	NEX	C7-C8	-2.02	1.28	1.32
26	r	602	CLA	CMC-C2C	-2.02	1.46	1.50
26	n	610	CLA	C3B-CAB	-2.02	1.43	1.47
26	2	610	CLA	C3B-CAB	-2.02	1.43	1.47
26	G	612	CLA	CMC-C2C	-2.02	1.46	1.50
26	6	603	CLA	CMC-C2C	-2.02	1.46	1.50
26	g	612	CLA	CMC-C2C	-2.02	1.46	1.50
25	Y	601	CHL	CMC-C2C	2.02	1.49	1.45
25	y	601	CHL	CMC-C2C	2.02	1.49	1.45
25	Y	609	CHL	C4C-C3C	2.01	1.48	1.45
26	g	604	CLA	CMC-C2C	-2.01	1.46	1.50
39	C	518	DGD	O4D-C4D	-2.01	1.38	1.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
39	c	518	DGD	O4D-C4D	-2.01	1.38	1.43
37	C	521	LMG	O7-C8	-2.01	1.41	1.46
37	c	521	LMG	O7-C8	-2.01	1.41	1.46
27	R	620	LUT	C22-C21	-2.01	1.52	1.54
26	2	603	CLA	C4B-CHC	-2.01	1.35	1.41
26	6	603	CLA	C4B-CHC	-2.01	1.35	1.41
26	R	603	CLA	CMC-C2C	-2.01	1.46	1.50
26	r	603	CLA	CMC-C2C	-2.01	1.46	1.50
26	b	617	CLA	MG-ND	-2.01	2.01	2.05
30	2	2630	LHG	P-O6	2.01	1.67	1.59
26	2	610	CLA	CMC-C2C	-2.01	1.46	1.50
26	G	603	CLA	CAA-C2A	-2.01	1.50	1.54
26	g	603	CLA	CAA-C2A	-2.01	1.50	1.54
31	c	514	BCR	C10-C9	-2.01	1.33	1.35
28	Y	1622	XAT	O4-C5	-2.01	1.43	1.46
25	s	601	CHL	C4B-CHC	2.01	1.46	1.41
30	6	2630	LHG	P-O6	2.01	1.67	1.59
25	g	601	CHL	C4B-CHC	2.01	1.46	1.41
25	R	608	CHL	C1B-CHB	2.01	1.46	1.41
25	r	608	CHL	C1B-CHB	2.01	1.46	1.41
26	6	612	CLA	CMC-C2C	-2.01	1.46	1.50
30	4	2630	LHG	P-O6	2.01	1.67	1.59
26	G	604	CLA	CMC-C2C	-2.01	1.46	1.50
26	r	613	CLA	C3B-CAB	-2.01	1.43	1.47
28	2	1622	XAT	O4-C5	-2.01	1.43	1.46
28	6	1622	XAT	O4-C5	-2.01	1.43	1.46
25	1	609	CHL	C4C-C3C	2.01	1.48	1.45
25	5	609	CHL	C4C-C3C	2.01	1.48	1.45
25	7	609	CHL	C4B-CHC	2.01	1.46	1.41
25	Y	607	CHL	C4C-C3C	2.01	1.48	1.45
28	Y	1622	XAT	O24-C25	-2.01	1.43	1.46
25	2	608	CHL	C2C-C1C	2.01	1.48	1.44
26	r	610	CLA	C3B-CAB	-2.00	1.43	1.47
26	b	614	CLA	C3B-C2B	-2.00	1.37	1.40
26	2	604	CLA	C4B-CHC	-2.00	1.35	1.41
26	6	604	CLA	C4B-CHC	-2.00	1.35	1.41
26	B	607	CLA	CMA-C3A	-2.00	1.48	1.53
26	B	616	CLA	C3B-CAB	-2.00	1.43	1.47
26	b	616	CLA	C3B-CAB	-2.00	1.43	1.47
26	7	611	CLA	CMC-C2C	-2.00	1.46	1.50
25	2	609	CHL	C4B-CHC	2.00	1.46	1.41
26	1	611	CLA	CMC-C2C	-2.00	1.46	1.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(Å)	Ideal(Å)
26	R	610	CLA	MG-ND	-2.00	2.01	2.05
25	2	607	CHL	C4D-CHA	2.00	1.45	1.38
25	6	607	CHL	C4D-CHA	2.00	1.45	1.38
26	R	609	CLA	CMC-C2C	-2.00	1.46	1.50
25	N	607	CHL	C4D-CHA	2.00	1.45	1.38
25	n	607	CHL	C4D-CHA	2.00	1.45	1.38
25	G	605	CHL	C2C-C1C	2.00	1.48	1.44
25	g	605	CHL	C2C-C1C	2.00	1.48	1.44

All (5990) bond angle outliers are listed below:

Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	N	607	CHL	C2C-C3C-C4C	-10.86	98.75	106.49
25	n	607	CHL	C2C-C3C-C4C	-10.86	98.75	106.49
25	y	601	CHL	CMD-C2D-C1D	10.85	143.84	124.71
25	Y	601	CHL	CMD-C2D-C1D	10.83	143.81	124.71
25	G	601	CHL	CMD-C2D-C1D	10.64	143.47	124.71
25	g	601	CHL	CMD-C2D-C1D	10.61	143.42	124.71
25	3	601	CHL	CMD-C2D-C1D	10.46	143.14	124.71
25	7	601	CHL	CMD-C2D-C1D	10.44	143.11	124.71
28	2	1622	XAT	O24-C25-C24	10.32	121.14	113.38
28	6	1622	XAT	O24-C25-C24	10.24	121.08	113.38
25	N	601	CHL	CMD-C2D-C1D	10.19	142.68	124.71
25	n	601	CHL	CMD-C2D-C1D	10.19	142.67	124.71
25	2	601	CHL	CMD-C2D-C1D	9.94	142.23	124.71
25	6	601	CHL	CMD-C2D-C1D	9.94	142.22	124.71
25	1	601	CHL	CMD-C2D-C1D	9.76	141.92	124.71
25	5	601	CHL	CMD-C2D-C1D	9.76	141.92	124.71
25	Y	607	CHL	C2C-C3C-C4C	-9.59	99.66	106.49
25	y	607	CHL	C2C-C3C-C4C	-9.57	99.67	106.49
25	G	608	CHL	CMD-C2D-C1D	9.55	141.54	124.71
25	g	608	CHL	CMD-C2D-C1D	9.54	141.52	124.71
25	R	608	CHL	CMD-C2D-C1D	9.49	141.44	124.71
25	r	608	CHL	CMD-C2D-C1D	9.47	141.41	124.71
25	1	607	CHL	C2C-C3C-C4C	-9.34	99.83	106.49
25	5	607	CHL	C2C-C3C-C4C	-9.33	99.84	106.49
26	s	604	CLA	C4A-NA-C1A	9.27	110.88	106.71
25	r	614	CHL	CMD-C2D-C1D	9.25	141.01	124.71
25	R	607	CHL	CMD-C2D-C1D	9.24	141.00	124.71
25	R	614	CHL	CMD-C2D-C1D	9.24	140.99	124.71
26	S	604	CLA	C4A-NA-C1A	9.23	110.86	106.71
25	r	607	CHL	CMD-C2D-C1D	9.22	140.96	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	606	CHL	CMD-C2D-C1D	9.21	140.95	124.71
25	r	606	CHL	CMD-C2D-C1D	9.21	140.94	124.71
29	1	1623	NEX	O24-C25-C24	9.19	120.29	113.38
25	N	608	CHL	CMD-C2D-C1D	9.17	140.88	124.71
25	n	608	CHL	CMD-C2D-C1D	9.17	140.88	124.71
25	G	601	CHL	C1D-ND-C4D	-9.17	99.82	106.33
25	S	608	CHL	C2C-C3C-C4C	-9.17	99.95	106.49
25	g	601	CHL	C1D-ND-C4D	-9.16	99.83	106.33
29	5	1623	NEX	O24-C25-C24	9.15	120.25	113.38
25	s	608	CHL	C2C-C3C-C4C	-9.14	99.97	106.49
28	1	1622	XAT	O24-C25-C24	9.13	120.24	113.38
28	5	1622	XAT	O24-C25-C24	9.11	120.23	113.38
28	2	1622	XAT	O4-C5-C4	9.04	120.17	113.38
25	8	608	CHL	C1D-ND-C4D	-9.04	99.91	106.33
25	S	606	CHL	C1D-ND-C4D	-9.00	99.94	106.33
25	s	606	CHL	C1D-ND-C4D	-9.00	99.94	106.33
28	6	1622	XAT	O4-C5-C4	8.99	120.14	113.38
25	4	608	CHL	C1D-ND-C4D	-8.96	99.97	106.33
29	2	1623	NEX	O24-C25-C24	8.95	120.11	113.38
25	y	605	CHL	C2C-C3C-C4C	-8.95	100.11	106.49
25	Y	605	CHL	C2C-C3C-C4C	-8.94	100.11	106.49
25	S	601	CHL	CMD-C2D-C1D	8.94	140.47	124.71
25	s	601	CHL	CMD-C2D-C1D	8.93	140.46	124.71
29	6	1623	NEX	O24-C25-C24	8.91	120.08	113.38
26	C	507	CLA	C4A-NA-C1A	8.87	110.70	106.71
25	Y	608	CHL	CMD-C2D-C1D	8.87	140.35	124.71
25	y	608	CHL	CMD-C2D-C1D	8.87	140.35	124.71
29	g	1623	NEX	O24-C25-C24	8.86	120.03	113.38
29	G	1623	NEX	O24-C25-C24	8.84	120.02	113.38
25	Y	606	CHL	C2C-C3C-C4C	-8.82	100.20	106.49
26	c	507	CLA	C4A-NA-C1A	8.79	110.66	106.71
25	5	608	CHL	CMD-C2D-C1D	8.78	140.18	124.71
25	y	606	CHL	C2C-C3C-C4C	-8.77	100.23	106.49
25	1	608	CHL	CMD-C2D-C1D	8.77	140.17	124.71
25	4	608	CHL	CMD-C2D-C1D	8.76	140.15	124.71
25	8	608	CHL	CMD-C2D-C1D	8.76	140.15	124.71
25	G	609	CHL	CMD-C2D-C1D	8.74	140.11	124.71
25	Y	605	CHL	C1D-ND-C4D	-8.73	100.13	106.33
25	g	609	CHL	CMD-C2D-C1D	8.73	140.10	124.71
25	6	608	CHL	CMD-C2D-C1D	8.73	140.09	124.71
25	2	608	CHL	CMD-C2D-C1D	8.72	140.07	124.71
25	y	605	CHL	C1D-ND-C4D	-8.71	100.15	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5	609	CHL	CMD-C2D-C1D	8.71	140.06	124.71
25	S	608	CHL	CMD-C2D-C1D	8.71	140.06	124.71
25	1	609	CHL	CMD-C2D-C1D	8.70	140.05	124.71
25	3	601	CHL	C1D-ND-C4D	-8.70	100.16	106.33
25	R	608	CHL	C2C-C3C-C4C	-8.69	100.29	106.49
25	s	608	CHL	CMD-C2D-C1D	8.69	140.03	124.71
25	r	607	CHL	C2C-C3C-C4C	-8.69	100.30	106.49
25	r	608	CHL	C2C-C3C-C4C	-8.68	100.30	106.49
25	G	605	CHL	CMD-C2D-C1D	8.68	140.00	124.71
28	g	1622	XAT	O24-C25-C24	8.68	119.90	113.38
25	g	605	CHL	CMD-C2D-C1D	8.67	139.99	124.71
25	R	607	CHL	C2C-C3C-C4C	-8.64	100.33	106.49
25	7	608	CHL	CMD-C2D-C1D	8.64	139.94	124.71
25	5	607	CHL	CMD-C2D-C1D	8.63	139.92	124.71
25	1	607	CHL	CMD-C2D-C1D	8.62	139.91	124.71
25	3	608	CHL	CMD-C2D-C1D	8.62	139.90	124.71
26	c	505	CLA	C4A-NA-C1A	8.61	110.58	106.71
25	2	608	CHL	C1D-ND-C4D	-8.61	100.22	106.33
25	7	601	CHL	C1D-ND-C4D	-8.61	100.22	106.33
28	G	1622	XAT	O24-C25-C24	8.59	119.83	113.38
26	C	505	CLA	C4A-NA-C1A	8.58	110.56	106.71
26	C	502	CLA	C4A-NA-C1A	8.58	110.56	106.71
25	6	608	CHL	C1D-ND-C4D	-8.57	100.25	106.33
25	1	608	CHL	C1D-ND-C4D	-8.56	100.26	106.33
25	g	601	CHL	CHD-C1D-ND	-8.55	116.59	124.45
25	g	607	CHL	CMD-C2D-C1D	8.54	139.76	124.71
26	c	502	CLA	C4A-NA-C1A	8.53	110.54	106.71
25	G	607	CHL	CMD-C2D-C1D	8.52	139.73	124.71
25	y	609	CHL	CMD-C2D-C1D	8.52	139.73	124.71
25	5	608	CHL	C2C-C3C-C4C	-8.52	100.42	106.49
25	8	609	CHL	CMD-C2D-C1D	8.52	139.72	124.71
25	y	605	CHL	CMD-C2D-C1D	8.52	139.72	124.71
25	Y	609	CHL	CMD-C2D-C1D	8.52	139.72	124.71
25	G	601	CHL	CHD-C1D-ND	-8.51	116.63	124.45
25	5	608	CHL	C1D-ND-C4D	-8.51	100.29	106.33
25	4	609	CHL	CMD-C2D-C1D	8.50	139.70	124.71
25	G	606	CHL	CMD-C2D-C1D	8.50	139.69	124.71
25	Y	605	CHL	CMD-C2D-C1D	8.49	139.68	124.71
25	1	608	CHL	C2C-C3C-C4C	-8.49	100.44	106.49
25	1	607	CHL	C1D-ND-C4D	-8.49	100.30	106.33
25	5	607	CHL	C1D-ND-C4D	-8.49	100.30	106.33
25	3	607	CHL	CMD-C2D-C1D	8.49	139.67	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	7	607	CHL	CMD-C2D-C1D	8.48	139.66	124.71
25	g	606	CHL	CMD-C2D-C1D	8.48	139.66	124.71
25	s	606	CHL	CMD-C2D-C1D	8.48	139.65	124.71
25	R	607	CHL	C1D-ND-C4D	-8.47	100.31	106.33
25	S	606	CHL	CMD-C2D-C1D	8.46	139.63	124.71
25	r	607	CHL	C1D-ND-C4D	-8.45	100.33	106.33
25	4	607	CHL	CMD-C2D-C1D	8.45	139.60	124.71
25	1	605	CHL	CMD-C2D-C1D	8.44	139.60	124.71
25	8	607	CHL	CMD-C2D-C1D	8.43	139.57	124.71
25	5	605	CHL	CMD-C2D-C1D	8.43	139.57	124.71
25	n	605	CHL	C2C-C3C-C4C	-8.42	100.49	106.49
25	y	601	CHL	C1D-ND-C4D	-8.42	100.35	106.33
25	g	607	CHL	C2C-C3C-C4C	-8.42	100.49	106.49
25	n	601	CHL	C1D-ND-C4D	-8.42	100.36	106.33
25	G	607	CHL	C2C-C3C-C4C	-8.41	100.49	106.49
25	r	606	CHL	C2C-C3C-C4C	-8.39	100.51	106.49
25	N	601	CHL	C1D-ND-C4D	-8.39	100.38	106.33
25	2	606	CHL	CMD-C2D-C1D	8.38	139.49	124.71
25	R	606	CHL	C2C-C3C-C4C	-8.38	100.51	106.49
25	6	606	CHL	CMD-C2D-C1D	8.38	139.49	124.71
25	s	607	CHL	C1D-ND-C4D	-8.38	100.38	106.33
25	3	605	CHL	CMD-C2D-C1D	8.38	139.48	124.71
25	N	605	CHL	C2C-C3C-C4C	-8.37	100.52	106.49
25	s	606	CHL	C2C-C3C-C4C	-8.37	100.52	106.49
25	S	606	CHL	C2C-C3C-C4C	-8.37	100.52	106.49
25	7	605	CHL	CMD-C2D-C1D	8.37	139.46	124.71
26	b	608	CLA	C4A-NA-C1A	8.36	110.46	106.71
25	Y	601	CHL	C1D-ND-C4D	-8.34	100.41	106.33
25	3	608	CHL	C1D-ND-C4D	-8.33	100.42	106.33
25	R	606	CHL	C1D-ND-C4D	-8.33	100.42	106.33
25	S	607	CHL	C1D-ND-C4D	-8.32	100.42	106.33
25	G	605	CHL	C2C-C3C-C4C	-8.32	100.56	106.49
26	B	608	CLA	C4A-NA-C1A	8.31	110.44	106.71
25	s	607	CHL	CMD-C2D-C1D	8.31	139.36	124.71
25	3	609	CHL	CMD-C2D-C1D	8.31	139.36	124.71
25	7	609	CHL	CMD-C2D-C1D	8.31	139.36	124.71
25	r	606	CHL	C1D-ND-C4D	-8.31	100.43	106.33
25	Y	601	CHL	CHD-C1D-ND	-8.31	116.82	124.45
25	y	601	CHL	CHD-C1D-ND	-8.31	116.82	124.45
25	4	606	CHL	CMD-C2D-C1D	8.30	139.35	124.71
25	8	606	CHL	CMD-C2D-C1D	8.30	139.35	124.71
25	S	607	CHL	CMD-C2D-C1D	8.30	139.34	124.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	7	606	CHL	C2C-C3C-C4C	-8.30	100.57	106.49
25	7	608	CHL	C1D-ND-C4D	-8.30	100.44	106.33
29	Y	1623	NEX	O24-C25-C24	8.28	119.60	113.38
25	g	605	CHL	C2C-C3C-C4C	-8.27	100.60	106.49
29	y	1623	NEX	O24-C25-C24	8.26	119.59	113.38
25	3	606	CHL	C2C-C3C-C4C	-8.26	100.60	106.49
26	d	402	CLA	C4A-NA-C1A	8.26	110.42	106.71
25	N	609	CHL	CMD-C2D-C1D	8.25	139.26	124.71
25	n	609	CHL	CMD-C2D-C1D	8.25	139.26	124.71
25	y	607	CHL	CMD-C2D-C1D	8.25	139.26	124.71
25	4	601	CHL	CMD-C2D-C1D	8.25	139.25	124.71
25	Y	607	CHL	CMD-C2D-C1D	8.25	139.25	124.71
25	Y	608	CHL	C1D-ND-C4D	-8.25	100.48	106.33
25	y	608	CHL	C1D-ND-C4D	-8.25	100.48	106.33
25	8	601	CHL	CMD-C2D-C1D	8.24	139.24	124.71
25	2	605	CHL	C1D-ND-C4D	-8.24	100.48	106.33
25	6	605	CHL	C1D-ND-C4D	-8.24	100.48	106.33
25	n	608	CHL	C1D-ND-C4D	-8.23	100.48	106.33
25	R	614	CHL	C1D-ND-C4D	-8.23	100.49	106.33
25	6	609	CHL	CMD-C2D-C1D	8.23	139.21	124.71
25	n	605	CHL	CMD-C2D-C1D	8.23	139.21	124.71
25	2	607	CHL	CMD-C2D-C1D	8.22	139.20	124.71
25	6	607	CHL	CMD-C2D-C1D	8.22	139.19	124.71
25	N	605	CHL	CMD-C2D-C1D	8.21	139.19	124.71
25	g	608	CHL	C1D-ND-C4D	-8.21	100.50	106.33
25	2	609	CHL	CMD-C2D-C1D	8.21	139.18	124.71
25	r	614	CHL	C1D-ND-C4D	-8.21	100.51	106.33
25	N	608	CHL	C1D-ND-C4D	-8.19	100.52	106.33
25	2	605	CHL	CMD-C2D-C1D	8.19	139.14	124.71
25	6	605	CHL	CMD-C2D-C1D	8.19	139.14	124.71
25	2	601	CHL	C1D-ND-C4D	-8.19	100.52	106.33
26	D	402	CLA	C4A-NA-C1A	8.19	110.39	106.71
25	G	608	CHL	C1D-ND-C4D	-8.18	100.53	106.33
25	2	607	CHL	C2C-C3C-C4C	-8.17	100.66	106.49
25	6	601	CHL	C1D-ND-C4D	-8.14	100.55	106.33
25	y	606	CHL	CMD-C2D-C1D	8.14	139.05	124.71
25	6	607	CHL	C2C-C3C-C4C	-8.14	100.69	106.49
25	2	606	CHL	C2C-C3C-C4C	-8.12	100.70	106.49
25	Y	606	CHL	CMD-C2D-C1D	8.11	139.01	124.71
25	n	607	CHL	C1D-ND-C4D	-8.11	100.57	106.33
25	6	606	CHL	C2C-C3C-C4C	-8.10	100.71	106.49
25	N	607	CHL	C1D-ND-C4D	-8.09	100.59	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5	606	CHL	CMD-C2D-C1D	8.08	138.95	124.71
25	g	605	CHL	C1D-ND-C4D	-8.07	100.60	106.33
25	7	606	CHL	CMD-C2D-C1D	8.07	138.94	124.71
25	G	605	CHL	C1D-ND-C4D	-8.07	100.60	106.33
25	3	606	CHL	CMD-C2D-C1D	8.07	138.93	124.71
25	1	606	CHL	CMD-C2D-C1D	8.06	138.92	124.71
25	y	605	CHL	C2D-C1D-ND	8.06	116.05	110.10
25	n	606	CHL	C2C-C3C-C4C	-8.04	100.76	106.49
25	n	609	CHL	C1D-ND-C4D	-8.04	100.62	106.33
25	R	614	CHL	CHD-C1D-ND	-8.03	117.07	124.45
25	r	614	CHL	CHD-C1D-ND	-8.03	117.07	124.45
25	N	606	CHL	C2C-C3C-C4C	-8.03	100.76	106.49
25	Y	605	CHL	C2D-C1D-ND	8.03	116.02	110.10
25	N	609	CHL	C1D-ND-C4D	-8.00	100.65	106.33
25	N	605	CHL	C1D-ND-C4D	-8.00	100.65	106.33
25	n	605	CHL	C1D-ND-C4D	-7.99	100.66	106.33
25	8	608	CHL	C2D-C1D-ND	7.99	115.99	110.10
25	1	605	CHL	C1D-ND-C4D	-7.98	100.67	106.33
25	1	606	CHL	C2C-C3C-C4C	-7.98	100.80	106.49
25	5	606	CHL	C2C-C3C-C4C	-7.98	100.80	106.49
25	N	607	CHL	C2D-C1D-ND	7.96	115.97	110.10
25	4	608	CHL	C2D-C1D-ND	7.95	115.96	110.10
25	5	605	CHL	C1D-ND-C4D	-7.93	100.70	106.33
25	n	607	CHL	C2D-C1D-ND	7.91	115.93	110.10
25	7	608	CHL	C2C-C3C-C4C	-7.91	100.85	106.49
25	3	608	CHL	C2C-C3C-C4C	-7.91	100.85	106.49
25	Y	608	CHL	C2C-C3C-C4C	-7.90	100.86	106.49
25	n	606	CHL	CMD-C2D-C1D	7.89	138.62	124.71
25	8	606	CHL	C1D-ND-C4D	-7.87	100.74	106.33
25	N	606	CHL	CMD-C2D-C1D	7.87	138.58	124.71
25	y	608	CHL	C2C-C3C-C4C	-7.85	100.89	106.49
25	s	601	CHL	C2C-C3C-C4C	-7.81	100.92	106.49
25	S	608	CHL	C1D-ND-C4D	-7.81	100.79	106.33
25	R	608	CHL	C1D-ND-C4D	-7.81	100.79	106.33
25	S	601	CHL	C2C-C3C-C4C	-7.80	100.93	106.49
25	4	606	CHL	C1D-ND-C4D	-7.80	100.80	106.33
25	Y	609	CHL	C1D-ND-C4D	-7.79	100.80	106.33
25	s	608	CHL	C1D-ND-C4D	-7.79	100.80	106.33
25	r	608	CHL	C1D-ND-C4D	-7.78	100.81	106.33
25	y	609	CHL	C1D-ND-C4D	-7.77	100.81	106.33
25	g	606	CHL	C1D-ND-C4D	-7.75	100.83	106.33
25	3	601	CHL	CHD-C1D-ND	-7.75	117.34	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	613	CLA	C4A-NA-C1A	7.74	110.19	106.71
25	G	606	CHL	C1D-ND-C4D	-7.74	100.84	106.33
25	8	609	CHL	CHD-C1D-ND	-7.72	117.36	124.45
25	7	601	CHL	CHD-C1D-ND	-7.72	117.36	124.45
26	B	613	CLA	C4A-NA-C1A	7.70	110.17	106.71
25	2	608	CHL	C2C-C3C-C4C	-7.70	101.00	106.49
25	3	608	CHL	C2D-C1D-ND	7.70	115.78	110.10
26	A	405	CLA	C4A-NA-C1A	7.69	110.17	106.71
25	7	608	CHL	C2D-C1D-ND	7.69	115.77	110.10
25	y	606	CHL	C1D-ND-C4D	-7.68	100.88	106.33
28	r	622	XAT	O4-C5-C4	7.68	119.15	113.38
25	6	608	CHL	C2C-C3C-C4C	-7.68	101.02	106.49
25	4	609	CHL	CHD-C1D-ND	-7.67	117.40	124.45
28	N	1622	XAT	O4-C5-C4	7.67	119.14	113.38
29	R	623	NEX	O24-C25-C24	7.66	119.14	113.38
29	r	623	NEX	O24-C25-C24	7.66	119.13	113.38
25	3	607	CHL	C2C-C3C-C4C	-7.65	101.03	106.49
28	n	1622	XAT	O4-C5-C4	7.65	119.13	113.38
25	Y	606	CHL	C1D-ND-C4D	-7.64	100.91	106.33
25	n	607	CHL	CMD-C2D-C1D	7.64	138.17	124.71
25	N	607	CHL	CMD-C2D-C1D	7.63	138.17	124.71
26	C	511	CLA	C4A-NA-C1A	7.63	110.14	106.71
25	3	607	CHL	CHD-C1D-ND	-7.63	117.44	124.45
28	R	622	XAT	O4-C5-C4	7.62	119.11	113.38
29	3	1623	NEX	O24-C25-C24	7.62	119.11	113.38
28	n	1622	XAT	O24-C25-C24	7.62	119.10	113.38
25	G	607	CHL	C1D-ND-C4D	-7.62	100.92	106.33
25	7	607	CHL	C2C-C3C-C4C	-7.62	101.06	106.49
25	s	607	CHL	C2D-C1D-ND	7.61	115.71	110.10
25	4	606	CHL	C2C-C3C-C4C	-7.60	101.08	106.49
25	N	608	CHL	C2C-C3C-C4C	-7.60	101.08	106.49
25	7	607	CHL	CHD-C1D-ND	-7.59	117.47	124.45
25	n	608	CHL	C2C-C3C-C4C	-7.59	101.08	106.49
25	g	607	CHL	C1D-ND-C4D	-7.59	100.94	106.33
25	n	606	CHL	C1D-ND-C4D	-7.59	100.94	106.33
25	5	605	CHL	C2C-C3C-C4C	-7.59	101.08	106.49
25	7	605	CHL	C1D-ND-C4D	-7.59	100.95	106.33
28	N	1622	XAT	O24-C25-C24	7.58	119.08	113.38
25	G	609	CHL	C1D-ND-C4D	-7.58	100.95	106.33
25	Y	607	CHL	C1D-ND-C4D	-7.58	100.95	106.33
25	y	607	CHL	C1D-ND-C4D	-7.58	100.95	106.33
25	N	606	CHL	C1D-ND-C4D	-7.58	100.95	106.33

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	8	622	XAT	O24-C25-C24	7.57	119.07	113.38
25	6	606	CHL	C1D-ND-C4D	-7.56	100.96	106.33
26	c	511	CLA	C4A-NA-C1A	7.56	110.11	106.71
25	1	609	CHL	C1D-ND-C4D	-7.56	100.97	106.33
25	8	601	CHL	CHD-C1D-ND	-7.56	117.51	124.45
26	a	405	CLA	C4A-NA-C1A	7.56	110.10	106.71
25	8	606	CHL	C2C-C3C-C4C	-7.55	101.11	106.49
25	1	605	CHL	C2C-C3C-C4C	-7.55	101.11	106.49
25	5	609	CHL	C1D-ND-C4D	-7.55	100.97	106.33
29	7	1623	NEX	O24-C25-C24	7.55	119.05	113.38
25	3	605	CHL	C1D-ND-C4D	-7.55	100.97	106.33
25	g	609	CHL	C1D-ND-C4D	-7.54	100.98	106.33
25	S	607	CHL	C2D-C1D-ND	7.54	115.66	110.10
25	g	608	CHL	C2C-C3C-C4C	-7.54	101.11	106.49
25	4	601	CHL	CHD-C1D-ND	-7.54	117.53	124.45
25	8	608	CHL	C2C-C3C-C4C	-7.54	101.12	106.49
26	B	611	CLA	C4A-NA-C1A	7.53	110.09	106.71
25	G	608	CHL	C2C-C3C-C4C	-7.52	101.12	106.49
25	1	606	CHL	C1D-ND-C4D	-7.52	100.99	106.33
28	4	622	XAT	O24-C25-C24	7.52	119.03	113.38
25	N	609	CHL	C2C-C3C-C4C	-7.51	101.13	106.49
28	Y	1622	XAT	O24-C25-C24	7.51	119.03	113.38
25	n	609	CHL	C2C-C3C-C4C	-7.51	101.13	106.49
25	5	606	CHL	C1D-ND-C4D	-7.51	101.00	106.33
25	S	601	CHL	C1D-ND-C4D	-7.51	101.00	106.33
29	n	1623	NEX	O24-C25-C24	7.51	119.02	113.38
25	2	606	CHL	C1D-ND-C4D	-7.50	101.00	106.33
31	8	623	BCR	C24-C23-C22	-7.50	114.90	126.23
31	4	623	BCR	C24-C23-C22	-7.50	114.91	126.23
25	s	601	CHL	C1D-ND-C4D	-7.49	101.01	106.33
29	N	1623	NEX	O24-C25-C24	7.49	119.01	113.38
26	b	611	CLA	C4A-NA-C1A	7.47	110.06	106.71
28	y	1622	XAT	O24-C25-C24	7.46	118.99	113.38
25	n	601	CHL	CHD-C1D-ND	-7.46	117.60	124.45
25	6	607	CHL	C1D-ND-C4D	-7.45	101.04	106.33
25	N	601	CHL	CHD-C1D-ND	-7.44	117.61	124.45
25	4	608	CHL	C2C-C3C-C4C	-7.44	101.19	106.49
25	G	606	CHL	C2C-C3C-C4C	-7.44	101.19	106.49
25	g	606	CHL	C2C-C3C-C4C	-7.44	101.19	106.49
25	1	608	CHL	C2D-C1D-ND	7.44	115.59	110.10
28	7	1622	XAT	O4-C5-C4	7.43	118.97	113.38
25	S	606	CHL	C2D-C1D-ND	7.42	115.57	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	s	606	CHL	C2D-C1D-ND	7.41	115.57	110.10
25	y	606	CHL	C2D-C1D-ND	7.41	115.57	110.10
25	7	606	CHL	C1D-ND-C4D	-7.41	101.07	106.33
25	5	608	CHL	C2D-C1D-ND	7.40	115.56	110.10
28	3	1622	XAT	O4-C5-C4	7.40	118.94	113.38
25	3	606	CHL	C1D-ND-C4D	-7.39	101.09	106.33
28	y	1622	XAT	C6-C7-C8	-7.37	110.40	125.99
25	2	607	CHL	C1D-ND-C4D	-7.37	101.10	106.33
25	Y	606	CHL	C2D-C1D-ND	7.37	115.54	110.10
28	Y	1622	XAT	C6-C7-C8	-7.37	110.41	125.99
25	R	607	CHL	C2D-C1D-ND	7.37	115.53	110.10
26	B	610	CLA	C4A-NA-C1A	7.35	110.01	106.71
25	6	609	CHL	C1D-ND-C4D	-7.35	101.12	106.33
25	G	601	CHL	C2D-C1D-ND	7.34	115.51	110.10
25	2	605	CHL	C2C-C3C-C4C	-7.33	101.26	106.49
25	6	605	CHL	C2C-C3C-C4C	-7.33	101.26	106.49
25	8	607	CHL	C1D-ND-C4D	-7.32	101.13	106.33
25	g	601	CHL	C2D-C1D-ND	7.32	115.50	110.10
25	2	609	CHL	C1D-ND-C4D	-7.31	101.14	106.33
25	r	607	CHL	C2D-C1D-ND	7.30	115.48	110.10
25	4	607	CHL	C1D-ND-C4D	-7.30	101.15	106.33
25	3	605	CHL	C2C-C3C-C4C	-7.28	101.30	106.49
26	b	610	CLA	C4A-NA-C1A	7.27	109.98	106.71
25	4	609	CHL	C2C-C3C-C4C	-7.27	101.31	106.49
26	N	613	CLA	C4A-NA-C1A	7.26	109.97	106.71
26	n	613	CLA	C4A-NA-C1A	7.26	109.97	106.71
25	6	608	CHL	C2D-C1D-ND	7.26	115.45	110.10
25	7	605	CHL	C2C-C3C-C4C	-7.26	101.31	106.49
25	8	609	CHL	C2C-C3C-C4C	-7.25	101.32	106.49
25	N	608	CHL	C2D-C1D-ND	7.25	115.44	110.10
25	2	608	CHL	C2D-C1D-ND	7.24	115.44	110.10
25	6	609	CHL	C2C-C3C-C4C	-7.24	101.33	106.49
25	n	608	CHL	C2D-C1D-ND	7.23	115.43	110.10
28	R	622	XAT	O24-C25-C24	7.22	118.81	113.38
25	2	609	CHL	C2C-C3C-C4C	-7.20	101.36	106.49
28	r	622	XAT	O24-C25-C24	7.20	118.79	113.38
25	2	601	CHL	CHD-C1D-ND	-7.19	117.85	124.45
25	6	601	CHL	CHD-C1D-ND	-7.19	117.85	124.45
25	y	607	CHL	C2D-C1D-ND	7.16	115.38	110.10
26	N	611	CLA	C4A-NA-C1A	7.16	109.92	106.71
25	n	609	CHL	C2D-C1D-ND	7.16	115.38	110.10
26	n	611	CLA	C4A-NA-C1A	7.14	109.92	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	607	CHL	C2D-C1D-ND	7.12	115.35	110.10
25	N	609	CHL	C2D-C1D-ND	7.12	115.35	110.10
26	B	602	CLA	C4A-NA-C1A	7.11	109.90	106.71
25	1	609	CHL	C2C-C3C-C4C	-7.10	101.43	106.49
26	S	603	CLA	C4A-NA-C1A	7.10	109.90	106.71
26	s	603	CLA	C4A-NA-C1A	7.10	109.90	106.71
26	R	612	CLA	C4A-NA-C1A	7.09	109.89	106.71
26	b	602	CLA	C4A-NA-C1A	7.08	109.89	106.71
25	8	609	CHL	C1D-ND-C4D	-7.08	101.30	106.33
25	5	609	CHL	C2C-C3C-C4C	-7.08	101.44	106.49
26	C	508	CLA	CMB-C2B-C1B	-7.05	117.62	128.46
26	c	508	CLA	CMB-C2B-C1B	-7.04	117.64	128.46
26	c	509	CLA	C4A-NA-C1A	7.04	109.87	106.71
26	g	611	CLA	C4A-NA-C1A	7.03	109.86	106.71
28	N	1622	XAT	C15-C14-C13	-7.02	117.29	127.31
25	y	609	CHL	C2D-C1D-ND	7.02	115.28	110.10
26	B	606	CLA	C4A-NA-C1A	7.02	109.86	106.71
28	n	1622	XAT	C15-C14-C13	-7.02	117.30	127.31
26	r	612	CLA	C4A-NA-C1A	7.01	109.86	106.71
25	Y	609	CHL	C2D-C1D-ND	7.00	115.27	110.10
26	C	509	CLA	C4A-NA-C1A	6.99	109.85	106.71
25	R	614	CHL	C2D-C1D-ND	6.98	115.25	110.10
25	r	614	CHL	C2D-C1D-ND	6.98	115.25	110.10
25	4	609	CHL	C1D-ND-C4D	-6.98	101.37	106.33
26	G	611	CLA	C4A-NA-C1A	6.97	109.84	106.71
26	r	609	CLA	C4A-NA-C1A	6.96	109.84	106.71
25	n	605	CHL	C2D-C1D-ND	6.96	115.23	110.10
26	b	606	CLA	C4A-NA-C1A	6.96	109.83	106.71
26	b	617	CLA	C4A-NA-C1A	6.95	109.83	106.71
26	R	609	CLA	C4A-NA-C1A	6.94	109.83	106.71
25	8	607	CHL	CHD-C1D-ND	-6.93	118.08	124.45
25	N	605	CHL	C2D-C1D-ND	6.92	115.20	110.10
31	t	101	BCR	C24-C23-C22	-6.92	115.78	126.23
25	S	607	CHL	C2C-C3C-C4C	-6.92	101.56	106.49
26	B	617	CLA	C4A-NA-C1A	6.91	109.81	106.71
25	4	607	CHL	CHD-C1D-ND	-6.90	118.11	124.45
29	s	1623	NEX	O24-C25-C24	6.90	118.57	113.38
31	T	101	BCR	C24-C23-C22	-6.90	115.81	126.23
26	r	602	CLA	C4A-NA-C1A	6.89	109.80	106.71
29	S	1623	NEX	O24-C25-C24	6.89	118.56	113.38
25	8	607	CHL	C2C-C3C-C4C	-6.89	101.58	106.49
25	s	607	CHL	C2C-C3C-C4C	-6.87	101.59	106.49

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	605	CHL	CHD-C1D-ND	-6.86	118.15	124.45
25	4	607	CHL	C2C-C3C-C4C	-6.86	101.60	106.49
25	y	609	CHL	CHD-C1D-ND	-6.85	118.16	124.45
26	b	609	CLA	C4A-NA-C1A	6.85	109.79	106.71
25	3	609	CHL	C2C-C3C-C4C	-6.85	101.61	106.49
26	B	612	CLA	C4A-NA-C1A	6.85	109.78	106.71
26	R	601	CLA	C4A-NA-C1A	6.85	109.78	106.71
25	7	609	CHL	C2C-C3C-C4C	-6.84	101.61	106.49
25	y	605	CHL	CHD-C1D-ND	-6.84	118.17	124.45
25	1	607	CHL	C2D-C1D-ND	6.84	115.14	110.10
25	1	601	CHL	CHD-C1D-ND	-6.83	118.17	124.45
25	2	605	CHL	C2D-C1D-ND	6.83	115.14	110.10
25	6	605	CHL	C2D-C1D-ND	6.83	115.14	110.10
25	5	607	CHL	C2D-C1D-ND	6.82	115.13	110.10
26	R	602	CLA	C4A-NA-C1A	6.82	109.77	106.71
25	1	601	CHL	C1D-ND-C4D	-6.81	101.50	106.33
25	Y	609	CHL	CHD-C1D-ND	-6.81	118.19	124.45
25	5	601	CHL	CHD-C1D-ND	-6.81	118.19	124.45
25	R	608	CHL	C2D-C1D-ND	6.81	115.12	110.10
26	r	601	CLA	C4A-NA-C1A	6.80	109.77	106.71
26	B	614	CLA	C4A-NA-C1A	6.80	109.76	106.71
26	b	612	CLA	C4A-NA-C1A	6.80	109.76	106.71
26	A	406	CLA	C4A-NA-C1A	6.79	109.76	106.71
26	R	611	CLA	C4A-NA-C1A	6.78	109.75	106.71
25	r	608	CHL	C2D-C1D-ND	6.77	115.09	110.10
26	B	609	CLA	C4A-NA-C1A	6.77	109.75	106.71
25	3	609	CHL	CHD-C1D-ND	-6.76	118.24	124.45
26	b	614	CLA	C4A-NA-C1A	6.75	109.74	106.71
25	5	601	CHL	C1D-ND-C4D	-6.75	101.54	106.33
26	a	406	CLA	C4A-NA-C1A	6.73	109.73	106.71
26	s	611	CLA	C4A-NA-C1A	6.73	109.73	106.71
25	S	606	CHL	CHD-C1D-ND	-6.72	118.28	124.45
25	r	614	CHL	C2C-C3C-C4C	-6.72	101.70	106.49
25	R	614	CHL	C2C-C3C-C4C	-6.72	101.70	106.49
25	7	609	CHL	CHD-C1D-ND	-6.72	118.28	124.45
25	8	601	CHL	C2C-C3C-C4C	-6.72	101.70	106.49
26	C	504	CLA	C4A-NA-C1A	6.72	109.72	106.71
26	r	611	CLA	C4A-NA-C1A	6.71	109.72	106.71
25	1	609	CHL	CHD-C1D-ND	-6.70	118.30	124.45
25	4	601	CHL	C2C-C3C-C4C	-6.69	101.72	106.49
25	R	606	CHL	CHD-C1D-ND	-6.69	118.31	124.45
25	r	606	CHL	CHD-C1D-ND	-6.67	118.32	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5	609	CHL	CHD-C1D-ND	-6.67	118.32	124.45
25	s	606	CHL	CHD-C1D-ND	-6.67	118.32	124.45
25	G	609	CHL	C2D-C1D-ND	6.65	115.00	110.10
26	S	611	CLA	C4A-NA-C1A	6.63	109.69	106.71
25	G	605	CHL	C2D-C1D-ND	6.63	114.99	110.10
25	g	608	CHL	C2D-C1D-ND	6.63	114.99	110.10
25	n	601	CHL	C2D-C1D-ND	6.63	114.99	110.10
26	c	504	CLA	C4A-NA-C1A	6.62	109.68	106.71
25	G	608	CHL	C2D-C1D-ND	6.62	114.98	110.10
25	g	605	CHL	C2D-C1D-ND	6.61	114.97	110.10
25	N	601	CHL	C2D-C1D-ND	6.61	114.97	110.10
25	g	609	CHL	C2D-C1D-ND	6.61	114.97	110.10
25	8	608	CHL	CHD-C1D-ND	-6.60	118.39	124.45
25	3	609	CHL	C1D-ND-C4D	-6.58	101.66	106.33
25	Y	608	CHL	C2D-C1D-ND	6.56	114.94	110.10
25	G	605	CHL	CHD-C1D-ND	-6.55	118.43	124.45
25	7	609	CHL	C1D-ND-C4D	-6.55	101.69	106.33
25	8	606	CHL	CHD-C1D-ND	-6.54	118.44	124.45
26	Y	611	CLA	C4A-NA-C1A	6.54	109.65	106.71
25	4	608	CHL	CHD-C1D-ND	-6.54	118.44	124.45
25	4	606	CHL	CHD-C1D-ND	-6.52	118.46	124.45
25	y	608	CHL	C2D-C1D-ND	6.52	114.91	110.10
25	g	605	CHL	CHD-C1D-ND	-6.51	118.47	124.45
26	n	604	CLA	CMB-C2B-C1B	-6.51	118.46	128.46
28	g	1622	XAT	C6-C7-C8	-6.50	112.24	125.99
25	N	607	CHL	C3C-C4C-NC	6.50	117.86	110.57
25	n	607	CHL	C3C-C4C-NC	6.50	117.86	110.57
28	G	1622	XAT	C6-C7-C8	-6.48	112.28	125.99
26	y	611	CLA	C4A-NA-C1A	6.48	109.62	106.71
25	1	605	CHL	C2D-C1D-ND	6.48	114.88	110.10
25	y	609	CHL	C2C-C3C-C4C	-6.47	101.87	106.49
25	5	601	CHL	C2C-C3C-C4C	-6.47	101.88	106.49
25	Y	606	CHL	C3C-C4C-NC	6.47	117.83	110.57
26	N	604	CLA	CMB-C2B-C1B	-6.47	118.52	128.46
25	y	606	CHL	C3C-C4C-NC	6.46	117.82	110.57
25	G	607	CHL	CHD-C1D-ND	-6.46	118.52	124.45
25	g	607	CHL	CHD-C1D-ND	-6.46	118.52	124.45
25	r	608	CHL	C3C-C4C-NC	6.46	117.81	110.57
25	2	609	CHL	CHD-C1D-ND	-6.45	118.52	124.45
25	8	606	CHL	C2D-C1D-ND	6.45	114.86	110.10
25	3	601	CHL	C2D-C1D-ND	6.45	114.86	110.10
25	R	608	CHL	C3C-C4C-NC	6.43	117.78	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	609	CHL	CHD-C1D-ND	-6.42	118.55	124.45
25	R	606	CHL	C2D-C1D-ND	6.42	114.84	110.10
25	5	605	CHL	C2D-C1D-ND	6.42	114.84	110.10
25	3	605	CHL	C2D-C1D-ND	6.41	114.83	110.10
25	7	605	CHL	C2D-C1D-ND	6.41	114.83	110.10
31	T	101	BCR	C20-C21-C22	-6.41	118.16	127.31
25	Y	609	CHL	C2C-C3C-C4C	-6.41	101.92	106.49
25	r	606	CHL	C2D-C1D-ND	6.41	114.83	110.10
31	C	516	BCR	C24-C23-C22	-6.40	116.56	126.23
25	1	601	CHL	C2C-C3C-C4C	-6.40	101.92	106.49
31	c	516	BCR	C24-C23-C22	-6.40	116.56	126.23
31	t	101	BCR	C20-C21-C22	-6.39	118.19	127.31
25	Y	605	CHL	C3C-C4C-NC	6.39	117.74	110.57
25	y	605	CHL	C3C-C4C-NC	6.39	117.74	110.57
25	4	606	CHL	C2D-C1D-ND	6.38	114.81	110.10
28	1	1622	XAT	O4-C5-C4	6.38	118.17	113.38
25	n	606	CHL	C2D-C1D-ND	6.37	114.80	110.10
28	5	1622	XAT	O4-C5-C4	6.36	118.16	113.38
25	7	601	CHL	C2D-C1D-ND	6.36	114.79	110.10
25	1	605	CHL	CHD-C1D-ND	-6.36	118.61	124.45
25	N	606	CHL	C2D-C1D-ND	6.36	114.79	110.10
25	8	601	CHL	C1D-ND-C4D	-6.36	101.82	106.33
25	y	601	CHL	C2D-C1D-ND	6.35	114.78	110.10
31	t	101	BCR	C16-C17-C18	-6.32	118.29	127.31
31	T	101	BCR	C16-C17-C18	-6.31	118.30	127.31
28	4	622	XAT	O4-C5-C4	6.31	118.12	113.38
25	n	609	CHL	CHD-C1D-ND	-6.30	118.66	124.45
25	5	605	CHL	CHD-C1D-ND	-6.30	118.66	124.45
26	y	603	CLA	C4A-NA-C1A	6.30	109.54	106.71
26	Y	603	CLA	C4A-NA-C1A	6.29	109.54	106.71
25	4	601	CHL	C1D-ND-C4D	-6.29	101.87	106.33
25	N	609	CHL	CHD-C1D-ND	-6.29	118.68	124.45
25	Y	601	CHL	C2D-C1D-ND	6.28	114.73	110.10
25	R	607	CHL	CHD-C1D-ND	-6.27	118.70	124.45
26	b	613	CLA	CMB-C2B-C1B	-6.26	118.84	128.46
26	y	604	CLA	CMB-C2B-C1B	-6.26	118.84	128.46
28	8	622	XAT	O4-C5-C4	6.26	118.08	113.38
26	C	510	CLA	C4A-NA-C1A	6.25	109.52	106.71
26	Y	604	CLA	CMB-C2B-C1B	-6.24	118.87	128.46
25	r	607	CHL	CHD-C1D-ND	-6.24	118.72	124.45
26	a	410	CLA	C4A-NA-C1A	6.24	109.51	106.71
28	7	1622	XAT	O24-C25-C24	6.23	118.06	113.38

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	613	CLA	CMB-C2B-C1B	-6.22	118.90	128.46
25	s	601	CHL	CHD-C1D-ND	-6.22	118.74	124.45
26	7	611	CLA	C4A-NA-C1A	6.22	109.50	106.71
28	3	1622	XAT	O24-C25-C24	6.21	118.05	113.38
25	S	601	CHL	CHD-C1D-ND	-6.21	118.75	124.45
25	G	609	CHL	C2C-C3C-C4C	-6.21	102.06	106.49
25	G	607	CHL	C2D-C1D-ND	6.21	114.68	110.10
25	g	607	CHL	C2D-C1D-ND	6.20	114.67	110.10
26	c	510	CLA	C4A-NA-C1A	6.20	109.49	106.71
25	1	607	CHL	CHD-C1D-ND	-6.20	118.76	124.45
25	5	607	CHL	CHD-C1D-ND	-6.20	118.76	124.45
25	g	609	CHL	C2C-C3C-C4C	-6.20	102.07	106.49
28	R	622	XAT	C26-C27-C28	-6.19	112.90	125.99
26	A	410	CLA	C4A-NA-C1A	6.19	109.49	106.71
28	r	622	XAT	C26-C27-C28	-6.18	112.92	125.99
26	C	506	CLA	C4A-NA-C1A	6.18	109.49	106.71
26	c	506	CLA	C4A-NA-C1A	6.18	109.49	106.71
25	6	609	CHL	C2D-C1D-ND	6.18	114.66	110.10
25	2	609	CHL	C2D-C1D-ND	6.17	114.65	110.10
28	n	1622	XAT	C31-C30-C29	-6.17	118.51	127.31
26	D	403	CLA	C4A-NA-C1A	6.17	109.48	106.71
26	3	611	CLA	C4A-NA-C1A	6.16	109.48	106.71
28	N	1622	XAT	C31-C30-C29	-6.16	118.52	127.31
25	2	607	CHL	C2D-C1D-ND	6.15	114.63	110.10
25	6	607	CHL	C2D-C1D-ND	6.14	114.63	110.10
25	7	605	CHL	CHD-C1D-ND	-6.14	118.81	124.45
31	8	623	BCR	C11-C10-C9	-6.13	118.56	127.31
25	1	609	CHL	C2D-C1D-ND	6.13	114.62	110.10
25	3	608	CHL	CHD-C1D-ND	-6.13	118.82	124.45
26	G	604	CLA	CMB-C2B-C1B	-6.12	119.06	128.46
26	g	604	CLA	CMB-C2B-C1B	-6.12	119.06	128.46
26	B	616	CLA	C4A-NA-C1A	6.11	109.45	106.71
31	4	623	BCR	C11-C10-C9	-6.11	118.59	127.31
25	3	605	CHL	CHD-C1D-ND	-6.11	118.84	124.45
25	5	609	CHL	C2D-C1D-ND	6.11	114.61	110.10
25	7	601	CHL	C2C-C3C-C4C	-6.10	102.14	106.49
25	y	607	CHL	C3C-C4C-NC	6.10	117.41	110.57
26	b	616	CLA	C4A-NA-C1A	6.10	109.45	106.71
25	G	609	CHL	CHD-C1D-ND	-6.09	118.86	124.45
25	7	608	CHL	CHD-C1D-ND	-6.08	118.86	124.45
26	d	403	CLA	C4A-NA-C1A	6.08	109.44	106.71
25	s	607	CHL	CHD-C1D-ND	-6.08	118.86	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	608	CHL	C2D-C1D-ND	6.08	114.58	110.10
25	s	608	CHL	C2D-C1D-ND	6.08	114.58	110.10
25	Y	607	CHL	C3C-C4C-NC	6.08	117.39	110.57
25	3	601	CHL	C2C-C3C-C4C	-6.05	102.17	106.49
26	b	603	CLA	C4A-NA-C1A	6.05	109.43	106.71
26	g	603	CLA	C4A-NA-C1A	6.05	109.43	106.71
26	G	613	CLA	C4A-NA-C1A	6.04	109.42	106.71
26	g	613	CLA	C4A-NA-C1A	6.04	109.42	106.71
25	S	607	CHL	CHD-C1D-ND	-6.04	118.91	124.45
26	G	603	CLA	C4A-NA-C1A	6.04	109.42	106.71
25	6	607	CHL	CHD-C1D-ND	-6.03	118.91	124.45
25	g	609	CHL	CHD-C1D-ND	-6.03	118.92	124.45
26	Y	604	CLA	C4A-NA-C1A	6.02	109.41	106.71
25	2	605	CHL	CHD-C1D-ND	-6.01	118.93	124.45
25	6	605	CHL	CHD-C1D-ND	-6.01	118.93	124.45
25	2	607	CHL	CHD-C1D-ND	-6.01	118.93	124.45
26	B	603	CLA	C4A-NA-C1A	6.01	109.41	106.71
26	b	609	CLA	CMB-C2B-C1B	-6.00	119.24	128.46
25	2	608	CHL	CHD-C1D-ND	-6.00	118.94	124.45
26	B	609	CLA	CMB-C2B-C1B	-5.99	119.25	128.46
28	y	1622	XAT	C15-C14-C13	-5.98	118.77	127.31
28	Y	1622	XAT	C15-C14-C13	-5.98	118.77	127.31
26	y	604	CLA	C4A-NA-C1A	5.98	109.39	106.71
25	6	608	CHL	CHD-C1D-ND	-5.97	118.97	124.45
26	Y	613	CLA	C4A-NA-C1A	5.97	109.39	106.71
25	3	606	CHL	C2D-C1D-ND	5.95	114.49	110.10
25	7	606	CHL	C2D-C1D-ND	5.95	114.49	110.10
25	2	601	CHL	C2D-C1D-ND	5.93	114.48	110.10
26	c	513	CLA	C4A-NA-C1A	5.93	109.37	106.71
25	3	608	CHL	C3D-C2D-C1D	-5.92	97.75	105.83
26	y	613	CLA	C4A-NA-C1A	5.92	109.37	106.71
26	B	612	CLA	CMB-C2B-C1B	-5.92	119.37	128.46
25	7	608	CHL	C3D-C2D-C1D	-5.92	97.76	105.83
26	B	605	CLA	CAA-C2A-C3A	-5.92	96.58	112.78
25	6	606	CHL	C2D-C1D-ND	5.91	114.46	110.10
26	C	503	CLA	C4A-NA-C1A	5.91	109.36	106.71
26	c	503	CLA	C4A-NA-C1A	5.91	109.36	106.71
26	A	407	CLA	C4A-NA-C1A	5.91	109.36	106.71
26	C	513	CLA	C4A-NA-C1A	5.91	109.36	106.71
26	b	605	CLA	CAA-C2A-C3A	-5.90	96.61	112.78
26	b	612	CLA	CMB-C2B-C1B	-5.90	119.39	128.46
25	6	601	CHL	C2D-C1D-ND	5.90	114.45	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	r	607	CHL	C3C-C4C-NC	5.89	117.18	110.57
28	G	1622	XAT	C15-C14-C13	-5.89	118.91	127.31
26	N	603	CLA	C4A-NA-C1A	5.88	109.35	106.71
25	g	606	CHL	CHD-C1D-ND	-5.88	119.05	124.45
25	R	607	CHL	C3C-C4C-NC	5.88	117.16	110.57
26	C	504	CLA	CMB-C2B-C1B	-5.87	119.44	128.46
26	b	607	CLA	C4A-NA-C1A	5.87	109.35	106.71
25	g	606	CHL	C2D-C1D-ND	5.87	114.43	110.10
25	Y	608	CHL	CHD-C1D-ND	-5.87	119.06	124.45
26	c	504	CLA	CMB-C2B-C1B	-5.86	119.46	128.46
26	S	613	CLA	C4A-NA-C1A	5.86	109.34	106.71
25	G	606	CHL	C2D-C1D-ND	5.86	114.42	110.10
26	B	615	CLA	C4A-NA-C1A	5.85	109.34	106.71
28	g	1622	XAT	C15-C14-C13	-5.85	118.95	127.31
25	2	606	CHL	C2D-C1D-ND	5.85	114.42	110.10
26	s	613	CLA	C4A-NA-C1A	5.85	109.34	106.71
25	N	605	CHL	CHD-C1D-ND	-5.85	119.08	124.45
29	Y	1623	NEX	C35-C34-C33	-5.85	118.96	127.31
25	n	605	CHL	C3C-C4C-NC	5.85	117.13	110.57
26	C	506	CLA	CMB-C2B-C1B	-5.85	119.47	128.46
29	y	1623	NEX	C35-C34-C33	-5.85	118.97	127.31
25	N	605	CHL	C3C-C4C-NC	5.85	117.13	110.57
26	b	615	CLA	C4A-NA-C1A	5.85	109.33	106.71
25	n	605	CHL	CHD-C1D-ND	-5.84	119.08	124.45
25	3	608	CHL	C3C-C4C-NC	5.84	117.12	110.57
31	d	404	BCR	C7-C8-C9	-5.84	117.41	126.23
25	N	608	CHL	C3D-C2D-C1D	-5.84	97.86	105.83
31	c	517	BCR	C24-C23-C22	-5.84	117.41	126.23
25	n	608	CHL	C3D-C2D-C1D	-5.84	97.86	105.83
26	N	602	CLA	CMB-C2B-C1B	-5.83	119.50	128.46
26	n	602	CLA	CMB-C2B-C1B	-5.83	119.50	128.46
25	y	608	CHL	CHD-C1D-ND	-5.83	119.09	124.45
31	c	517	BCR	C7-C8-C9	-5.83	117.42	126.23
26	c	506	CLA	CMB-C2B-C1B	-5.83	119.50	128.46
25	G	606	CHL	CHD-C1D-ND	-5.83	119.09	124.45
31	D	404	BCR	C7-C8-C9	-5.83	117.42	126.23
31	C	517	BCR	C7-C8-C9	-5.83	117.42	126.23
25	g	608	CHL	CHD-C1D-ND	-5.83	119.10	124.45
26	n	603	CLA	C4A-NA-C1A	5.83	109.33	106.71
26	1	603	CLA	C4A-NA-C1A	5.82	109.32	106.71
26	5	603	CLA	C4A-NA-C1A	5.82	109.32	106.71
25	8	607	CHL	C2D-C1D-ND	5.82	114.39	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	s	612	CLA	CMB-C2B-C1B	-5.82	119.52	128.46
25	7	608	CHL	C3C-C4C-NC	5.81	117.09	110.57
31	C	517	BCR	C24-C23-C22	-5.81	117.45	126.23
26	2	611	CLA	C4A-NA-C1A	5.81	109.32	106.71
26	S	612	CLA	CMB-C2B-C1B	-5.81	119.54	128.46
29	3	1623	NEX	C15-C14-C13	-5.81	119.03	127.31
26	a	407	CLA	C4A-NA-C1A	5.80	109.31	106.71
25	G	608	CHL	CHD-C1D-ND	-5.80	119.12	124.45
25	s	608	CHL	C3C-C4C-NC	5.79	117.07	110.57
25	5	606	CHL	C2D-C1D-ND	5.79	114.37	110.10
25	n	606	CHL	C3C-C4C-NC	5.79	117.06	110.57
29	7	1623	NEX	C15-C14-C13	-5.79	119.05	127.31
25	1	606	CHL	C2D-C1D-ND	5.79	114.37	110.10
25	4	607	CHL	C2D-C1D-ND	5.79	114.37	110.10
28	G	1622	XAT	O4-C5-C4	5.79	117.73	113.38
26	B	607	CLA	C4A-NA-C1A	5.78	109.31	106.71
26	6	611	CLA	C4A-NA-C1A	5.78	109.31	106.71
25	5	608	CHL	C3C-C4C-NC	5.78	117.05	110.57
25	S	608	CHL	C3C-C4C-NC	5.78	117.05	110.57
25	4	608	CHL	C3D-C2D-C1D	-5.77	97.96	105.83
25	6	606	CHL	CHD-C1D-ND	-5.76	119.16	124.45
28	g	1622	XAT	O4-C5-C4	5.76	117.71	113.38
26	C	508	CLA	C4A-NA-C1A	5.76	109.30	106.71
25	R	608	CHL	C3D-C2D-C1D	-5.76	97.97	105.83
26	n	614	CLA	C4A-NA-C1A	5.75	109.29	106.71
25	8	608	CHL	C3D-C2D-C1D	-5.75	97.98	105.83
25	1	608	CHL	C3C-C4C-NC	5.75	117.02	110.57
25	N	606	CHL	C3C-C4C-NC	5.75	117.02	110.57
25	y	605	CHL	C3D-C2D-C1D	-5.75	97.99	105.83
25	r	608	CHL	C3D-C2D-C1D	-5.75	97.99	105.83
25	Y	605	CHL	C3D-C2D-C1D	-5.74	98.00	105.83
26	c	508	CLA	C4A-NA-C1A	5.73	109.28	106.71
26	R	604	CLA	C4A-NA-C1A	5.73	109.28	106.71
26	r	604	CLA	C4A-NA-C1A	5.73	109.28	106.71
25	6	608	CHL	C3C-C4C-NC	5.73	117.00	110.57
26	C	512	CLA	C4A-NA-C1A	5.73	109.28	106.71
25	2	608	CHL	C3C-C4C-NC	5.72	116.98	110.57
25	2	606	CHL	CHD-C1D-ND	-5.72	119.20	124.45
25	4	601	CHL	C1B-CHB-C4A	-5.72	118.80	130.12
25	8	601	CHL	C1B-CHB-C4A	-5.71	118.80	130.12
25	G	601	CHL	C3D-C2D-C1D	-5.71	98.04	105.83
26	B	605	CLA	C4A-NA-C1A	5.71	109.27	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	605	CLA	C4A-NA-C1A	5.71	109.27	106.71
25	g	601	CHL	C3D-C2D-C1D	-5.70	98.06	105.83
25	N	607	CHL	C3D-C2D-C1D	-5.70	98.06	105.83
26	c	512	CLA	C4A-NA-C1A	5.70	109.27	106.71
25	G	605	CHL	C3C-C4C-NC	5.70	116.96	110.57
25	3	607	CHL	C1D-ND-C4D	-5.70	102.29	106.33
28	3	1622	XAT	C6-C7-C8	-5.69	113.96	125.99
28	7	1622	XAT	C6-C7-C8	-5.69	113.96	125.99
31	t	101	BCR	C11-C10-C9	-5.69	119.19	127.31
25	g	605	CHL	C3C-C4C-NC	5.69	116.95	110.57
25	7	607	CHL	C1D-ND-C4D	-5.69	102.30	106.33
25	N	605	CHL	O2D-CGD-CBD	5.67	121.35	111.27
25	n	605	CHL	O2D-CGD-CBD	5.67	121.35	111.27
25	1	608	CHL	CHD-C1D-ND	-5.67	119.24	124.45
25	n	607	CHL	C3D-C2D-C1D	-5.66	98.10	105.83
31	T	101	BCR	C11-C10-C9	-5.65	119.25	127.31
26	N	614	CLA	C4A-NA-C1A	5.65	109.25	106.71
25	1	608	CHL	C3D-C2D-C1D	-5.65	98.12	105.83
28	y	1622	XAT	C31-C30-C29	-5.65	119.25	127.31
25	R	608	CHL	O2D-CGD-CBD	5.64	121.30	111.27
25	5	608	CHL	C3D-C2D-C1D	-5.64	98.13	105.83
25	n	608	CHL	CHD-C1D-ND	-5.64	119.27	124.45
25	5	608	CHL	CHD-C1D-ND	-5.64	119.27	124.45
25	N	601	CHL	C2C-C3C-C4C	-5.64	102.47	106.49
28	Y	1622	XAT	C31-C30-C29	-5.63	119.28	127.31
25	2	609	CHL	O2D-CGD-CBD	5.63	121.27	111.27
25	r	608	CHL	O2D-CGD-CBD	5.63	121.27	111.27
25	N	608	CHL	CHD-C1D-ND	-5.63	119.28	124.45
25	6	609	CHL	O2D-CGD-CBD	5.63	121.27	111.27
28	y	1622	XAT	O4-C5-C4	5.62	117.60	113.38
26	7	603	CLA	C4A-NA-C1A	5.62	109.23	106.71
28	Y	1622	XAT	O4-C5-C4	5.62	117.60	113.38
25	n	609	CHL	C3D-C2D-C1D	-5.62	98.17	105.83
31	h	101	BCR	C11-C10-C9	-5.61	119.30	127.31
31	H	101	BCR	C11-C10-C9	-5.61	119.31	127.31
25	n	601	CHL	C2C-C3C-C4C	-5.61	102.49	106.49
25	S	606	CHL	C3C-C4C-NC	5.60	116.85	110.57
25	N	609	CHL	C3D-C2D-C1D	-5.60	98.19	105.83
26	3	603	CLA	C4A-NA-C1A	5.59	109.22	106.71
25	s	606	CHL	C3C-C4C-NC	5.58	116.83	110.57
25	y	609	CHL	O2D-CGD-CBD	5.58	121.18	111.27
25	y	609	CHL	C3D-C2D-C1D	-5.58	98.22	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	609	CHL	O2D-CGD-CBD	5.57	121.16	111.27
25	Y	609	CHL	C3D-C2D-C1D	-5.57	98.23	105.83
25	y	601	CHL	C3D-C2D-C1D	-5.56	98.24	105.83
25	y	606	CHL	C3D-C2D-C1D	-5.56	98.24	105.83
25	Y	601	CHL	C3D-C2D-C1D	-5.55	98.25	105.83
28	r	622	XAT	C38-C25-C26	-5.55	112.95	122.26
28	R	622	XAT	C38-C25-C26	-5.55	112.96	122.26
25	R	607	CHL	C3D-C2D-C1D	-5.54	98.27	105.83
26	Y	614	CLA	C4A-NA-C1A	5.53	109.19	106.71
25	1	606	CHL	CHD-C1D-ND	-5.53	119.37	124.45
28	4	622	XAT	C6-C7-C8	-5.53	114.30	125.99
25	Y	606	CHL	C3D-C2D-C1D	-5.53	98.29	105.83
28	8	622	XAT	C6-C7-C8	-5.53	114.30	125.99
26	y	614	CLA	C4A-NA-C1A	5.53	109.19	106.71
25	n	608	CHL	C3C-C4C-NC	5.52	116.77	110.57
26	4	603	CLA	C4A-NA-C1A	5.52	109.19	106.71
25	G	608	CHL	C3D-C2D-C1D	-5.52	98.30	105.83
25	g	608	CHL	C3D-C2D-C1D	-5.51	98.31	105.83
25	g	607	CHL	C3C-C4C-NC	5.51	116.75	110.57
25	r	607	CHL	C3D-C2D-C1D	-5.51	98.31	105.83
25	G	607	CHL	C3C-C4C-NC	5.51	116.75	110.57
25	N	608	CHL	C3C-C4C-NC	5.51	116.75	110.57
25	s	607	CHL	C3D-C2D-C1D	-5.50	98.32	105.83
25	n	601	CHL	C3D-C2D-C1D	-5.50	98.32	105.83
31	C	515	BCR	C7-C8-C9	-5.50	117.92	126.23
25	N	601	CHL	C3D-C2D-C1D	-5.50	98.32	105.83
25	5	606	CHL	CHD-C1D-ND	-5.50	119.40	124.45
28	n	1622	XAT	C6-C7-C8	-5.50	114.37	125.99
25	S	607	CHL	C3D-C2D-C1D	-5.50	98.33	105.83
25	2	608	CHL	C3D-C2D-C1D	-5.49	98.33	105.83
25	6	608	CHL	C3D-C2D-C1D	-5.49	98.33	105.83
25	8	601	CHL	C2D-C1D-ND	5.49	114.15	110.10
25	r	614	CHL	C3D-C2D-C1D	-5.49	98.34	105.83
25	8	608	CHL	C3C-C4C-NC	5.48	116.72	110.57
25	s	608	CHL	CHD-C1D-ND	-5.48	119.42	124.45
28	N	1622	XAT	C6-C7-C8	-5.48	114.41	125.99
25	8	609	CHL	C2D-C1D-ND	5.47	114.14	110.10
31	c	515	BCR	C7-C8-C9	-5.47	117.96	126.23
25	R	614	CHL	C3D-C2D-C1D	-5.47	98.36	105.83
28	3	1622	XAT	C31-C30-C29	-5.47	119.51	127.31
28	7	1622	XAT	C31-C30-C29	-5.47	119.51	127.31
25	4	601	CHL	C2D-C1D-ND	5.47	114.13	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	2	601	CHL	C2C-C3C-C4C	-5.47	102.59	106.49
26	n	614	CLA	CMB-C2B-C1B	-5.46	120.07	128.46
26	1	604	CLA	CMB-C2B-C1B	-5.46	120.08	128.46
26	8	603	CLA	C4A-NA-C1A	5.45	109.16	106.71
25	S	608	CHL	CHD-C1D-ND	-5.45	119.45	124.45
26	r	616	CLA	C4A-NA-C1A	5.45	109.16	106.71
25	1	606	CHL	C3C-C4C-NC	5.44	116.68	110.57
26	N	614	CLA	CMB-C2B-C1B	-5.44	120.10	128.46
26	5	604	CLA	CMB-C2B-C1B	-5.44	120.10	128.46
31	8	623	BCR	C16-C17-C18	-5.44	119.54	127.31
31	4	623	BCR	C16-C17-C18	-5.44	119.55	127.31
26	R	603	CLA	CMB-C2B-C1B	-5.44	120.10	128.46
25	6	601	CHL	C2C-C3C-C4C	-5.44	102.61	106.49
26	r	603	CLA	CMB-C2B-C1B	-5.43	120.12	128.46
25	4	608	CHL	C3C-C4C-NC	5.42	116.65	110.57
25	R	606	CHL	C3C-C4C-NC	5.42	116.65	110.57
29	r	623	NEX	C15-C14-C13	-5.42	119.57	127.31
26	C	509	CLA	CMB-C2B-C1B	-5.42	120.14	128.46
26	c	509	CLA	CMB-C2B-C1B	-5.42	120.14	128.46
25	5	606	CHL	C3C-C4C-NC	5.42	116.65	110.57
25	7	609	CHL	O2D-CGD-CBD	5.42	120.89	111.27
25	r	606	CHL	C3C-C4C-NC	5.41	116.64	110.57
25	3	609	CHL	O2D-CGD-CBD	5.40	120.87	111.27
25	1	605	CHL	C3C-C4C-NC	5.40	116.63	110.57
28	y	1622	XAT	C11-C10-C9	-5.40	119.61	127.31
25	4	609	CHL	C2D-C1D-ND	5.40	114.08	110.10
25	G	608	CHL	C3C-C4C-NC	5.40	116.62	110.57
25	7	606	CHL	C3C-C4C-NC	5.40	116.62	110.57
28	Y	1622	XAT	C11-C10-C9	-5.39	119.61	127.31
29	R	623	NEX	C15-C14-C13	-5.39	119.62	127.31
25	6	606	CHL	C3C-C4C-NC	5.39	116.61	110.57
26	S	604	CLA	CMB-C2B-C1B	-5.38	120.19	128.46
25	5	605	CHL	C3C-C4C-NC	5.38	116.60	110.57
25	N	606	CHL	CHD-C1D-ND	-5.38	119.51	124.45
25	2	606	CHL	C3C-C4C-NC	5.38	116.60	110.57
26	A	405	CLA	CMB-C2B-C1B	-5.38	120.20	128.46
26	Y	612	CLA	C4A-NA-C1A	5.37	109.12	106.71
26	s	604	CLA	CMB-C2B-C1B	-5.37	120.21	128.46
26	R	616	CLA	C4A-NA-C1A	5.37	109.12	106.71
25	g	608	CHL	C3C-C4C-NC	5.37	116.59	110.57
26	a	405	CLA	CMB-C2B-C1B	-5.37	120.22	128.46
25	G	605	CHL	O2D-CGD-CBD	5.35	120.78	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	g	605	CHL	O2D-CGD-CBD	5.35	120.78	111.27
26	y	612	CLA	C4A-NA-C1A	5.35	109.11	106.71
25	4	606	CHL	O2D-CGD-CBD	5.35	120.77	111.27
25	3	606	CHL	C3C-C4C-NC	5.35	116.57	110.57
25	n	606	CHL	CHD-C1D-ND	-5.34	119.54	124.45
25	Y	608	CHL	C3D-C2D-C1D	-5.34	98.54	105.83
25	8	606	CHL	O2D-CGD-CBD	5.33	120.75	111.27
26	B	604	CLA	CMB-C2B-C1B	-5.33	120.27	128.46
26	b	605	CLA	C2D-C1D-ND	-5.33	106.18	110.10
40	D	401	BCT	O2-C-O1	5.33	133.36	119.55
25	N	601	CHL	O2D-CGD-CBD	5.32	120.73	111.27
25	y	608	CHL	C3D-C2D-C1D	-5.32	98.57	105.83
25	G	609	CHL	C3D-C2D-C1D	-5.32	98.57	105.83
25	g	609	CHL	C3D-C2D-C1D	-5.32	98.57	105.83
25	Y	607	CHL	C3D-C2D-C1D	-5.31	98.58	105.83
40	d	401	BCT	O2-C-O1	5.31	133.32	119.55
31	b	618	BCR	C15-C14-C13	-5.31	119.73	127.31
31	B	618	BCR	C15-C14-C13	-5.31	119.73	127.31
26	B	605	CLA	C2D-C1D-ND	-5.31	106.19	110.10
25	N	608	CHL	O2D-CGD-CBD	5.30	120.69	111.27
26	b	604	CLA	CMB-C2B-C1B	-5.30	120.32	128.46
25	n	601	CHL	O2D-CGD-CBD	5.30	120.68	111.27
26	y	602	CLA	C4A-NA-C1A	5.30	109.09	106.71
25	y	607	CHL	C3D-C2D-C1D	-5.30	98.60	105.83
31	T	101	BCR	C7-C8-C9	-5.29	118.23	126.23
25	n	608	CHL	O2D-CGD-CBD	5.29	120.67	111.27
26	S	613	CLA	CMB-C2B-C1B	-5.29	120.33	128.46
26	s	613	CLA	CMB-C2B-C1B	-5.29	120.33	128.46
26	S	612	CLA	C4A-NA-C1A	5.28	109.08	106.71
25	2	605	CHL	C3C-C4C-NC	5.28	116.50	110.57
25	6	605	CHL	C3C-C4C-NC	5.28	116.50	110.57
28	N	1622	XAT	C38-C25-C26	-5.28	113.41	122.26
26	G	602	CLA	CMB-C2B-C1B	-5.28	120.34	128.46
26	D	403	CLA	CMB-C2B-C1B	-5.28	120.34	128.46
26	D	402	CLA	CMB-C2B-C1B	-5.28	120.35	128.46
26	d	402	CLA	CMB-C2B-C1B	-5.28	120.35	128.46
26	r	603	CLA	C4A-NA-C1A	5.28	109.08	106.71
29	r	623	NEX	C11-C10-C9	-5.28	119.77	127.31
25	1	607	CHL	C3C-C4C-NC	5.28	116.49	110.57
25	5	607	CHL	C3C-C4C-NC	5.28	116.49	110.57
25	3	605	CHL	O2D-CGD-CBD	5.28	120.64	111.27
28	3	1622	XAT	C38-C25-C26	-5.28	113.42	122.26

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	7	606	CHL	O2D-CGD-CBD	5.28	120.64	111.27
26	R	603	CLA	C4A-NA-C1A	5.27	109.08	106.71
28	3	1622	XAT	C15-C14-C13	-5.27	119.79	127.31
28	n	1622	XAT	C38-C25-C26	-5.27	113.42	122.26
29	R	623	NEX	C11-C10-C9	-5.27	119.79	127.31
25	R	606	CHL	O2D-CGD-CBD	5.27	120.63	111.27
26	g	602	CLA	CMB-C2B-C1B	-5.27	120.37	128.46
25	Y	608	CHL	O2D-CGD-CBD	5.26	120.62	111.27
28	7	1622	XAT	C38-C25-C26	-5.26	113.44	122.26
26	C	510	CLA	CMB-C2B-C1B	-5.26	120.38	128.46
25	3	606	CHL	O2D-CGD-CBD	5.26	120.61	111.27
25	r	606	CHL	O2D-CGD-CBD	5.26	120.61	111.27
28	5	1622	XAT	C31-C30-C29	-5.26	119.81	127.31
25	S	606	CHL	O2D-CGD-CBD	5.26	120.61	111.27
26	b	613	CLA	CMB-C2B-C3B	5.25	134.51	124.68
31	t	101	BCR	C7-C8-C9	-5.25	118.30	126.23
25	y	608	CHL	O2D-CGD-CBD	5.25	120.60	111.27
26	d	403	CLA	CMB-C2B-C1B	-5.25	120.39	128.46
25	7	605	CHL	O2D-CGD-CBD	5.25	120.60	111.27
28	7	1622	XAT	C15-C14-C13	-5.25	119.82	127.31
25	s	606	CHL	C3D-C4D-ND	5.25	118.72	110.24
25	S	606	CHL	C3D-C4D-ND	5.24	118.72	110.24
25	s	606	CHL	O2D-CGD-CBD	5.24	120.58	111.27
26	g	611	CLA	CMB-C2B-C1B	-5.24	120.41	128.46
26	c	510	CLA	CMB-C2B-C1B	-5.24	120.42	128.46
26	s	612	CLA	C4A-NA-C1A	5.23	109.06	106.71
28	1	1622	XAT	C31-C30-C29	-5.23	119.84	127.31
26	Y	602	CLA	C4A-NA-C1A	5.23	109.06	106.71
25	G	606	CHL	C3C-C4C-NC	5.23	116.43	110.57
25	g	606	CHL	C3C-C4C-NC	5.23	116.43	110.57
26	B	613	CLA	CMB-C2B-C3B	5.23	134.45	124.68
25	2	607	CHL	O2D-CGD-CBD	5.22	120.55	111.27
28	4	622	XAT	C18-C5-C6	-5.22	113.51	122.26
28	8	622	XAT	C18-C5-C6	-5.22	113.52	122.26
25	y	606	CHL	O2D-CGD-CBD	5.21	120.53	111.27
25	6	607	CHL	O2D-CGD-CBD	5.21	120.53	111.27
26	G	611	CLA	CMB-C2B-C1B	-5.21	120.45	128.46
25	Y	606	CHL	O2D-CGD-CBD	5.21	120.52	111.27
25	3	601	CHL	C3D-C2D-C1D	-5.20	98.74	105.83
25	R	606	CHL	C3D-C2D-C1D	-5.19	98.74	105.83
28	5	1622	XAT	C15-C14-C13	-5.19	119.90	127.31
28	G	1622	XAT	C31-C30-C29	-5.18	119.91	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	r	606	CHL	C3D-C2D-C1D	-5.18	98.76	105.83
25	7	601	CHL	C3D-C2D-C1D	-5.18	98.76	105.83
28	1	1622	XAT	C15-C14-C13	-5.18	119.92	127.31
26	R	602	CLA	CMB-C2B-C1B	-5.17	120.52	128.46
25	1	607	CHL	C3D-C2D-C1D	-5.17	98.78	105.83
29	Y	1623	NEX	C17-C1-C6	-5.17	105.84	110.47
25	5	607	CHL	C3D-C2D-C1D	-5.16	98.79	105.83
25	Y	606	CHL	CHD-C4C-C3C	-5.16	117.26	124.84
31	4	623	BCR	C28-C27-C26	-5.15	104.87	114.08
26	c	513	CLA	CMB-C2B-C1B	-5.15	120.54	128.46
25	Y	601	CHL	O2D-CGD-CBD	5.15	120.43	111.27
28	y	1622	XAT	C15-C35-C34	-5.15	112.92	123.47
26	r	602	CLA	CMB-C2B-C1B	-5.15	120.55	128.46
28	g	1622	XAT	C31-C30-C29	-5.15	119.96	127.31
31	8	623	BCR	C28-C27-C26	-5.15	104.89	114.08
25	y	606	CHL	CHD-C4C-C3C	-5.14	117.28	124.84
25	S	606	CHL	C3D-C2D-C1D	-5.14	98.81	105.83
28	Y	1622	XAT	C15-C35-C34	-5.14	112.95	123.47
25	8	608	CHL	CHD-C4C-C3C	-5.14	117.29	124.84
25	s	606	CHL	C3D-C2D-C1D	-5.14	98.82	105.83
29	y	1623	NEX	C17-C1-C6	-5.13	105.88	110.47
25	y	601	CHL	O2D-CGD-CBD	5.13	120.39	111.27
26	C	513	CLA	CMB-C2B-C1B	-5.13	120.58	128.46
29	n	1623	NEX	C35-C34-C33	-5.13	119.99	127.31
26	c	508	CLA	CMB-C2B-C3B	5.13	134.27	124.68
26	C	508	CLA	CMB-C2B-C3B	5.12	134.26	124.68
25	2	607	CHL	C3C-C4C-NC	5.12	116.32	110.57
29	N	1623	NEX	C35-C34-C33	-5.12	120.00	127.31
29	6	1623	NEX	C15-C14-C13	-5.12	120.00	127.31
28	Y	1622	XAT	O4-C5-C18	5.12	121.19	115.06
28	y	1622	XAT	O4-C5-C18	5.12	121.19	115.06
25	4	608	CHL	CHD-C4C-C3C	-5.11	117.33	124.84
29	2	1623	NEX	C15-C14-C13	-5.11	120.02	127.31
29	3	1623	NEX	C38-C25-C26	-5.10	113.71	122.26
28	1	1622	XAT	C38-C25-C26	-5.09	113.72	122.26
28	5	1622	XAT	C38-C25-C26	-5.09	113.73	122.26
26	b	608	CLA	CMB-C2B-C1B	-5.09	120.64	128.46
26	S	614	CLA	CMB-C2B-C1B	-5.09	120.65	128.46
25	6	607	CHL	C3C-C4C-NC	5.08	116.27	110.57
26	8	602	CLA	C4A-NA-C1A	5.08	108.99	106.71
28	g	1622	XAT	C15-C35-C34	-5.08	113.07	123.47
26	s	614	CLA	CMB-C2B-C1B	-5.08	120.66	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	7	1623	NEX	C38-C25-C26	-5.08	113.75	122.26
25	Y	608	CHL	C3C-C4C-NC	5.07	116.26	110.57
25	y	608	CHL	C3C-C4C-NC	5.07	116.26	110.57
28	r	622	XAT	C6-C7-C8	-5.07	115.27	125.99
26	B	608	CLA	CMB-C2B-C1B	-5.07	120.67	128.46
26	G	602	CLA	C4A-NA-C1A	5.07	108.98	106.71
25	6	609	CHL	C3C-C4C-NC	5.07	116.25	110.57
25	N	609	CHL	O2D-CGD-CBD	5.06	120.27	111.27
26	r	613	CLA	C4A-NA-C1A	5.06	108.98	106.71
25	8	606	CHL	C3D-C2D-C1D	-5.06	98.92	105.83
28	G	1622	XAT	C15-C35-C34	-5.06	113.10	123.47
28	R	622	XAT	C6-C7-C8	-5.06	115.29	125.99
25	S	601	CHL	C3D-C4D-ND	5.06	118.42	110.24
25	2	609	CHL	C3C-C4C-NC	5.05	116.24	110.57
25	n	609	CHL	O2D-CGD-CBD	5.05	120.24	111.27
25	s	601	CHL	C3D-C4D-ND	5.05	118.41	110.24
25	4	606	CHL	C3D-C2D-C1D	-5.05	98.94	105.83
25	2	605	CHL	C3D-C2D-C1D	-5.05	98.94	105.83
25	6	605	CHL	C3D-C2D-C1D	-5.05	98.94	105.83
25	5	605	CHL	C3D-C2D-C1D	-5.05	98.95	105.83
25	5	609	CHL	O2D-CGD-CBD	5.04	120.23	111.27
25	G	609	CHL	O2D-CGD-CBD	5.04	120.23	111.27
29	y	1623	NEX	C27-C28-C29	-5.04	117.71	125.53
25	3	606	CHL	CHD-C1D-ND	-5.04	119.82	124.45
29	Y	1623	NEX	C27-C28-C29	-5.04	117.71	125.53
25	1	609	CHL	C3D-C2D-C1D	-5.04	98.96	105.83
25	g	609	CHL	O2D-CGD-CBD	5.04	120.22	111.27
25	1	605	CHL	C3D-C2D-C1D	-5.03	98.96	105.83
25	5	605	CHL	O2D-CGD-CBD	5.03	120.20	111.27
29	R	623	NEX	C27-C28-C29	-5.03	117.73	125.53
29	r	623	NEX	C27-C28-C29	-5.03	117.73	125.53
25	7	605	CHL	C3C-C4C-NC	5.03	116.21	110.57
29	5	1623	NEX	C27-C28-C29	-5.02	117.73	125.53
25	5	609	CHL	C3D-C2D-C1D	-5.02	98.98	105.83
25	g	605	CHL	C3D-C2D-C1D	-5.02	98.98	105.83
29	1	1623	NEX	C27-C28-C29	-5.02	117.74	125.53
25	1	609	CHL	O2D-CGD-CBD	5.02	120.18	111.27
25	N	606	CHL	O2D-CGD-CBD	5.02	120.18	111.27
25	7	606	CHL	CHD-C1D-ND	-5.02	119.84	124.45
25	1	605	CHL	O2D-CGD-CBD	5.01	120.17	111.27
26	7	613	CLA	C4A-NA-C1A	5.01	108.96	106.71
25	n	606	CHL	O2D-CGD-CBD	5.01	120.17	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	G	605	CHL	C3D-C2D-C1D	-5.01	99.00	105.83
26	s	612	CLA	CMB-C2B-C3B	5.01	134.04	124.68
25	7	605	CHL	C3D-C2D-C1D	-5.00	99.00	105.83
25	3	605	CHL	C3C-C4C-NC	5.00	116.18	110.57
25	3	609	CHL	C2D-C1D-ND	5.00	113.79	110.10
25	7	609	CHL	C2D-C1D-ND	5.00	113.79	110.10
26	S	612	CLA	CMB-C2B-C3B	5.00	134.03	124.68
25	3	605	CHL	C3D-C2D-C1D	-5.00	99.01	105.83
31	8	623	BCR	C15-C14-C13	-5.00	120.18	127.31
25	3	601	CHL	C3D-C4D-ND	4.99	118.32	110.24
26	g	602	CLA	C4A-NA-C1A	4.99	108.95	106.71
25	n	605	CHL	C3D-C2D-C1D	-4.98	99.03	105.83
25	6	601	CHL	C3D-C2D-C1D	-4.98	99.04	105.83
29	s	1623	NEX	C11-C10-C9	-4.97	120.21	127.31
31	4	623	BCR	C15-C14-C13	-4.97	120.21	127.31
29	n	1623	NEX	C27-C28-C29	-4.97	117.82	125.53
25	2	601	CHL	C3D-C2D-C1D	-4.97	99.05	105.83
29	S	1623	NEX	C11-C10-C9	-4.97	120.22	127.31
26	N	612	CLA	C4A-NA-C1A	4.96	108.94	106.71
26	n	612	CLA	C4A-NA-C1A	4.96	108.94	106.71
26	A	406	CLA	CMB-C2B-C1B	-4.96	120.83	128.46
26	a	406	CLA	CMB-C2B-C1B	-4.96	120.84	128.46
25	N	605	CHL	C3D-C2D-C1D	-4.96	99.06	105.83
25	7	601	CHL	C3D-C4D-ND	4.95	118.24	110.24
29	g	1623	NEX	C11-C10-C9	-4.95	120.25	127.31
28	4	622	XAT	O4-C5-C18	4.95	120.98	115.06
28	g	1622	XAT	C38-C25-C26	-4.95	113.97	122.26
29	N	1623	NEX	C27-C28-C29	-4.95	117.86	125.53
29	G	1623	NEX	C38-C25-C26	-4.94	113.97	122.26
26	2	604	CLA	C4A-NA-C1A	4.94	108.93	106.71
26	R	613	CLA	C4A-NA-C1A	4.94	108.93	106.71
26	6	604	CLA	C4A-NA-C1A	4.94	108.93	106.71
25	7	606	CHL	CAC-C3C-C4C	4.94	131.22	124.81
28	8	622	XAT	O4-C5-C18	4.94	120.98	115.06
29	g	1623	NEX	C38-C25-C26	-4.94	113.98	122.26
28	n	1622	XAT	C15-C35-C34	-4.94	113.36	123.47
26	4	602	CLA	C4A-NA-C1A	4.93	108.92	106.71
28	G	1622	XAT	C38-C25-C26	-4.93	114.00	122.26
26	B	603	CLA	CMB-C2B-C1B	-4.93	120.89	128.46
26	3	613	CLA	C4A-NA-C1A	4.92	108.92	106.71
25	4	606	CHL	C3C-C4C-NC	4.92	116.09	110.57
28	N	1622	XAT	C15-C35-C34	-4.92	113.40	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	606	CHL	C3D-C4D-ND	4.92	118.19	110.24
25	Y	606	CHL	CHD-C1D-ND	-4.92	119.94	124.45
29	G	1623	NEX	C11-C10-C9	-4.92	120.29	127.31
25	y	606	CHL	CHD-C1D-ND	-4.91	119.94	124.45
25	3	606	CHL	CAC-C3C-C4C	4.90	131.17	124.81
26	b	603	CLA	CMB-C2B-C1B	-4.90	120.93	128.46
25	5	607	CHL	C3D-C4D-ND	4.90	118.17	110.24
25	1	607	CHL	C3D-C4D-ND	4.90	118.16	110.24
25	G	607	CHL	C3D-C2D-C1D	-4.90	99.15	105.83
25	n	606	CHL	C3D-C2D-C1D	-4.90	99.15	105.83
26	Y	602	CLA	CMB-C2B-C1B	-4.90	120.94	128.46
25	7	607	CHL	O2D-CGD-CBD	4.90	119.97	111.27
25	G	601	CHL	C3D-C4D-ND	4.90	118.16	110.24
25	2	601	CHL	C3D-C4D-ND	4.90	118.16	110.24
25	g	607	CHL	C3D-C2D-C1D	-4.89	99.15	105.83
25	3	607	CHL	O2D-CGD-CBD	4.89	119.96	111.27
25	r	606	CHL	C3D-C4D-ND	4.89	118.15	110.24
25	g	601	CHL	C3D-C4D-ND	4.89	118.15	110.24
25	N	606	CHL	C3D-C2D-C1D	-4.89	99.16	105.83
25	4	601	CHL	C3D-C2D-C1D	-4.89	99.16	105.83
26	G	604	CLA	C4A-NA-C1A	4.89	108.90	106.71
25	8	601	CHL	C3D-C2D-C1D	-4.89	99.16	105.83
25	5	605	CHL	C3D-C4D-ND	4.89	118.14	110.24
25	8	607	CHL	O2D-CGD-CBD	4.89	119.95	111.27
26	S	614	CLA	C4A-NA-C1A	4.88	108.90	106.71
26	B	610	CLA	CMB-C2B-C1B	-4.88	120.96	128.46
25	8	606	CHL	C3C-C4C-NC	4.88	116.04	110.57
26	c	501	CLA	C4A-NA-C1A	4.88	108.90	106.71
26	b	610	CLA	CMB-C2B-C1B	-4.88	120.97	128.46
26	y	602	CLA	CMB-C2B-C1B	-4.88	120.97	128.46
25	6	601	CHL	C3D-C4D-ND	4.88	118.13	110.24
25	1	605	CHL	C3D-C4D-ND	4.87	118.12	110.24
25	2	605	CHL	C3D-C4D-ND	4.87	118.12	110.24
25	6	605	CHL	C3D-C4D-ND	4.87	118.12	110.24
36	a	418	SQD	O7-S-C6	4.87	112.73	106.94
25	8	606	CHL	C3D-C4D-ND	4.87	118.12	110.24
25	G	608	CHL	O2D-CGD-CBD	4.87	119.92	111.27
25	g	608	CHL	O2D-CGD-CBD	4.87	119.92	111.27
25	S	601	CHL	C2D-C1D-ND	4.87	113.69	110.10
29	2	1623	NEX	C38-C25-C26	-4.87	114.10	122.26
25	7	606	CHL	C3D-C2D-C1D	-4.87	99.19	105.83
25	4	607	CHL	O2D-CGD-CBD	4.86	119.91	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	609	CHL	C3D-C2D-C1D	-4.86	99.20	105.83
29	6	1623	NEX	C38-C25-C26	-4.86	114.11	122.26
25	G	601	CHL	C2C-C3C-C4C	-4.86	103.03	106.49
28	4	622	XAT	C26-C27-C28	-4.86	115.72	125.99
27	2	1620	LUT	C35-C34-C33	-4.86	120.38	127.31
25	g	601	CHL	O2D-CGD-CBD	4.86	119.90	111.27
26	c	512	CLA	CMB-C2B-C1B	-4.86	121.00	128.46
25	8	609	CHL	C3D-C4D-ND	4.85	118.09	110.24
28	Y	1622	XAT	C38-C25-C26	-4.85	114.13	122.26
25	g	606	CHL	C3D-C4D-ND	4.85	118.08	110.24
25	s	601	CHL	C2D-C1D-ND	4.85	113.68	110.10
25	y	605	CHL	CHD-C4C-C3C	-4.85	117.72	124.84
25	1	609	CHL	C3C-C4C-NC	4.85	116.01	110.57
25	5	609	CHL	C3C-C4C-NC	4.85	116.01	110.57
26	C	512	CLA	CMB-C2B-C1B	-4.85	121.02	128.46
25	2	609	CHL	C3D-C2D-C1D	-4.85	99.22	105.83
25	G	606	CHL	C3D-C4D-ND	4.84	118.08	110.24
26	R	604	CLA	CMB-C2B-C1B	-4.84	121.02	128.46
26	r	604	CLA	CMB-C2B-C1B	-4.84	121.02	128.46
25	3	607	CHL	C2D-C1D-ND	4.84	113.67	110.10
25	4	609	CHL	C3D-C4D-ND	4.84	118.07	110.24
25	Y	605	CHL	CHD-C4C-C3C	-4.84	117.72	124.84
28	y	1622	XAT	C38-C25-C26	-4.84	114.15	122.26
28	8	622	XAT	C26-C27-C28	-4.84	115.76	125.99
25	3	606	CHL	C3D-C2D-C1D	-4.84	99.23	105.83
36	A	418	SQD	O7-S-C6	4.84	112.69	106.94
27	6	1620	LUT	C35-C34-C33	-4.84	120.40	127.31
25	4	606	CHL	C3D-C4D-ND	4.84	118.06	110.24
36	a	412	SQD	O6-C1-C2	4.84	115.85	108.30
25	g	601	CHL	C2C-C3C-C4C	-4.83	103.04	106.49
26	B	609	CLA	CMB-C2B-C3B	4.83	133.72	124.68
25	R	614	CHL	C3D-C4D-ND	4.83	118.06	110.24
26	C	501	CLA	C4A-NA-C1A	4.83	108.88	106.71
26	b	609	CLA	CMB-C2B-C3B	4.83	133.72	124.68
25	G	601	CHL	O2D-CGD-CBD	4.83	119.85	111.27
26	N	602	CLA	CMB-C2B-C3B	4.83	133.71	124.68
36	A	412	SQD	O6-C1-C2	4.82	115.83	108.30
25	1	609	CHL	C3D-C4D-ND	4.82	118.04	110.24
31	b	620	BCR	C7-C8-C9	-4.82	118.95	126.23
26	s	610	CLA	CMB-C2B-C1B	-4.82	121.05	128.46
25	r	614	CHL	C3D-C4D-ND	4.82	118.04	110.24
25	3	607	CHL	C3D-C2D-C1D	-4.82	99.25	105.83

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	607	CLA	CMB-C2B-C1B	-4.82	121.06	128.46
25	5	609	CHL	C3D-C4D-ND	4.82	118.03	110.24
29	3	1623	NEX	C11-C10-C9	-4.82	120.43	127.31
26	n	602	CLA	CMB-C2B-C3B	4.81	133.68	124.68
26	R	601	CLA	CMB-C2B-C1B	-4.81	121.07	128.46
26	N	604	CLA	C4A-NA-C1A	4.81	108.87	106.71
26	n	604	CLA	C4A-NA-C1A	4.81	108.87	106.71
25	8	607	CHL	C3D-C2D-C1D	-4.81	99.27	105.83
26	r	601	CLA	CMB-C2B-C1B	-4.81	121.07	128.46
31	B	620	BCR	C7-C8-C9	-4.81	118.97	126.23
26	S	610	CLA	CMB-C2B-C1B	-4.80	121.08	128.46
25	4	607	CHL	C3D-C2D-C1D	-4.80	99.28	105.83
25	1	601	CHL	C3D-C4D-ND	4.80	118.01	110.24
26	b	607	CLA	CMB-C2B-C1B	-4.80	121.08	128.46
35	A	409	PHO	CMB-C2B-C3B	4.80	133.66	124.68
31	c	515	BCR	C21-C20-C19	-4.80	108.25	123.22
29	7	1623	NEX	C11-C10-C9	-4.79	120.47	127.31
31	C	515	BCR	C21-C20-C19	-4.79	108.27	123.22
25	7	607	CHL	C3D-C2D-C1D	-4.79	99.29	105.83
25	R	614	CHL	C3C-C4C-NC	4.79	115.94	110.57
25	8	609	CHL	C3D-C2D-C1D	-4.79	99.30	105.83
25	5	601	CHL	C3D-C4D-ND	4.78	117.97	110.24
26	s	614	CLA	C4A-NA-C1A	4.78	108.86	106.71
25	y	608	CHL	C3D-C4D-ND	4.78	117.97	110.24
35	a	409	PHO	CMB-C2B-C3B	4.78	133.62	124.68
25	7	607	CHL	C2D-C1D-ND	4.78	113.63	110.10
25	5	606	CHL	C3D-C4D-ND	4.78	117.97	110.24
25	y	601	CHL	C3D-C4D-ND	4.78	117.97	110.24
25	6	607	CHL	C3D-C2D-C1D	-4.78	99.31	105.83
25	1	606	CHL	C3D-C4D-ND	4.78	117.97	110.24
26	g	604	CLA	C4A-NA-C1A	4.78	108.85	106.71
25	N	601	CHL	C3D-C4D-ND	4.78	117.96	110.24
27	G	1621	LUT	C15-C14-C13	-4.78	120.50	127.31
25	r	614	CHL	C3C-C4C-NC	4.77	115.92	110.57
38	D	405	PL9	C7-C3-C4	4.77	120.75	116.88
25	N	607	CHL	CHD-C1D-ND	-4.77	120.07	124.45
25	6	606	CHL	C3D-C4D-ND	4.77	117.95	110.24
25	2	607	CHL	C3D-C2D-C1D	-4.77	99.32	105.83
25	4	607	CHL	C3D-C4D-ND	4.77	117.95	110.24
25	4	609	CHL	C3D-C2D-C1D	-4.76	99.33	105.83
28	1	1622	XAT	C6-C7-C8	-4.76	115.92	125.99
25	3	601	CHL	O2D-CGD-CBD	4.76	119.73	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	7	601	CHL	O2D-CGD-CBD	4.76	119.73	111.27
25	Y	608	CHL	C3D-C4D-ND	4.76	117.94	110.24
25	n	601	CHL	C3D-C4D-ND	4.76	117.94	110.24
28	7	1622	XAT	O24-C25-C38	4.76	120.76	115.06
28	5	1622	XAT	C6-C7-C8	-4.76	115.93	125.99
26	8	611	CLA	C4A-NA-C1A	4.76	108.84	106.71
29	n	1623	NEX	C38-C25-C26	-4.76	114.29	122.26
25	Y	601	CHL	C3D-C4D-ND	4.76	117.93	110.24
25	S	608	CHL	C3D-C2D-C1D	-4.76	99.34	105.83
25	8	608	CHL	C3D-C4D-ND	4.75	117.93	110.24
29	N	1623	NEX	C38-C25-C26	-4.75	114.29	122.26
25	2	606	CHL	C3D-C4D-ND	4.75	117.93	110.24
28	2	1622	XAT	C38-C25-C26	-4.75	114.29	122.26
25	s	607	CHL	C3C-C4C-NC	4.75	115.90	110.57
26	6	603	CLA	C4A-NA-C1A	4.75	108.84	106.71
28	3	1622	XAT	O24-C25-C38	4.75	120.75	115.06
26	n	614	CLA	CMB-C2B-C3B	4.75	133.57	124.68
25	s	608	CHL	C3D-C2D-C1D	-4.75	99.35	105.83
26	R	603	CLA	CMB-C2B-C3B	4.75	133.57	124.68
25	S	607	CHL	C3C-C4C-NC	4.75	115.90	110.57
27	S	1621	LUT	C35-C34-C33	-4.75	120.53	127.31
25	Y	605	CHL	C3D-C4D-ND	4.75	117.92	110.24
28	6	1622	XAT	C38-C25-C26	-4.75	114.30	122.26
25	8	607	CHL	C3D-C4D-ND	4.75	117.92	110.24
27	s	1621	LUT	C35-C34-C33	-4.75	120.54	127.31
25	8	609	CHL	O2D-CGD-CBD	4.74	119.70	111.27
31	4	623	BCR	C7-C8-C9	-4.74	119.08	126.23
27	g	1621	LUT	C15-C14-C13	-4.74	120.55	127.31
25	g	605	CHL	C3D-C4D-ND	4.74	117.90	110.24
25	3	609	CHL	C3D-C4D-ND	4.74	117.90	110.24
25	G	605	CHL	C3D-C4D-ND	4.74	117.90	110.24
25	4	609	CHL	O2D-CGD-CBD	4.73	119.68	111.27
26	r	603	CLA	CMB-C2B-C3B	4.73	133.53	124.68
29	s	1623	NEX	C38-C25-C26	-4.73	114.33	122.26
28	N	1622	XAT	C27-C28-C29	-4.73	118.19	125.53
26	N	614	CLA	CMB-C2B-C3B	4.73	133.53	124.68
25	4	608	CHL	C3D-C4D-ND	4.73	117.89	110.24
25	n	607	CHL	CHD-C1D-ND	-4.73	120.11	124.45
25	N	607	CHL	CHD-C4C-C3C	-4.73	117.89	124.84
38	d	405	PL9	C7-C3-C4	4.72	120.72	116.88
31	8	623	BCR	C7-C8-C9	-4.72	119.10	126.23
25	n	607	CHL	CHD-C4C-C3C	-4.72	117.90	124.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	605	CHL	C3D-C4D-ND	4.72	117.88	110.24
25	5	608	CHL	CHD-C4C-C3C	-4.72	117.90	124.84
28	n	1622	XAT	C27-C28-C29	-4.72	118.21	125.53
25	7	609	CHL	C3D-C4D-ND	4.72	117.87	110.24
25	y	601	CHL	C1C-C2C-C3C	-4.72	103.37	107.11
25	S	608	CHL	C3D-C4D-ND	4.72	117.87	110.24
25	2	608	CHL	C3D-C4D-ND	4.72	117.87	110.24
25	1	601	CHL	O2D-CGD-CBD	4.72	119.65	111.27
25	5	601	CHL	O2D-CGD-CBD	4.71	119.64	111.27
28	2	1622	XAT	C31-C30-C29	-4.71	120.58	127.31
31	C	514	BCR	C15-C14-C13	-4.71	120.59	127.31
29	S	1623	NEX	C38-C25-C26	-4.71	114.37	122.26
25	6	608	CHL	C3D-C4D-ND	4.70	117.85	110.24
26	C	504	CLA	CMB-C2B-C3B	4.70	133.48	124.68
25	1	608	CHL	CHD-C4C-C3C	-4.70	117.93	124.84
39	C	518	DGD	O3G-C3G-C2G	-4.70	99.55	110.90
31	c	514	BCR	C15-C14-C13	-4.70	120.60	127.31
25	r	607	CHL	C3D-C4D-ND	4.70	117.84	110.24
39	c	518	DGD	O3G-C3G-C2G	-4.70	99.56	110.90
26	2	603	CLA	C4A-NA-C1A	4.70	108.82	106.71
28	6	1622	XAT	C31-C30-C29	-4.69	120.61	127.31
25	Y	601	CHL	C1C-C2C-C3C	-4.69	103.39	107.11
25	7	605	CHL	C3D-C4D-ND	4.69	117.83	110.24
25	g	607	CHL	C3D-C4D-ND	4.69	117.83	110.24
36	a	412	SQD	O9-S-C6	4.69	112.51	106.94
25	G	609	CHL	C3C-C4C-NC	4.69	115.83	110.57
26	c	504	CLA	CMB-C2B-C3B	4.69	133.45	124.68
28	R	622	XAT	O4-C5-C18	4.69	120.67	115.06
25	3	608	CHL	O2D-CGD-CBD	4.69	119.59	111.27
25	G	607	CHL	C3D-C4D-ND	4.69	117.82	110.24
25	6	606	CHL	C3D-C2D-C1D	-4.69	99.44	105.83
29	1	1623	NEX	C38-C25-C26	-4.68	114.41	122.26
25	s	608	CHL	C3D-C4D-ND	4.68	117.81	110.24
29	n	1623	NEX	C15-C14-C13	-4.68	120.63	127.31
25	Y	609	CHL	C3C-C4C-NC	4.68	115.82	110.57
36	A	412	SQD	O9-S-C6	4.68	112.50	106.94
25	y	609	CHL	C3C-C4C-NC	4.68	115.82	110.57
25	R	607	CHL	C3D-C4D-ND	4.68	117.81	110.24
26	C	508	CLA	O2D-CGD-O1D	-4.67	114.70	123.84
31	c	517	BCR	C15-C14-C13	-4.67	120.65	127.31
25	g	609	CHL	C1C-C2C-C3C	-4.66	103.41	107.11
31	C	517	BCR	C15-C14-C13	-4.66	120.65	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	605	CHL	O2D-CGD-CBD	4.66	119.55	111.27
25	7	608	CHL	O2D-CGD-CBD	4.66	119.55	111.27
25	g	609	CHL	C3C-C4C-NC	4.66	115.80	110.57
26	C	510	CLA	CMB-C2B-C3B	4.66	133.39	124.68
29	5	1623	NEX	C38-C25-C26	-4.66	114.45	122.26
25	2	605	CHL	O2D-CGD-CBD	4.66	119.54	111.27
25	3	605	CHL	C3D-C4D-ND	4.66	117.77	110.24
25	R	608	CHL	CHD-C1D-ND	-4.65	120.18	124.45
25	r	608	CHL	CHD-C1D-ND	-4.65	120.18	124.45
25	7	609	CHL	C3C-C4C-NC	4.65	115.79	110.57
28	r	622	XAT	O4-C5-C18	4.65	120.63	115.06
25	2	606	CHL	C3D-C2D-C1D	-4.65	99.49	105.83
28	3	1622	XAT	C18-C5-C6	-4.64	114.48	122.26
26	c	508	CLA	O2D-CGD-O1D	-4.64	114.76	123.84
25	N	609	CHL	C3C-C4C-NC	4.64	115.77	110.57
25	2	606	CHL	O2D-CGD-CBD	4.64	119.50	111.27
26	4	611	CLA	C4A-NA-C1A	4.63	108.79	106.71
25	N	609	CHL	C3D-C4D-ND	4.63	117.73	110.24
25	n	609	CHL	C3D-C4D-ND	4.63	117.73	110.24
25	4	609	CHL	C3C-C4C-NC	4.63	115.77	110.57
29	N	1623	NEX	C15-C14-C13	-4.63	120.70	127.31
25	n	609	CHL	C3C-C4C-NC	4.63	115.77	110.57
26	c	510	CLA	CMB-C2B-C3B	4.63	133.34	124.68
26	5	613	CLA	C4A-NA-C1A	4.63	108.79	106.71
28	7	1622	XAT	C18-C5-C6	-4.63	114.50	122.26
31	H	101	BCR	C16-C17-C18	-4.63	120.71	127.31
25	6	606	CHL	O2D-CGD-CBD	4.63	119.49	111.27
25	3	609	CHL	C3C-C4C-NC	4.62	115.76	110.57
25	6	609	CHL	C3D-C4D-ND	4.62	117.72	110.24
28	2	1622	XAT	C18-C5-C6	-4.62	114.51	122.26
28	G	1622	XAT	O4-C5-C18	4.62	120.59	115.06
26	7	604	CLA	CMB-C2B-C1B	-4.62	121.37	128.46
25	G	609	CHL	C1C-C2C-C3C	-4.62	103.45	107.11
26	1	613	CLA	C4A-NA-C1A	4.62	108.78	106.71
28	g	1622	XAT	O4-C5-C18	4.62	120.59	115.06
25	2	608	CHL	CHD-C4C-C3C	-4.61	118.06	124.84
25	R	607	CHL	O2D-CGD-CBD	4.61	119.47	111.27
25	Y	601	CHL	CAC-C3C-C4C	4.61	130.79	124.81
26	3	604	CLA	CMB-C2B-C1B	-4.61	121.38	128.46
25	Y	609	CHL	C3D-C4D-ND	4.61	117.69	110.24
31	h	101	BCR	C16-C17-C18	-4.60	120.74	127.31
25	r	607	CHL	O2D-CGD-CBD	4.60	119.45	111.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	6	1622	XAT	C18-C5-C6	-4.60	114.55	122.26
25	y	601	CHL	CAC-C3C-C4C	4.60	130.78	124.81
29	1	1623	NEX	C31-C30-C29	-4.60	120.75	127.31
25	8	609	CHL	C3C-C4C-NC	4.60	115.73	110.57
25	6	608	CHL	CHD-C4C-C3C	-4.60	118.08	124.84
25	g	601	CHL	C1C-C2C-C3C	-4.59	103.47	107.11
25	Y	601	CHL	C2C-C3C-C4C	-4.59	103.22	106.49
29	y	1623	NEX	C11-C10-C9	-4.59	120.76	127.31
29	Y	1623	NEX	C11-C10-C9	-4.58	120.77	127.31
25	2	609	CHL	C3D-C4D-ND	4.58	117.65	110.24
29	5	1623	NEX	C31-C30-C29	-4.58	120.78	127.31
25	5	606	CHL	O2D-CGD-CBD	4.58	119.40	111.27
26	2	612	CLA	C4A-NA-C1A	4.58	108.76	106.71
25	6	607	CHL	C3D-C4D-ND	4.57	117.64	110.24
25	y	609	CHL	C3D-C4D-ND	4.57	117.64	110.24
31	c	517	BCR	C11-C10-C9	-4.57	120.78	127.31
28	g	1622	XAT	C27-C28-C29	-4.57	118.44	125.53
25	s	601	CHL	C3C-C4C-NC	4.57	115.70	110.57
26	R	601	CLA	CAC-C3C-C4C	4.57	130.74	124.81
25	7	606	CHL	C3D-C4D-ND	4.57	117.63	110.24
25	G	606	CHL	C3D-C2D-C1D	-4.57	99.60	105.83
25	g	606	CHL	C3D-C2D-C1D	-4.57	99.60	105.83
25	n	605	CHL	C3D-C4D-ND	4.57	117.62	110.24
25	G	601	CHL	C1C-C2C-C3C	-4.57	103.49	107.11
25	S	601	CHL	C3C-C4C-NC	4.57	115.69	110.57
25	N	605	CHL	C3D-C4D-ND	4.56	117.62	110.24
25	1	606	CHL	O2D-CGD-CBD	4.56	119.38	111.27
25	3	606	CHL	C3D-C4D-ND	4.56	117.62	110.24
25	7	609	CHL	C3D-C2D-C1D	-4.56	99.61	105.83
26	C	513	CLA	CMB-C2B-C3B	4.56	133.21	124.68
26	c	513	CLA	CMB-C2B-C3B	4.56	133.21	124.68
26	d	403	CLA	CMB-C2B-C3B	4.56	133.21	124.68
25	1	601	CHL	C2D-C1D-ND	4.56	113.46	110.10
26	D	403	CLA	CMB-C2B-C3B	4.55	133.20	124.68
26	r	601	CLA	CAC-C3C-C4C	4.55	130.72	124.81
25	n	606	CHL	C3D-C4D-ND	4.55	117.60	110.24
31	C	517	BCR	C11-C10-C9	-4.55	120.82	127.31
28	G	1622	XAT	C27-C28-C29	-4.54	118.48	125.53
25	2	607	CHL	C3D-C4D-ND	4.54	117.59	110.24
25	y	601	CHL	C2C-C3C-C4C	-4.54	103.25	106.49
31	B	619	BCR	C15-C14-C13	-4.54	120.83	127.31
26	G	614	CLA	C4A-NA-C1A	4.54	108.75	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S	602	CLA	CMB-C2B-C1B	-4.54	121.49	128.46
25	3	609	CHL	C3D-C2D-C1D	-4.53	99.64	105.83
26	g	614	CLA	C4A-NA-C1A	4.53	108.74	106.71
25	6	601	CHL	O2D-CGD-CBD	4.53	119.32	111.27
25	n	601	CHL	CAC-C3C-C4C	4.53	130.69	124.81
25	s	601	CHL	O2D-CGD-CBD	4.53	119.31	111.27
25	s	607	CHL	O2D-CGD-CBD	4.53	119.31	111.27
25	N	606	CHL	C3D-C4D-ND	4.52	117.56	110.24
29	7	1623	NEX	C27-C28-C29	-4.52	118.51	125.53
25	S	601	CHL	O2D-CGD-CBD	4.52	119.31	111.27
26	s	602	CLA	CMB-C2B-C1B	-4.52	121.51	128.46
31	c	515	BCR	C15-C14-C13	-4.52	120.86	127.31
26	8	612	CLA	C4A-NA-C1A	4.52	108.74	106.71
28	8	622	XAT	C38-C25-C26	-4.52	114.69	122.26
29	R	623	NEX	C38-C25-C26	-4.52	114.69	122.26
28	1	1622	XAT	C18-C5-C6	-4.52	114.69	122.26
25	S	607	CHL	O2D-CGD-CBD	4.51	119.29	111.27
26	4	612	CLA	C4A-NA-C1A	4.51	108.73	106.71
25	2	601	CHL	O2D-CGD-CBD	4.51	119.28	111.27
29	r	623	NEX	C38-C25-C26	-4.51	114.70	122.26
25	S	601	CHL	C4A-NA-C1A	-4.51	104.68	106.71
29	3	1623	NEX	C27-C28-C29	-4.51	118.53	125.53
25	s	607	CHL	C3D-C4D-ND	4.51	117.53	110.24
26	b	614	CLA	CMB-C2B-C1B	-4.51	121.54	128.46
25	y	607	CHL	CHD-C1D-ND	-4.50	120.31	124.45
25	N	601	CHL	CAC-C3C-C4C	4.50	130.65	124.81
26	a	410	CLA	C1-C2-C3	-4.50	118.25	126.04
26	n	610	CLA	CMB-C2B-C1B	-4.50	121.54	128.46
26	N	610	CLA	CMB-C2B-C1B	-4.50	121.55	128.46
31	T	101	BCR	C20-C19-C18	-4.50	113.78	126.42
25	S	607	CHL	C3D-C4D-ND	4.50	117.52	110.24
28	4	622	XAT	C38-C25-C26	-4.50	114.72	122.26
31	b	619	BCR	C15-C14-C13	-4.50	120.89	127.31
26	6	612	CLA	C4A-NA-C1A	4.50	108.73	106.71
25	5	601	CHL	C2D-C1D-ND	4.49	113.41	110.10
39	C	519	DGD	O3G-C3G-C2G	-4.49	100.06	110.90
31	t	101	BCR	C20-C19-C18	-4.49	113.80	126.42
28	5	1622	XAT	C18-C5-C6	-4.49	114.74	122.26
39	c	519	DGD	O3G-C3G-C2G	-4.49	100.08	110.90
25	1	608	CHL	C3D-C4D-ND	4.48	117.49	110.24
25	5	608	CHL	C3D-C4D-ND	4.48	117.49	110.24
29	S	1623	NEX	O24-C25-C38	4.48	120.43	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	s	1623	NEX	O24-C25-C38	4.48	120.43	115.06
26	A	410	CLA	C1-C2-C3	-4.48	118.29	126.04
25	G	608	CHL	C3D-C4D-ND	4.48	117.49	110.24
26	B	614	CLA	CMB-C2B-C1B	-4.48	121.58	128.46
28	r	622	XAT	C18-C5-C6	-4.48	114.75	122.26
25	g	609	CHL	C3B-C4B-NB	4.48	115.00	109.21
31	C	515	BCR	C15-C14-C13	-4.48	120.92	127.31
28	R	622	XAT	C18-C5-C6	-4.47	114.76	122.26
28	r	622	XAT	C35-C34-C33	-4.47	120.93	127.31
29	l	1623	NEX	C35-C34-C33	-4.47	120.93	127.31
25	R	608	CHL	CHD-C4C-C3C	-4.47	118.27	124.84
27	S	1620	LUT	C35-C34-C33	-4.47	120.94	127.31
25	g	606	CHL	O2D-CGD-CBD	4.46	119.20	111.27
25	g	608	CHL	C3D-C4D-ND	4.46	117.46	110.24
25	r	608	CHL	CHD-C4C-C3C	-4.46	118.28	124.84
25	s	601	CHL	C4A-NA-C1A	-4.46	104.70	106.71
25	G	606	CHL	O2D-CGD-CBD	4.46	119.19	111.27
27	s	1620	LUT	C35-C34-C33	-4.46	120.95	127.31
26	6	602	CLA	CMB-C2B-C1B	-4.45	121.62	128.46
29	Y	1623	NEX	C38-C25-C26	-4.45	114.80	122.26
28	R	622	XAT	C35-C34-C33	-4.45	120.96	127.31
29	y	1623	NEX	C38-C25-C26	-4.45	114.81	122.26
29	5	1623	NEX	C35-C34-C33	-4.45	120.96	127.31
25	2	608	CHL	O2D-CGD-CBD	4.45	119.17	111.27
31	C	516	BCR	C16-C17-C18	-4.45	120.97	127.31
26	S	614	CLA	CMB-C2B-C3B	4.45	133.00	124.68
26	s	614	CLA	CMB-C2B-C3B	4.45	133.00	124.68
25	Y	607	CHL	CHD-C1D-ND	-4.45	120.37	124.45
25	G	609	CHL	C3B-C4B-NB	4.44	114.96	109.21
25	g	607	CHL	O2D-CGD-CBD	4.44	119.17	111.27
25	r	607	CHL	CHD-C4C-C3C	-4.44	118.32	124.84
31	H	101	BCR	C24-C23-C22	-4.44	119.53	126.23
28	Y	1622	XAT	C18-C5-C6	-4.44	114.83	122.26
25	6	608	CHL	O2D-CGD-CBD	4.44	119.15	111.27
25	R	607	CHL	CHD-C4C-C3C	-4.44	118.32	124.84
31	h	101	BCR	C24-C23-C22	-4.43	119.53	126.23
26	2	602	CLA	CMB-C2B-C1B	-4.43	121.65	128.46
25	5	606	CHL	C3D-C2D-C1D	-4.43	99.78	105.83
28	y	1622	XAT	C18-C5-C6	-4.43	114.83	122.26
26	n	602	CLA	C4A-NA-C1A	4.43	108.70	106.71
25	l	606	CHL	C3D-C2D-C1D	-4.43	99.78	105.83
29	Y	1623	NEX	C15-C14-C13	-4.43	120.99	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	G	607	CHL	O2D-CGD-CBD	4.42	119.13	111.27
29	y	1623	NEX	C15-C14-C13	-4.41	121.02	127.31
31	c	516	BCR	C16-C17-C18	-4.41	121.02	127.31
27	1	1620	LUT	C35-C34-C33	-4.41	121.02	127.31
26	5	614	CLA	C4A-NA-C1A	4.41	108.69	106.71
25	3	608	CHL	C3D-C4D-ND	4.41	117.37	110.24
26	a	406	CLA	CMB-C2B-C3B	4.40	132.92	124.68
25	4	607	CHL	C3C-C4C-NC	4.40	115.51	110.57
31	b	618	BCR	C16-C17-C18	-4.40	121.03	127.31
25	1	601	CHL	C3D-C2D-C1D	-4.40	99.83	105.83
26	N	602	CLA	C4A-NA-C1A	4.40	108.68	106.71
26	A	406	CLA	CMB-C2B-C3B	4.40	132.91	124.68
25	7	608	CHL	C3D-C4D-ND	4.40	117.35	110.24
25	n	608	CHL	C3D-C4D-ND	4.39	117.34	110.24
29	7	1623	NEX	O24-C25-C38	4.39	120.31	115.06
26	A	405	CLA	CMB-C2B-C3B	4.38	132.88	124.68
31	B	618	BCR	C16-C17-C18	-4.38	121.05	127.31
25	8	607	CHL	C3C-C4C-NC	4.38	115.48	110.57
26	G	602	CLA	CMB-C2B-C3B	4.38	132.87	124.68
25	4	601	CHL	C3D-C4D-ND	4.38	117.32	110.24
27	5	1620	LUT	C35-C34-C33	-4.38	121.06	127.31
28	6	1622	XAT	C15-C14-C13	-4.38	121.06	127.31
26	1	614	CLA	C4A-NA-C1A	4.38	108.67	106.71
29	3	1623	NEX	O24-C25-C38	4.37	120.30	115.06
25	8	601	CHL	C3D-C4D-ND	4.37	117.31	110.24
29	S	1623	NEX	C27-C28-C29	-4.37	118.75	125.53
26	C	509	CLA	CMB-C2B-C3B	4.37	132.86	124.68
25	G	609	CHL	C3D-C4D-ND	4.37	117.31	110.24
26	B	604	CLA	C4A-NA-C1A	4.37	108.67	106.71
27	Y	1621	LUT	C15-C14-C13	-4.37	121.08	127.31
25	5	601	CHL	C3D-C2D-C1D	-4.37	99.87	105.83
26	a	405	CLA	CMB-C2B-C3B	4.36	132.84	124.68
29	s	1623	NEX	C27-C28-C29	-4.36	118.76	125.53
25	N	608	CHL	C3D-C4D-ND	4.36	117.29	110.24
27	n	1621	LUT	C15-C14-C13	-4.36	121.09	127.31
31	c	517	BCR	C33-C5-C6	-4.36	119.64	124.53
37	D	411	LMG	C1-C2-C3	-4.36	100.92	110.00
26	g	602	CLA	CMB-C2B-C3B	4.35	132.82	124.68
25	g	609	CHL	C3D-C4D-ND	4.35	117.28	110.24
26	c	509	CLA	CMB-C2B-C3B	4.35	132.82	124.68
26	B	617	CLA	CMB-C2B-C1B	-4.35	121.78	128.46
28	2	1622	XAT	C15-C14-C13	-4.35	121.10	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	N	605	CHL	O2D-CGD-O1D	-4.35	115.34	123.84
25	n	605	CHL	O2D-CGD-O1D	-4.35	115.34	123.84
27	y	1621	LUT	C15-C14-C13	-4.35	121.11	127.31
37	d	411	LMG	C1-C2-C3	-4.34	100.97	110.00
25	S	608	CHL	CHD-C4C-C3C	-4.34	118.47	124.84
27	N	1621	LUT	C15-C14-C13	-4.33	121.13	127.31
26	C	504	CLA	O2D-CGD-O1D	-4.33	115.37	123.84
26	c	504	CLA	O2D-CGD-O1D	-4.33	115.37	123.84
26	R	601	CLA	CBC-CAC-C3C	4.33	124.37	112.43
26	b	617	CLA	CMB-C2B-C1B	-4.33	121.81	128.46
26	r	601	CLA	CBC-CAC-C3C	4.33	124.36	112.43
25	3	607	CHL	C3C-C4C-NC	4.33	115.42	110.57
29	G	1623	NEX	C15-C14-C13	-4.33	121.14	127.31
25	s	608	CHL	CHD-C4C-C3C	-4.32	118.49	124.84
29	g	1623	NEX	C15-C14-C13	-4.32	121.14	127.31
26	b	604	CLA	C4A-NA-C1A	4.32	108.65	106.71
25	5	607	CHL	O2D-CGD-CBD	4.32	118.94	111.27
31	C	517	BCR	C33-C5-C6	-4.31	119.68	124.53
28	7	1622	XAT	C15-C35-C34	-4.31	114.64	123.47
30	L	101	LHG	O4-P-O5	4.31	133.57	112.24
30	l	101	LHG	O4-P-O5	4.31	133.56	112.24
28	y	1622	XAT	O24-C25-C38	4.31	120.22	115.06
30	4	2630	LHG	O4-P-O5	4.31	133.55	112.24
28	3	1622	XAT	C15-C35-C34	-4.31	114.64	123.47
25	1	607	CHL	O2D-CGD-CBD	4.31	118.93	111.27
29	r	623	NEX	C35-C34-C33	-4.31	121.16	127.31
30	c	523	LHG	O4-P-O5	4.30	133.52	112.24
25	N	601	CHL	C3C-C4C-NC	4.30	115.40	110.57
30	C	523	LHG	O4-P-O5	4.30	133.51	112.24
30	8	2630	LHG	O4-P-O5	4.30	133.50	112.24
27	Y	1621	LUT	C35-C34-C33	-4.30	121.17	127.31
29	2	1623	NEX	C27-C28-C29	-4.30	118.86	125.53
29	6	1623	NEX	C27-C28-C29	-4.30	118.86	125.53
29	R	623	NEX	C35-C34-C33	-4.30	121.17	127.31
25	7	601	CHL	C3C-C4C-NC	4.30	115.39	110.57
25	7	607	CHL	C3C-C4C-NC	4.30	115.39	110.57
31	B	619	BCR	C11-C10-C9	-4.30	121.18	127.31
25	3	601	CHL	C3C-C4C-NC	4.29	115.39	110.57
28	1	1622	XAT	C11-C10-C9	-4.29	121.19	127.31
31	b	619	BCR	C11-C10-C9	-4.29	121.19	127.31
25	n	601	CHL	C3C-C4C-NC	4.29	115.38	110.57
25	3	607	CHL	C1B-CHB-C4A	-4.29	121.63	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	N	610	CLA	C4A-NA-C1A	4.28	108.63	106.71
26	n	610	CLA	C4A-NA-C1A	4.28	108.63	106.71
25	G	605	CHL	CHD-C4C-C3C	-4.28	118.54	124.84
26	4	602	CLA	O2D-CGD-O1D	-4.28	115.46	123.84
26	B	612	CLA	CMB-C2B-C3B	4.28	132.69	124.68
28	5	1622	XAT	C11-C10-C9	-4.28	121.20	127.31
31	C	516	BCR	C28-C27-C26	-4.28	106.43	114.08
25	n	609	CHL	C3B-C4B-NB	4.28	114.74	109.21
25	S	601	CHL	C3D-C2D-C1D	-4.28	99.99	105.83
30	D	408	LHG	O4-P-O5	4.28	133.39	112.24
26	C	508	CLA	O2D-CGD-CBD	4.27	118.86	111.27
26	b	612	CLA	CMB-C2B-C3B	4.27	132.68	124.68
26	d	403	CLA	O2D-CGD-O1D	-4.27	115.48	123.84
30	d	408	LHG	O4-P-O5	4.27	133.36	112.24
31	c	515	BCR	C11-C10-C9	-4.27	121.22	127.31
25	7	607	CHL	C1B-CHB-C4A	-4.27	121.66	130.12
25	N	609	CHL	C3B-C4B-NB	4.27	114.73	109.21
25	s	601	CHL	C3D-C2D-C1D	-4.27	100.01	105.83
28	Y	1622	XAT	O24-C25-C38	4.27	120.17	115.06
30	s	2630	LHG	O4-P-O5	4.27	133.33	112.24
26	c	508	CLA	O2D-CGD-CBD	4.27	118.85	111.27
25	7	608	CHL	CHD-C4C-C3C	-4.26	118.57	124.84
25	4	601	CHL	C3C-C4C-NC	4.26	115.35	110.57
30	S	2630	LHG	O4-P-O5	4.26	133.31	112.24
36	B	621	SQD	O9-S-C6	4.26	112.00	106.94
27	y	1621	LUT	C35-C34-C33	-4.26	121.23	127.31
26	8	602	CLA	O2D-CGD-O1D	-4.26	115.51	123.84
26	D	403	CLA	O2D-CGD-O1D	-4.26	115.51	123.84
31	c	516	BCR	C28-C27-C26	-4.25	106.48	114.08
26	4	604	CLA	C4A-NA-C1A	4.25	108.62	106.71
29	Y	1623	NEX	C2-C1-C6	4.25	113.34	109.21
25	g	605	CHL	CHD-C4C-C3C	-4.25	118.59	124.84
25	Y	605	CHL	O2D-CGD-CBD	4.25	118.82	111.27
30	Y	2630	LHG	O4-P-O5	4.25	133.25	112.24
30	y	2630	LHG	O4-P-O5	4.25	133.25	112.24
30	D	409	LHG	O4-P-O5	4.25	133.25	112.24
25	3	608	CHL	CHD-C4C-C3C	-4.25	118.59	124.84
30	d	409	LHG	O4-P-O5	4.25	133.25	112.24
26	3	604	CLA	C4A-NA-C1A	4.25	108.62	106.71
36	B	623	SQD	C1-O5-C5	4.25	122.03	113.69
29	y	1623	NEX	C2-C1-C6	4.25	113.34	109.21
36	b	623	SQD	O47-C7-C8	4.25	120.65	111.50

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	n	2630	LHG	O4-P-O5	4.24	133.22	112.24
25	8	601	CHL	C3C-C4C-NC	4.24	115.33	110.57
31	C	515	BCR	C11-C10-C9	-4.24	121.25	127.31
25	n	609	CHL	CAC-C3C-C4C	4.24	130.31	124.81
26	Y	610	CLA	CMB-C2B-C1B	-4.24	121.94	128.46
26	y	610	CLA	CMB-C2B-C1B	-4.24	121.94	128.46
30	N	2630	LHG	O4-P-O5	4.24	133.20	112.24
36	b	621	SQD	O9-S-C6	4.24	111.98	106.94
25	y	605	CHL	O2D-CGD-CBD	4.24	118.80	111.27
28	r	622	XAT	O24-C25-C38	4.24	120.13	115.06
36	B	623	SQD	O47-C7-C8	4.23	120.63	111.50
25	N	609	CHL	CAC-C3C-C4C	4.23	130.30	124.81
36	b	623	SQD	C1-O5-C5	4.23	121.99	113.69
26	s	613	CLA	CMB-C2B-C3B	4.23	132.59	124.68
26	R	602	CLA	CMB-C2B-C3B	4.22	132.58	124.68
30	r	2630	LHG	O4-P-O5	4.22	133.11	112.24
28	N	1622	XAT	O24-C25-C38	4.22	120.11	115.06
28	n	1622	XAT	O24-C25-C38	4.22	120.11	115.06
30	C	522	LHG	O4-P-O5	4.22	133.08	112.24
30	R	2630	LHG	O4-P-O5	4.22	133.08	112.24
25	y	601	CHL	CMD-C2D-C3D	-4.21	117.92	127.61
29	S	1623	NEX	C15-C14-C13	-4.21	121.30	127.31
26	S	613	CLA	CMB-C2B-C3B	4.21	132.56	124.68
36	b	621	SQD	O47-C7-C8	4.21	120.58	111.50
30	c	522	LHG	O4-P-O5	4.21	133.06	112.24
28	R	622	XAT	O24-C25-C38	4.21	120.10	115.06
25	Y	601	CHL	CMD-C2D-C3D	-4.20	117.94	127.61
36	B	621	SQD	O47-C7-C8	4.20	120.56	111.50
30	1	2630	LHG	O4-P-O5	4.20	133.02	112.24
26	r	602	CLA	CMB-C2B-C3B	4.20	132.54	124.68
26	7	604	CLA	C4A-NA-C1A	4.20	108.59	106.71
25	s	607	CHL	C3B-C4B-NB	4.20	114.64	109.21
30	5	2630	LHG	O4-P-O5	4.20	133.01	112.24
26	c	511	CLA	CMB-C2B-C1B	-4.20	122.01	128.46
30	g	2630	LHG	O4-P-O5	4.20	133.00	112.24
31	b	620	BCR	C16-C17-C18	-4.20	121.32	127.31
25	7	607	CHL	C3D-C4D-ND	4.20	117.03	110.24
26	s	604	CLA	CMB-C2B-C3B	4.20	132.53	124.68
25	G	605	CHL	O2D-CGD-O1D	-4.20	115.63	123.84
30	d	410	LHG	O4-P-O5	4.20	132.99	112.24
31	B	620	BCR	C16-C17-C18	-4.20	121.32	127.31
25	g	605	CHL	O2D-CGD-O1D	-4.20	115.64	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	s	1623	NEX	C15-C14-C13	-4.20	121.32	127.31
29	N	1623	NEX	O24-C25-C38	4.19	120.08	115.06
25	S	607	CHL	C3B-C4B-NB	4.19	114.63	109.21
30	D	410	LHG	O4-P-O5	4.19	132.97	112.24
31	t	101	BCR	C15-C14-C13	-4.19	121.33	127.31
31	T	101	BCR	C15-C14-C13	-4.19	121.33	127.31
30	G	2630	LHG	O4-P-O5	4.19	132.96	112.24
25	2	605	CHL	CHD-C4C-C3C	-4.19	118.68	124.84
26	8	604	CLA	C4A-NA-C1A	4.19	108.59	106.71
25	y	601	CHL	C3B-C4B-NB	4.18	114.62	109.21
25	6	605	CHL	CHD-C4C-C3C	-4.18	118.69	124.84
26	C	511	CLA	CMB-C2B-C1B	-4.18	122.04	128.46
26	S	604	CLA	CMB-C2B-C3B	4.18	132.50	124.68
25	r	606	CHL	CHD-C4C-C3C	-4.18	118.70	124.84
25	3	607	CHL	C3D-C4D-ND	4.18	116.99	110.24
25	Y	601	CHL	C3B-C4B-NB	4.17	114.61	109.21
29	n	1623	NEX	O24-C25-C38	4.17	120.05	115.06
30	C	2630	LHG	O4-P-O5	4.17	132.85	112.24
26	b	603	CLA	CMB-C2B-C3B	4.17	132.47	124.68
30	c	2630	LHG	O4-P-O5	4.17	132.84	112.24
29	6	1623	NEX	C11-C10-C9	-4.16	121.37	127.31
26	B	603	CLA	CMB-C2B-C3B	4.16	132.47	124.68
26	g	614	CLA	CMB-C2B-C1B	-4.16	122.07	128.46
25	S	606	CHL	CAC-C3C-C4C	4.15	130.20	124.81
25	r	608	CHL	C3D-C4D-ND	4.15	116.96	110.24
26	S	610	CLA	C4A-NA-C1A	4.15	108.57	106.71
29	2	1623	NEX	C11-C10-C9	-4.15	121.39	127.31
25	R	606	CHL	CHD-C4C-C3C	-4.15	118.74	124.84
30	B	2630	LHG	O4-P-O5	4.15	132.74	112.24
26	G	612	CLA	C4A-NA-C1A	4.15	108.57	106.71
27	G	1621	LUT	C35-C34-C33	-4.15	121.39	127.31
25	n	607	CHL	C3D-C4D-ND	4.15	116.94	110.24
31	A	411	BCR	C7-C8-C9	-4.14	119.97	126.23
26	g	612	CLA	C4A-NA-C1A	4.14	108.57	106.71
30	b	2630	LHG	O4-P-O5	4.14	132.71	112.24
27	g	1621	LUT	C2-C3-C4	4.14	115.97	110.30
26	G	614	CLA	CMB-C2B-C1B	-4.14	122.10	128.46
26	s	614	CLA	O2D-CGD-O1D	-4.14	115.75	123.84
25	s	606	CHL	CAC-C3C-C4C	4.14	130.18	124.81
27	g	1621	LUT	C35-C34-C33	-4.13	121.41	127.31
25	Y	607	CHL	C3D-C4D-ND	4.13	116.92	110.24
30	2	2630	LHG	O4-P-O5	4.13	132.67	112.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	6	2630	LHG	O4-P-O5	4.13	132.67	112.24
27	1	1621	LUT	C15-C14-C13	-4.13	121.41	127.31
27	2	1620	LUT	C35-C15-C14	-4.13	115.02	123.47
25	N	607	CHL	C3D-C4D-ND	4.13	116.92	110.24
25	R	608	CHL	C3D-C4D-ND	4.13	116.92	110.24
25	3	601	CHL	CMD-C2D-C3D	-4.13	118.12	127.61
27	G	1621	LUT	C2-C3-C4	4.12	115.95	110.30
25	G	608	CHL	CHD-C4C-C3C	-4.12	118.78	124.84
25	7	601	CHL	CMD-C2D-C3D	-4.12	118.13	127.61
30	B	2631	LHG	O4-P-O5	4.12	132.61	112.24
30	b	2631	LHG	O4-P-O5	4.12	132.61	112.24
25	y	607	CHL	C3D-C4D-ND	4.12	116.90	110.24
26	S	614	CLA	O2D-CGD-O1D	-4.12	115.79	123.84
39	C	520	DGD	O3G-C3G-C2G	-4.12	100.97	110.90
27	5	1621	LUT	C15-C14-C13	-4.11	121.44	127.31
26	C	512	CLA	CMB-C2B-C3B	4.11	132.37	124.68
26	c	512	CLA	CMB-C2B-C3B	4.11	132.37	124.68
26	B	606	CLA	CMB-C2B-C1B	-4.11	122.15	128.46
25	g	608	CHL	CHD-C4C-C3C	-4.11	118.80	124.84
27	6	1620	LUT	C35-C15-C14	-4.11	115.06	123.47
25	Y	609	CHL	C3B-C4B-NB	4.11	114.52	109.21
39	c	520	DGD	O3G-C3G-C2G	-4.11	100.99	110.90
31	a	411	BCR	C7-C8-C9	-4.10	120.03	126.23
25	y	609	CHL	C3B-C4B-NB	4.10	114.52	109.21
26	R	604	CLA	O2D-CGD-CBD	4.10	118.56	111.27
26	b	606	CLA	CMB-C2B-C1B	-4.10	122.16	128.46
28	G	1622	XAT	C4-C3-C2	-4.10	102.85	110.77
25	G	607	CHL	CHD-C4C-C3C	-4.10	118.82	124.84
25	5	601	CHL	CMD-C2D-C3D	-4.09	118.20	127.61
28	r	622	XAT	C15-C14-C13	-4.09	121.47	127.31
26	r	604	CLA	O2D-CGD-CBD	4.09	118.54	111.27
26	5	612	CLA	C4A-NA-C1A	4.09	108.54	106.71
31	c	515	BCR	C16-C17-C18	-4.09	121.48	127.31
26	C	506	CLA	CMB-C2B-C3B	4.08	132.32	124.68
27	2	1621	LUT	C15-C14-C13	-4.08	121.48	127.31
26	s	610	CLA	C4A-NA-C1A	4.08	108.54	106.71
25	2	607	CHL	CAC-C3C-C4C	4.08	130.10	124.81
30	7	2630	LHG	O4-P-O5	4.08	132.40	112.24
31	D	404	BCR	C11-C10-C9	-4.08	121.49	127.31
31	d	404	BCR	C11-C10-C9	-4.08	121.49	127.31
25	g	607	CHL	CHD-C4C-C3C	-4.08	118.85	124.84
26	3	602	CLA	CMB-C2B-C1B	-4.07	122.20	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	7	602	CLA	CMB-C2B-C1B	-4.07	122.20	128.46
26	c	506	CLA	CMB-C2B-C3B	4.07	132.30	124.68
25	1	601	CHL	CMD-C2D-C3D	-4.07	118.25	127.61
28	g	1622	XAT	C4-C3-C2	-4.07	102.91	110.77
30	3	2630	LHG	O4-P-O5	4.07	132.36	112.24
25	G	601	CHL	C3C-C4C-NC	4.07	115.14	110.57
25	g	601	CHL	C3C-C4C-NC	4.07	115.14	110.57
28	R	622	XAT	C15-C14-C13	-4.07	121.50	127.31
31	C	515	BCR	C16-C17-C18	-4.07	121.51	127.31
27	6	1621	LUT	C15-C14-C13	-4.06	121.51	127.31
26	b	611	CLA	CMB-C2B-C1B	-4.06	122.22	128.46
26	5	610	CLA	C1B-CHB-C4A	-4.06	122.08	130.12
29	R	623	NEX	C26-C27-C28	-4.06	117.41	125.99
29	r	623	NEX	C26-C27-C28	-4.06	117.41	125.99
26	y	614	CLA	O2D-CGD-O1D	-4.05	115.91	123.84
26	Y	602	CLA	CMB-C2B-C3B	4.05	132.26	124.68
26	1	611	CLA	C4A-NA-C1A	4.05	108.53	106.71
26	5	611	CLA	C4A-NA-C1A	4.05	108.53	106.71
26	N	612	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
26	n	612	CLA	CMB-C2B-C1B	-4.05	122.24	128.46
25	Y	607	CHL	CHD-C4C-C3C	-4.05	118.89	124.84
26	1	610	CLA	C1B-CHB-C4A	-4.05	122.11	130.12
25	6	607	CHL	CAC-C3C-C4C	4.04	130.06	124.81
26	2	613	CLA	C4A-NA-C1A	4.04	108.52	106.71
25	S	607	CHL	CAC-C3C-C4C	4.04	130.05	124.81
26	y	602	CLA	CMB-C2B-C3B	4.03	132.22	124.68
26	Y	614	CLA	O2D-CGD-O1D	-4.03	115.95	123.84
26	1	612	CLA	C4A-NA-C1A	4.03	108.52	106.71
25	y	607	CHL	CHD-C4C-C3C	-4.03	118.92	124.84
26	B	611	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
26	6	604	CLA	CMB-C2B-C1B	-4.03	122.27	128.46
25	s	607	CHL	CAC-C3C-C4C	4.02	130.03	124.81
26	R	601	CLA	CMB-C2B-C3B	4.02	132.21	124.68
25	y	607	CHL	CAC-C3C-C4C	4.02	130.03	124.81
28	3	1622	XAT	C27-C28-C29	-4.02	119.30	125.53
26	b	615	CLA	O2D-CGD-O1D	-4.02	115.98	123.84
25	n	606	CHL	CHD-C4C-C3C	-4.02	118.94	124.84
26	B	610	CLA	CMB-C2B-C3B	4.02	132.19	124.68
28	7	1622	XAT	C27-C28-C29	-4.02	119.30	125.53
25	Y	607	CHL	CAC-C3C-C4C	4.01	130.02	124.81
25	N	607	CHL	CHB-C4A-NA	4.01	130.06	124.51
26	r	601	CLA	CMB-C2B-C3B	4.01	132.18	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	2	604	CLA	CMB-C2B-C1B	-4.01	122.31	128.46
26	G	610	CLA	CMB-C2B-C1B	-4.01	122.31	128.46
25	n	607	CHL	CHB-C4A-NA	4.00	130.05	124.51
25	n	608	CHL	CHD-C4C-C3C	-4.00	118.95	124.84
26	b	610	CLA	CMB-C2B-C3B	4.00	132.17	124.68
25	r	608	CHL	CAC-C3C-C4C	4.00	130.00	124.81
25	r	614	CHL	O2D-CGD-CBD	3.99	118.37	111.27
26	s	610	CLA	CMB-C2B-C3B	3.99	132.15	124.68
26	g	610	CLA	CMB-C2B-C1B	-3.99	122.33	128.46
25	N	606	CHL	CHD-C4C-C3C	-3.99	118.98	124.84
26	B	615	CLA	O2D-CGD-O1D	-3.99	116.05	123.84
31	d	404	BCR	C24-C23-C22	-3.98	120.21	126.23
25	N	608	CHL	CHD-C4C-C3C	-3.98	118.98	124.84
26	n	610	CLA	CMB-C2B-C3B	3.98	132.13	124.68
31	D	404	BCR	C24-C23-C22	-3.98	120.22	126.23
25	y	606	CHL	C3D-C4D-ND	3.98	116.67	110.24
25	Y	609	CHL	C1C-C2C-C3C	-3.98	103.96	107.11
26	S	610	CLA	CMB-C2B-C3B	3.98	132.12	124.68
25	R	608	CHL	CAC-C3C-C4C	3.97	129.97	124.81
29	N	1623	NEX	C17-C1-C6	-3.97	106.92	110.47
25	R	614	CHL	O2D-CGD-CBD	3.97	118.33	111.27
25	Y	608	CHL	CHD-C4C-C3C	-3.97	119.01	124.84
26	A	407	CLA	CMB-C2B-C1B	-3.97	122.37	128.46
25	G	601	CHL	CMD-C2D-C3D	-3.97	118.49	127.61
28	N	1622	XAT	C11-C10-C9	-3.96	121.65	127.31
26	N	610	CLA	CMB-C2B-C3B	3.96	132.09	124.68
25	y	607	CHL	CHB-C4A-NA	3.96	129.99	124.51
25	Y	606	CHL	C3D-C4D-ND	3.96	116.64	110.24
31	H	101	BCR	C15-C14-C13	-3.96	121.66	127.31
31	h	101	BCR	C15-C14-C13	-3.96	121.66	127.31
26	N	613	CLA	CMB-C2B-C1B	-3.96	122.39	128.46
26	b	617	CLA	CMB-C2B-C3B	3.95	132.07	124.68
25	n	608	CHL	CAC-C3C-C4C	3.95	129.94	124.81
25	g	601	CHL	CMD-C2D-C3D	-3.95	118.53	127.61
36	b	623	SQD	O9-S-C6	3.95	111.63	106.94
25	N	608	CHL	CAC-C3C-C4C	3.95	129.94	124.81
26	a	407	CLA	CMB-C2B-C1B	-3.95	122.40	128.46
25	5	605	CHL	CHD-C4C-C3C	-3.95	119.04	124.84
26	a	410	CLA	O2D-CGD-O1D	-3.94	116.12	123.84
26	B	617	CLA	CMB-C2B-C3B	3.94	132.06	124.68
25	y	608	CHL	CHD-C4C-C3C	-3.94	119.05	124.84
28	1	1622	XAT	O4-C5-C18	3.94	119.78	115.06

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	606	CHL	CHD-C4C-C3C	-3.94	119.05	124.84
28	Y	1622	XAT	C27-C28-C29	-3.94	119.42	125.53
25	5	601	CHL	C3C-C4C-NC	3.94	114.99	110.57
28	n	1622	XAT	C11-C10-C9	-3.94	121.69	127.31
26	c	507	CLA	CMB-C2B-C1B	-3.94	122.41	128.46
28	5	1622	XAT	O4-C5-C18	3.94	119.77	115.06
28	y	1622	XAT	C27-C28-C29	-3.93	119.42	125.53
36	B	623	SQD	O9-S-C6	3.93	111.61	106.94
25	y	609	CHL	C1C-C2C-C3C	-3.93	103.99	107.11
29	n	1623	NEX	C17-C1-C6	-3.93	106.95	110.47
26	A	410	CLA	O2D-CGD-O1D	-3.93	116.15	123.84
26	C	507	CLA	CMB-C2B-C1B	-3.93	122.42	128.46
25	s	606	CHL	CHD-C4C-C3C	-3.93	119.06	124.84
27	N	1620	LUT	C35-C34-C33	-3.93	121.71	127.31
26	b	605	CLA	C1D-ND-C4D	3.93	109.12	106.33
25	1	605	CHL	CHD-C4C-C3C	-3.92	119.07	124.84
25	Y	607	CHL	CHB-C4A-NA	3.92	129.94	124.51
26	G	612	CLA	CMB-C2B-C1B	-3.92	122.44	128.46
26	g	612	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
26	n	613	CLA	CMB-C2B-C1B	-3.91	122.45	128.46
26	6	613	CLA	C4A-NA-C1A	3.91	108.47	106.71
25	S	607	CHL	CHD-C4C-C3C	-3.91	119.10	124.84
26	8	603	CLA	CMB-C2B-C1B	-3.91	122.46	128.46
27	n	1620	LUT	C35-C34-C33	-3.91	121.74	127.31
25	s	607	CHL	CHD-C4C-C3C	-3.90	119.10	124.84
36	A	418	SQD	O9-S-O7	-3.90	100.44	113.95
36	a	418	SQD	O9-S-O7	-3.90	100.44	113.95
25	n	601	CHL	C1C-C2C-C3C	-3.90	104.02	107.11
31	c	517	BCR	C16-C17-C18	-3.90	121.74	127.31
26	B	605	CLA	C1D-ND-C4D	3.90	109.11	106.33
26	y	613	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
26	a	410	CLA	CMB-C2B-C1B	-3.90	122.47	128.46
26	Y	604	CLA	CMB-C2B-C3B	3.90	131.97	124.68
26	r	610	CLA	C1B-CHB-C4A	-3.90	122.40	130.12
26	R	610	CLA	C1B-CHB-C4A	-3.89	122.40	130.12
26	D	402	CLA	CAA-CBA-CGA	-3.89	101.87	113.25
25	1	601	CHL	C3C-C4C-NC	3.89	114.94	110.57
26	R	604	CLA	CMB-C2B-C3B	3.89	131.96	124.68
26	n	604	CLA	CMB-C2B-C3B	3.89	131.96	124.68
26	Y	613	CLA	CMB-C2B-C1B	-3.89	122.49	128.46
31	H	101	BCR	C7-C8-C9	-3.89	120.36	126.23
26	4	603	CLA	CMB-C2B-C1B	-3.89	122.49	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	d	402	CLA	CAA-CBA-CGA	-3.89	101.89	113.25
28	8	622	XAT	C35-C34-C33	-3.89	121.76	127.31
31	B	620	BCR	C11-C10-C9	-3.88	121.77	127.31
26	y	604	CLA	CMB-C2B-C3B	3.88	131.94	124.68
31	h	101	BCR	C7-C8-C9	-3.88	120.37	126.23
31	b	620	BCR	C11-C10-C9	-3.88	121.77	127.31
26	C	505	CLA	O2D-CGD-O1D	-3.88	116.25	123.84
25	N	601	CHL	C1C-C2C-C3C	-3.88	104.03	107.11
36	b	623	SQD	O9-S-O7	-3.88	100.52	113.95
28	4	622	XAT	C35-C34-C33	-3.88	121.77	127.31
26	r	604	CLA	CMB-C2B-C3B	3.88	131.93	124.68
36	B	623	SQD	O9-S-O7	-3.87	100.54	113.95
31	C	517	BCR	C16-C17-C18	-3.87	121.78	127.31
26	A	410	CLA	CMB-C2B-C1B	-3.87	122.51	128.46
25	2	601	CHL	CMD-C2D-C3D	-3.87	118.71	127.61
26	N	604	CLA	CMB-C2B-C3B	3.87	131.91	124.68
28	y	1622	XAT	C35-C34-C33	-3.87	121.79	127.31
25	4	608	CHL	O2D-CGD-CBD	3.86	118.13	111.27
25	6	601	CHL	CMD-C2D-C3D	-3.86	118.73	127.61
25	1	608	CHL	O2D-CGD-CBD	3.86	118.13	111.27
25	5	608	CHL	O2D-CGD-CBD	3.86	118.13	111.27
26	3	614	CLA	C4A-NA-C1A	3.86	108.44	106.71
26	c	505	CLA	O2D-CGD-O1D	-3.86	116.29	123.84
26	Y	611	CLA	O2D-CGD-O1D	-3.86	116.29	123.84
31	T	101	BCR	C33-C5-C6	-3.86	120.20	124.53
25	8	608	CHL	O2D-CGD-CBD	3.86	118.12	111.27
25	7	606	CHL	CHD-C4C-C3C	-3.85	119.18	124.84
27	S	1620	LUT	C35-C15-C14	-3.85	115.59	123.47
27	s	1620	LUT	C35-C15-C14	-3.85	115.59	123.47
26	S	602	CLA	C4A-NA-C1A	3.84	108.43	106.71
31	c	516	BCR	C20-C21-C22	-3.84	121.83	127.31
28	Y	1622	XAT	C35-C34-C33	-3.84	121.83	127.31
36	a	418	SQD	O9-S-C6	3.84	111.50	106.94
26	N	604	CLA	O2D-CGD-O1D	-3.84	116.33	123.84
27	3	1621	LUT	C15-C14-C13	-3.84	121.83	127.31
27	7	1621	LUT	C15-C14-C13	-3.84	121.83	127.31
36	A	418	SQD	O9-S-C6	3.84	111.50	106.94
26	b	613	CLA	CMD-C2D-C1D	-3.84	117.95	124.71
25	1	606	CHL	CHD-C4C-C3C	-3.84	119.20	124.84
25	5	606	CHL	CHD-C4C-C3C	-3.84	119.20	124.84
26	2	614	CLA	C4A-NA-C1A	3.83	108.43	106.71
26	6	614	CLA	C4A-NA-C1A	3.83	108.43	106.71

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	y	611	CLA	O2D-CGD-O1D	-3.83	116.35	123.84
26	7	614	CLA	C4A-NA-C1A	3.83	108.43	106.71
25	3	606	CHL	CHD-C4C-C3C	-3.83	119.22	124.84
26	Y	603	CLA	CMB-C2B-C1B	-3.83	122.58	128.46
26	B	613	CLA	CMD-C2D-C1D	-3.82	117.97	124.71
25	n	605	CHL	CAC-C3C-C4C	3.82	129.77	124.81
26	n	604	CLA	O2D-CGD-O1D	-3.82	116.36	123.84
26	S	602	CLA	CMB-C2B-C3B	3.82	131.83	124.68
26	s	602	CLA	CMB-C2B-C3B	3.82	131.83	124.68
25	2	601	CHL	C3C-C4C-NC	3.82	114.86	110.57
26	y	603	CLA	CMB-C2B-C1B	-3.82	122.60	128.46
28	3	1622	XAT	C26-C27-C28	-3.82	117.92	125.99
28	g	1622	XAT	C18-C5-C6	-3.82	115.86	122.26
31	b	620	BCR	C15-C14-C13	-3.82	121.86	127.31
25	4	609	CHL	CAC-C3C-C4C	3.82	129.76	124.81
25	N	607	CHL	CAC-C3C-C4C	3.82	129.76	124.81
25	n	607	CHL	CAC-C3C-C4C	3.82	129.76	124.81
28	G	1622	XAT	C18-C5-C6	-3.81	115.87	122.26
31	B	620	BCR	C15-C14-C13	-3.81	121.87	127.31
25	N	607	CHL	C3B-C4B-NB	3.81	114.14	109.21
35	a	408	PHO	CMC-C2C-C3C	3.81	132.12	124.94
25	y	609	CHL	CAC-C3C-C4C	3.81	129.75	124.81
25	n	607	CHL	C3B-C4B-NB	3.81	114.14	109.21
31	C	516	BCR	C20-C21-C22	-3.81	121.87	127.31
26	5	614	CLA	CMB-C2B-C1B	-3.81	122.61	128.46
36	b	621	SQD	C4-C3-C2	3.81	117.47	110.82
31	T	101	BCR	C28-C27-C26	-3.81	107.28	114.08
25	S	607	CHL	CHB-C4A-NA	3.81	129.77	124.51
31	t	101	BCR	C33-C5-C6	-3.81	120.25	124.53
35	A	408	PHO	CMC-C2C-C3C	3.80	132.11	124.94
25	G	606	CHL	CHD-C4C-C3C	-3.80	119.25	124.84
26	B	605	CLA	CBC-CAC-C3C	3.80	122.92	112.43
25	g	606	CHL	CHD-C4C-C3C	-3.80	119.25	124.84
25	n	609	CHL	CHB-C4A-NA	3.80	129.76	124.51
28	7	1622	XAT	C26-C27-C28	-3.80	117.96	125.99
25	N	605	CHL	CAC-C3C-C4C	3.80	129.74	124.81
26	1	614	CLA	CMB-C2B-C1B	-3.80	122.63	128.46
26	s	602	CLA	C4A-NA-C1A	3.80	108.41	106.71
25	5	601	CHL	CAC-C3C-C4C	3.79	129.73	124.81
26	8	602	CLA	CMB-C2B-C1B	-3.79	122.64	128.46
26	b	613	CLA	O2D-CGD-O1D	-3.79	116.42	123.84
25	1	601	CHL	CAC-C3C-C4C	3.79	129.73	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	601	CHL	C3C-C4C-NC	3.79	114.82	110.57
36	B	621	SQD	C4-C3-C2	3.79	117.43	110.82
26	b	605	CLA	CBC-CAC-C3C	3.79	122.87	112.43
25	8	609	CHL	CAC-C3C-C4C	3.79	129.72	124.81
31	C	514	BCR	C15-C16-C17	-3.79	115.72	123.47
29	G	1623	NEX	C35-C34-C33	-3.79	121.91	127.31
25	1	607	CHL	CHB-C4A-NA	3.78	129.75	124.51
27	r	620	LUT	C30-C31-C32	-3.78	111.41	123.22
26	4	602	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
29	g	1623	NEX	C35-C34-C33	-3.78	121.91	127.31
39	C	518	DGD	O6D-C1D-O3G	-3.78	101.02	109.97
27	R	620	LUT	C30-C31-C32	-3.78	111.41	123.22
31	t	101	BCR	C28-C27-C26	-3.78	107.32	114.08
25	N	609	CHL	CHB-C4A-NA	3.78	129.74	124.51
26	s	603	CLA	CMB-C2B-C1B	-3.78	122.65	128.46
25	Y	609	CHL	CAC-C3C-C4C	3.78	129.72	124.81
26	N	613	CLA	O2D-CGD-CBD	3.78	117.98	111.27
27	G	1620	LUT	C35-C34-C33	-3.78	121.92	127.31
25	5	607	CHL	CHB-C4A-NA	3.78	129.73	124.51
25	s	607	CHL	CHB-C4A-NA	3.77	129.73	124.51
31	c	514	BCR	C15-C16-C17	-3.77	115.75	123.47
26	B	606	CLA	O2D-CGD-O1D	-3.77	116.47	123.84
39	c	518	DGD	O6D-C1D-O3G	-3.77	101.05	109.97
26	B	613	CLA	O2D-CGD-O1D	-3.77	116.47	123.84
31	C	514	BCR	C20-C21-C22	-3.77	121.93	127.31
26	1	603	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
26	5	603	CLA	CMB-C2B-C1B	-3.77	122.67	128.46
26	5	604	CLA	CMB-C2B-C3B	3.77	131.72	124.68
26	7	610	CLA	C1B-CHB-C4A	-3.76	122.67	130.12
36	b	621	SQD	O9-S-O7	-3.76	100.94	113.95
28	n	1622	XAT	C18-C5-C6	-3.76	115.96	122.26
39	C	520	DGD	O6D-C1D-O3G	-3.76	101.08	109.97
26	6	614	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
26	7	613	CLA	CMB-C2B-C1B	-3.76	122.69	128.46
26	n	613	CLA	O2D-CGD-CBD	3.76	117.94	111.27
25	1	609	CHL	C3B-C4B-NB	3.75	114.06	109.21
28	N	1622	XAT	C18-C5-C6	-3.75	115.97	122.26
25	5	607	CHL	CHD-C4C-C3C	-3.75	119.32	124.84
26	b	606	CLA	O2D-CGD-O1D	-3.75	116.50	123.84
31	c	514	BCR	C20-C21-C22	-3.75	121.95	127.31
26	2	614	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
26	G	604	CLA	CMB-C2B-C3B	3.75	131.69	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	G	601	CHL	C3B-C4B-NB	3.75	114.06	109.21
25	5	609	CHL	C3B-C4B-NB	3.75	114.06	109.21
26	S	603	CLA	CMB-C2B-C1B	-3.75	122.70	128.46
25	N	601	CHL	CMD-C2D-C3D	-3.75	119.00	127.61
26	1	604	CLA	CMB-C2B-C3B	3.75	131.69	124.68
26	3	610	CLA	C1B-CHB-C4A	-3.75	122.70	130.12
27	1	1620	LUT	C30-C31-C32	-3.75	111.53	123.22
36	B	621	SQD	O9-S-O7	-3.75	100.98	113.95
39	c	520	DGD	O6D-C1D-O3G	-3.74	101.11	109.97
26	B	604	CLA	CMB-C2B-C3B	3.74	131.68	124.68
26	C	509	CLA	O2D-CGD-O1D	-3.74	116.53	123.84
25	n	601	CHL	CMD-C2D-C3D	-3.74	119.01	127.61
26	B	605	CLA	CAA-C2A-C1A	3.74	124.23	111.97
25	1	607	CHL	CHD-C4C-C3C	-3.74	119.34	124.84
25	n	607	CHL	O2D-CGD-CBD	3.74	117.91	111.27
26	r	609	CLA	CMB-C2B-C1B	-3.74	122.72	128.46
27	g	1620	LUT	C35-C34-C33	-3.74	121.98	127.31
27	5	1620	LUT	C30-C31-C32	-3.73	111.57	123.22
26	C	503	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
26	c	503	CLA	CMB-C2B-C1B	-3.73	122.73	128.46
28	G	1622	XAT	O24-C25-C38	3.73	119.52	115.06
26	c	512	CLA	O2D-CGD-O1D	-3.73	116.55	123.84
26	c	509	CLA	O2D-CGD-O1D	-3.73	116.55	123.84
26	3	613	CLA	CMB-C2B-C1B	-3.73	122.74	128.46
31	C	516	BCR	C33-C5-C6	-3.73	120.34	124.53
26	b	605	CLA	CAA-C2A-C1A	3.73	124.18	111.97
26	Y	614	CLA	CMB-C2B-C1B	-3.72	122.74	128.46
28	y	1622	XAT	C10-C11-C12	-3.72	111.60	123.22
26	y	614	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
28	5	1622	XAT	C27-C28-C29	-3.72	119.76	125.53
26	g	604	CLA	CMB-C2B-C3B	3.72	131.63	124.68
26	b	604	CLA	CMB-C2B-C3B	3.72	131.63	124.68
28	Y	1622	XAT	C10-C11-C12	-3.72	111.62	123.22
31	D	404	BCR	C16-C17-C18	-3.72	122.01	127.31
26	R	609	CLA	CMB-C2B-C1B	-3.72	122.75	128.46
25	N	607	CHL	O2D-CGD-CBD	3.72	117.87	111.27
29	g	1623	NEX	C27-C28-C29	-3.71	119.77	125.53
26	B	605	CLA	CHB-C4A-NA	3.71	129.65	124.51
26	G	611	CLA	O2D-CGD-O1D	-3.71	116.58	123.84
25	Y	607	CHL	O2D-CGD-CBD	3.71	117.86	111.27
25	y	607	CHL	O2D-CGD-CBD	3.71	117.86	111.27
26	C	512	CLA	O2D-CGD-O1D	-3.71	116.58	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	a	412	SQD	O47-C7-C8	3.71	119.50	111.50
25	g	601	CHL	C3B-C4B-NB	3.71	114.00	109.21
31	a	411	BCR	C15-C14-C13	-3.71	122.02	127.31
26	R	610	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
26	r	610	CLA	CMB-C2B-C1B	-3.71	122.77	128.46
26	g	611	CLA	O2D-CGD-O1D	-3.71	116.59	123.84
31	c	516	BCR	C33-C5-C6	-3.70	120.37	124.53
26	C	502	CLA	CMB-C2B-C1B	-3.70	122.77	128.46
25	2	601	CHL	C3B-C4B-NB	3.70	114.00	109.21
28	g	1622	XAT	O24-C25-C38	3.70	119.49	115.06
31	d	404	BCR	C16-C17-C18	-3.70	122.03	127.31
36	A	412	SQD	O47-C7-C8	3.70	119.48	111.50
27	4	620	LUT	C15-C14-C13	-3.70	122.03	127.31
28	1	1622	XAT	C27-C28-C29	-3.70	119.79	125.53
29	G	1623	NEX	C27-C28-C29	-3.70	119.80	125.53
27	N	1620	LUT	C35-C15-C14	-3.69	115.91	123.47
26	b	605	CLA	CHB-C4A-NA	3.69	129.62	124.51
28	G	1622	XAT	C10-C11-C12	-3.69	111.70	123.22
26	6	602	CLA	CMB-C2B-C3B	3.69	131.58	124.68
26	c	511	CLA	CMB-C2B-C3B	3.69	131.58	124.68
31	A	411	BCR	C15-C14-C13	-3.69	122.05	127.31
25	1	607	CHL	C3B-C4B-NB	3.69	113.97	109.21
27	3	1620	LUT	C35-C34-C33	-3.68	122.05	127.31
26	c	501	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
26	c	502	CLA	CMB-C2B-C1B	-3.68	122.81	128.46
26	c	513	CLA	O2D-CGD-O1D	-3.68	116.64	123.84
27	n	1620	LUT	C35-C15-C14	-3.68	115.94	123.47
27	4	620	LUT	C7-C8-C9	-3.68	120.68	126.23
25	g	606	CHL	CAC-C3C-C4C	3.68	129.58	124.81
25	6	601	CHL	C3B-C4B-NB	3.68	113.96	109.21
28	g	1622	XAT	C10-C11-C12	-3.68	111.74	123.22
29	2	1623	NEX	O24-C25-C38	3.67	119.46	115.06
25	5	607	CHL	C3B-C4B-NB	3.67	113.96	109.21
29	g	1623	NEX	O24-C25-C38	3.67	119.46	115.06
26	C	511	CLA	CMB-C2B-C3B	3.67	131.55	124.68
26	2	602	CLA	CMB-C2B-C3B	3.67	131.54	124.68
26	C	501	CLA	O2D-CGD-O1D	-3.67	116.66	123.84
27	7	1620	LUT	C35-C34-C33	-3.67	122.07	127.31
27	3	1620	LUT	C15-C14-C13	-3.67	122.08	127.31
25	S	608	CHL	O2D-CGD-CBD	3.67	117.78	111.27
28	6	1622	XAT	C11-C10-C9	-3.67	122.08	127.31
27	8	620	LUT	C15-C14-C13	-3.67	122.08	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	2	1622	XAT	C11-C10-C9	-3.67	122.08	127.31
26	C	513	CLA	O2D-CGD-O1D	-3.66	116.67	123.84
27	2	1621	LUT	C35-C34-C33	-3.66	122.08	127.31
27	6	1621	LUT	C35-C34-C33	-3.66	122.08	127.31
39	h	102	DGD	O3G-C3G-C2G	-3.66	102.06	110.90
26	r	612	CLA	CMB-C2B-C1B	-3.66	122.84	128.46
26	y	604	CLA	C1B-CHB-C4A	-3.66	122.87	130.12
27	8	620	LUT	C7-C8-C9	-3.66	120.70	126.23
26	n	603	CLA	C2D-C1D-ND	-3.66	107.41	110.10
26	7	604	CLA	CMB-C2B-C3B	3.66	131.52	124.68
26	g	614	CLA	CMB-C2B-C3B	3.66	131.52	124.68
25	G	606	CHL	CAC-C3C-C4C	3.65	129.55	124.81
26	C	505	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
26	c	505	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
25	r	607	CHL	C3B-C4B-NB	3.65	113.93	109.21
26	8	604	CLA	CMB-C2B-C1B	-3.65	122.85	128.46
27	N	1621	LUT	C10-C11-C12	-3.65	111.83	123.22
29	G	1623	NEX	O24-C25-C38	3.65	119.43	115.06
28	7	1622	XAT	C4-C3-C2	-3.65	103.72	110.77
25	Y	601	CHL	CHB-C4A-NA	3.65	129.56	124.51
25	g	606	CHL	CMB-C2B-C3B	3.65	131.50	124.68
25	1	605	CHL	C3B-C4B-NB	3.65	113.93	109.21
27	7	1620	LUT	C15-C14-C13	-3.65	122.10	127.31
39	H	102	DGD	O3G-C3G-C2G	-3.65	102.10	110.90
25	s	608	CHL	O2D-CGD-CBD	3.65	117.75	111.27
27	n	1621	LUT	C10-C11-C12	-3.65	111.84	123.22
26	R	612	CLA	CMB-C2B-C1B	-3.65	122.86	128.46
29	6	1623	NEX	C31-C30-C29	-3.64	122.11	127.31
26	7	610	CLA	CMB-C2B-C1B	-3.64	122.86	128.46
26	Y	604	CLA	C1B-CHB-C4A	-3.64	122.90	130.12
25	5	605	CHL	C3B-C4B-NB	3.64	113.92	109.21
26	b	603	CLA	O2D-CGD-O1D	-3.64	116.72	123.84
26	3	610	CLA	CMB-C2B-C1B	-3.64	122.87	128.46
26	b	607	CLA	CMB-C2B-C3B	3.64	131.49	124.68
31	C	514	BCR	C10-C11-C12	-3.64	111.86	123.22
26	G	614	CLA	CMB-C2B-C3B	3.64	131.49	124.68
29	6	1623	NEX	O24-C25-C38	3.64	119.42	115.06
25	6	601	CHL	C1C-C2C-C3C	-3.64	104.23	107.11
29	2	1623	NEX	C31-C30-C29	-3.64	122.12	127.31
28	3	1622	XAT	C4-C3-C2	-3.63	103.75	110.77
26	N	603	CLA	C2D-C1D-ND	-3.63	107.43	110.10
31	A	411	BCR	C20-C21-C22	-3.63	122.13	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
36	A	412	SQD	O9-S-O7	-3.63	101.38	113.95
26	4	604	CLA	CMB-C2B-C1B	-3.63	122.88	128.46
26	3	602	CLA	CMB-C2B-C3B	3.63	131.47	124.68
26	3	604	CLA	CMB-C2B-C3B	3.63	131.47	124.68
26	B	607	CLA	CMB-C2B-C3B	3.63	131.47	124.68
26	1	613	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
26	B	605	CLA	CAA-CBA-CGA	-3.63	102.65	113.25
31	c	517	BCR	C15-C16-C17	-3.63	116.04	123.47
31	A	411	BCR	C16-C17-C18	-3.63	122.13	127.31
25	G	606	CHL	CMB-C2B-C3B	3.63	131.47	124.68
26	7	602	CLA	CMB-C2B-C3B	3.63	131.47	124.68
31	c	514	BCR	C10-C11-C12	-3.63	111.89	123.22
26	6	613	CLA	CMB-C2B-C1B	-3.63	122.89	128.46
36	A	418	SQD	C45-O47-C7	3.63	126.72	117.79
31	C	517	BCR	C15-C16-C17	-3.63	116.05	123.47
36	a	418	SQD	C45-O47-C7	3.63	126.72	117.79
36	a	412	SQD	O9-S-O7	-3.63	101.40	113.95
25	R	607	CHL	C3B-C4B-NB	3.62	113.89	109.21
25	2	601	CHL	C1C-C2C-C3C	-3.62	104.24	107.11
26	s	610	CLA	C1B-CHB-C4A	-3.62	122.94	130.12
26	Y	613	CLA	CMB-C2B-C3B	3.62	131.45	124.68
26	y	613	CLA	CMB-C2B-C3B	3.62	131.45	124.68
26	B	603	CLA	O2D-CGD-O1D	-3.62	116.76	123.84
26	b	605	CLA	CAA-CBA-CGA	-3.62	102.67	113.25
31	a	411	BCR	C20-C21-C22	-3.62	122.14	127.31
26	S	610	CLA	C1B-CHB-C4A	-3.62	122.95	130.12
31	a	411	BCR	C16-C17-C18	-3.62	122.14	127.31
37	A	413	LMG	O6-C1-O1	-3.62	101.41	109.97
25	s	608	CHL	C3B-C4B-NB	3.62	113.89	109.21
31	a	411	BCR	C11-C10-C9	-3.61	122.15	127.31
25	y	601	CHL	CHB-C4A-NA	3.61	129.51	124.51
26	d	403	CLA	O2D-CGD-CBD	3.61	117.69	111.27
26	n	612	CLA	CMB-C2B-C3B	3.61	131.43	124.68
37	a	413	LMG	O6-C1-O1	-3.61	101.43	109.97
26	N	613	CLA	CMB-C2B-C3B	3.61	131.43	124.68
25	y	607	CHL	C3B-C4B-NB	3.61	113.87	109.21
31	c	514	BCR	C16-C17-C18	-3.61	122.16	127.31
31	A	411	BCR	C11-C10-C9	-3.61	122.17	127.31
29	1	1623	NEX	C15-C14-C13	-3.60	122.17	127.31
26	5	613	CLA	CMB-C2B-C1B	-3.60	122.93	128.46
31	C	514	BCR	C16-C17-C18	-3.60	122.17	127.31
26	B	607	CLA	O2D-CGD-O1D	-3.60	116.80	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	Y	1620	LUT	C10-C11-C12	-3.60	111.98	123.22
27	5	1621	LUT	C2-C3-C4	3.60	115.23	110.30
27	y	1620	LUT	C10-C11-C12	-3.60	111.99	123.22
26	s	604	CLA	CHB-C4A-NA	3.60	129.49	124.51
26	R	603	CLA	O2D-CGD-O1D	-3.60	116.80	123.84
26	C	508	CLA	C1B-CHB-C4A	-3.60	123.00	130.12
26	N	612	CLA	CMB-C2B-C3B	3.60	131.41	124.68
26	2	613	CLA	CMB-C2B-C1B	-3.60	122.94	128.46
26	D	403	CLA	O2D-CGD-CBD	3.59	117.66	111.27
25	S	608	CHL	C3B-C4B-NB	3.59	113.86	109.21
26	n	613	CLA	CMB-C2B-C3B	3.59	131.40	124.68
28	N	1622	XAT	C4-C3-C2	-3.59	103.84	110.77
26	b	607	CLA	O2D-CGD-O1D	-3.59	116.82	123.84
29	5	1623	NEX	C15-C14-C13	-3.59	122.19	127.31
25	Y	607	CHL	C3B-C4B-NB	3.59	113.85	109.21
27	3	1620	LUT	C10-C11-C12	-3.59	112.01	123.22
26	c	507	CLA	CMB-C2B-C3B	3.59	131.39	124.68
25	n	605	CHL	CHD-C4C-C3C	-3.59	119.56	124.84
26	y	610	CLA	C1B-CHB-C4A	-3.59	123.01	130.12
27	7	1620	LUT	C10-C11-C12	-3.59	112.02	123.22
26	c	508	CLA	C1B-CHB-C4A	-3.59	123.01	130.12
26	B	604	CLA	O2D-CGD-O1D	-3.59	116.83	123.84
25	r	608	CHL	C3B-C4B-NB	3.59	113.85	109.21
26	S	604	CLA	CHB-C4A-NA	3.59	129.47	124.51
26	r	603	CLA	O2D-CGD-O1D	-3.58	116.83	123.84
26	8	610	CLA	C1B-CHB-C4A	-3.58	123.02	130.12
28	n	1622	XAT	C4-C3-C2	-3.58	103.86	110.77
26	C	507	CLA	CMB-C2B-C3B	3.58	131.37	124.68
27	G	1620	LUT	C15-C14-C13	-3.58	122.20	127.31
26	N	604	CLA	C1B-CHB-C4A	-3.58	123.03	130.12
25	7	608	CHL	CAC-C3C-C4C	3.58	129.45	124.81
29	5	1623	NEX	O24-C25-C38	3.58	119.34	115.06
25	3	608	CHL	CAC-C3C-C4C	3.57	129.45	124.81
27	1	1621	LUT	C2-C3-C4	3.57	115.20	110.30
26	b	604	CLA	O2D-CGD-O1D	-3.57	116.85	123.84
26	7	612	CLA	CMB-C2B-C1B	-3.57	122.97	128.46
25	N	605	CHL	CHD-C4C-C3C	-3.57	119.59	124.84
31	B	619	BCR	C16-C17-C18	-3.57	122.21	127.31
31	b	619	BCR	C16-C17-C18	-3.57	122.21	127.31
26	Y	610	CLA	C1B-CHB-C4A	-3.57	123.05	130.12
26	6	612	CLA	CMB-C2B-C1B	-3.57	122.98	128.46
26	2	612	CLA	CMB-C2B-C1B	-3.57	122.98	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	7	605	CHL	CHD-C4C-C3C	-3.57	119.59	124.84
25	g	608	CHL	C3B-C4B-NB	3.56	113.82	109.21
26	A	410	CLA	CMB-C2B-C3B	3.56	131.34	124.68
28	n	1622	XAT	O4-C5-C18	3.56	119.32	115.06
25	R	608	CHL	C3B-C4B-NB	3.56	113.81	109.21
28	N	1622	XAT	O4-C5-C18	3.56	119.32	115.06
26	n	604	CLA	C1B-CHB-C4A	-3.56	123.07	130.12
26	4	610	CLA	C1B-CHB-C4A	-3.56	123.07	130.12
26	b	613	CLA	CHB-C4A-NA	3.56	129.43	124.51
26	4	612	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
26	a	410	CLA	CMB-C2B-C3B	3.56	131.33	124.68
26	G	603	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
26	g	603	CLA	CMB-C2B-C1B	-3.56	123.00	128.46
29	1	1623	NEX	O24-C25-C38	3.56	119.32	115.06
27	S	1620	LUT	C15-C14-C13	-3.56	122.24	127.31
26	B	611	CLA	O2D-CGD-O1D	-3.56	116.89	123.84
25	G	605	CHL	CAC-C3C-C4C	3.55	129.42	124.81
27	g	1621	LUT	C7-C8-C9	-3.55	120.87	126.23
27	s	1620	LUT	C15-C14-C13	-3.55	122.24	127.31
29	Y	1623	NEX	O24-C25-C38	3.55	119.31	115.06
26	b	611	CLA	O2D-CGD-O1D	-3.55	116.91	123.84
26	8	612	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
26	3	612	CLA	CMB-C2B-C1B	-3.54	123.02	128.46
25	3	605	CHL	CHD-C4C-C3C	-3.54	119.63	124.84
25	g	605	CHL	CAC-C3C-C4C	3.54	129.41	124.81
25	n	601	CHL	C3B-C4B-NB	3.54	113.79	109.21
28	3	1622	XAT	O4-C5-C18	3.54	119.30	115.06
27	G	1621	LUT	C10-C11-C12	-3.54	112.17	123.22
27	g	1620	LUT	C15-C14-C13	-3.54	122.26	127.31
26	C	507	CLA	CHB-C4A-NA	3.54	129.41	124.51
26	c	509	CLA	CHB-C4A-NA	3.54	129.40	124.51
27	G	1621	LUT	C7-C8-C9	-3.54	120.89	126.23
25	2	606	CHL	CHD-C4C-C3C	-3.54	119.64	124.84
27	g	1621	LUT	C10-C11-C12	-3.54	112.18	123.22
25	G	608	CHL	C3B-C4B-NB	3.53	113.78	109.21
26	B	613	CLA	CHB-C4A-NA	3.53	129.40	124.51
36	a	412	SQD	C4-C3-C2	3.53	116.99	110.82
31	b	619	BCR	C28-C27-C26	-3.53	107.77	114.08
31	B	619	BCR	C28-C27-C26	-3.53	107.77	114.08
26	y	610	CLA	CMB-C2B-C3B	3.53	131.28	124.68
41	f	101	HEM	CBA-CAA-C2A	-3.53	106.60	112.62
31	B	620	BCR	C28-C27-C26	-3.53	107.77	114.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	3	613	CLA	C1B-CHB-C4A	-3.53	123.13	130.12
26	5	611	CLA	CMB-C2B-C1B	-3.53	123.05	128.46
29	y	1623	NEX	O24-C25-C38	3.52	119.28	115.06
27	r	620	LUT	C35-C15-C14	-3.52	116.26	123.47
26	7	602	CLA	C1B-CHB-C4A	-3.52	123.14	130.12
25	G	609	CHL	CAC-C3C-C4C	3.52	129.38	124.81
25	g	609	CHL	CAC-C3C-C4C	3.52	129.37	124.81
26	1	611	CLA	CMB-C2B-C1B	-3.52	123.06	128.46
26	B	605	CLA	CAC-C3C-C4C	3.52	129.37	124.81
26	Y	610	CLA	CMB-C2B-C3B	3.51	131.25	124.68
25	3	601	CHL	CAC-C3C-C4C	3.51	129.37	124.81
25	6	606	CHL	CHD-C4C-C3C	-3.51	119.68	124.84
29	g	1623	NEX	C31-C30-C29	-3.51	122.30	127.31
25	N	601	CHL	C3B-C4B-NB	3.51	113.75	109.21
25	S	601	CHL	CMD-C2D-C3D	-3.51	119.53	127.61
25	s	601	CHL	CMD-C2D-C3D	-3.51	119.53	127.61
26	3	602	CLA	C1B-CHB-C4A	-3.51	123.16	130.12
28	7	1622	XAT	O4-C5-C18	3.51	119.26	115.06
27	6	1620	LUT	C30-C31-C32	-3.51	112.26	123.22
27	R	620	LUT	C35-C15-C14	-3.51	116.28	123.47
31	b	620	BCR	C28-C27-C26	-3.51	107.81	114.08
26	C	509	CLA	CHB-C4A-NA	3.51	129.37	124.51
26	c	507	CLA	CHB-C4A-NA	3.51	129.37	124.51
26	7	613	CLA	C1B-CHB-C4A	-3.51	123.17	130.12
27	r	620	LUT	C35-C34-C33	-3.51	122.30	127.31
41	F	101	HEM	CBA-CAA-C2A	-3.51	106.63	112.62
26	D	402	CLA	CMB-C2B-C3B	3.51	131.24	124.68
36	A	412	SQD	C4-C3-C2	3.51	116.94	110.82
27	2	1620	LUT	C30-C31-C32	-3.51	112.28	123.22
25	G	608	CHL	CAC-C3C-C4C	3.50	129.36	124.81
26	R	610	CLA	C4A-NA-C1A	3.50	108.28	106.71
26	b	611	CLA	CMB-C2B-C3B	3.50	131.23	124.68
25	G	609	CHL	CHB-C4A-NA	3.50	129.35	124.51
26	d	402	CLA	CMB-C2B-C3B	3.50	131.23	124.68
25	7	601	CHL	CAC-C3C-C4C	3.50	129.35	124.81
26	2	610	CLA	C1B-CHB-C4A	-3.50	123.19	130.12
26	C	505	CLA	O2D-CGD-CBD	3.50	117.49	111.27
25	y	606	CHL	C3B-C4B-NB	3.50	113.73	109.21
27	N	1621	LUT	C16-C1-C6	-3.50	104.63	110.30
26	b	605	CLA	CAC-C3C-C4C	3.50	129.35	124.81
25	8	607	CHL	CAC-C3C-C4C	3.50	129.35	124.81
26	B	606	CLA	CMB-C2B-C3B	3.49	131.22	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	606	CLA	CMB-C2B-C3B	3.49	131.22	124.68
26	C	502	CLA	O2D-CGD-O1D	-3.49	117.00	123.84
26	c	502	CLA	O2D-CGD-O1D	-3.49	117.00	123.84
26	r	602	CLA	O2D-CGD-O1D	-3.49	117.01	123.84
26	c	503	CLA	CMB-C2B-C3B	3.49	131.21	124.68
26	s	603	CLA	CMB-C2B-C3B	3.49	131.21	124.68
29	G	1623	NEX	C31-C30-C29	-3.49	122.33	127.31
26	c	505	CLA	O2D-CGD-CBD	3.49	117.47	111.27
26	C	503	CLA	CMB-C2B-C3B	3.49	131.21	124.68
25	4	607	CHL	CAC-C3C-C4C	3.49	129.34	124.81
28	5	1622	XAT	O24-C25-C38	3.48	119.23	115.06
26	B	611	CLA	CMB-C2B-C3B	3.48	131.20	124.68
27	n	1621	LUT	C16-C1-C6	-3.48	104.65	110.30
26	6	610	CLA	C1B-CHB-C4A	-3.48	123.22	130.12
26	R	602	CLA	O2D-CGD-O1D	-3.48	117.03	123.84
25	R	614	CHL	C3B-C4B-NB	3.48	113.71	109.21
25	g	608	CHL	CAC-C3C-C4C	3.48	129.32	124.81
25	R	607	CHL	CHB-C4A-NA	3.48	129.32	124.51
25	g	609	CHL	CHB-C4A-NA	3.48	129.32	124.51
26	8	611	CLA	CMB-C2B-C1B	-3.48	123.12	128.46
26	S	603	CLA	CMB-C2B-C3B	3.48	131.18	124.68
26	4	602	CLA	O2D-CGD-CBD	3.47	117.44	111.27
26	G	610	CLA	C4A-NA-C1A	3.47	108.27	106.71
25	6	609	CHL	C1B-CHB-C4A	-3.47	123.24	130.12
38	d	405	PL9	C7-C8-C9	-3.47	121.01	126.79
25	r	607	CHL	CHB-C4A-NA	3.47	129.31	124.51
27	R	620	LUT	C35-C34-C33	-3.47	122.36	127.31
25	3	605	CHL	C3B-C4B-NB	3.47	113.69	109.21
25	R	614	CHL	CAC-C3C-C4C	3.47	129.31	124.81
29	r	623	NEX	C15-C35-C34	-3.47	116.37	123.47
29	R	623	NEX	C15-C35-C34	-3.47	116.38	123.47
25	Y	606	CHL	C3B-C4B-NB	3.46	113.69	109.21
38	D	405	PL9	C7-C8-C9	-3.46	121.03	126.79
26	r	610	CLA	C4A-NA-C1A	3.46	108.26	106.71
25	N	608	CHL	C3B-C4B-NB	3.46	113.68	109.21
25	r	614	CHL	CAC-C3C-C4C	3.46	129.30	124.81
28	n	1622	XAT	C35-C34-C33	-3.46	122.37	127.31
25	n	606	CHL	CAC-C3C-C4C	3.46	129.30	124.81
28	1	1622	XAT	O24-C25-C38	3.46	119.20	115.06
25	r	614	CHL	C3B-C4B-NB	3.46	113.68	109.21
26	4	611	CLA	CMB-C2B-C1B	-3.46	123.15	128.46
25	2	609	CHL	C1B-CHB-C4A	-3.46	123.27	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	6	609	CHL	C3B-C4B-NB	3.46	113.68	109.21
25	n	608	CHL	C3B-C4B-NB	3.46	113.68	109.21
26	A	407	CLA	CMB-C2B-C3B	3.45	131.14	124.68
36	B	623	SQD	O7-S-C6	3.45	111.04	106.94
25	7	605	CHL	C3B-C4B-NB	3.45	113.67	109.21
26	C	505	CLA	C2D-C1D-ND	-3.45	107.56	110.10
26	c	505	CLA	C2D-C1D-ND	-3.45	107.56	110.10
25	2	607	CHL	C3B-C4B-NB	3.45	113.67	109.21
27	5	1620	LUT	C10-C11-C12	-3.45	112.44	123.22
36	b	623	SQD	O7-S-C6	3.45	111.04	106.94
27	s	1621	LUT	C35-C15-C14	-3.45	116.41	123.47
26	G	603	CLA	CHB-C4A-NA	3.45	129.28	124.51
25	Y	608	CHL	CAC-C3C-C4C	3.45	129.29	124.81
26	8	602	CLA	O2D-CGD-CBD	3.45	117.39	111.27
38	d	405	PL9	C7-C3-C2	-3.45	118.77	123.30
36	B	621	SQD	O6-C1-C2	3.45	113.69	108.30
27	N	1621	LUT	C7-C8-C9	-3.45	121.03	126.23
26	B	609	CLA	O2D-CGD-O1D	-3.45	117.10	123.84
26	A	406	CLA	CHD-C1D-ND	-3.45	121.29	124.45
27	1	1620	LUT	C10-C11-C12	-3.45	112.47	123.22
26	G	613	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
26	g	613	CLA	CMB-C2B-C1B	-3.45	123.17	128.46
29	g	1623	NEX	C16-C1-C6	3.44	113.56	110.47
38	D	405	PL9	C7-C3-C2	-3.44	118.77	123.30
26	y	604	CLA	O2D-CGD-O1D	-3.44	117.11	123.84
29	G	1623	NEX	C16-C1-C6	3.44	113.55	110.47
25	Y	608	CHL	C3B-C4B-NB	3.44	113.66	109.21
26	a	407	CLA	CMB-C2B-C3B	3.44	131.11	124.68
36	b	621	SQD	O6-C1-C2	3.44	113.67	108.30
25	2	609	CHL	C3B-C4B-NB	3.44	113.65	109.21
26	8	602	CLA	CMB-C2B-C3B	3.44	131.11	124.68
25	3	608	CHL	C3B-C4B-NB	3.44	113.65	109.21
26	C	513	CLA	CAA-C2A-C3A	-3.43	103.37	112.78
25	6	607	CHL	C3B-C4B-NB	3.43	113.65	109.21
26	6	610	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
27	S	1621	LUT	C35-C15-C14	-3.43	116.44	123.47
28	N	1622	XAT	C35-C34-C33	-3.43	122.41	127.31
26	2	610	CLA	CMB-C2B-C1B	-3.43	123.19	128.46
26	b	609	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
26	b	616	CLA	O2D-CGD-O1D	-3.43	117.14	123.84
26	R	613	CLA	CMB-C2B-C1B	-3.43	123.20	128.46
26	g	603	CLA	CHB-C4A-NA	3.43	129.25	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	406	CLA	CHD-C1D-ND	-3.43	121.31	124.45
25	N	606	CHL	CAC-C3C-C4C	3.43	129.25	124.81
25	7	608	CHL	C3B-C4B-NB	3.43	113.64	109.21
25	5	605	CHL	CAC-C3C-C4C	3.42	129.25	124.81
25	1	606	CHL	C3B-C4B-NB	3.42	113.64	109.21
27	1	1620	LUT	C35-C15-C14	-3.42	116.46	123.47
26	c	513	CLA	CAA-C2A-C3A	-3.42	103.41	112.78
26	B	616	CLA	O2D-CGD-O1D	-3.42	117.15	123.84
28	N	1622	XAT	C10-C11-C12	-3.42	112.54	123.22
26	1	604	CLA	C4A-NA-C1A	3.42	108.24	106.71
26	2	603	CLA	CMB-C2B-C1B	-3.42	123.21	128.46
28	y	1622	XAT	C4-C3-C2	-3.42	104.17	110.77
28	n	1622	XAT	C10-C11-C12	-3.42	112.55	123.22
25	N	605	CHL	C3B-C4B-NB	3.42	113.63	109.21
26	4	602	CLA	CMB-C2B-C3B	3.42	131.07	124.68
25	S	606	CHL	O2D-CGD-O1D	-3.42	117.16	123.84
25	y	608	CHL	CAC-C3C-C4C	3.42	129.24	124.81
28	Y	1622	XAT	C4-C3-C2	-3.41	104.18	110.77
26	Y	604	CLA	O2D-CGD-O1D	-3.41	117.16	123.84
26	6	603	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
26	r	613	CLA	CMB-C2B-C1B	-3.41	123.22	128.46
25	y	608	CHL	C3B-C4B-NB	3.41	113.62	109.21
27	n	1621	LUT	C7-C8-C9	-3.41	121.08	126.23
27	5	1620	LUT	C35-C15-C14	-3.41	116.48	123.47
25	2	607	CHL	CHD-C4C-C3C	-3.41	119.83	124.84
25	8	606	CHL	CHD-C4C-C3C	-3.41	119.83	124.84
29	2	1623	NEX	C16-C1-C6	3.41	113.52	110.47
25	5	606	CHL	C3B-C4B-NB	3.41	113.62	109.21
25	R	607	CHL	C4-C3-C5	3.41	121.00	115.27
39	B	626	DGD	O6D-C1D-O3G	-3.41	101.90	109.97
26	b	614	CLA	CMB-C2B-C3B	3.41	131.05	124.68
25	1	605	CHL	CAC-C3C-C4C	3.41	129.23	124.81
26	B	608	CLA	C1B-CHB-C4A	-3.40	123.38	130.12
25	4	606	CHL	CHD-C4C-C3C	-3.40	119.84	124.84
25	n	605	CHL	C3B-C4B-NB	3.40	113.61	109.21
25	s	606	CHL	O2D-CGD-O1D	-3.40	117.18	123.84
26	r	616	CLA	CMB-C2B-C1B	-3.40	123.23	128.46
26	g	602	CLA	C1-C2-C3	-3.40	120.16	126.04
26	B	614	CLA	CMB-C2B-C3B	3.40	131.04	124.68
26	G	602	CLA	C1-C2-C3	-3.40	120.16	126.04
28	Y	1622	XAT	C26-C27-C28	-3.40	118.80	125.99
26	b	608	CLA	C1B-CHB-C4A	-3.40	123.38	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	y	1622	XAT	C26-C27-C28	-3.40	118.81	125.99
26	1	610	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
26	5	610	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
36	A	412	SQD	O5-C5-C4	3.40	115.86	109.69
26	1	612	CLA	CMB-C2B-C1B	-3.40	123.24	128.46
29	N	1623	NEX	C11-C10-C9	-3.39	122.47	127.31
26	g	612	CLA	CMB-C2B-C3B	3.39	131.03	124.68
26	g	610	CLA	C4A-NA-C1A	3.39	108.23	106.71
26	R	616	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
31	b	619	BCR	C20-C21-C22	-3.39	122.47	127.31
25	r	607	CHL	C4-C3-C5	3.39	120.98	115.27
26	G	604	CLA	C1B-CHB-C4A	-3.39	123.40	130.12
39	b	626	DGD	O6D-C1D-O3G	-3.39	101.94	109.97
25	N	606	CHL	C3B-C4B-NB	3.39	113.59	109.21
26	A	407	CLA	C1B-CHB-C4A	-3.39	123.40	130.12
26	5	602	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
26	s	609	CLA	CMB-C2B-C1B	-3.39	123.25	128.46
26	B	608	CLA	CMB-C2B-C3B	3.39	131.02	124.68
26	b	608	CLA	CMB-C2B-C3B	3.39	131.02	124.68
26	B	605	CLA	C1B-CHB-C4A	-3.39	123.41	130.12
25	g	601	CHL	CHD-C4C-C3C	-3.39	119.86	124.84
26	7	603	CLA	CHB-C4A-NA	3.39	129.20	124.51
31	B	619	BCR	C20-C21-C22	-3.39	122.48	127.31
26	7	612	CLA	O2D-CGD-O1D	-3.39	117.22	123.84
26	N	610	CLA	C1B-CHB-C4A	-3.38	123.42	130.12
29	n	1623	NEX	C11-C10-C9	-3.38	122.48	127.31
25	7	605	CHL	CAC-C3C-C4C	3.38	129.20	124.81
26	3	612	CLA	O2D-CGD-O1D	-3.38	117.23	123.84
26	a	407	CLA	C1B-CHB-C4A	-3.38	123.42	130.12
25	6	607	CHL	CHD-C4C-C3C	-3.38	119.87	124.84
26	5	612	CLA	CMB-C2B-C1B	-3.38	123.27	128.46
26	A	406	CLA	C1B-CHB-C4A	-3.38	123.42	130.12
25	G	601	CHL	CHD-C4C-C3C	-3.38	119.87	124.84
26	G	612	CLA	CMB-C2B-C3B	3.38	131.00	124.68
26	5	604	CLA	C1B-CHB-C4A	-3.38	123.43	130.12
25	1	601	CHL	C3B-C4B-NB	3.38	113.58	109.21
25	5	601	CHL	C3B-C4B-NB	3.38	113.58	109.21
25	7	607	CHL	C4A-NA-C1A	3.38	108.22	106.71
26	g	604	CLA	C1B-CHB-C4A	-3.38	123.43	130.12
26	S	609	CLA	CMB-C2B-C1B	-3.38	123.28	128.46
27	5	1621	LUT	C35-C34-C33	-3.38	122.49	127.31
25	n	606	CHL	C3B-C4B-NB	3.37	113.57	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	C	515	BCR	C15-C16-C17	-3.37	116.56	123.47
25	y	601	CHL	C4-C3-C5	3.37	120.95	115.27
36	a	412	SQD	O5-C5-C4	3.37	115.82	109.69
26	a	406	CLA	C1B-CHB-C4A	-3.37	123.44	130.12
31	c	515	BCR	C15-C16-C17	-3.37	116.57	123.47
26	b	611	CLA	CAA-CBA-CGA	-3.37	103.40	113.25
26	l	602	CLA	CMB-C2B-C1B	-3.37	123.28	128.46
26	n	610	CLA	C1B-CHB-C4A	-3.37	123.44	130.12
38	A	414	PL9	C7-C3-C2	-3.37	118.87	123.30
26	b	605	CLA	C1B-CHB-C4A	-3.37	123.45	130.12
26	5	602	CLA	CMB-C2B-C3B	3.37	130.98	124.68
26	B	612	CLA	C1B-CHB-C4A	-3.37	123.45	130.12
26	B	611	CLA	CAA-CBA-CGA	-3.37	103.42	113.25
26	b	612	CLA	C1B-CHB-C4A	-3.37	123.45	130.12
25	7	609	CHL	C1C-C2C-C3C	-3.37	104.44	107.11
26	A	410	CLA	C1B-CHB-C4A	-3.36	123.45	130.12
26	l	604	CLA	C1B-CHB-C4A	-3.36	123.45	130.12
26	N	603	CLA	CHB-C4A-NA	3.36	129.16	124.51
26	n	603	CLA	CHB-C4A-NA	3.36	129.16	124.51
38	a	414	PL9	C7-C3-C2	-3.36	118.88	123.30
26	a	410	CLA	O2D-CGD-CBD	3.36	117.24	111.27
27	l	1621	LUT	C35-C34-C33	-3.36	122.51	127.31
25	N	606	CHL	CMB-C2B-C3B	3.36	130.97	124.68
25	3	609	CHL	C1C-C2C-C3C	-3.36	104.45	107.11
26	a	406	CLA	O2D-CGD-O1D	-3.36	117.27	123.84
29	6	1623	NEX	C16-C1-C6	3.36	113.48	110.47
26	s	603	CLA	CHB-C4A-NA	3.36	129.16	124.51
29	7	1623	NEX	C39-C29-C30	-3.36	118.22	122.92
26	5	604	CLA	C4A-NA-C1A	3.36	108.22	106.71
26	G	611	CLA	C1B-CHB-C4A	-3.36	123.47	130.12
25	3	605	CHL	CAC-C3C-C4C	3.36	129.16	124.81
26	6	614	CLA	CMB-C2B-C3B	3.36	130.96	124.68
25	8	607	CHL	C3B-C4B-NB	3.36	113.55	109.21
31	B	620	BCR	C1-C6-C5	-3.35	117.89	122.61
31	b	620	BCR	C1-C6-C5	-3.35	117.89	122.61
26	a	410	CLA	C1B-CHB-C4A	-3.35	123.48	130.12
26	3	603	CLA	CHB-C4A-NA	3.35	129.14	124.51
26	r	610	CLA	O2D-CGD-O1D	-3.35	117.29	123.84
31	T	101	BCR	C33-C5-C4	3.35	120.05	113.62
26	5	613	CLA	C1B-CHB-C4A	-3.35	123.49	130.12
25	Y	601	CHL	C4-C3-C5	3.35	120.90	115.27
26	A	406	CLA	O2D-CGD-O1D	-3.34	117.30	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	A	410	CLA	O2D-CGD-CBD	3.34	117.21	111.27
25	Y	601	CHL	C3C-C4C-NC	3.34	114.32	110.57
26	S	603	CLA	CHB-C4A-NA	3.34	129.13	124.51
25	4	607	CHL	C3B-C4B-NB	3.34	113.53	109.21
26	6	611	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
36	a	412	SQD	O8-S-C6	3.34	111.06	105.74
26	B	606	CLA	C1B-CHB-C4A	-3.34	123.51	130.12
26	2	611	CLA	CMB-C2B-C1B	-3.34	123.33	128.46
25	n	606	CHL	CMB-C2B-C3B	3.34	130.92	124.68
39	C	519	DGD	O6D-C1D-O3G	-3.34	102.07	109.97
36	A	412	SQD	O8-S-C6	3.34	111.06	105.74
31	t	101	BCR	C33-C5-C4	3.34	120.02	113.62
28	3	1622	XAT	C24-C23-C22	-3.34	104.33	110.77
26	B	611	CLA	CHB-C4A-NA	3.34	129.12	124.51
25	6	609	CHL	CAC-C3C-C4C	3.33	129.14	124.81
26	1	602	CLA	CMB-C2B-C3B	3.33	130.92	124.68
26	8	610	CLA	CMB-C2B-C1B	-3.33	123.34	128.46
25	3	609	CHL	C3B-C4B-NB	3.33	113.52	109.21
26	g	611	CLA	C1B-CHB-C4A	-3.33	123.52	130.12
26	2	614	CLA	CMB-C2B-C3B	3.33	130.91	124.68
39	c	519	DGD	O6D-C1D-O3G	-3.33	102.08	109.97
26	R	610	CLA	O2D-CGD-O1D	-3.33	117.32	123.84
26	b	606	CLA	C1B-CHB-C4A	-3.33	123.52	130.12
29	3	1623	NEX	C39-C29-C30	-3.33	118.26	122.92
31	b	620	BCR	C33-C5-C4	3.33	120.02	113.62
26	C	509	CLA	O2D-CGD-CBD	3.33	117.19	111.27
26	1	613	CLA	C1B-CHB-C4A	-3.33	123.52	130.12
27	3	1620	LUT	C30-C31-C32	-3.33	112.84	123.22
25	2	601	CHL	CAC-C3C-C4C	3.33	129.12	124.81
26	D	403	CLA	CHB-C4A-NA	3.32	129.11	124.51
25	6	601	CHL	CAC-C3C-C4C	3.32	129.12	124.81
26	s	609	CLA	C1B-CHB-C4A	-3.32	123.54	130.12
27	7	1620	LUT	C30-C31-C32	-3.32	112.85	123.22
26	c	509	CLA	O2D-CGD-CBD	3.32	117.17	111.27
25	5	609	CHL	C1C-C2C-C3C	-3.32	104.48	107.11
28	7	1622	XAT	C24-C23-C22	-3.32	104.36	110.77
26	4	610	CLA	CMB-C2B-C1B	-3.32	123.36	128.46
28	8	622	XAT	O24-C25-C38	3.32	119.03	115.06
26	b	611	CLA	CHB-C4A-NA	3.32	129.10	124.51
25	1	607	CHL	CAC-C3C-C4C	3.31	129.11	124.81
25	5	607	CHL	CAC-C3C-C4C	3.31	129.11	124.81
26	G	610	CLA	CMB-C2B-C3B	3.31	130.88	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	B	620	BCR	C24-C23-C22	-3.31	121.23	126.23
25	7	609	CHL	C3B-C4B-NB	3.31	113.49	109.21
26	7	602	CLA	O2D-CGD-O1D	-3.31	117.36	123.84
28	4	622	XAT	O24-C25-C38	3.31	119.02	115.06
31	B	620	BCR	C33-C5-C4	3.31	119.98	113.62
26	R	610	CLA	CHB-C4A-NA	3.31	129.09	124.51
27	S	1621	LUT	C30-C31-C32	-3.31	112.89	123.22
25	s	608	CHL	C1B-CHB-C4A	-3.31	123.56	130.12
26	S	609	CLA	C1B-CHB-C4A	-3.31	123.56	130.12
27	g	1620	LUT	C10-C11-C12	-3.31	112.89	123.22
25	y	601	CHL	C3C-C4C-NC	3.31	114.28	110.57
25	3	607	CHL	C4A-NA-C1A	3.31	108.19	106.71
26	g	610	CLA	CMB-C2B-C3B	3.31	130.87	124.68
27	s	1621	LUT	C30-C31-C32	-3.31	112.90	123.22
31	b	620	BCR	C24-C23-C22	-3.30	121.24	126.23
26	B	602	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
29	3	1623	NEX	C11-C12-C13	-3.30	117.14	126.42
26	b	617	CLA	O2D-CGD-O1D	-3.30	117.39	123.84
29	7	1623	NEX	C11-C12-C13	-3.30	117.15	126.42
26	S	611	CLA	CMB-C2B-C1B	-3.30	123.39	128.46
25	1	609	CHL	C1C-C2C-C3C	-3.30	104.50	107.11
25	2	606	CHL	C3B-C4B-NB	3.30	113.47	109.21
25	6	606	CHL	C3B-C4B-NB	3.30	113.47	109.21
25	2	609	CHL	CAC-C3C-C4C	3.30	129.09	124.81
26	d	403	CLA	CHB-C4A-NA	3.30	129.07	124.51
27	G	1620	LUT	C10-C11-C12	-3.30	112.93	123.22
25	5	608	CHL	C3B-C4B-NB	3.30	113.47	109.21
28	R	622	XAT	C10-C11-C12	-3.30	112.93	123.22
26	B	617	CLA	O2D-CGD-O1D	-3.29	117.40	123.84
26	b	602	CLA	CMB-C2B-C1B	-3.29	123.40	128.46
25	1	608	CHL	C3B-C4B-NB	3.29	113.47	109.21
28	r	622	XAT	C10-C11-C12	-3.29	112.94	123.22
28	6	1622	XAT	C27-C28-C29	-3.29	120.43	125.53
27	4	620	LUT	C11-C10-C9	-3.29	122.62	127.31
28	2	1622	XAT	C27-C28-C29	-3.29	120.43	125.53
26	r	610	CLA	CHB-C4A-NA	3.29	129.06	124.51
28	2	1622	XAT	C7-C8-C9	-3.29	120.43	125.53
26	6	611	CLA	O2D-CGD-O1D	-3.29	117.41	123.84
31	b	619	BCR	C8-C7-C6	-3.28	117.98	127.20
26	G	610	CLA	C1B-CHB-C4A	-3.28	123.61	130.12
26	r	604	CLA	CBA-CAA-C2A	3.28	123.56	113.86
25	7	601	CHL	C3B-C4B-NB	3.28	113.45	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	R	604	CLA	CBA-CAA-C2A	3.28	123.55	113.86
26	C	511	CLA	CHB-C4A-NA	3.28	129.05	124.51
27	Y	1620	LUT	C35-C15-C14	-3.28	116.75	123.47
26	r	611	CLA	O2D-CGD-O1D	-3.28	117.42	123.84
25	S	608	CHL	C1B-CHB-C4A	-3.28	123.62	130.12
26	c	511	CLA	CHB-C4A-NA	3.28	129.05	124.51
25	r	606	CHL	C3B-C4B-NB	3.28	113.45	109.21
29	3	1623	NEX	C24-C23-C22	-3.28	104.44	110.77
26	s	611	CLA	CMB-C2B-C1B	-3.28	123.43	128.46
25	R	606	CHL	C3B-C4B-NB	3.27	113.44	109.21
31	B	619	BCR	C8-C7-C6	-3.27	118.01	127.20
26	R	611	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
26	n	613	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
26	3	602	CLA	O2D-CGD-O1D	-3.27	117.44	123.84
27	8	620	LUT	C11-C10-C9	-3.27	122.64	127.31
28	5	1622	XAT	C35-C34-C33	-3.27	122.64	127.31
26	1	614	CLA	CMB-C2B-C3B	3.27	130.79	124.68
26	5	614	CLA	CMB-C2B-C3B	3.27	130.79	124.68
26	N	613	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
28	1	1622	XAT	C35-C34-C33	-3.27	122.65	127.31
26	Y	602	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
26	2	611	CLA	O2D-CGD-O1D	-3.27	117.45	123.84
29	r	623	NEX	C31-C30-C29	-3.26	122.65	127.31
25	3	601	CHL	C3B-C4B-NB	3.26	113.43	109.21
25	6	608	CHL	CAC-C3C-C4C	3.26	129.04	124.81
26	Y	614	CLA	CMB-C2B-C3B	3.26	130.78	124.68
29	7	1623	NEX	C24-C23-C22	-3.26	104.47	110.77
25	2	608	CHL	C3B-C4B-NB	3.26	113.43	109.21
27	y	1620	LUT	C35-C15-C14	-3.26	116.80	123.47
26	C	502	CLA	CHB-C4A-NA	3.26	129.02	124.51
25	5	608	CHL	CAC-C3C-C4C	3.26	129.04	124.81
25	y	606	CHL	CMB-C2B-C3B	3.26	130.77	124.68
25	7	601	CHL	C4A-NA-C1A	-3.26	105.24	106.71
26	D	403	CLA	C1B-CHB-C4A	-3.26	123.67	130.12
27	Y	1620	LUT	C15-C14-C13	-3.26	122.66	127.31
26	g	610	CLA	C1B-CHB-C4A	-3.25	123.67	130.12
25	7	609	CHL	CAC-C3C-C4C	3.25	129.03	124.81
25	2	608	CHL	CAC-C3C-C4C	3.25	129.03	124.81
28	6	1622	XAT	C7-C8-C9	-3.25	120.49	125.53
26	y	602	CLA	O2D-CGD-O1D	-3.25	117.48	123.84
26	y	614	CLA	CMB-C2B-C3B	3.25	130.75	124.68
28	r	622	XAT	C35-C15-C14	-3.25	116.82	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	606	CHL	CMB-C2B-C3B	3.25	130.75	124.68
28	G	1622	XAT	C11-C10-C9	-3.25	122.68	127.31
25	Y	601	CHL	O2D-CGD-O1D	-3.25	117.49	123.84
25	y	601	CHL	O2D-CGD-O1D	-3.25	117.49	123.84
26	B	615	CLA	CMB-C2B-C1B	-3.24	123.48	128.46
25	g	609	CHL	CMB-C2B-C3B	3.24	130.75	124.68
26	G	603	CLA	CAA-C2A-C3A	-3.24	103.90	112.78
26	g	603	CLA	CAA-C2A-C3A	-3.24	103.90	112.78
29	R	623	NEX	C31-C30-C29	-3.24	122.68	127.31
25	l	608	CHL	CAC-C3C-C4C	3.24	129.02	124.81
27	r	620	LUT	C15-C14-C13	-3.24	122.68	127.31
26	d	403	CLA	C1B-CHB-C4A	-3.24	123.70	130.12
29	S	1623	NEX	C26-C27-C28	-3.24	119.14	125.99
26	c	508	CLA	CMC-C2C-C1C	-3.24	120.11	125.04
25	G	608	CHL	CMD-C2D-C3D	-3.24	120.16	127.61
26	6	603	CLA	CHB-C4A-NA	3.24	128.99	124.51
26	b	615	CLA	CMB-C2B-C1B	-3.24	123.49	128.46
25	g	608	CHL	CMD-C2D-C3D	-3.24	120.17	127.61
26	5	603	CLA	CMB-C2B-C3B	3.24	130.73	124.68
27	R	620	LUT	C15-C14-C13	-3.23	122.69	127.31
26	7	613	CLA	CMB-C2B-C3B	3.23	130.73	124.68
25	y	609	CHL	CHB-C4A-NA	3.23	128.98	124.51
28	R	622	XAT	C35-C15-C14	-3.23	116.85	123.47
26	g	603	CLA	O2D-CGD-O1D	-3.23	117.52	123.84
25	6	608	CHL	C3B-C4B-NB	3.23	113.39	109.21
25	G	609	CHL	CMB-C2B-C3B	3.23	130.72	124.68
25	8	609	CHL	C3B-C4B-NB	3.23	113.38	109.21
25	3	609	CHL	CAC-C3C-C4C	3.23	129.00	124.81
26	n	602	CLA	C1B-CHB-C4A	-3.23	123.73	130.12
25	N	605	CHL	C4D-CHA-C1A	-3.23	117.32	121.25
25	n	605	CHL	C4D-CHA-C1A	-3.23	117.32	121.25
27	8	620	LUT	C18-C5-C6	-3.22	120.91	124.53
25	3	607	CHL	C3B-C4B-NB	3.22	113.38	109.21
26	N	602	CLA	C1B-CHB-C4A	-3.22	123.73	130.12
26	3	603	CLA	CMB-C2B-C1B	-3.22	123.51	128.46
27	y	1620	LUT	C15-C14-C13	-3.22	122.71	127.31
26	C	507	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
26	1	603	CLA	CMB-C2B-C3B	3.22	130.71	124.68
26	c	507	CLA	O2D-CGD-O1D	-3.22	117.54	123.84
27	N	1621	LUT	C35-C34-C33	-3.22	122.72	127.31
26	3	614	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
27	s	1621	LUT	C10-C11-C12	-3.22	113.17	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	8	620	LUT	C18-C5-C4	3.22	120.32	114.36
26	G	603	CLA	O2D-CGD-O1D	-3.22	117.55	123.84
26	g	614	CLA	C1B-CHB-C4A	-3.22	123.75	130.12
26	c	502	CLA	CHB-C4A-NA	3.22	128.96	124.51
25	2	605	CHL	C3B-C4B-NB	3.22	113.37	109.21
29	s	1623	NEX	C26-C27-C28	-3.22	119.19	125.99
25	Y	609	CHL	CHB-C4A-NA	3.22	128.96	124.51
25	7	606	CHL	C3B-C4B-NB	3.21	113.36	109.21
29	6	1623	NEX	C15-C35-C34	-3.21	116.89	123.47
31	T	101	BCR	C16-C15-C14	-3.21	116.89	123.47
26	3	613	CLA	CMB-C2B-C3B	3.21	130.69	124.68
31	t	101	BCR	C16-C15-C14	-3.21	116.89	123.47
25	s	601	CHL	CAC-C3C-C4C	3.21	128.98	124.81
26	2	603	CLA	CHB-C4A-NA	3.21	128.95	124.51
27	N	1620	LUT	C10-C11-C12	-3.21	113.20	123.22
27	S	1621	LUT	C10-C11-C12	-3.21	113.20	123.22
27	n	1620	LUT	C10-C11-C12	-3.21	113.20	123.22
26	C	508	CLA	CMC-C2C-C1C	-3.21	120.15	125.04
26	r	610	CLA	CMB-C2B-C3B	3.21	130.69	124.68
28	g	1622	XAT	C11-C10-C9	-3.21	122.73	127.31
25	r	614	CHL	CHD-C4C-C3C	-3.21	120.12	124.84
25	S	601	CHL	CAC-C3C-C4C	3.21	128.97	124.81
28	g	1622	XAT	C35-C34-C33	-3.21	122.73	127.31
25	g	605	CHL	C4A-NA-C1A	-3.21	105.26	106.71
27	n	1621	LUT	C35-C34-C33	-3.21	122.73	127.31
25	6	605	CHL	C3B-C4B-NB	3.21	113.36	109.21
25	N	607	CHL	CMB-C2B-C3B	3.21	130.68	124.68
26	G	614	CLA	C1B-CHB-C4A	-3.20	123.77	130.12
25	3	606	CHL	C3B-C4B-NB	3.20	113.35	109.21
27	r	620	LUT	C10-C11-C12	-3.20	113.22	123.22
25	8	601	CHL	C3B-C4B-NB	3.20	113.35	109.21
25	G	605	CHL	C4A-NA-C1A	-3.20	105.27	106.71
26	2	611	CLA	C1B-CHB-C4A	-3.20	123.77	130.12
26	7	614	CLA	O2D-CGD-O1D	-3.20	117.58	123.84
26	r	604	CLA	C1B-CHB-C4A	-3.20	123.79	130.12
25	n	607	CHL	CMB-C2B-C3B	3.20	130.66	124.68
26	R	610	CLA	CMB-C2B-C3B	3.20	130.66	124.68
27	4	620	LUT	C18-C5-C6	-3.20	120.94	124.53
27	4	620	LUT	C18-C5-C4	3.20	120.28	114.36
29	2	1623	NEX	C15-C35-C34	-3.19	116.93	123.47
28	4	622	XAT	C4-C3-C2	-3.19	104.61	110.77
25	7	607	CHL	C3B-C4B-NB	3.19	113.34	109.21

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	8	622	XAT	C4-C3-C2	-3.19	104.61	110.77
25	r	606	CHL	CMD-C2D-C3D	-3.19	120.27	127.61
26	7	603	CLA	CMB-C2B-C1B	-3.19	123.56	128.46
25	n	609	CHL	CMB-C2B-C3B	3.19	130.65	124.68
26	N	602	CLA	C1-C2-C3	-3.19	120.53	126.04
25	R	606	CHL	CMD-C2D-C3D	-3.19	120.28	127.61
26	6	611	CLA	C1B-CHB-C4A	-3.19	123.80	130.12
26	y	603	CLA	O2D-CGD-O1D	-3.19	117.61	123.84
27	R	620	LUT	C10-C11-C12	-3.19	113.27	123.22
31	a	411	BCR	C24-C23-C22	-3.19	121.42	126.23
29	S	1623	NEX	C35-C34-C33	-3.19	122.76	127.31
29	1	1623	NEX	C11-C10-C9	-3.18	122.77	127.31
26	b	610	CLA	C7-C6-C5	-3.18	104.71	113.36
26	c	501	CLA	CMB-C2B-C1B	-3.18	123.57	128.46
38	d	405	PL9	C40-C39-C41	3.18	120.63	115.27
25	N	609	CHL	CMB-C2B-C3B	3.18	130.63	124.68
25	R	614	CHL	CHD-C4C-C3C	-3.18	120.16	124.84
26	C	504	CLA	CHB-C4A-NA	3.18	128.91	124.51
28	8	622	XAT	C15-C14-C13	-3.18	122.77	127.31
26	n	602	CLA	C1-C2-C3	-3.18	120.54	126.04
26	C	501	CLA	CMB-C2B-C1B	-3.18	123.58	128.46
29	5	1623	NEX	C11-C10-C9	-3.18	122.77	127.31
26	n	613	CLA	C1B-CHB-C4A	-3.18	123.82	130.12
26	B	610	CLA	C7-C6-C5	-3.18	104.72	113.36
28	4	622	XAT	C15-C14-C13	-3.18	122.77	127.31
29	s	1623	NEX	C35-C34-C33	-3.18	122.77	127.31
26	S	602	CLA	O2D-CGD-O1D	-3.18	117.62	123.84
25	4	609	CHL	C3B-C4B-NB	3.18	113.32	109.21
25	y	606	CHL	CAC-C3C-C4C	3.18	128.93	124.81
26	6	602	CLA	C4A-NA-C1A	3.18	108.13	106.71
28	G	1622	XAT	C35-C34-C33	-3.17	122.78	127.31
25	g	601	CHL	CHB-C4A-NA	3.17	128.90	124.51
26	N	603	CLA	CMB-C2B-C1B	-3.17	123.59	128.46
26	s	602	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
26	C	505	CLA	C7-C6-C5	-3.17	104.75	113.36
26	c	505	CLA	C7-C6-C5	-3.17	104.75	113.36
26	D	402	CLA	CHD-C1D-ND	-3.17	121.54	124.45
26	Y	603	CLA	O2D-CGD-O1D	-3.17	117.64	123.84
26	3	610	CLA	CMB-C2B-C3B	3.17	130.60	124.68
26	7	610	CLA	CMB-C2B-C3B	3.17	130.60	124.68
26	n	603	CLA	O2D-CGD-O1D	-3.17	117.65	123.84
26	R	604	CLA	C1B-CHB-C4A	-3.17	123.85	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	D	405	PL9	C40-C39-C41	3.16	120.59	115.27
26	n	603	CLA	CMB-C2B-C1B	-3.16	123.60	128.46
26	2	613	CLA	C1B-CHB-C4A	-3.16	123.85	130.12
27	7	1621	LUT	C15-C35-C34	-3.16	116.99	123.47
25	Y	606	CHL	CAC-C3C-C4C	3.16	128.91	124.81
25	4	601	CHL	C3B-C4B-NB	3.16	113.30	109.21
26	4	604	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
25	3	601	CHL	C1C-C2C-C3C	-3.16	104.61	107.11
27	4	620	LUT	C35-C34-C33	-3.16	122.80	127.31
26	B	611	CLA	CAA-C2A-C3A	-3.16	104.12	112.78
28	3	1622	XAT	C11-C10-C9	-3.16	122.80	127.31
26	6	613	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
26	r	609	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
26	R	609	CLA	C1B-CHB-C4A	-3.16	123.86	130.12
26	N	603	CLA	O2D-CGD-O1D	-3.16	117.67	123.84
27	8	620	LUT	C35-C34-C33	-3.16	122.81	127.31
26	b	611	CLA	CAA-C2A-C3A	-3.15	104.14	112.78
31	A	411	BCR	C24-C23-C22	-3.15	121.47	126.23
26	N	613	CLA	C1B-CHB-C4A	-3.15	123.87	130.12
26	b	607	CLA	C1B-CHB-C4A	-3.15	123.87	130.12
25	6	601	CHL	C4A-NA-C1A	-3.15	105.29	106.71
26	A	407	CLA	CHB-C4A-NA	3.15	128.87	124.51
26	s	614	CLA	O2D-CGD-CBD	3.15	116.87	111.27
31	C	515	BCR	C24-C23-C22	-3.15	121.48	126.23
26	y	611	CLA	CMB-C2B-C1B	-3.15	123.63	128.46
26	c	504	CLA	CHB-C4A-NA	3.15	128.86	124.51
26	S	614	CLA	O2D-CGD-CBD	3.15	116.86	111.27
26	B	607	CLA	C1B-CHB-C4A	-3.14	123.89	130.12
26	8	604	CLA	C1B-CHB-C4A	-3.14	123.89	130.12
27	Y	1620	LUT	C30-C31-C32	-3.14	113.40	123.22
26	C	501	CLA	C1B-CHB-C4A	-3.14	123.89	130.12
28	6	1622	XAT	C35-C34-C33	-3.14	122.82	127.31
25	1	606	CHL	CAC-C3C-C4C	3.14	128.89	124.81
26	c	501	CLA	C1B-CHB-C4A	-3.14	123.89	130.12
26	A	406	CLA	O2D-CGD-CBD	3.14	116.85	111.27
26	8	603	CLA	CMB-C2B-C3B	3.14	130.55	124.68
26	r	611	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
26	C	502	CLA	C1B-CHB-C4A	-3.14	123.90	130.12
35	A	408	PHO	O1D-CGD-CBD	3.14	129.97	124.74
27	3	1621	LUT	C15-C35-C34	-3.14	117.04	123.47
26	4	603	CLA	CMB-C2B-C3B	3.14	130.55	124.68
39	C	518	DGD	C1E-O6E-C5E	3.14	119.85	113.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	y	603	CLA	CHB-C4A-NA	3.14	128.85	124.51
26	S	609	CLA	C4A-NA-C1A	3.14	108.12	106.71
26	y	602	CLA	C1-C2-C3	-3.14	120.61	126.04
27	n	1620	LUT	C15-C14-C13	-3.14	122.83	127.31
31	c	515	BCR	C24-C23-C22	-3.14	121.49	126.23
26	Y	611	CLA	CMB-C2B-C1B	-3.14	123.64	128.46
35	a	408	PHO	O1D-CGD-CBD	3.14	129.96	124.74
25	G	601	CHL	CHB-C4A-NA	3.14	128.85	124.51
31	B	618	BCR	C7-C8-C9	-3.14	121.50	126.23
26	6	610	CLA	C4A-NA-C1A	3.13	108.11	106.71
25	3	601	CHL	C4A-NA-C1A	-3.13	105.30	106.71
27	y	1620	LUT	C30-C31-C32	-3.13	113.44	123.22
31	d	404	BCR	C38-C26-C25	-3.13	121.01	124.53
26	B	604	CLA	C1B-CHB-C4A	-3.13	123.92	130.12
28	2	1622	XAT	C35-C34-C33	-3.13	122.84	127.31
25	y	607	CHL	CMB-C2B-C3B	3.13	130.53	124.68
26	2	602	CLA	C4A-NA-C1A	3.13	108.11	106.71
27	N	1620	LUT	C15-C14-C13	-3.13	122.85	127.31
25	3	607	CHL	CAC-C3C-C4C	3.13	128.87	124.81
26	2	610	CLA	O2D-CGD-O1D	-3.12	117.73	123.84
25	3	601	CHL	CHD-C4C-C3C	-3.12	120.25	124.84
25	7	601	CHL	CHD-C4C-C3C	-3.12	120.25	124.84
26	d	402	CLA	CHD-C1D-ND	-3.12	121.58	124.45
31	T	101	BCR	C1-C6-C7	3.12	124.61	115.78
28	7	1622	XAT	C11-C10-C9	-3.12	122.85	127.31
26	a	406	CLA	O2D-CGD-CBD	3.12	116.81	111.27
25	r	614	CHL	C1C-C2C-C3C	-3.12	104.64	107.11
25	5	606	CHL	CAC-C3C-C4C	3.12	128.86	124.81
26	S	603	CLA	O2D-CGD-O1D	-3.12	117.74	123.84
31	b	618	BCR	C7-C8-C9	-3.12	121.52	126.23
26	6	603	CLA	C1B-CHB-C4A	-3.12	123.94	130.12
26	c	502	CLA	C1B-CHB-C4A	-3.12	123.94	130.12
26	R	611	CLA	CMB-C2B-C1B	-3.12	123.67	128.46
31	t	101	BCR	C1-C6-C7	3.12	124.60	115.78
26	a	407	CLA	CHB-C4A-NA	3.12	128.82	124.51
26	Y	602	CLA	C1-C2-C3	-3.12	120.66	126.04
26	b	609	CLA	C1B-CHB-C4A	-3.11	123.95	130.12
26	b	615	CLA	O2D-CGD-CBD	3.11	116.80	111.27
26	Y	603	CLA	CHB-C4A-NA	3.11	128.82	124.51
39	c	518	DGD	C1E-O6E-C5E	3.11	119.80	113.69
26	B	609	CLA	O2D-CGD-CBD	3.11	116.80	111.27
26	R	611	CLA	CHB-C4A-NA	3.11	128.82	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	604	CLA	C1B-CHB-C4A	-3.11	123.95	130.12
26	N	602	CLA	O2D-CGD-O1D	-3.11	117.75	123.84
26	5	603	CLA	CHB-C4A-NA	3.11	128.81	124.51
26	A	405	CLA	C1B-CHB-C4A	-3.11	123.96	130.12
26	B	615	CLA	O2D-CGD-CBD	3.11	116.79	111.27
25	7	601	CHL	C1C-C2C-C3C	-3.11	104.65	107.11
25	6	609	CHL	C1C-C2C-C3C	-3.11	104.65	107.11
26	2	603	CLA	C1B-CHB-C4A	-3.11	123.96	130.12
28	r	622	XAT	C4-C3-C2	-3.11	104.77	110.77
26	s	604	CLA	C1B-CHB-C4A	-3.11	123.97	130.12
26	8	602	CLA	C1B-CHB-C4A	-3.11	123.97	130.12
26	a	405	CLA	C1B-CHB-C4A	-3.11	123.97	130.12
25	6	609	CHL	CHD-C4C-C3C	-3.10	120.28	124.84
25	Y	607	CHL	CMB-C2B-C3B	3.10	130.49	124.68
31	D	404	BCR	C38-C26-C25	-3.10	121.04	124.53
27	8	620	LUT	C30-C31-C32	-3.10	113.53	123.22
25	7	607	CHL	CAC-C3C-C4C	3.10	128.84	124.81
26	B	610	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
26	6	610	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
26	b	610	CLA	O2D-CGD-O1D	-3.10	117.77	123.84
36	b	621	SQD	C44-O6-C1	3.10	119.80	113.74
27	4	620	LUT	C30-C31-C32	-3.10	113.54	123.22
25	4	606	CHL	C3B-C4B-NB	3.10	113.22	109.21
26	s	603	CLA	O2D-CGD-O1D	-3.10	117.78	123.84
28	8	622	XAT	C24-C23-C22	-3.10	104.79	110.77
26	1	603	CLA	CHB-C4A-NA	3.10	128.80	124.51
26	g	611	CLA	CMB-C2B-C3B	3.10	130.47	124.68
36	B	621	SQD	C44-O6-C1	3.10	119.79	113.74
26	7	603	CLA	CBC-CAC-C3C	-3.10	103.89	112.43
26	G	611	CLA	CMB-C2B-C3B	3.10	130.47	124.68
26	3	603	CLA	CBC-CAC-C3C	-3.10	103.90	112.43
26	1	610	CLA	CMB-C2B-C3B	3.10	130.47	124.68
28	R	622	XAT	C4-C3-C2	-3.09	104.80	110.77
26	5	610	CLA	CMB-C2B-C3B	3.09	130.47	124.68
25	8	606	CHL	C3B-C4B-NB	3.09	113.21	109.21
26	b	609	CLA	O2D-CGD-CBD	3.09	116.76	111.27
26	B	609	CLA	C1B-CHB-C4A	-3.09	123.99	130.12
26	2	610	CLA	C4A-NA-C1A	3.09	108.10	106.71
26	Y	612	CLA	CMB-C2B-C1B	-3.09	123.71	128.46
26	g	613	CLA	CMB-C2B-C3B	3.09	130.46	124.68
27	R	620	LUT	C39-C29-C28	3.09	122.95	118.08
26	n	602	CLA	O2D-CGD-O1D	-3.09	117.80	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	R	614	CHL	C1C-C2C-C3C	-3.09	104.66	107.11
26	4	602	CLA	C1B-CHB-C4A	-3.09	124.00	130.12
25	Y	609	CHL	CMB-C2B-C3B	3.09	130.46	124.68
26	S	604	CLA	C1B-CHB-C4A	-3.09	124.00	130.12
31	8	623	BCR	C11-C12-C13	-3.09	117.74	126.42
27	r	620	LUT	C39-C29-C28	3.09	122.94	118.08
25	2	609	CHL	C1C-C2C-C3C	-3.09	104.66	107.11
27	S	1620	LUT	C10-C11-C12	-3.09	113.59	123.22
26	1	614	CLA	C1B-CHB-C4A	-3.08	124.02	130.12
25	r	606	CHL	O2A-CGA-CBA	3.08	121.58	111.91
26	b	608	CLA	CHB-C4A-NA	3.08	128.77	124.51
25	s	601	CHL	CHD-C4C-C3C	-3.08	120.31	124.84
31	4	623	BCR	C11-C12-C13	-3.08	117.76	126.42
31	b	618	BCR	C15-C16-C17	-3.08	117.17	123.47
25	4	608	CHL	C3B-C4B-NB	3.08	113.19	109.21
25	1	609	CHL	CHD-C4C-C3C	-3.08	120.32	124.84
31	B	618	BCR	C15-C16-C17	-3.08	117.17	123.47
25	8	608	CHL	C3B-C4B-NB	3.08	113.19	109.21
31	b	620	BCR	C4-C5-C6	-3.08	118.27	122.73
26	G	613	CLA	CMB-C2B-C3B	3.08	130.43	124.68
25	S	601	CHL	CHD-C4C-C3C	-3.08	120.32	124.84
25	S	601	CHL	C3B-C4B-NB	3.08	113.19	109.21
25	S	601	CHL	CMB-C2B-C3B	3.07	130.43	124.68
25	s	601	CHL	CMB-C2B-C3B	3.07	130.43	124.68
26	s	609	CLA	C4A-NA-C1A	3.07	108.09	106.71
27	s	1620	LUT	C10-C11-C12	-3.07	113.62	123.22
26	y	613	CLA	O2D-CGD-CBD	3.07	116.73	111.27
26	A	405	CLA	CHB-C4A-NA	3.07	128.76	124.51
28	4	622	XAT	C24-C23-C22	-3.07	104.84	110.77
26	r	611	CLA	CHB-C4A-NA	3.07	128.76	124.51
26	Y	610	CLA	C4A-NA-C1A	3.07	108.09	106.71
26	2	604	CLA	C1B-CHB-C4A	-3.07	124.03	130.12
25	R	606	CHL	O2A-CGA-CBA	3.07	121.55	111.91
25	2	609	CHL	CHD-C4C-C3C	-3.07	120.33	124.84
25	y	609	CHL	CMB-C2B-C3B	3.07	130.42	124.68
26	1	611	CLA	C1B-CHB-C4A	-3.07	124.04	130.12
26	5	611	CLA	C1B-CHB-C4A	-3.07	124.04	130.12
26	Y	613	CLA	O2D-CGD-CBD	3.07	116.72	111.27
36	A	418	SQD	O6-C1-C2	3.07	113.09	108.30
31	H	101	BCR	C20-C21-C22	-3.07	122.93	127.31
36	a	418	SQD	O6-C1-C2	3.07	113.09	108.30
26	N	611	CLA	CMB-C2B-C1B	-3.07	123.75	128.46

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	n	611	CLA	CMB-C2B-C1B	-3.07	123.75	128.46
31	h	101	BCR	C20-C21-C22	-3.07	122.93	127.31
26	c	506	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
26	C	506	CLA	C1B-CHB-C4A	-3.06	124.05	130.12
26	y	612	CLA	CMB-C2B-C1B	-3.06	123.75	128.46
26	3	604	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
26	1	613	CLA	CMB-C2B-C3B	3.06	130.40	124.68
26	5	613	CLA	CMB-C2B-C3B	3.06	130.40	124.68
25	S	608	CHL	CMD-C2D-C3D	-3.06	120.58	127.61
26	R	611	CLA	C2C-C1C-NC	3.06	112.84	109.97
28	Y	1622	XAT	C24-C23-C22	-3.06	104.86	110.77
25	s	601	CHL	C3B-C4B-NB	3.06	113.16	109.21
26	a	405	CLA	CHB-C4A-NA	3.06	128.74	124.51
26	B	611	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
31	B	620	BCR	C4-C5-C6	-3.06	118.29	122.73
31	b	618	BCR	C21-C20-C19	-3.06	113.68	123.22
26	5	614	CLA	C1B-CHB-C4A	-3.06	124.06	130.12
26	B	608	CLA	CHB-C4A-NA	3.06	128.74	124.51
25	R	608	CHL	CMD-C2D-C3D	-3.05	120.59	127.61
31	B	618	BCR	C21-C20-C19	-3.05	113.69	123.22
26	r	611	CLA	C2C-C1C-NC	3.05	112.83	109.97
26	6	604	CLA	C1B-CHB-C4A	-3.05	124.07	130.12
25	y	609	CHL	C4-C3-C5	3.05	120.41	115.27
26	B	616	CLA	CHB-C4A-NA	3.05	128.73	124.51
26	b	616	CLA	CHB-C4A-NA	3.05	128.73	124.51
27	g	1621	LUT	C18-C5-C6	-3.05	121.10	124.53
25	s	608	CHL	CMD-C2D-C3D	-3.05	120.60	127.61
26	7	604	CLA	C1B-CHB-C4A	-3.05	124.08	130.12
31	d	404	BCR	C15-C14-C13	-3.05	122.96	127.31
25	r	608	CHL	CMD-C2D-C3D	-3.05	120.60	127.61
26	s	611	CLA	O2D-CGD-O1D	-3.05	117.88	123.84
26	2	610	CLA	CMB-C2B-C3B	3.05	130.38	124.68
31	c	517	BCR	C21-C20-C19	-3.05	113.71	123.22
26	2	602	CLA	C1B-CHB-C4A	-3.05	124.09	130.12
26	6	602	CLA	C1B-CHB-C4A	-3.05	124.09	130.12
36	a	418	SQD	C4-C3-C2	3.05	116.14	110.82
26	y	614	CLA	O2D-CGD-CBD	3.05	116.68	111.27
25	5	609	CHL	CHD-C4C-C3C	-3.04	120.36	124.84
31	a	411	BCR	C16-C15-C14	-3.04	117.24	123.47
36	A	418	SQD	C4-C3-C2	3.04	116.13	110.82
35	A	408	PHO	CAA-CBA-CGA	-3.04	104.36	113.25
29	S	1623	NEX	C31-C30-C29	-3.04	122.97	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	1	1623	NEX	C24-C23-C22	-3.04	104.90	110.77
31	D	404	BCR	C15-C14-C13	-3.04	122.97	127.31
28	y	1622	XAT	C24-C23-C22	-3.04	104.90	110.77
35	a	408	PHO	CAA-CBA-CGA	-3.04	104.37	113.25
27	G	1621	LUT	C18-C5-C6	-3.04	121.11	124.53
25	g	606	CHL	C3B-C4B-NB	3.04	113.14	109.21
26	b	609	CLA	CHB-C4A-NA	3.04	128.71	124.51
27	s	1621	LUT	C17-C1-C6	3.04	115.22	110.30
31	C	517	BCR	C21-C20-C19	-3.04	113.74	123.22
26	Y	614	CLA	O2D-CGD-CBD	3.04	116.66	111.27
26	b	611	CLA	C1B-CHB-C4A	-3.04	124.11	130.12
29	s	1623	NEX	C31-C30-C29	-3.03	122.98	127.31
31	A	411	BCR	C16-C15-C14	-3.03	117.26	123.47
29	Y	1623	NEX	C5-C4-C3	-3.03	108.15	111.75
29	y	1623	NEX	C5-C4-C3	-3.03	108.15	111.75
25	G	606	CHL	C3B-C4B-NB	3.03	113.13	109.21
27	4	620	LUT	C8-C7-C6	-3.03	118.68	127.20
25	Y	609	CHL	C4-C3-C5	3.03	120.37	115.27
25	N	601	CHL	C1-C2-C3	-3.03	120.80	126.04
25	2	601	CHL	C4A-NA-C1A	-3.03	105.34	106.71
26	y	610	CLA	C4A-NA-C1A	3.03	108.07	106.71
25	2	601	CHL	CHD-C4C-C3C	-3.03	120.39	124.84
25	r	614	CHL	CMD-C2D-C3D	-3.03	120.64	127.61
25	G	608	CHL	C1-C2-C3	-3.03	120.80	126.04
25	R	614	CHL	CMD-C2D-C3D	-3.03	120.65	127.61
28	3	1622	XAT	C31-C32-C33	-3.03	117.91	126.42
25	n	601	CHL	C1-C2-C3	-3.03	120.81	126.04
27	8	620	LUT	C8-C7-C6	-3.03	118.71	127.20
26	S	611	CLA	O2D-CGD-O1D	-3.02	117.93	123.84
26	a	406	CLA	CAC-C3C-C4C	-3.02	120.89	124.81
27	n	1620	LUT	C30-C31-C32	-3.02	113.78	123.22
25	N	601	CHL	CHD-C4C-C3C	-3.02	120.40	124.84
25	Y	608	CHL	O2A-CGA-CBA	3.02	121.39	111.91
25	y	608	CHL	O2A-CGA-CBA	3.02	121.39	111.91
27	N	1620	LUT	C30-C31-C32	-3.02	113.79	123.22
25	y	605	CHL	CAC-C3C-C4C	3.02	128.73	124.81
26	Y	603	CLA	CMB-C2B-C3B	3.02	130.33	124.68
25	g	608	CHL	C1-C2-C3	-3.02	120.82	126.04
26	R	604	CLA	CAA-C2A-C3A	-3.02	104.51	112.78
25	n	601	CHL	CHD-C4C-C3C	-3.02	120.40	124.84
26	4	612	CLA	CMB-C2B-C3B	3.02	130.33	124.68
26	7	612	CLA	CMB-C2B-C3B	3.02	130.33	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	6	610	CLA	CMB-C2B-C3B	3.02	130.33	124.68
27	r	620	LUT	C28-C29-C30	-3.02	114.31	118.94
27	S	1621	LUT	C17-C1-C6	3.02	115.19	110.30
26	B	606	CLA	C1-C2-C3	-3.02	120.82	126.04
26	r	604	CLA	CAA-C2A-C3A	-3.02	104.52	112.78
29	5	1623	NEX	C24-C23-C22	-3.02	104.95	110.77
26	C	505	CLA	CMB-C2B-C3B	3.02	130.32	124.68
26	g	611	CLA	CHB-C4A-NA	3.02	128.68	124.51
25	6	601	CHL	CHD-C4C-C3C	-3.01	120.41	124.84
26	b	606	CLA	C1-C2-C3	-3.01	120.83	126.04
39	B	626	DGD	CDB-CCB-CBB	-3.01	99.12	114.42
28	7	1622	XAT	C31-C32-C33	-3.01	117.95	126.42
39	b	626	DGD	CDB-CCB-CBB	-3.01	99.13	114.42
31	b	618	BCR	C20-C21-C22	-3.01	123.01	127.31
26	6	604	CLA	CMB-C2B-C3B	3.01	130.31	124.68
41	f	101	HEM	CMC-C2C-C3C	3.01	130.31	124.68
26	G	611	CLA	CHB-C4A-NA	3.01	128.67	124.51
26	2	604	CLA	CMB-C2B-C3B	3.01	130.31	124.68
26	G	613	CLA	O2D-CGD-CBD	3.01	116.62	111.27
25	r	614	CHL	C1B-CHB-C4A	-3.01	124.16	130.12
26	c	505	CLA	CMB-C2B-C3B	3.01	130.31	124.68
26	B	609	CLA	CHB-C4A-NA	3.01	128.67	124.51
41	F	101	HEM	CMC-C2C-C3C	3.01	130.31	124.68
26	c	511	CLA	O2D-CGD-O1D	-3.01	117.96	123.84
26	y	603	CLA	CMB-C2B-C3B	3.01	130.30	124.68
26	4	611	CLA	C1B-CHB-C4A	-3.01	124.17	130.12
26	8	611	CLA	C1B-CHB-C4A	-3.01	124.17	130.12
26	R	613	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
26	6	614	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
26	G	603	CLA	C1B-CHB-C4A	-3.00	124.17	130.12
26	c	512	CLA	O2D-CGD-CBD	3.00	116.61	111.27
25	S	608	CHL	CAC-C3C-C4C	3.00	128.71	124.81
27	Y	1620	LUT	C35-C34-C33	-3.00	123.02	127.31
26	A	406	CLA	CAC-C3C-C4C	-3.00	120.91	124.81
26	6	613	CLA	CMB-C2B-C3B	3.00	130.30	124.68
26	8	612	CLA	CMB-C2B-C3B	3.00	130.30	124.68
26	C	511	CLA	O2D-CGD-O1D	-3.00	117.97	123.84
25	R	614	CHL	C1B-CHB-C4A	-3.00	124.17	130.12
26	3	612	CLA	CMB-C2B-C3B	3.00	130.29	124.68
27	y	1620	LUT	C35-C34-C33	-3.00	123.03	127.31
25	G	606	CHL	CMD-C2D-C3D	-3.00	120.72	127.61
26	r	613	CLA	C1B-CHB-C4A	-3.00	124.18	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	2	601	CHL	C4D-CHA-C1A	-3.00	117.60	121.25
26	2	613	CLA	CMB-C2B-C3B	3.00	130.28	124.68
26	g	604	CLA	O2D-CGD-O1D	-2.99	117.98	123.84
27	R	620	LUT	C28-C29-C30	-2.99	114.35	118.94
25	R	607	CHL	CMD-C2D-C3D	-2.99	120.73	127.61
25	r	607	CHL	CMD-C2D-C3D	-2.99	120.73	127.61
26	C	509	CLA	C2D-C1D-ND	-2.99	107.90	110.10
27	G	1621	LUT	C30-C31-C32	-2.99	113.88	123.22
25	s	608	CHL	CAC-C3C-C4C	2.99	128.69	124.81
31	B	619	BCR	C15-C16-C17	-2.99	117.35	123.47
26	2	614	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
27	N	1620	LUT	C38-C25-C24	-2.99	117.17	123.56
31	b	619	BCR	C15-C16-C17	-2.99	117.36	123.47
25	g	606	CHL	CMD-C2D-C3D	-2.99	120.74	127.61
26	R	611	CLA	C1B-CHB-C4A	-2.99	124.20	130.12
26	C	512	CLA	O2D-CGD-CBD	2.99	116.57	111.27
25	6	601	CHL	C4D-CHA-C1A	-2.98	117.62	121.25
26	y	612	CLA	O2D-CGD-O1D	-2.98	118.00	123.84
26	g	613	CLA	O2D-CGD-CBD	2.98	116.57	111.27
25	Y	605	CHL	CAC-C3C-C4C	2.98	128.68	124.81
31	A	411	BCR	C38-C26-C25	-2.98	121.18	124.53
26	R	604	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
26	g	604	CLA	C1-C2-C3	-2.98	121.93	126.75
26	g	613	CLA	C1B-CHB-C4A	-2.98	124.21	130.12
25	r	614	CHL	O2D-CGD-O1D	-2.98	118.01	123.84
26	g	603	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
26	Y	612	CLA	O2D-CGD-O1D	-2.98	118.01	123.84
31	B	618	BCR	C20-C21-C22	-2.98	123.06	127.31
26	G	604	CLA	C1-C2-C3	-2.98	121.94	126.75
29	R	623	NEX	C38-C25-C24	2.98	117.63	114.28
29	r	623	NEX	C38-C25-C24	2.98	117.63	114.28
26	r	604	CLA	O2D-CGD-O1D	-2.98	118.02	123.84
27	S	1621	LUT	C19-C9-C8	2.98	122.77	118.08
36	B	623	SQD	C44-O6-C1	2.98	119.55	113.74
26	y	614	CLA	C1B-CHB-C4A	-2.98	124.22	130.12
26	G	604	CLA	O2D-CGD-O1D	-2.97	118.02	123.84
26	G	613	CLA	C1B-CHB-C4A	-2.97	124.23	130.12
27	s	1621	LUT	C19-C9-C8	2.97	122.76	118.08
27	S	1620	LUT	C30-C31-C32	-2.97	113.94	123.22
27	s	1620	LUT	C30-C31-C32	-2.97	113.94	123.22
26	l	612	CLA	CMB-C2B-C3B	2.97	130.24	124.68
27	g	1621	LUT	C30-C31-C32	-2.97	113.94	123.22

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	n	1621	LUT	C21-C26-C27	-2.97	108.94	112.70
25	R	614	CHL	O2D-CGD-O1D	-2.97	118.03	123.84
25	Y	606	CHL	O2D-CGD-O1D	-2.97	118.03	123.84
25	y	606	CHL	O2D-CGD-O1D	-2.97	118.03	123.84
26	3	603	CLA	CMB-C2B-C3B	2.97	130.23	124.68
31	a	411	BCR	C38-C26-C25	-2.97	121.19	124.53
25	G	601	CHL	CAC-C3C-C4C	2.97	128.66	124.81
25	g	601	CHL	CAC-C3C-C4C	2.97	128.66	124.81
36	b	623	SQD	C44-O6-C1	2.97	119.54	113.74
27	2	1620	LUT	C10-C11-C12	-2.97	113.96	123.22
26	A	407	CLA	O2D-CGD-O1D	-2.97	118.04	123.84
37	C	521	LMG	C1-C2-C3	-2.96	103.82	110.00
26	Y	614	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
25	6	606	CHL	CAC-C3C-C4C	2.96	128.65	124.81
26	1	602	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
25	n	609	CHL	C4-C3-C5	2.96	120.25	115.27
26	1	604	CLA	O2D-CGD-O1D	-2.96	118.05	123.84
26	n	603	CLA	C1B-CHB-C4A	-2.96	124.25	130.12
27	6	1620	LUT	C10-C11-C12	-2.96	113.98	123.22
26	5	612	CLA	CMB-C2B-C3B	2.96	130.22	124.68
26	5	602	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
26	A	410	CLA	CHB-C4A-NA	2.96	128.60	124.51
27	7	1621	LUT	C35-C34-C33	-2.96	123.09	127.31
26	r	611	CLA	C1B-CHB-C4A	-2.96	124.26	130.12
26	N	614	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
26	n	614	CLA	O2D-CGD-O1D	-2.96	118.06	123.84
25	g	607	CHL	CHB-C4A-NA	2.95	128.60	124.51
25	Y	605	CHL	C3B-C4B-NB	2.95	113.03	109.21
28	2	1622	XAT	C6-C7-C8	-2.95	119.75	125.99
27	n	1620	LUT	C38-C25-C24	-2.95	117.24	123.56
25	2	606	CHL	CAC-C3C-C4C	2.95	128.64	124.81
25	n	609	CHL	C1-O2A-CGA	2.95	124.19	116.44
26	a	410	CLA	CHB-C4A-NA	2.95	128.59	124.51
26	N	603	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
26	5	604	CLA	O2D-CGD-O1D	-2.95	118.07	123.84
26	b	607	CLA	CHB-C4A-NA	2.95	128.59	124.51
26	a	407	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
27	g	1620	LUT	C35-C15-C14	-2.95	117.44	123.47
26	B	603	CLA	C1B-CHB-C4A	-2.95	124.28	130.12
39	B	626	DGD	O5D-C1E-C2E	2.95	112.90	108.30
27	G	1620	LUT	C35-C15-C14	-2.95	117.44	123.47
26	S	602	CLA	C1B-CHB-C4A	-2.95	124.28	130.12

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	C	506	CLA	O2D-CGD-O1D	-2.95	118.08	123.84
25	N	609	CHL	C1-O2A-CGA	2.94	124.17	116.44
37	c	521	LMG	C1-C2-C3	-2.94	103.86	110.00
25	N	609	CHL	C4-C3-C5	2.94	120.22	115.27
39	b	626	DGD	O5D-C1E-C2E	2.94	112.90	108.30
26	b	603	CLA	C1B-CHB-C4A	-2.94	124.29	130.12
26	c	509	CLA	C2D-C1D-ND	-2.94	107.94	110.10
26	8	611	CLA	CMB-C2B-C3B	2.94	130.18	124.68
26	B	613	CLA	CMA-C3A-C4A	-2.94	103.87	111.77
27	Y	1620	LUT	C39-C29-C28	2.94	122.71	118.08
26	7	603	CLA	CMB-C2B-C3B	2.94	130.18	124.68
26	s	602	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
26	Y	602	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
26	5	611	CLA	CMB-C2B-C3B	2.94	130.17	124.68
26	B	607	CLA	CHB-C4A-NA	2.94	128.57	124.51
26	b	605	CLA	CMB-C2B-C1B	-2.94	123.95	128.46
26	b	610	CLA	C1B-CHB-C4A	-2.94	124.30	130.12
26	A	406	CLA	CHB-C4A-NA	2.94	128.57	124.51
38	a	414	PL9	C7-C3-C4	2.94	121.79	118.08
30	d	410	LHG	O8-C23-C24	2.94	121.12	111.91
27	5	1621	LUT	C18-C5-C6	-2.93	121.23	124.53
28	1	1622	XAT	C31-C32-C33	-2.93	118.17	126.42
25	G	601	CHL	C4D-CHA-C1A	-2.93	117.68	121.25
25	g	601	CHL	C4D-CHA-C1A	-2.93	117.68	121.25
26	5	614	CLA	O2D-CGD-O1D	-2.93	118.10	123.84
26	a	406	CLA	CHB-C4A-NA	2.93	128.57	124.51
26	b	613	CLA	CMA-C3A-C4A	-2.93	103.89	111.77
26	b	613	CLA	CMD-C2D-C3D	2.93	134.36	127.61
27	2	1621	LUT	C10-C11-C12	-2.93	114.07	123.22
27	s	1620	LUT	C21-C26-C27	-2.93	109.00	112.70
28	5	1622	XAT	C31-C32-C33	-2.93	118.18	126.42
27	N	1621	LUT	C21-C26-C27	-2.93	109.00	112.70
25	G	607	CHL	CHB-C4A-NA	2.93	128.56	124.51
26	1	611	CLA	CMB-C2B-C3B	2.93	130.16	124.68
28	6	1622	XAT	C6-C7-C8	-2.93	119.80	125.99
26	1	614	CLA	O2D-CGD-O1D	-2.93	118.11	123.84
35	a	409	PHO	O2D-CGD-O1D	-2.93	118.11	123.84
26	S	611	CLA	CMB-C2B-C3B	2.93	130.16	124.68
31	C	516	BCR	C10-C11-C12	-2.93	114.08	123.22
26	C	504	CLA	O2D-CGD-CBD	2.93	116.47	111.27
30	D	408	LHG	O8-C23-C24	2.93	121.10	111.91
26	B	602	CLA	O2D-CGD-O1D	-2.93	118.11	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
31	c	516	BCR	C10-C11-C12	-2.93	114.08	123.22
26	y	602	CLA	C1B-CHB-C4A	-2.93	124.32	130.12
26	B	615	CLA	CMB-C2B-C3B	2.93	130.15	124.68
26	c	505	CLA	CGD-CBD-CAD	2.93	120.21	110.73
30	d	408	LHG	O8-C23-C24	2.93	121.09	111.91
25	y	605	CHL	C3B-C4B-NB	2.92	112.99	109.21
26	B	606	CLA	CHB-C4A-NA	2.92	128.56	124.51
39	h	102	DGD	O6D-C1D-O3G	-2.92	103.05	109.97
26	c	506	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
26	g	612	CLA	O2D-CGD-O1D	-2.92	118.12	123.84
26	n	614	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
27	3	1621	LUT	C35-C34-C33	-2.92	123.14	127.31
26	B	617	CLA	O2D-CGD-CBD	2.92	116.46	111.27
26	3	611	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
25	G	609	CHL	C1-O2A-CGA	2.92	124.11	116.44
26	S	610	CLA	CHB-C4A-NA	2.92	128.55	124.51
26	C	505	CLA	CGD-CBD-CAD	2.92	120.19	110.73
37	B	2633	LMG	O2-C2-C1	-2.92	102.95	110.05
26	R	602	CLA	C1B-CHB-C4A	-2.92	124.33	130.12
26	s	611	CLA	CMB-C2B-C3B	2.92	130.14	124.68
39	H	102	DGD	O6D-C1D-O3G	-2.92	103.06	109.97
26	C	502	CLA	CMB-C2B-C3B	2.92	130.14	124.68
26	C	504	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
26	G	614	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
26	c	504	CLA	O2D-CGD-CBD	2.92	116.45	111.27
27	S	1620	LUT	C11-C10-C9	-2.92	123.14	127.31
30	D	410	LHG	O8-C23-C24	2.92	121.06	111.91
26	c	504	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
27	7	1621	LUT	C10-C11-C12	-2.92	114.11	123.22
27	s	1620	LUT	C11-C10-C9	-2.92	123.15	127.31
26	5	612	CLA	O2D-CGD-O1D	-2.92	118.13	123.84
31	c	516	BCR	C16-C15-C14	-2.92	117.50	123.47
26	b	606	CLA	CHB-C4A-NA	2.92	128.55	124.51
26	N	614	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
28	2	1622	XAT	O24-C25-C38	2.92	118.55	115.06
26	Y	613	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
26	B	610	CLA	C1B-CHB-C4A	-2.92	124.34	130.12
26	b	602	CLA	O2D-CGD-O1D	-2.92	118.14	123.84
27	6	1621	LUT	C10-C11-C12	-2.91	114.12	123.22
25	8	607	CHL	CHD-C4C-C3C	-2.91	120.56	124.84
26	s	604	CLA	O2D-CGD-O1D	-2.91	118.14	123.84
37	b	2633	LMG	O2-C2-C1	-2.91	102.97	110.05

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	y	613	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
25	7	606	CHL	OMC-CMC-C2C	-2.91	119.10	125.69
26	G	602	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
26	8	610	CLA	CMB-C2B-C3B	2.91	130.13	124.68
26	c	503	CLA	CHB-C4A-NA	2.91	128.54	124.51
26	4	611	CLA	CMB-C2B-C3B	2.91	130.12	124.68
26	B	605	CLA	C1-C2-C3	-2.91	121.01	126.04
26	7	611	CLA	C1B-CHB-C4A	-2.91	124.35	130.12
26	8	612	CLA	CHB-C4A-NA	2.91	128.54	124.51
27	G	1620	LUT	C38-C25-C24	-2.91	117.33	123.56
25	3	606	CHL	OMC-CMC-C2C	-2.91	119.11	125.69
31	c	517	BCR	C20-C21-C22	-2.91	123.16	127.31
26	c	510	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
31	8	623	BCR	C3-C4-C5	-2.91	108.88	114.08
28	6	1622	XAT	O24-C25-C38	2.91	118.54	115.06
26	r	602	CLA	C1B-CHB-C4A	-2.91	124.36	130.12
26	b	617	CLA	O2D-CGD-CBD	2.91	116.44	111.27
26	G	612	CLA	O2D-CGD-O1D	-2.91	118.15	123.84
26	B	613	CLA	CMD-C2D-C3D	2.91	134.30	127.61
26	s	610	CLA	CHB-C4A-NA	2.91	128.53	124.51
31	b	619	BCR	C24-C23-C22	-2.91	121.84	126.23
26	R	601	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
31	C	516	BCR	C16-C15-C14	-2.91	117.52	123.47
26	r	601	CLA	O2D-CGD-O1D	-2.91	118.16	123.84
28	N	1622	XAT	C24-C23-C22	-2.90	105.16	110.77
28	n	1622	XAT	C24-C23-C22	-2.90	105.16	110.77
26	d	402	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
26	g	614	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
35	A	409	PHO	O2D-CGD-O1D	-2.90	118.16	123.84
25	N	601	CHL	CHB-C4A-NA	2.90	128.53	124.51
25	S	601	CHL	CHB-C4A-NA	2.90	128.53	124.51
38	a	414	PL9	O2-C1-C2	-2.90	117.26	121.41
25	g	609	CHL	C1-O2A-CGA	2.90	124.06	116.44
26	S	604	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
26	b	605	CLA	C1-C2-C3	-2.90	121.02	126.04
25	4	606	CHL	CAC-C3C-C4C	2.90	128.58	124.81
26	g	602	CLA	CAC-C3C-C4C	2.90	128.58	124.81
27	3	1621	LUT	C10-C11-C12	-2.90	114.16	123.22
26	1	612	CLA	O2D-CGD-O1D	-2.90	118.16	123.84
26	g	610	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
28	1	1622	XAT	C4-C3-C2	-2.90	105.17	110.77
27	y	1620	LUT	C39-C29-C28	2.90	122.64	118.08

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	605	CLA	CMB-C2B-C1B	-2.90	124.01	128.46
38	A	414	PL9	O2-C1-C2	-2.90	117.26	121.41
29	5	1623	NEX	C26-C27-C28	-2.90	119.86	125.99
25	8	606	CHL	CAC-C3C-C4C	2.90	128.57	124.81
31	B	619	BCR	C24-C23-C22	-2.90	121.86	126.23
38	A	414	PL9	C7-C3-C4	2.90	121.74	118.08
26	r	609	CLA	CMB-C2B-C3B	2.90	130.10	124.68
29	s	1623	NEX	C24-C23-C22	-2.90	105.18	110.77
29	1	1623	NEX	C26-C27-C28	-2.90	119.87	125.99
26	C	510	CLA	O2D-CGD-O1D	-2.90	118.17	123.84
31	C	517	BCR	C20-C21-C22	-2.90	123.18	127.31
27	g	1620	LUT	C38-C25-C24	-2.90	117.36	123.56
28	4	622	XAT	C10-C11-C12	-2.90	114.18	123.22
35	a	409	PHO	O1D-CGD-CBD	2.90	129.56	124.74
26	g	602	CLA	C1B-CHB-C4A	-2.90	124.38	130.12
31	4	623	BCR	C3-C4-C5	-2.90	108.91	114.08
26	4	610	CLA	CMB-C2B-C3B	2.89	130.09	124.68
26	r	604	CLA	CHB-C4A-NA	2.89	128.51	124.51
26	G	610	CLA	O2D-CGD-O1D	-2.89	118.18	123.84
29	S	1623	NEX	C24-C23-C22	-2.89	105.19	110.77
26	c	502	CLA	CMB-C2B-C3B	2.89	130.09	124.68
27	S	1620	LUT	C21-C26-C27	-2.89	109.05	112.70
26	b	615	CLA	CMB-C2B-C3B	2.89	130.09	124.68
31	T	101	BCR	C11-C12-C13	-2.89	118.29	126.42
26	2	612	CLA	C1B-CHB-C4A	-2.89	124.39	130.12
31	B	618	BCR	C11-C10-C9	-2.89	123.18	127.31
25	N	601	CHL	O2D-CGD-O1D	-2.89	118.19	123.84
25	5	609	CHL	CMD-C2D-C3D	-2.89	120.96	127.61
27	1	1621	LUT	C18-C5-C6	-2.89	121.28	124.53
25	4	607	CHL	CHD-C4C-C3C	-2.89	120.59	124.84
28	6	1622	XAT	O4-C5-C18	2.89	118.52	115.06
28	R	622	XAT	C19-C9-C8	2.89	122.63	118.08
31	t	101	BCR	C11-C12-C13	-2.89	118.30	126.42
28	5	1622	XAT	C4-C3-C2	-2.89	105.20	110.77
25	4	609	CHL	CMD-C2D-C3D	-2.89	120.97	127.61
25	8	609	CHL	CMD-C2D-C3D	-2.89	120.97	127.61
28	8	622	XAT	C10-C11-C12	-2.89	114.21	123.22
26	g	603	CLA	CMB-C2B-C3B	2.89	130.08	124.68
25	s	601	CHL	CHB-C4A-NA	2.89	128.50	124.51
27	8	620	LUT	C31-C30-C29	-2.88	123.19	127.31
26	G	602	CLA	CAC-C3C-C4C	2.88	128.55	124.81
26	C	503	CLA	CHB-C4A-NA	2.88	128.50	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	G	603	CLA	CBC-CAC-C3C	-2.88	104.49	112.43
26	b	608	CLA	O2D-CGD-O1D	-2.88	118.20	123.84
26	R	609	CLA	CMB-C2B-C3B	2.88	130.07	124.68
26	g	603	CLA	CBC-CAC-C3C	-2.88	104.49	112.43
27	1	1621	LUT	C22-C23-C24	-2.88	108.46	111.74
25	1	609	CHL	CMD-C2D-C3D	-2.88	120.99	127.61
25	3	609	CHL	CMD-C2D-C3D	-2.88	120.99	127.61
26	6	612	CLA	C1B-CHB-C4A	-2.88	124.42	130.12
25	n	601	CHL	CHB-C4A-NA	2.88	128.49	124.51
25	G	605	CHL	CMD-C2D-C3D	-2.88	121.00	127.61
27	S	1621	LUT	C8-C9-C10	-2.88	114.53	118.94
26	B	608	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
26	G	603	CLA	CMB-C2B-C3B	2.87	130.06	124.68
28	4	622	XAT	C38-C25-C24	2.87	117.51	114.28
26	n	613	CLA	CHB-C4A-NA	2.87	128.49	124.51
25	n	601	CHL	O2D-CGD-O1D	-2.87	118.22	123.84
26	R	604	CLA	CHB-C4A-NA	2.87	128.49	124.51
27	g	1620	LUT	C30-C31-C32	-2.87	114.25	123.22
26	7	603	CLA	C1B-CHB-C4A	-2.87	124.43	130.12
27	s	1621	LUT	C8-C9-C10	-2.87	114.53	118.94
27	G	1620	LUT	C30-C31-C32	-2.87	114.25	123.22
26	D	402	CLA	O2D-CGD-O1D	-2.87	118.22	123.84
29	g	1623	NEX	C39-C29-C30	-2.87	118.91	122.92
30	c	523	LHG	O8-C23-C24	2.87	120.90	111.91
25	2	606	CHL	CMD-C2D-C3D	-2.87	121.02	127.61
35	A	409	PHO	O1D-CGD-CBD	2.87	129.51	124.74
27	5	1621	LUT	C22-C23-C24	-2.87	108.48	111.74
28	8	622	XAT	C38-C25-C24	2.86	117.50	114.28
28	r	622	XAT	C19-C9-C8	2.86	122.59	118.08
26	A	407	CLA	CHD-C1D-ND	-2.86	121.82	124.45
25	G	607	CHL	CMB-C2B-C3B	2.86	130.03	124.68
25	g	605	CHL	CMD-C2D-C3D	-2.86	121.03	127.61
26	2	603	CLA	CMB-C2B-C3B	2.86	130.03	124.68
25	7	609	CHL	CMD-C2D-C3D	-2.86	121.03	127.61
31	c	517	BCR	C33-C5-C4	2.86	119.11	113.62
26	4	612	CLA	CHB-C4A-NA	2.86	128.47	124.51
25	5	606	CHL	CMB-C2B-C3B	2.86	130.03	124.68
30	C	523	LHG	O8-C23-C24	2.86	120.88	111.91
26	a	407	CLA	CHD-C1D-ND	-2.86	121.83	124.45
25	7	607	CHL	CMD-C2D-C3D	-2.86	121.04	127.61
26	6	603	CLA	CMB-C2B-C3B	2.86	130.02	124.68
25	4	601	CHL	CAC-C3C-C4C	2.86	128.52	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	8	603	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
26	s	613	CLA	O2D-CGD-O1D	-2.86	118.25	123.84
26	4	603	CLA	C1B-CHB-C4A	-2.86	124.46	130.12
26	R	611	CLA	CMB-C2B-C3B	2.85	130.02	124.68
26	S	602	CLA	CMD-C2D-C1D	-2.85	119.68	124.71
28	2	1622	XAT	O4-C5-C18	2.85	118.48	115.06
26	n	602	CLA	CAC-C3C-C4C	2.85	128.51	124.81
29	r	623	NEX	O24-C25-C38	2.85	118.47	115.06
26	B	602	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
26	b	602	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
26	S	612	CLA	O2D-CGD-O1D	-2.85	118.26	123.84
29	G	1623	NEX	C39-C29-C30	-2.85	118.93	122.92
27	4	620	LUT	C31-C30-C29	-2.85	123.24	127.31
26	8	604	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
26	3	614	CLA	C1B-CHB-C4A	-2.85	124.47	130.12
26	b	617	CLA	CHB-C4A-NA	2.85	128.45	124.51
26	s	612	CLA	O2D-CGD-O1D	-2.85	118.27	123.84
27	3	1621	LUT	C22-C23-C24	-2.85	108.50	111.74
30	D	409	LHG	O8-C23-C24	2.85	120.84	111.91
36	b	623	SQD	O48-C23-C24	2.85	120.84	111.91
25	1	606	CHL	CMB-C2B-C3B	2.85	130.00	124.68
25	4	607	CHL	C1C-C2C-C3C	-2.85	104.86	107.11
25	5	609	CHL	C1B-CHB-C4A	-2.85	124.48	130.12
26	3	603	CLA	C1B-CHB-C4A	-2.85	124.48	130.12
25	3	607	CHL	CMD-C2D-C3D	-2.85	121.07	127.61
31	b	618	BCR	C11-C10-C9	-2.85	123.25	127.31
36	B	623	SQD	O48-C23-C24	2.85	120.84	111.91
25	g	607	CHL	CMB-C2B-C3B	2.84	130.00	124.68
30	d	409	LHG	O8-C23-C24	2.84	120.83	111.91
27	2	1620	LUT	C15-C14-C13	-2.84	123.25	127.31
25	y	608	CHL	CMD-C2D-C3D	-2.84	121.08	127.61
26	s	602	CLA	CMD-C2D-C1D	-2.84	119.70	124.71
25	6	606	CHL	CMD-C2D-C3D	-2.84	121.08	127.61
36	a	418	SQD	O8-S-C6	2.84	110.27	105.74
26	6	613	CLA	O2D-CGD-O1D	-2.84	118.28	123.84
26	7	614	CLA	C1B-CHB-C4A	-2.84	124.49	130.12
25	7	606	CHL	CMB-C2B-C3B	2.84	129.99	124.68
25	8	601	CHL	CAC-C3C-C4C	2.84	128.50	124.81
26	C	509	CLA	CAA-C2A-C3A	-2.84	105.00	112.78
27	Y	1621	LUT	C10-C11-C12	-2.84	114.36	123.22
26	r	611	CLA	CMB-C2B-C3B	2.84	129.99	124.68
26	2	602	CLA	O2D-CGD-O1D	-2.84	118.29	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S	613	CLA	O2D-CGD-O1D	-2.84	118.29	123.84
25	1	609	CHL	C1B-CHB-C4A	-2.84	124.50	130.12
36	B	621	SQD	O7-S-C6	2.84	110.31	106.94
36	A	418	SQD	O8-S-C6	2.84	110.26	105.74
27	7	1621	LUT	C22-C23-C24	-2.84	108.51	111.74
25	3	607	CHL	O2A-CGA-CBA	2.84	120.81	111.91
27	y	1621	LUT	C10-C11-C12	-2.84	114.37	123.22
26	B	617	CLA	CHB-C4A-NA	2.84	128.43	124.51
25	7	605	CHL	C1B-CHB-C4A	-2.84	124.50	130.12
25	g	607	CHL	CMD-C2D-C3D	-2.84	121.09	127.61
31	C	517	BCR	C33-C5-C4	2.84	119.06	113.62
25	g	605	CHL	CMB-C2B-C3B	2.84	129.98	124.68
26	6	602	CLA	O2D-CGD-O1D	-2.84	118.30	123.84
26	S	603	CLA	C2A-C1A-CHA	2.83	128.81	123.86
37	z	101	LMG	O8-C28-O10	-2.83	116.44	123.59
26	N	612	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
27	6	1620	LUT	C15-C14-C13	-2.83	123.27	127.31
25	G	606	CHL	O2A-CGA-CBA	2.83	120.80	111.91
26	4	604	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
37	Z	101	LMG	O8-C28-O10	-2.83	116.44	123.59
37	C	521	LMG	O6-C1-O1	-2.83	103.26	109.97
26	3	612	CLA	C1B-CHB-C4A	-2.83	124.51	130.12
25	1	601	CHL	CMB-C2B-C3B	2.83	129.98	124.68
25	1	601	CHL	C1C-C2C-C3C	-2.83	104.87	107.11
37	c	521	LMG	O1-C7-C8	-2.83	104.06	110.90
25	5	601	CHL	CMB-C2B-C3B	2.83	129.98	124.68
26	3	613	CLA	O2D-CGD-O1D	-2.83	118.30	123.84
29	N	1623	NEX	C39-C29-C30	-2.83	118.96	122.92
39	c	519	DGD	O5D-C6D-C5D	-2.83	103.81	109.05
29	R	623	NEX	O24-C25-C38	2.83	118.45	115.06
37	d	411	LMG	O6-C1-O1	-2.83	103.27	109.97
26	N	602	CLA	CAC-C3C-C4C	2.83	128.48	124.81
37	D	411	LMG	O6-C1-O1	-2.83	103.27	109.97
25	Y	608	CHL	CMD-C2D-C3D	-2.83	121.10	127.61
37	C	521	LMG	O1-C7-C8	-2.83	104.07	110.90
26	2	613	CLA	O2D-CGD-O1D	-2.83	118.31	123.84
26	s	603	CLA	C2A-C1A-CHA	2.83	128.81	123.86
25	G	601	CHL	C1-C2-C3	-2.83	121.15	126.04
26	B	606	CLA	O2D-CGD-CBD	2.83	116.30	111.27
26	b	606	CLA	O2D-CGD-CBD	2.83	116.29	111.27
25	4	606	CHL	CAA-C2A-C3A	-2.83	105.03	112.78
26	5	603	CLA	O2D-CGD-O1D	-2.83	118.31	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	509	CLA	CAA-C2A-C3A	-2.83	105.04	112.78
25	3	605	CHL	C1B-CHB-C4A	-2.83	124.52	130.12
26	B	615	CLA	C2D-C1D-ND	-2.83	108.02	110.10
26	b	615	CLA	C2D-C1D-ND	-2.83	108.02	110.10
26	N	613	CLA	CHB-C4A-NA	2.82	128.42	124.51
36	b	621	SQD	O7-S-C6	2.82	110.30	106.94
25	G	607	CHL	CMD-C2D-C3D	-2.82	121.12	127.61
31	C	514	BCR	C21-C20-C19	-2.82	114.41	123.22
26	7	613	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
25	7	607	CHL	O2A-CGA-CBA	2.82	120.77	111.91
25	4	607	CHL	CMD-C2D-C3D	-2.82	121.12	127.61
29	n	1623	NEX	C39-C29-C30	-2.82	118.97	122.92
25	4	601	CHL	CMB-C2B-C3B	2.82	129.96	124.68
27	y	1620	LUT	C38-C25-C24	-2.82	117.52	123.56
26	5	602	CLA	O2D-CGD-O1D	-2.82	118.32	123.84
25	8	607	CHL	C1B-CHB-C4A	-2.82	124.53	130.12
26	c	509	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
25	8	606	CHL	CAA-C2A-C3A	-2.82	105.06	112.78
26	1	612	CLA	C1B-CHB-C4A	-2.82	124.53	130.12
31	c	514	BCR	C21-C20-C19	-2.82	114.42	123.22
25	G	605	CHL	CMB-C2B-C3B	2.82	129.95	124.68
39	C	518	DGD	O3E-C3E-C2E	-2.82	103.83	110.35
39	c	518	DGD	O3E-C3E-C2E	-2.82	103.83	110.35
37	c	521	LMG	O6-C1-O1	-2.82	103.30	109.97
25	g	606	CHL	O2A-CGA-CBA	2.82	120.75	111.91
26	c	507	CLA	C2A-C1A-CHA	2.82	128.78	123.86
36	A	418	SQD	O47-C7-C8	2.82	117.57	111.50
26	7	612	CLA	C1B-CHB-C4A	-2.81	124.54	130.12
25	3	606	CHL	CMB-C2B-C3B	2.81	129.94	124.68
25	G	607	CHL	CAC-C3C-C4C	2.81	128.46	124.81
26	C	509	CLA	C1B-CHB-C4A	-2.81	124.55	130.12
26	B	614	CLA	C4-C3-C5	2.81	120.00	115.27
25	2	605	CHL	C1C-C2C-C3C	-2.81	104.88	107.11
26	1	603	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
26	n	612	CLA	O2D-CGD-O1D	-2.81	118.34	123.84
25	G	605	CHL	C4D-CHA-C1A	-2.81	117.83	121.25
25	8	608	CHL	OMC-CMC-C2C	-2.81	119.34	125.69
26	3	603	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
26	7	603	CLA	O2D-CGD-O1D	-2.81	118.35	123.84
26	5	612	CLA	C1B-CHB-C4A	-2.81	124.56	130.12
25	8	601	CHL	CMB-C2B-C3B	2.81	129.93	124.68
25	n	609	CHL	C1C-C2C-C3C	-2.81	104.89	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	8	607	CHL	CMD-C2D-C3D	-2.81	121.16	127.61
29	g	1623	NEX	C26-C27-C28	-2.81	120.06	125.99
25	g	601	CHL	C1-C2-C3	-2.81	121.19	126.04
39	C	519	DGD	O5D-C6D-C5D	-2.81	103.86	109.05
26	G	602	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
26	N	603	CLA	CAA-C2A-C3A	-2.80	105.10	112.78
26	C	507	CLA	C2A-C1A-CHA	2.80	128.76	123.86
25	S	606	CHL	OMC-CMC-C2C	-2.80	119.35	125.69
26	6	603	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
26	n	603	CLA	CMB-C2B-C3B	2.80	129.92	124.68
36	a	418	SQD	O47-C7-C8	2.80	117.53	111.50
29	r	623	NEX	C39-C29-C30	-2.80	119.00	122.92
26	g	602	CLA	O2D-CGD-O1D	-2.80	118.36	123.84
26	b	613	CLA	O2D-CGD-CBD	2.80	116.24	111.27
26	b	614	CLA	C4-C3-C5	2.80	119.98	115.27
25	N	608	CHL	O2A-CGA-CBA	2.80	120.69	111.91
25	8	607	CHL	C1C-C2C-C3C	-2.80	104.89	107.11
25	4	607	CHL	C1B-CHB-C4A	-2.80	124.58	130.12
26	C	507	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
25	6	608	CHL	CMB-C2B-C3B	2.80	129.91	124.68
26	S	603	CLA	C1B-CHB-C4A	-2.80	124.58	130.12
26	1	602	CLA	O2D-CGD-O1D	-2.79	118.37	123.84
25	n	608	CHL	O2A-CGA-CBA	2.79	120.68	111.91
26	n	603	CLA	CAA-C2A-C3A	-2.79	105.13	112.78
27	N	1621	LUT	C22-C23-C24	-2.79	108.56	111.74
29	G	1623	NEX	C26-C27-C28	-2.79	120.09	125.99
25	N	609	CHL	C1C-C2C-C3C	-2.79	104.90	107.11
25	2	608	CHL	CMB-C2B-C3B	2.79	129.90	124.68
26	1	603	CLA	CBC-CAC-C3C	-2.79	104.74	112.43
25	s	606	CHL	OMC-CMC-C2C	-2.79	119.38	125.69
26	s	603	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
25	7	605	CHL	C1C-C2C-C3C	-2.79	104.90	107.11
26	B	612	CLA	CHB-C4A-NA	2.79	128.37	124.51
25	g	607	CHL	CAC-C3C-C4C	2.79	128.43	124.81
26	R	603	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
26	r	603	CLA	C1B-CHB-C4A	-2.79	124.59	130.12
31	c	516	BCR	C15-C14-C13	-2.79	123.33	127.31
26	2	612	CLA	CHB-C4A-NA	2.79	128.37	124.51
25	4	608	CHL	OMC-CMC-C2C	-2.79	119.38	125.69
28	1	1622	XAT	C18-C5-C4	2.79	117.42	114.28
26	5	603	CLA	CBC-CAC-C3C	-2.79	104.75	112.43
25	7	601	CHL	C2A-C1A-CHA	-2.79	118.99	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	y	1623	NEX	C26-C27-C28	-2.79	120.10	125.99
26	6	612	CLA	O2D-CGD-O1D	-2.79	118.39	123.84
25	3	601	CHL	C2A-C1A-CHA	-2.79	118.99	123.86
27	Y	1620	LUT	C38-C25-C24	-2.79	117.60	123.56
25	5	601	CHL	C1C-C2C-C3C	-2.79	104.90	107.11
28	g	1622	XAT	C24-C23-C22	-2.79	105.39	110.77
25	7	609	CHL	CMB-C2B-C3B	2.79	129.89	124.68
26	2	611	CLA	CMB-C2B-C3B	2.79	129.89	124.68
25	g	609	CHL	C4-C3-C5	2.79	119.96	115.27
25	G	605	CHL	C3B-C4B-NB	2.79	112.81	109.21
25	g	605	CHL	C4D-CHA-C1A	-2.78	117.86	121.25
27	3	1620	LUT	C7-C8-C9	-2.78	122.03	126.23
26	3	603	CLA	C2A-C1A-CHA	2.78	128.73	123.86
26	B	613	CLA	O2D-CGD-CBD	2.78	116.21	111.27
26	b	605	CLA	CBA-CAA-C2A	2.78	122.08	113.86
26	2	603	CLA	O2D-CGD-O1D	-2.78	118.40	123.84
27	n	1621	LUT	C15-C35-C34	-2.78	117.77	123.47
26	N	612	CLA	CHB-C4A-NA	2.78	128.36	124.51
26	n	612	CLA	CHB-C4A-NA	2.78	128.36	124.51
29	7	1623	NEX	C15-C35-C34	-2.78	117.78	123.47
25	6	605	CHL	C1C-C2C-C3C	-2.78	104.91	107.11
26	C	501	CLA	O2D-CGD-CBD	2.78	116.21	111.27
25	G	609	CHL	C4-C3-C5	2.78	119.94	115.27
26	c	501	CLA	O2D-CGD-CBD	2.78	116.20	111.27
25	4	601	CHL	C1C-C2C-C3C	-2.78	104.91	107.11
26	c	507	CLA	C1B-CHB-C4A	-2.78	124.62	130.12
26	2	612	CLA	O2D-CGD-O1D	-2.78	118.41	123.84
27	N	1621	LUT	C15-C35-C34	-2.78	117.79	123.47
25	3	609	CHL	CMB-C2B-C3B	2.78	129.87	124.68
39	h	102	DGD	C3D-C4D-C5D	-2.78	105.29	110.24
31	c	515	BCR	C3-C4-C5	-2.78	109.12	114.08
26	8	612	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
28	5	1622	XAT	C18-C5-C4	2.77	117.40	114.28
26	S	614	CLA	C1B-CHB-C4A	-2.77	124.62	130.12
31	C	515	BCR	C3-C4-C5	-2.77	109.12	114.08
26	2	612	CLA	CAA-C2A-C3A	-2.77	105.18	112.78
26	N	603	CLA	CMB-C2B-C3B	2.77	129.87	124.68
26	6	611	CLA	CMB-C2B-C3B	2.77	129.87	124.68
26	b	612	CLA	CHB-C4A-NA	2.77	128.34	124.51
26	8	604	CLA	CMB-C2B-C3B	2.77	129.86	124.68
39	B	626	DGD	C3G-C2G-C1G	-2.77	105.24	111.79
29	Y	1623	NEX	C26-C27-C28	-2.77	120.14	125.99

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	r	608	CHL	O1D-CGD-CBD	-2.77	118.82	124.48
26	y	603	CLA	CHD-C1D-ND	-2.77	121.91	124.45
26	S	609	CLA	CMB-C2B-C3B	2.77	129.86	124.68
27	n	1621	LUT	C30-C31-C32	-2.77	114.58	123.22
26	C	513	CLA	C1B-CHB-C4A	-2.77	124.63	130.12
28	G	1622	XAT	C24-C23-C22	-2.77	105.43	110.77
27	2	1620	LUT	C20-C13-C12	2.77	122.44	118.08
26	B	605	CLA	CBA-CAA-C2A	2.77	122.03	113.86
25	R	608	CHL	O1D-CGD-CBD	-2.77	118.82	124.48
25	3	605	CHL	C1C-C2C-C3C	-2.77	104.92	107.11
26	4	604	CLA	CMB-C2B-C3B	2.77	129.85	124.68
31	B	618	BCR	C33-C5-C6	-2.77	121.42	124.53
31	b	618	BCR	C33-C5-C6	-2.77	121.42	124.53
27	n	1621	LUT	C22-C23-C24	-2.77	108.59	111.74
29	R	623	NEX	C39-C29-C30	-2.77	119.05	122.92
25	n	608	CHL	CMD-C2D-C3D	-2.77	121.25	127.61
25	n	605	CHL	O2A-CGA-CBA	2.77	120.59	111.91
25	G	606	CHL	C4D-CHA-C1A	-2.77	117.88	121.25
29	3	1623	NEX	C15-C35-C34	-2.76	117.81	123.47
25	N	608	CHL	CMD-C2D-C3D	-2.76	121.25	127.61
25	g	601	CHL	O2D-CGD-O1D	-2.76	118.43	123.84
26	s	614	CLA	C1B-CHB-C4A	-2.76	124.64	130.12
25	s	608	CHL	CMB-C2B-C3B	2.76	129.85	124.68
27	7	1620	LUT	C7-C8-C9	-2.76	122.06	126.23
26	7	603	CLA	C2A-C1A-CHA	2.76	128.69	123.86
25	6	606	CHL	C1C-C2C-C3C	-2.76	104.92	107.11
25	S	608	CHL	CMB-C2B-C3B	2.76	129.85	124.68
26	7	611	CLA	CHB-C4A-NA	2.76	128.33	124.51
25	7	601	CHL	O2A-CGA-CBA	2.76	120.58	111.91
25	5	606	CHL	CMD-C2D-C3D	-2.76	121.26	127.61
26	6	612	CLA	CAA-C2A-C3A	-2.76	105.22	112.78
25	R	607	CHL	CAC-C3C-C4C	2.76	128.39	124.81
26	r	609	CLA	O2D-CGD-O1D	-2.76	118.44	123.84
39	b	626	DGD	C3G-C2G-C1G	-2.76	105.26	111.79
25	g	605	CHL	C3B-C4B-NB	2.76	112.78	109.21
35	a	408	PHO	CMB-C2B-C3B	2.76	129.84	124.68
31	C	516	BCR	C15-C14-C13	-2.76	123.37	127.31
36	b	623	SQD	O5-C1-C2	2.76	116.19	110.35
26	c	513	CLA	C1B-CHB-C4A	-2.76	124.66	130.12
26	r	603	CLA	CHB-C4A-NA	2.76	128.32	124.51
27	N	1621	LUT	C30-C31-C32	-2.76	114.62	123.22
39	H	102	DGD	C3D-C4D-C5D	-2.75	105.33	110.24

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	s	609	CLA	CMB-C2B-C3B	2.75	129.83	124.68
26	3	611	CLA	CHB-C4A-NA	2.75	128.32	124.51
36	B	623	SQD	O5-C1-C2	2.75	116.18	110.35
25	6	609	CHL	C1-C2-C3	-2.75	121.28	126.04
25	3	601	CHL	O2A-CGA-CBA	2.75	120.55	111.91
25	N	608	CHL	CHB-C4A-NA	2.75	128.32	124.51
25	N	605	CHL	O2A-CGA-CBA	2.75	120.55	111.91
29	n	1623	NEX	C26-C27-C28	-2.75	120.17	125.99
25	G	601	CHL	O2D-CGD-O1D	-2.75	118.46	123.84
25	n	607	CHL	CED-O2D-CGD	2.75	122.16	115.94
26	S	610	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
26	s	610	CLA	O2D-CGD-O1D	-2.75	118.46	123.84
26	4	612	CLA	C1B-CHB-C4A	-2.75	124.67	130.12
28	2	1622	XAT	C4-C3-C2	-2.75	105.46	110.77
25	1	606	CHL	CMD-C2D-C3D	-2.75	121.29	127.61
26	6	612	CLA	CHB-C4A-NA	2.75	128.31	124.51
25	5	607	CHL	CMD-C2D-C3D	-2.75	121.30	127.61
27	Y	1621	LUT	C30-C31-C32	-2.75	114.65	123.22
25	y	609	CHL	CHD-C4C-C3C	-2.75	120.80	124.84
26	B	616	CLA	CMB-C2B-C1B	-2.75	124.24	128.46
26	n	611	CLA	O2D-CGD-O1D	-2.75	118.47	123.84
26	Y	603	CLA	CHD-C1D-ND	-2.75	121.93	124.45
31	C	514	BCR	C8-C9-C10	-2.74	114.73	118.94
25	g	606	CHL	C4D-CHA-C1A	-2.74	117.91	121.25
26	r	612	CLA	CMB-C2B-C3B	2.74	129.81	124.68
29	N	1623	NEX	C24-C23-C22	-2.74	105.47	110.77
26	3	614	CLA	CMB-C2B-C1B	-2.74	124.25	128.46
26	c	513	CLA	CHB-C4A-NA	2.74	128.31	124.51
25	R	606	CHL	O2D-CGD-O1D	-2.74	118.48	123.84
27	y	1621	LUT	C30-C31-C32	-2.74	114.66	123.22
25	s	607	CHL	C1C-C2C-C3C	-2.74	104.94	107.11
31	C	515	BCR	C37-C22-C23	2.74	122.40	118.08
31	c	515	BCR	C37-C22-C23	2.74	122.40	118.08
29	N	1623	NEX	C26-C27-C28	-2.74	120.20	125.99
31	c	514	BCR	C8-C9-C10	-2.74	114.73	118.94
26	S	612	CLA	CHB-C4A-NA	2.74	128.30	124.51
28	6	1622	XAT	C4-C3-C2	-2.74	105.48	110.77
26	3	613	CLA	CHB-C4A-NA	2.74	128.30	124.51
26	8	602	CLA	CHB-C4A-NA	2.74	128.30	124.51
25	1	607	CHL	CMD-C2D-C3D	-2.74	121.31	127.61
27	6	1620	LUT	C20-C13-C12	2.74	122.39	118.08
26	N	610	CLA	O2A-CGA-O1A	-2.74	116.68	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	N	612	CLA	C1B-CHB-C4A	-2.74	124.69	130.12
28	r	622	XAT	C8-C9-C10	-2.74	114.74	118.94
25	N	607	CHL	CED-O2D-CGD	2.74	122.13	115.94
39	c	518	DGD	CDB-CCB-CBB	-2.74	100.53	114.42
31	B	619	BCR	C39-C30-C25	-2.74	105.86	110.30
26	Y	611	CLA	CHB-C4A-NA	2.74	128.30	124.51
26	7	613	CLA	CHB-C4A-NA	2.74	128.30	124.51
26	Y	603	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
26	y	603	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
25	G	609	CHL	CMD-C2D-C3D	-2.74	121.32	127.61
39	C	518	DGD	CDB-CCB-CBB	-2.74	100.53	114.42
26	n	612	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
31	8	623	BCR	C29-C30-C25	2.74	114.69	110.48
26	y	611	CLA	C1B-CHB-C4A	-2.74	124.70	130.12
25	r	607	CHL	CAC-C3C-C4C	2.74	128.36	124.81
28	3	1622	XAT	C40-C33-C32	2.73	122.39	118.08
29	n	1623	NEX	C24-C23-C22	-2.73	105.49	110.77
26	R	613	CLA	CMB-C2B-C3B	2.73	129.79	124.68
26	r	613	CLA	CMB-C2B-C3B	2.73	129.79	124.68
25	g	609	CHL	CMD-C2D-C3D	-2.73	121.33	127.61
25	r	606	CHL	O2D-CGD-O1D	-2.73	118.49	123.84
26	C	513	CLA	CHB-C4A-NA	2.73	128.29	124.51
35	A	408	PHO	CMB-C2B-C3B	2.73	129.79	124.68
25	n	608	CHL	CHB-C4A-NA	2.73	128.29	124.51
26	R	609	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
39	h	102	DGD	CDB-CCB-CBB	-2.73	100.56	114.42
26	Y	611	CLA	C1B-CHB-C4A	-2.73	124.71	130.12
31	b	620	BCR	C20-C21-C22	-2.73	123.41	127.31
25	2	606	CHL	C1C-C2C-C3C	-2.73	104.95	107.11
31	B	620	BCR	C20-C21-C22	-2.73	123.41	127.31
31	4	623	BCR	C29-C30-C25	2.73	114.69	110.48
26	R	603	CLA	CHB-C4A-NA	2.73	128.29	124.51
26	6	603	CLA	CBC-CAC-C3C	-2.73	104.90	112.43
26	2	614	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
26	y	611	CLA	CHB-C4A-NA	2.73	128.29	124.51
31	H	101	BCR	C3-C4-C5	-2.73	109.20	114.08
26	s	612	CLA	CHB-C4A-NA	2.73	128.29	124.51
26	4	611	CLA	O2D-CGD-O1D	-2.73	118.50	123.84
26	8	603	CLA	CAA-C2A-C3A	-2.73	105.31	112.78
25	8	601	CHL	C1C-C2C-C3C	-2.73	104.95	107.11
39	C	520	DGD	O5D-C6D-C5D	-2.73	104.00	109.05
29	Y	1623	NEX	C39-C29-C30	-2.73	119.10	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	R	622	XAT	C8-C9-C10	-2.73	114.76	118.94
26	N	611	CLA	O2D-CGD-O1D	-2.73	118.51	123.84
27	7	1621	LUT	C19-C9-C8	2.72	122.37	118.08
27	S	1620	LUT	C7-C8-C9	-2.72	122.12	126.23
25	2	609	CHL	C1-C2-C3	-2.72	121.33	126.04
25	7	607	CHL	C4-C3-C5	2.72	119.85	115.27
26	2	603	CLA	CBC-CAC-C3C	-2.72	104.92	112.43
28	2	1622	XAT	C26-C27-C28	-2.72	120.23	125.99
29	r	623	NEX	C30-C31-C32	-2.72	114.72	123.22
25	6	605	CHL	C1B-CHB-C4A	-2.72	124.72	130.12
30	6	2630	LHG	O8-C23-C24	2.72	120.45	111.91
30	2	2630	LHG	O8-C23-C24	2.72	120.45	111.91
25	1	609	CHL	CAC-C3C-C4C	2.72	128.34	124.81
31	h	101	BCR	C3-C4-C5	-2.72	109.22	114.08
31	b	619	BCR	C39-C30-C25	-2.72	105.88	110.30
39	c	520	DGD	O5D-C6D-C5D	-2.72	104.01	109.05
27	s	1620	LUT	C7-C8-C9	-2.72	122.12	126.23
39	H	102	DGD	CDB-CCB-CBB	-2.72	100.61	114.42
26	n	610	CLA	O2A-CGA-O1A	-2.72	116.72	123.59
26	s	613	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
29	R	623	NEX	C30-C31-C32	-2.72	114.73	123.22
27	G	1621	LUT	C28-C29-C30	-2.72	114.77	118.94
26	7	614	CLA	CMB-C2B-C1B	-2.72	124.28	128.46
27	g	1621	LUT	C28-C29-C30	-2.72	114.77	118.94
26	b	616	CLA	C1B-CHB-C4A	-2.72	124.73	130.12
28	7	1622	XAT	C40-C33-C32	2.72	122.36	118.08
25	g	609	CHL	CAA-C2A-C3A	-2.72	105.33	112.78
25	Y	609	CHL	CHD-C4C-C3C	-2.72	120.84	124.84
25	1	605	CHL	CMB-C2B-C3B	2.72	129.76	124.68
27	3	1621	LUT	C19-C9-C8	2.72	122.36	118.08
26	4	603	CLA	CAA-C2A-C3A	-2.72	105.34	112.78
25	g	607	CHL	C3B-C4B-NB	2.72	112.72	109.21
25	Y	607	CHL	CAA-CBA-CGA	-2.72	105.31	113.25
25	Y	601	CHL	C4D-CHA-C1A	-2.72	117.94	121.25
26	R	612	CLA	CMB-C2B-C3B	2.72	129.76	124.68
26	c	508	CLA	CHB-C4A-NA	2.72	128.27	124.51
26	c	510	CLA	CHB-C4A-NA	2.71	128.27	124.51
26	6	604	CLA	O2D-CGD-O1D	-2.71	118.53	123.84
25	2	605	CHL	C1B-CHB-C4A	-2.71	124.75	130.12
26	b	616	CLA	CMB-C2B-C1B	-2.71	124.30	128.46
26	4	602	CLA	CHB-C4A-NA	2.71	128.26	124.51
26	R	602	CLA	CHB-C4A-NA	2.71	128.26	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	r	602	CLA	CHB-C4A-NA	2.71	128.26	124.51
26	a	410	CLA	CAA-CBA-CGA	-2.71	105.33	113.25
26	6	614	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
26	8	611	CLA	O2D-CGD-O1D	-2.71	118.54	123.84
25	3	607	CHL	C4-C3-C5	2.71	119.83	115.27
25	y	607	CHL	CAA-CBA-CGA	-2.71	105.33	113.25
26	G	612	CLA	C1B-CHB-C4A	-2.71	124.75	130.12
25	5	605	CHL	CMB-C2B-C3B	2.71	129.75	124.68
26	y	604	CLA	C1-C2-C3	-2.71	122.37	126.75
25	Y	609	CHL	CBC-CAC-C3C	-2.71	104.96	112.43
25	G	609	CHL	CAA-C2A-C3A	-2.71	105.36	112.78
26	B	602	CLA	CMB-C2B-C3B	2.71	129.75	124.68
25	y	609	CHL	CBC-CAC-C3C	-2.71	104.97	112.43
29	y	1623	NEX	C39-C29-C30	-2.71	119.13	122.92
28	6	1622	XAT	C26-C27-C28	-2.71	120.27	125.99
26	Y	604	CLA	C1-C2-C3	-2.71	122.37	126.75
26	y	612	CLA	CHB-C4A-NA	2.71	128.25	124.51
27	4	620	LUT	C10-C11-C12	-2.70	114.78	123.22
28	7	1622	XAT	C35-C34-C33	-2.70	123.45	127.31
26	g	612	CLA	C1B-CHB-C4A	-2.70	124.76	130.12
31	C	515	BCR	C38-C26-C25	-2.70	121.49	124.53
26	S	613	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
36	A	412	SQD	C3-C4-C5	2.70	115.06	110.24
26	b	602	CLA	CMB-C2B-C3B	2.70	129.73	124.68
26	A	410	CLA	CAA-CBA-CGA	-2.70	105.36	113.25
26	B	616	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
25	S	607	CHL	C1C-C2C-C3C	-2.70	104.97	107.11
26	1	603	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
26	5	603	CLA	C1B-CHB-C4A	-2.70	124.77	130.12
26	C	508	CLA	CHB-C4A-NA	2.70	128.24	124.51
25	n	601	CHL	C1-O2A-CGA	2.70	123.52	116.44
25	r	607	CHL	O2A-CGA-CBA	2.70	120.37	111.91
36	a	412	SQD	C3-C4-C5	2.70	115.05	110.24
28	3	1622	XAT	C35-C34-C33	-2.70	123.46	127.31
26	2	604	CLA	O2D-CGD-O1D	-2.70	118.57	123.84
26	n	614	CLA	CHB-C4A-NA	2.70	128.24	124.51
28	3	1622	XAT	C10-C11-C12	-2.69	114.81	123.22
25	N	601	CHL	C4D-CHA-C1A	-2.69	117.97	121.25
28	r	622	XAT	C31-C32-C33	-2.69	118.85	126.42
26	C	503	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
31	B	618	BCR	C10-C11-C12	-2.69	114.81	123.22
28	R	622	XAT	C31-C32-C33	-2.69	118.85	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	7	1622	XAT	C10-C11-C12	-2.69	114.81	123.22
26	s	611	CLA	CHB-C4A-NA	2.69	128.24	124.51
26	c	503	CLA	C1B-CHB-C4A	-2.69	124.78	130.12
25	n	601	CHL	C4D-CHA-C1A	-2.69	117.97	121.25
25	y	606	CHL	O2A-CGA-CBA	2.69	120.36	111.91
25	g	609	CHL	CHD-C4C-C3C	-2.69	120.88	124.84
27	8	620	LUT	C10-C11-C12	-2.69	114.82	123.22
26	8	611	CLA	CHB-C4A-NA	2.69	128.23	124.51
26	7	610	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
25	5	609	CHL	CAC-C3C-C4C	2.69	128.30	124.81
26	3	610	CLA	O2D-CGD-O1D	-2.69	118.58	123.84
25	G	607	CHL	C3B-C4B-NB	2.69	112.69	109.21
26	B	602	CLA	CHB-C4A-NA	2.69	128.23	124.51
26	C	510	CLA	CHB-C4A-NA	2.69	128.23	124.51
25	3	601	CHL	C4D-CHA-C1A	-2.69	117.98	121.25
25	2	605	CHL	CMB-C2B-C3B	2.69	129.71	124.68
25	5	601	CHL	C4D-CHA-C1A	-2.69	117.98	121.25
27	2	1621	LUT	C19-C9-C8	2.69	122.31	118.08
25	2	608	CHL	C1C-C2C-C3C	-2.69	104.98	107.11
30	N	2630	LHG	C20-C19-C18	-2.69	100.79	114.42
25	y	601	CHL	C4D-CHA-C1A	-2.69	117.98	121.25
25	N	601	CHL	C1-O2A-CGA	2.68	123.49	116.44
25	7	608	CHL	CHB-C4A-NA	2.68	128.22	124.51
26	n	603	CLA	C3C-C4C-NC	-2.68	107.56	110.57
25	R	607	CHL	O2A-CGA-CBA	2.68	120.33	111.91
25	Y	606	CHL	O2A-CGA-CBA	2.68	120.33	111.91
28	6	1622	XAT	C15-C35-C34	-2.68	117.98	123.47
25	1	605	CHL	CMD-C2D-C3D	-2.68	121.44	127.61
26	b	602	CLA	CHB-C4A-NA	2.68	128.22	124.51
26	G	612	CLA	CHB-C4A-NA	2.68	128.22	124.51
25	7	609	CHL	O2A-CGA-CBA	2.68	120.32	111.91
26	7	612	CLA	CAA-C2A-C3A	-2.68	105.44	112.78
26	S	611	CLA	CHB-C4A-NA	2.68	128.22	124.51
26	Y	612	CLA	CHB-C4A-NA	2.68	128.22	124.51
25	1	601	CHL	C4D-CHA-C1A	-2.68	117.99	121.25
26	5	613	CLA	O2D-CGD-O1D	-2.68	118.60	123.84
25	N	605	CHL	CHB-C4A-NA	2.68	128.22	124.51
25	7	601	CHL	C4D-CHA-C1A	-2.68	117.99	121.25
29	Y	1623	NEX	C24-C23-C22	-2.68	105.60	110.77
25	3	609	CHL	O2A-CGA-CBA	2.68	120.32	111.91
28	2	1622	XAT	C15-C35-C34	-2.68	117.99	123.47
25	y	601	CHL	C1-O2A-CGA	2.68	123.47	116.44

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	n	2630	LHG	C20-C19-C18	-2.68	100.83	114.42
29	1	1623	NEX	C5-C4-C3	-2.68	108.57	111.75
27	2	1620	LUT	C11-C10-C9	-2.68	123.49	127.31
31	b	618	BCR	C10-C11-C12	-2.68	114.87	123.22
26	4	611	CLA	CHB-C4A-NA	2.68	128.21	124.51
27	G	1620	LUT	C39-C29-C28	2.68	122.29	118.08
27	6	1621	LUT	C19-C9-C8	2.68	122.29	118.08
25	4	609	CHL	CMB-C2B-C3B	2.68	129.68	124.68
29	S	1623	NEX	O4-C5-C18	-2.67	104.63	109.39
29	s	1623	NEX	O4-C5-C18	-2.67	104.63	109.39
25	Y	601	CHL	C1-O2A-CGA	2.67	123.46	116.44
25	G	609	CHL	CHD-C4C-C3C	-2.67	120.91	124.84
25	G	609	CHL	O2D-CGD-O1D	-2.67	118.61	123.84
25	6	605	CHL	CMB-C2B-C3B	2.67	129.68	124.68
25	3	608	CHL	CHB-C4A-NA	2.67	128.21	124.51
25	8	609	CHL	CMB-C2B-C3B	2.67	129.68	124.68
31	a	411	BCR	C21-C20-C19	-2.67	114.88	123.22
26	N	603	CLA	C3C-C4C-NC	-2.67	107.58	110.57
25	n	606	CHL	O2A-CGA-CBA	2.67	120.29	111.91
26	g	612	CLA	CHB-C4A-NA	2.67	128.21	124.51
25	1	601	CHL	CHD-C4C-C3C	-2.67	120.91	124.84
26	3	612	CLA	CAA-C2A-C3A	-2.67	105.46	112.78
31	c	515	BCR	C38-C26-C25	-2.67	121.53	124.53
25	n	605	CHL	CHB-C4A-NA	2.67	128.21	124.51
25	2	607	CHL	CMD-C2D-C3D	-2.67	121.47	127.61
25	3	605	CHL	CAA-C2A-C3A	-2.67	105.47	112.78
29	y	1623	NEX	C24-C23-C22	-2.67	105.62	110.77
27	g	1620	LUT	C39-C29-C28	2.67	122.28	118.08
26	R	610	CLA	C1-C2-C3	-2.67	121.43	126.04
25	g	609	CHL	O2D-CGD-O1D	-2.67	118.62	123.84
26	N	614	CLA	CHB-C4A-NA	2.67	128.20	124.51
26	r	610	CLA	O2A-CGA-O1A	-2.67	116.86	123.59
31	A	411	BCR	C21-C20-C19	-2.66	114.90	123.22
25	5	605	CHL	CMD-C2D-C3D	-2.66	121.48	127.61
38	a	414	PL9	C8-C7-C3	2.66	119.51	111.98
25	7	605	CHL	CAA-C2A-C3A	-2.66	105.48	112.78
25	8	609	CHL	C1B-CHB-C4A	-2.66	124.84	130.12
26	y	602	CLA	C6-C7-C8	-2.66	107.32	115.92
25	N	606	CHL	O2A-CGA-CBA	2.66	120.25	111.91
25	5	601	CHL	CHD-C4C-C3C	-2.66	120.93	124.84
25	6	607	CHL	CMD-C2D-C3D	-2.66	121.50	127.61
31	c	515	BCR	C23-C22-C21	-2.66	114.86	118.94

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	b	612	CLA	O2D-CGD-O1D	-2.66	118.64	123.84
26	Y	602	CLA	C6-C7-C8	-2.66	107.33	115.92
25	Y	605	CHL	CMB-C2B-C3B	2.66	129.65	124.68
25	6	608	CHL	C1C-C2C-C3C	-2.65	105.01	107.11
25	3	605	CHL	CMD-C2D-C3D	-2.65	121.51	127.61
29	6	1623	NEX	C26-C27-C28	-2.65	120.38	125.99
26	1	613	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
26	B	612	CLA	O2D-CGD-O1D	-2.65	118.65	123.84
27	2	1620	LUT	C39-C29-C28	2.65	122.25	118.08
25	y	608	CHL	CMB-C2B-C3B	2.65	129.64	124.68
26	R	610	CLA	O2A-CGA-O1A	-2.65	116.91	123.59
26	r	610	CLA	C1-C2-C3	-2.65	121.46	126.04
30	L	101	LHG	C11-C10-C9	-2.65	100.98	114.42
30	l	101	LHG	C11-C10-C9	-2.65	100.98	114.42
25	6	601	CHL	CMB-C2B-C3B	2.65	129.63	124.68
29	5	1623	NEX	C5-C4-C3	-2.65	108.61	111.75
38	A	414	PL9	C8-C7-C3	2.65	119.46	111.98
29	2	1623	NEX	C26-C27-C28	-2.65	120.40	125.99
25	s	606	CHL	CMD-C2D-C3D	-2.65	121.53	127.61
26	2	611	CLA	CHB-C4A-NA	2.65	128.17	124.51
31	C	515	BCR	C23-C22-C21	-2.65	114.88	118.94
26	N	603	CLA	CBC-CAC-C3C	-2.65	105.14	112.43
31	C	516	BCR	C29-C30-C25	2.64	114.55	110.48
26	C	507	CLA	CAA-C2A-C3A	-2.64	105.54	112.78
27	6	1620	LUT	C39-C29-C28	2.64	122.24	118.08
26	1	612	CLA	CHB-C4A-NA	2.64	128.17	124.51
25	7	605	CHL	CMD-C2D-C3D	-2.64	121.53	127.61
26	6	611	CLA	CHB-C4A-NA	2.64	128.17	124.51
26	c	507	CLA	CAA-C2A-C3A	-2.64	105.54	112.78
28	1	1622	XAT	C26-C27-C28	-2.64	120.41	125.99
25	4	609	CHL	C1B-CHB-C4A	-2.64	124.89	130.12
35	A	408	PHO	O2A-CGA-O1A	-2.64	116.93	123.59
36	a	412	SQD	O48-C23-O10	-2.64	116.93	123.59
28	5	1622	XAT	C26-C27-C28	-2.64	120.41	125.99
25	4	606	CHL	C1C-C2C-C3C	-2.64	105.02	107.11
25	7	608	CHL	CMB-C2B-C3B	2.64	129.62	124.68
26	n	603	CLA	CBC-CAC-C3C	-2.64	105.16	112.43
25	y	605	CHL	CMB-C2B-C3B	2.64	129.61	124.68
31	H	101	BCR	C38-C26-C25	-2.64	121.57	124.53
25	G	607	CHL	CAA-C2A-C3A	-2.64	105.56	112.78
26	g	603	CLA	C3C-C4C-NC	-2.64	107.61	110.57
27	6	1620	LUT	C11-C10-C9	-2.64	123.55	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	G	605	CHL	C2A-C3A-C4A	-2.64	97.61	101.87
25	y	608	CHL	C4A-NA-C1A	-2.64	105.52	106.71
37	D	411	LMG	C6-C5-C4	-2.64	106.83	113.00
26	y	613	CLA	C16-C15-C13	-2.63	107.40	115.92
25	S	606	CHL	CMD-C2D-C3D	-2.63	121.55	127.61
26	B	604	CLA	O2D-CGD-CBD	2.63	115.95	111.27
39	h	102	DGD	O3E-C3E-C2E	-2.63	104.26	110.35
26	N	610	CLA	C2A-C1A-CHA	2.63	128.46	123.86
25	Y	608	CHL	CMB-C2B-C3B	2.63	129.60	124.68
39	c	519	DGD	O3E-C3E-C2E	-2.63	104.26	110.35
35	a	408	PHO	O2A-CGA-O1A	-2.63	116.95	123.59
26	r	609	CLA	CHB-C4A-NA	2.63	128.15	124.51
40	D	401	BCT	O3-C-O1	-2.63	112.72	119.55
26	3	604	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
26	R	601	CLA	CHB-C4A-NA	2.63	128.15	124.51
31	H	101	BCR	C16-C15-C14	-2.63	118.09	123.47
31	C	514	BCR	C34-C9-C8	2.63	122.22	118.08
25	g	605	CHL	C2A-C3A-C4A	-2.63	97.63	101.87
30	c	2630	LHG	C18-C17-C16	-2.63	101.09	114.42
26	5	612	CLA	CHB-C4A-NA	2.63	128.14	124.51
25	3	608	CHL	CMB-C2B-C3B	2.63	129.59	124.68
25	R	608	CHL	CMB-C2B-C3B	2.63	129.59	124.68
25	r	608	CHL	CMB-C2B-C3B	2.63	129.59	124.68
39	H	102	DGD	O3E-C3E-C2E	-2.63	104.28	110.35
27	6	1621	LUT	C39-C29-C28	2.63	122.22	118.08
31	h	101	BCR	C38-C26-C25	-2.63	121.58	124.53
30	n	2630	LHG	C11-C10-C9	-2.63	101.09	114.42
25	N	608	CHL	CMB-C2B-C3B	2.63	129.59	124.68
25	g	607	CHL	CAA-C2A-C3A	-2.63	105.59	112.78
25	6	608	CHL	CMD-C2D-C3D	-2.63	121.57	127.61
26	5	611	CLA	O2D-CGD-O1D	-2.63	118.70	123.84
26	G	603	CLA	C3C-C4C-NC	-2.63	107.63	110.57
36	A	412	SQD	O48-C23-O10	-2.62	116.97	123.59
27	2	1621	LUT	C39-C29-C28	2.62	122.21	118.08
26	4	603	CLA	CHB-C4A-NA	2.62	128.14	124.51
26	Y	613	CLA	C16-C15-C13	-2.62	107.44	115.92
25	5	609	CHL	O2A-CGA-CBA	2.62	120.14	111.91
30	N	2630	LHG	C11-C10-C9	-2.62	101.11	114.42
25	2	601	CHL	CMB-C2B-C3B	2.62	129.59	124.68
27	R	620	LUT	C20-C13-C12	2.62	122.21	118.08
25	1	609	CHL	O2A-CGA-CBA	2.62	120.14	111.91
25	n	608	CHL	CMB-C2B-C3B	2.62	129.58	124.68

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	N	606	CHL	O2D-CGD-O1D	-2.62	118.71	123.84
25	4	601	CHL	CMD-C2D-C3D	-2.62	121.58	127.61
25	6	609	CHL	CMD-C2D-C3D	-2.62	121.59	127.61
26	b	604	CLA	O2D-CGD-CBD	2.62	115.92	111.27
37	d	411	LMG	C6-C5-C4	-2.62	106.87	113.00
29	7	1623	NEX	C30-C31-C32	-2.62	115.04	123.22
31	b	618	BCR	C3-C4-C5	-2.62	109.40	114.08
28	3	1622	XAT	C18-C5-C4	2.62	117.23	114.28
25	8	601	CHL	CMD-C2D-C3D	-2.62	121.59	127.61
26	S	614	CLA	CHD-C1D-ND	-2.62	122.05	124.45
26	s	614	CLA	CHD-C1D-ND	-2.62	122.05	124.45
30	C	2630	LHG	C18-C17-C16	-2.62	101.14	114.42
27	r	620	LUT	C19-C9-C8	2.62	122.20	118.08
29	3	1623	NEX	C30-C31-C32	-2.62	115.05	123.22
25	2	608	CHL	CMD-C2D-C3D	-2.62	121.59	127.61
26	6	612	CLA	CMB-C2B-C3B	2.62	129.57	124.68
25	2	609	CHL	CMD-C2D-C3D	-2.62	121.60	127.61
25	n	606	CHL	O2D-CGD-O1D	-2.62	118.72	123.84
39	C	519	DGD	O3E-C3E-C2E	-2.62	104.30	110.35
25	1	605	CHL	C1C-C2C-C3C	-2.61	105.04	107.11
40	d	401	BCT	O3-C-O1	-2.61	112.76	119.55
26	n	610	CLA	C2A-C1A-CHA	2.61	128.43	123.86
31	B	618	BCR	C3-C4-C5	-2.61	109.41	114.08
31	B	620	BCR	C16-C15-C14	-2.61	118.12	123.47
26	7	604	CLA	O2D-CGD-O1D	-2.61	118.73	123.84
26	1	603	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
26	5	603	CLA	CAA-C2A-C3A	-2.61	105.62	112.78
31	c	516	BCR	C29-C30-C25	2.61	114.50	110.48
25	6	601	CHL	C2A-C1A-CHA	-2.61	119.29	123.86
27	r	620	LUT	C20-C13-C12	2.61	122.19	118.08
25	8	606	CHL	C1C-C2C-C3C	-2.61	105.04	107.11
25	2	605	CHL	CAC-C3C-C4C	2.61	128.20	124.81
25	6	605	CHL	CAC-C3C-C4C	2.61	128.20	124.81
31	b	620	BCR	C33-C5-C6	-2.61	121.60	124.53
31	h	101	BCR	C16-C15-C14	-2.61	118.13	123.47
25	7	608	CHL	C1C-C2C-C3C	-2.61	105.04	107.11
26	g	610	CLA	C1-C2-C3	-2.61	121.53	126.04
26	S	611	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
26	s	611	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
27	R	620	LUT	C19-C9-C8	2.61	122.19	118.08
31	c	514	BCR	C34-C9-C8	2.61	122.19	118.08
30	C	522	LHG	O8-C23-C24	2.61	120.09	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	r	607	CHL	C5-C3-C2	-2.61	115.84	121.12
26	Y	612	CLA	C1B-CHB-C4A	-2.61	124.95	130.12
26	2	612	CLA	CMB-C2B-C3B	2.61	129.55	124.68
31	b	620	BCR	C16-C15-C14	-2.61	118.14	123.47
26	R	609	CLA	CHB-C4A-NA	2.61	128.12	124.51
26	8	603	CLA	CHB-C4A-NA	2.61	128.12	124.51
36	a	418	SQD	O47-C45-C44	2.61	117.83	108.40
26	y	612	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
36	A	418	SQD	O47-C45-C44	2.60	117.83	108.40
26	C	505	CLA	C1B-CHB-C4A	-2.60	124.96	130.12
25	3	608	CHL	C1C-C2C-C3C	-2.60	105.05	107.11
25	1	601	CHL	C4A-NA-C1A	-2.60	105.54	106.71
30	c	522	LHG	O8-C23-C24	2.60	120.07	111.91
26	r	612	CLA	O2D-CGD-O1D	-2.60	118.75	123.84
28	7	1622	XAT	C18-C5-C4	2.60	117.21	114.28
31	B	618	BCR	C37-C22-C23	2.60	122.17	118.08
26	1	614	CLA	CHB-C4A-NA	2.60	128.11	124.51
26	N	611	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
26	n	611	CLA	O2A-CGA-O1A	-2.60	117.03	123.59
29	5	1623	NEX	C15-C35-C34	-2.60	118.15	123.47
25	R	607	CHL	C5-C3-C2	-2.60	115.86	121.12
31	B	620	BCR	C33-C5-C6	-2.60	121.61	124.53
28	Y	1622	XAT	C40-C33-C32	2.60	122.17	118.08
25	1	606	CHL	CHB-C4A-NA	2.60	128.10	124.51
36	b	623	SQD	O8-S-C6	2.60	109.88	105.74
25	G	608	CHL	C1C-C2C-C3C	-2.60	105.05	107.11
26	R	612	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
27	R	620	LUT	C38-C25-C24	-2.60	118.01	123.56
26	1	611	CLA	O2D-CGD-O1D	-2.60	118.76	123.84
26	c	505	CLA	C1B-CHB-C4A	-2.60	124.98	130.12
30	c	2630	LHG	C20-C19-C18	-2.59	101.25	114.42
25	g	608	CHL	C1C-C2C-C3C	-2.59	105.06	107.11
25	2	601	CHL	C2A-C1A-CHA	-2.59	119.33	123.86
27	3	1620	LUT	C35-C15-C14	-2.59	118.16	123.47
26	G	610	CLA	C1-C2-C3	-2.59	121.56	126.04
25	g	601	CHL	C4-C3-C5	2.59	119.63	115.27
27	r	620	LUT	C38-C25-C24	-2.59	118.02	123.56
30	C	2630	LHG	C20-C19-C18	-2.59	101.28	114.42
25	5	609	CHL	C1-C2-C3	-2.59	121.56	126.04
31	D	404	BCR	C21-C20-C19	-2.59	115.14	123.22
31	d	404	BCR	C21-C20-C19	-2.59	115.14	123.22
26	r	601	CLA	CHB-C4A-NA	2.59	128.09	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	n	609	CHL	O2D-CGD-O1D	-2.59	118.78	123.84
29	1	1623	NEX	C15-C35-C34	-2.59	118.17	123.47
26	5	614	CLA	CHB-C4A-NA	2.59	128.09	124.51
25	5	605	CHL	C1C-C2C-C3C	-2.59	105.06	107.11
26	5	613	CLA	CHB-C4A-NA	2.58	128.09	124.51
28	y	1622	XAT	C40-C33-C32	2.58	122.15	118.08
27	4	620	LUT	C15-C35-C34	-2.58	118.18	123.47
25	3	601	CHL	CHB-C4A-NA	2.58	128.09	124.51
25	y	609	CHL	O2D-CGD-O1D	-2.58	118.79	123.84
25	G	601	CHL	C4-C3-C5	2.58	119.62	115.27
31	b	618	BCR	C37-C22-C23	2.58	122.14	118.08
26	C	511	CLA	C1B-CHB-C4A	-2.58	125.00	130.12
27	7	1620	LUT	C35-C15-C14	-2.58	118.19	123.47
30	b	2630	LHG	C11-C10-C9	-2.58	101.32	114.42
25	4	609	CHL	CHD-C4C-C3C	-2.58	121.05	124.84
27	8	620	LUT	C15-C35-C34	-2.58	118.19	123.47
25	g	606	CHL	CHB-C4A-NA	2.58	128.08	124.51
26	3	602	CLA	C4A-NA-C1A	2.58	107.86	106.71
29	y	1623	NEX	C31-C30-C29	-2.58	123.63	127.31
26	c	511	CLA	C1B-CHB-C4A	-2.58	125.01	130.12
29	R	623	NEX	C17-C1-C6	-2.58	108.17	110.47
25	s	607	CHL	CBC-CAC-C3C	-2.58	105.33	112.43
25	8	609	CHL	CHD-C4C-C3C	-2.58	121.05	124.84
25	5	608	CHL	CMD-C2D-C3D	-2.58	121.69	127.61
25	N	609	CHL	O2D-CGD-O1D	-2.58	118.80	123.84
25	5	601	CHL	C4A-NA-C1A	-2.58	105.55	106.71
25	6	609	CHL	C4-C3-C5	2.58	119.60	115.27
25	g	608	CHL	CHB-C4A-NA	2.58	128.07	124.51
30	B	2630	LHG	C11-C10-C9	-2.58	101.35	114.42
25	1	609	CHL	C1-C2-C3	-2.57	121.59	126.04
27	5	1621	LUT	C10-C11-C12	-2.57	115.19	123.22
25	y	608	CHL	O2D-CGD-O1D	-2.57	118.81	123.84
26	1	602	CLA	C4A-NA-C1A	2.57	107.86	106.71
26	5	602	CLA	C4A-NA-C1A	2.57	107.86	106.71
27	G	1621	LUT	C31-C30-C29	-2.57	123.64	127.31
30	3	2630	LHG	C11-C10-C9	-2.57	101.36	114.42
30	7	2630	LHG	C11-C10-C9	-2.57	101.37	114.42
26	3	611	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
26	g	603	CLA	CHD-C1D-ND	-2.57	122.09	124.45
27	3	1620	LUT	C15-C35-C34	-2.57	118.21	123.47
25	S	607	CHL	CBC-CAC-C3C	-2.57	105.34	112.43
29	Y	1623	NEX	C31-C30-C29	-2.57	123.64	127.31

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	5	607	CHL	CAA-C2A-C3A	-2.57	105.74	112.78
25	1	608	CHL	CMD-C2D-C3D	-2.57	121.70	127.61
26	7	611	CLA	CAA-C2A-C3A	-2.57	105.74	112.78
27	1	1621	LUT	C10-C11-C12	-2.57	115.20	123.22
30	g	2630	LHG	C11-C10-C9	-2.57	101.39	114.42
25	4	606	CHL	CMD-C2D-C3D	-2.57	121.71	127.61
26	S	612	CLA	C1B-CHB-C4A	-2.57	125.03	130.12
25	1	607	CHL	CAA-C2A-C3A	-2.57	105.75	112.78
36	B	623	SQD	O8-S-C6	2.57	109.83	105.74
28	4	622	XAT	C35-C15-C14	-2.57	118.22	123.47
26	b	606	CLA	CMC-C2C-C1C	-2.57	121.13	125.04
25	Y	608	CHL	O2D-CGD-O1D	-2.57	118.82	123.84
25	n	606	CHL	C1C-C2C-C3C	-2.56	105.08	107.11
30	G	2630	LHG	C11-C10-C9	-2.56	101.41	114.42
29	g	1623	NEX	C24-C23-C22	-2.56	105.83	110.77
27	7	1621	LUT	C38-C25-C24	-2.56	118.08	123.56
28	8	622	XAT	C35-C15-C14	-2.56	118.23	123.47
39	c	519	DGD	CDB-CCB-CBB	-2.56	101.43	114.42
26	b	603	CLA	CHB-C4A-NA	2.56	128.05	124.51
26	2	613	CLA	CHD-C1D-ND	-2.56	122.10	124.45
25	5	606	CHL	CHB-C4A-NA	2.56	128.05	124.51
25	Y	609	CHL	O2D-CGD-O1D	-2.56	118.83	123.84
25	8	601	CHL	CHD-C4C-C3C	-2.56	121.08	124.84
27	4	620	LUT	C35-C15-C14	-2.56	118.23	123.47
26	G	603	CLA	CHD-C1D-ND	-2.56	122.10	124.45
29	G	1623	NEX	C24-C23-C22	-2.56	105.83	110.77
26	G	613	CLA	CHB-C4A-NA	2.56	128.05	124.51
26	g	613	CLA	CHB-C4A-NA	2.56	128.05	124.51
25	8	606	CHL	CMD-C2D-C3D	-2.56	121.73	127.61
27	N	1621	LUT	C8-C9-C10	-2.56	115.02	118.94
26	3	604	CLA	CHB-C4A-NA	2.56	128.05	124.51
27	7	1620	LUT	C15-C35-C34	-2.56	118.24	123.47
29	N	1623	NEX	C31-C30-C29	-2.56	123.66	127.31
25	5	605	CHL	CHB-C4A-NA	2.56	128.05	124.51
26	6	614	CLA	CHB-C4A-NA	2.56	128.05	124.51
26	1	613	CLA	CHB-C4A-NA	2.56	128.05	124.51
39	C	519	DGD	CDB-CCB-CBB	-2.56	101.45	114.42
29	r	623	NEX	C17-C1-C6	-2.56	108.19	110.47
26	s	612	CLA	C1B-CHB-C4A	-2.56	125.06	130.12
26	c	510	CLA	C6-C7-C8	-2.55	107.66	115.92
26	C	510	CLA	C6-C7-C8	-2.55	107.66	115.92
25	2	609	CHL	C4-C3-C5	2.55	119.57	115.27

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	g	1621	LUT	C31-C30-C29	-2.55	123.67	127.31
25	2	607	CHL	CAA-C2A-C3A	-2.55	105.79	112.78
31	T	101	BCR	C35-C13-C12	2.55	122.10	118.08
26	4	603	CLA	O2D-CGD-O1D	-2.55	118.85	123.84
26	c	513	CLA	CBA-CAA-C2A	2.55	121.39	113.86
25	N	605	CHL	CMD-C2D-C3D	-2.55	121.75	127.61
31	C	516	BCR	C8-C7-C6	-2.55	120.04	127.20
25	R	607	CHL	CMB-C2B-C3B	2.55	129.45	124.68
26	2	614	CLA	CHB-C4A-NA	2.55	128.04	124.51
28	5	1622	XAT	C11-C12-C13	-2.55	119.26	126.42
27	2	1620	LUT	C38-C25-C24	-2.55	118.11	123.56
26	a	406	CLA	C3C-C4C-NC	-2.55	107.71	110.57
31	c	516	BCR	C8-C7-C6	-2.55	120.05	127.20
26	B	606	CLA	CMC-C2C-C1C	-2.55	121.16	125.04
25	6	607	CHL	CAA-C2A-C3A	-2.55	105.80	112.78
26	2	610	CLA	CHB-C4A-NA	2.55	128.03	124.51
26	2	613	CLA	CHB-C4A-NA	2.55	128.03	124.51
31	D	404	BCR	C10-C11-C12	-2.55	115.27	123.22
31	d	404	BCR	C10-C11-C12	-2.55	115.27	123.22
26	B	603	CLA	CHB-C4A-NA	2.55	128.03	124.51
26	n	603	CLA	C1-C2-C3	-2.55	121.64	126.04
25	y	605	CHL	OMC-CMC-C2C	-2.54	119.93	125.69
26	6	610	CLA	CHB-C4A-NA	2.54	128.03	124.51
25	n	605	CHL	CMD-C2D-C3D	-2.54	121.76	127.61
25	Y	608	CHL	C4A-NA-C1A	-2.54	105.56	106.71
26	c	510	CLA	CHD-C1D-ND	-2.54	122.12	124.45
26	C	513	CLA	CBA-CAA-C2A	2.54	121.37	113.86
25	1	605	CHL	CHB-C4A-NA	2.54	128.03	124.51
27	8	620	LUT	C35-C15-C14	-2.54	118.27	123.47
25	r	608	CHL	CMA-C3A-C4A	2.54	118.60	111.77
25	G	606	CHL	CHB-C4A-NA	2.54	128.03	124.51
25	7	601	CHL	CHB-C4A-NA	2.54	128.03	124.51
27	3	1621	LUT	C38-C25-C24	-2.54	118.12	123.56
29	7	1623	NEX	C20-C13-C14	-2.54	119.36	122.92
27	n	1621	LUT	C8-C9-C10	-2.54	115.04	118.94
30	B	2630	LHG	O8-C23-C24	2.54	119.88	111.91
25	G	608	CHL	CHB-C4A-NA	2.54	128.02	124.51
31	c	515	BCR	C16-C15-C14	-2.54	118.27	123.47
25	R	608	CHL	CMA-C3A-C4A	2.54	118.59	111.77
28	1	1622	XAT	C11-C12-C13	-2.54	119.29	126.42
25	N	606	CHL	C1C-C2C-C3C	-2.54	105.10	107.11
29	6	1623	NEX	C39-C29-C30	-2.54	119.37	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	r	616	CLA	O2D-CGD-O1D	-2.54	118.88	123.84
26	6	613	CLA	CHB-C4A-NA	2.54	128.02	124.51
27	6	1620	LUT	C38-C25-C24	-2.54	118.13	123.56
39	h	102	DGD	C1D-C2D-C3D	-2.54	104.72	110.00
26	C	510	CLA	CHD-C1D-ND	-2.54	122.12	124.45
26	B	613	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
26	b	613	CLA	C1B-CHB-C4A	-2.53	125.10	130.12
25	r	607	CHL	CMB-C2B-C3B	2.53	129.42	124.68
26	n	602	CLA	CHB-C4A-NA	2.53	128.02	124.51
29	2	1623	NEX	C24-C23-C22	-2.53	105.88	110.77
30	b	2630	LHG	O8-C23-C24	2.53	119.86	111.91
26	S	602	CLA	CMD-C2D-C3D	2.53	133.44	127.61
26	s	602	CLA	CMD-C2D-C3D	2.53	133.44	127.61
26	7	604	CLA	CHB-C4A-NA	2.53	128.01	124.51
25	2	607	CHL	O2A-CGA-CBA	2.53	119.85	111.91
25	4	601	CHL	CHD-C4C-C3C	-2.53	121.12	124.84
26	2	602	CLA	C1-C2-C3	-2.53	121.67	126.04
26	8	603	CLA	O2D-CGD-O1D	-2.53	118.89	123.84
25	n	608	CHL	C7-C6-C5	2.53	120.22	113.36
25	n	609	CHL	CHD-C4C-C3C	-2.53	121.12	124.84
29	2	1623	NEX	C39-C29-C30	-2.53	119.38	122.92
25	7	609	CHL	CHD-C4C-C3C	-2.53	121.12	124.84
25	N	601	CHL	CMB-C2B-C3B	2.53	129.41	124.68
26	7	602	CLA	C4A-NA-C1A	2.53	107.84	106.71
25	N	608	CHL	C7-C6-C5	2.53	120.22	113.36
26	N	602	CLA	CHB-C4A-NA	2.53	128.00	124.51
29	n	1623	NEX	C31-C30-C29	-2.53	123.70	127.31
26	N	603	CLA	C1-C2-C3	-2.53	121.67	126.04
25	Y	605	CHL	OMC-CMC-C2C	-2.53	119.98	125.69
25	6	607	CHL	O2A-CGA-CBA	2.52	119.83	111.91
26	b	614	CLA	O2D-CGD-O1D	-2.52	118.90	123.84
29	6	1623	NEX	C24-C23-C22	-2.52	105.90	110.77
26	6	602	CLA	C1-C2-C3	-2.52	121.68	126.04
31	C	515	BCR	C16-C15-C14	-2.52	118.31	123.47
31	t	101	BCR	C35-C13-C12	2.52	122.05	118.08
25	N	609	CHL	CHD-C4C-C3C	-2.52	121.14	124.84
26	R	616	CLA	O2D-CGD-O1D	-2.52	118.91	123.84
27	1	1620	LUT	C15-C14-C13	-2.52	123.71	127.31
25	N	608	CHL	C1C-C2C-C3C	-2.52	105.11	107.11
26	A	406	CLA	C3C-C4C-NC	-2.52	107.75	110.57
36	a	412	SQD	O48-C23-C24	2.52	119.81	111.91
39	H	102	DGD	C1D-C2D-C3D	-2.52	104.75	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	6	613	CLA	CHD-C1D-ND	-2.52	122.14	124.45
26	B	614	CLA	O2D-CGD-O1D	-2.52	118.92	123.84
29	3	1623	NEX	C20-C13-C14	-2.52	119.40	122.92
25	N	606	CHL	CHB-C4A-NA	2.52	127.99	124.51
25	n	608	CHL	C1-C2-C3	-2.51	121.70	126.04
37	A	413	LMG	O3-C3-C2	-2.51	104.54	110.35
26	n	611	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
27	3	1620	LUT	C3-C4-C5	2.51	116.86	111.85
26	R	616	CLA	C1B-CHB-C4A	-2.51	125.14	130.12
27	Y	1621	LUT	C37-C21-C22	-2.51	104.68	109.44
25	5	609	CHL	C4-C3-C5	2.51	119.49	115.27
25	3	606	CHL	CMD-C2D-C3D	-2.51	121.84	127.61
27	5	1621	LUT	C38-C25-C24	-2.51	118.19	123.56
26	B	615	CLA	C4-C3-C5	2.51	119.49	115.27
25	R	608	CHL	O2A-CGA-CBA	2.51	119.78	111.91
25	5	605	CHL	O2D-CGD-O1D	-2.51	118.93	123.84
25	3	609	CHL	CHD-C4C-C3C	-2.51	121.15	124.84
29	6	1623	NEX	C11-C12-C13	-2.51	119.38	126.42
25	n	601	CHL	CMB-C2B-C3B	2.51	129.37	124.68
26	Y	612	CLA	CMB-C2B-C3B	2.51	129.37	124.68
36	A	412	SQD	O48-C23-C24	2.51	119.77	111.91
30	g	2630	LHG	C20-C19-C18	-2.50	101.71	114.42
27	1	1621	LUT	C38-C25-C24	-2.50	118.20	123.56
26	y	604	CLA	CHB-C4A-NA	2.50	127.97	124.51
30	G	2630	LHG	C20-C19-C18	-2.50	101.72	114.42
25	6	607	CHL	CMB-C2B-C3B	2.50	129.36	124.68
27	7	1620	LUT	C3-C4-C5	2.50	116.84	111.85
29	G	1623	NEX	C15-C35-C34	-2.50	118.35	123.47
26	r	616	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
27	5	1620	LUT	C15-C14-C13	-2.50	123.74	127.31
27	S	1620	LUT	C38-C25-C24	-2.50	118.21	123.56
27	s	1620	LUT	C38-C25-C24	-2.50	118.21	123.56
26	g	612	CLA	CAA-C2A-C3A	-2.50	105.93	112.78
37	b	622	LMG	O6-C1-O1	-2.50	104.05	109.97
26	N	611	CLA	C1B-CHB-C4A	-2.50	125.16	130.12
26	s	613	CLA	CHB-C4A-NA	2.50	127.97	124.51
25	s	607	CHL	O2A-CGA-CBA	2.50	119.75	111.91
26	G	612	CLA	CAA-C2A-C3A	-2.50	105.93	112.78
39	c	518	DGD	O6E-C5E-C6E	-2.50	100.22	106.44
39	C	518	DGD	O6E-C5E-C6E	-2.50	100.22	106.44
25	G	606	CHL	C1C-C2C-C3C	-2.50	105.13	107.11
26	n	610	CLA	O2D-CGD-O1D	-2.50	118.95	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	r	608	CHL	O2A-CGA-CBA	2.50	119.75	111.91
25	l	609	CHL	C4-C3-C5	2.50	119.47	115.27
26	r	613	CLA	CHB-C4A-NA	2.50	127.97	124.51
27	y	1621	LUT	C37-C21-C22	-2.50	104.71	109.44
31	B	620	BCR	C29-C30-C25	2.50	114.32	110.48
25	n	606	CHL	CHB-C4A-NA	2.50	127.96	124.51
37	a	413	LMG	O3-C3-C2	-2.50	104.58	110.35
31	a	411	BCR	C33-C5-C6	-2.50	121.72	124.53
25	8	608	CHL	CMD-C2D-C3D	-2.50	121.87	127.61
41	F	101	HEM	CMB-C2B-C1B	-2.50	121.24	125.04
41	f	101	HEM	CMB-C2B-C1B	-2.50	121.24	125.04
29	2	1623	NEX	C11-C12-C13	-2.50	119.41	126.42
25	7	606	CHL	CMD-C2D-C3D	-2.50	121.87	127.61
26	b	615	CLA	C4-C3-C5	2.50	119.47	115.27
25	y	607	CHL	CED-O2D-CGD	2.50	121.58	115.94
25	6	606	CHL	CMB-C2B-C3B	2.49	129.35	124.68
25	2	606	CHL	CMB-C2B-C3B	2.49	129.34	124.68
25	N	608	CHL	C1-C2-C3	-2.49	121.73	126.04
25	l	605	CHL	O2D-CGD-O1D	-2.49	118.96	123.84
25	G	607	CHL	O2A-CGA-CBA	2.49	119.73	111.91
25	g	607	CHL	O2A-CGA-CBA	2.49	119.73	111.91
25	Y	607	CHL	CED-O2D-CGD	2.49	121.57	115.94
25	y	608	CHL	C4-C3-C5	2.49	119.46	115.27
25	S	607	CHL	O2A-CGA-CBA	2.49	119.72	111.91
27	Y	1621	LUT	C19-C9-C8	2.49	122.00	118.08
25	8	608	CHL	CMB-C2B-C3B	2.49	129.34	124.68
27	G	1620	LUT	C28-C29-C30	-2.49	115.12	118.94
31	A	411	BCR	C33-C5-C6	-2.49	121.73	124.53
25	g	606	CHL	C1C-C2C-C3C	-2.49	105.14	107.11
26	r	601	CLA	CHD-C1D-ND	-2.49	122.17	124.45
37	B	622	LMG	O6-C1-O1	-2.49	104.08	109.97
39	H	102	DGD	C1E-O6E-C5E	2.49	118.57	113.69
30	c	522	LHG	C11-C10-C9	-2.49	101.80	114.42
28	1	1622	XAT	C15-C35-C34	-2.49	118.38	123.47
28	5	1622	XAT	C15-C35-C34	-2.49	118.38	123.47
25	4	608	CHL	CMD-C2D-C3D	-2.49	121.90	127.61
25	2	607	CHL	CMB-C2B-C3B	2.48	129.33	124.68
26	B	603	CLA	O2D-CGD-CBD	2.48	115.68	111.27
27	l	1621	LUT	C7-C8-C9	-2.48	122.48	126.23
26	Y	604	CLA	CHB-C4A-NA	2.48	127.94	124.51
29	6	1623	NEX	C35-C34-C33	-2.48	123.77	127.31
26	4	612	CLA	O2D-CGD-O1D	-2.48	118.99	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	C	522	LHG	C11-C10-C9	-2.48	101.83	114.42
25	n	608	CHL	C1C-C2C-C3C	-2.48	105.15	107.11
29	g	1623	NEX	C15-C35-C34	-2.48	118.39	123.47
26	R	613	CLA	CHB-C4A-NA	2.48	127.94	124.51
25	2	605	CHL	CMD-C2D-C3D	-2.48	121.91	127.61
37	Z	101	LMG	C1-C2-C3	-2.48	104.83	110.00
25	6	605	CHL	CMD-C2D-C3D	-2.48	121.91	127.61
31	b	620	BCR	C29-C30-C25	2.48	114.30	110.48
26	4	604	CLA	CHD-C1D-ND	-2.48	122.18	124.45
26	8	612	CLA	O2D-CGD-O1D	-2.48	118.99	123.84
25	4	608	CHL	CMB-C2B-C3B	2.48	129.31	124.68
26	Y	603	CLA	O2D-CGD-CBD	2.48	115.67	111.27
26	b	603	CLA	O2D-CGD-CBD	2.48	115.67	111.27
26	y	603	CLA	O2D-CGD-CBD	2.48	115.67	111.27
27	y	1621	LUT	C19-C9-C8	2.48	121.98	118.08
25	Y	608	CHL	C4-C3-C5	2.48	119.44	115.27
39	h	102	DGD	C1E-O6E-C5E	2.48	118.55	113.69
31	b	619	BCR	C29-C30-C25	2.47	114.29	110.48
28	2	1622	XAT	C18-C5-C4	2.47	117.06	114.28
28	6	1622	XAT	C18-C5-C4	2.47	117.06	114.28
25	3	605	CHL	CMB-C2B-C3B	2.47	129.31	124.68
26	N	610	CLA	O2D-CGD-O1D	-2.47	119.00	123.84
26	B	607	CLA	O2D-CGD-CBD	2.47	115.67	111.27
27	3	1621	LUT	C3-C4-C5	-2.47	106.92	111.85
26	y	612	CLA	CMB-C2B-C3B	2.47	129.31	124.68
26	g	603	CLA	C1-C2-C3	-2.47	121.76	126.04
27	7	1621	LUT	C3-C4-C5	-2.47	106.93	111.85
26	Y	614	CLA	CHB-C4A-NA	2.47	127.93	124.51
26	y	614	CLA	CHB-C4A-NA	2.47	127.93	124.51
25	7	609	CHL	C1B-CHB-C4A	-2.47	125.22	130.12
25	s	606	CHL	C2A-C1A-CHA	-2.47	119.53	123.86
26	S	613	CLA	CHB-C4A-NA	2.47	127.93	124.51
25	4	606	CHL	CAA-CBA-CGA	-2.47	105.95	112.51
27	n	1620	LUT	C8-C9-C10	-2.47	115.15	118.94
27	s	1621	LUT	C39-C29-C28	2.47	121.97	118.08
26	b	607	CLA	O2D-CGD-CBD	2.47	115.66	111.27
25	N	605	CHL	C1C-C2C-C3C	-2.47	105.15	107.11
28	3	1622	XAT	C32-C33-C34	-2.47	115.15	118.94
28	7	1622	XAT	C32-C33-C34	-2.47	115.15	118.94
28	g	1622	XAT	C40-C33-C32	2.47	121.97	118.08
39	c	518	DGD	C3G-C2G-C1G	-2.47	105.95	111.79
37	z	101	LMG	C1-C2-C3	-2.47	104.85	110.00

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	511	CLA	C1-C2-C3	-2.47	121.77	126.04
25	1	607	CHL	CMB-C2B-C3B	2.47	129.30	124.68
25	5	607	CHL	CMB-C2B-C3B	2.47	129.30	124.68
25	4	606	CHL	O2D-CGD-O1D	-2.47	119.01	123.84
26	C	511	CLA	C1-C2-C3	-2.47	121.77	126.04
26	b	612	CLA	CHD-C1D-ND	-2.47	122.19	124.45
39	C	518	DGD	C3G-C2G-C1G	-2.47	105.95	111.79
26	8	612	CLA	CAA-C2A-C3A	-2.47	106.02	112.78
27	g	1620	LUT	C28-C29-C30	-2.47	115.16	118.94
25	y	608	CHL	C1-C2-C3	-2.47	121.78	126.04
26	r	611	CLA	C2A-C1A-CHA	2.47	128.17	123.86
27	6	1620	LUT	C7-C8-C9	-2.47	122.51	126.23
26	B	608	CLA	CMC-C2C-C1C	-2.47	121.28	125.04
25	7	605	CHL	CMB-C2B-C3B	2.47	129.29	124.68
26	R	601	CLA	CHD-C1D-ND	-2.46	122.19	124.45
27	2	1620	LUT	C7-C8-C9	-2.46	122.51	126.23
25	5	607	CHL	O2A-CGA-CBA	2.46	119.64	111.91
26	c	510	CLA	C1B-CHB-C4A	-2.46	125.24	130.12
26	G	602	CLA	CHB-C4A-NA	2.46	127.92	124.51
25	8	606	CHL	O2D-CGD-O1D	-2.46	119.02	123.84
26	b	605	CLA	C16-C17-C18	-2.46	104.37	115.98
26	b	607	CLA	CAA-CBA-CGA	-2.46	106.06	113.25
26	7	612	CLA	CHB-C4A-NA	2.46	127.92	124.51
26	B	605	CLA	C16-C17-C18	-2.46	104.38	115.98
26	r	602	CLA	O2D-CGD-CBD	2.46	115.64	111.27
27	S	1621	LUT	C39-C29-C28	2.46	121.96	118.08
26	G	603	CLA	C1-C2-C3	-2.46	121.78	126.04
25	1	605	CHL	C4A-NA-C1A	-2.46	105.60	106.71
26	R	611	CLA	C2A-C1A-CHA	2.46	128.16	123.86
29	n	1623	NEX	C15-C35-C34	-2.46	118.43	123.47
26	4	612	CLA	CAA-C2A-C3A	-2.46	106.04	112.78
26	3	612	CLA	CHB-C4A-NA	2.46	127.92	124.51
27	N	1620	LUT	C8-C9-C10	-2.46	115.16	118.94
26	3	611	CLA	O2D-CGD-O1D	-2.46	119.03	123.84
26	C	510	CLA	C1B-CHB-C4A	-2.46	125.25	130.12
25	8	606	CHL	CAA-CBA-CGA	-2.46	105.98	112.51
39	B	626	DGD	C1D-C2D-C3D	-2.46	104.88	110.00
26	B	607	CLA	CAA-CBA-CGA	-2.46	106.07	113.25
31	B	619	BCR	C29-C30-C25	2.46	114.27	110.48
25	3	609	CHL	C1B-CHB-C4A	-2.46	125.25	130.12
27	5	1621	LUT	C30-C31-C32	-2.46	115.55	123.22
26	5	610	CLA	O2D-CGD-O1D	-2.46	119.03	123.84

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	4	620	LUT	C21-C26-C27	-2.46	109.59	112.70
26	R	602	CLA	O2D-CGD-CBD	2.46	115.63	111.27
25	S	606	CHL	C2A-C1A-CHA	-2.46	119.56	123.86
25	n	605	CHL	C1C-C2C-C3C	-2.46	105.17	107.11
25	g	608	CHL	O2A-CGA-CBA	2.46	119.61	111.91
30	1	2630	LHG	C11-C10-C9	-2.46	101.96	114.42
25	7	601	CHL	CMB-C2B-C3B	2.45	129.27	124.68
39	b	626	DGD	C1D-C2D-C3D	-2.45	104.89	110.00
25	G	608	CHL	O2A-CGA-CBA	2.45	119.61	111.91
29	2	1623	NEX	C35-C34-C33	-2.45	123.81	127.31
31	c	515	BCR	C11-C12-C13	-2.45	119.52	126.42
27	5	1621	LUT	C7-C8-C9	-2.45	122.53	126.23
26	Y	602	CLA	CAC-C3C-C4C	2.45	127.99	124.81
25	1	607	CHL	O2A-CGA-CBA	2.45	119.61	111.91
26	B	612	CLA	CHD-C1D-ND	-2.45	122.20	124.45
30	5	2630	LHG	C11-C10-C9	-2.45	101.97	114.42
29	N	1623	NEX	C15-C35-C34	-2.45	118.45	123.47
27	8	620	LUT	C21-C26-C27	-2.45	109.60	112.70
26	B	608	CLA	CHC-C1C-NC	2.45	127.92	124.20
26	b	611	CLA	CHD-C1D-ND	-2.45	122.20	124.45
28	G	1622	XAT	C40-C33-C32	2.45	121.94	118.08
25	G	605	CHL	CHB-C4A-NA	2.45	127.90	124.51
26	r	612	CLA	CHB-C4A-NA	2.45	127.90	124.51
25	Y	608	CHL	C1-C2-C3	-2.45	121.81	126.04
26	1	610	CLA	O2D-CGD-O1D	-2.45	119.06	123.84
25	g	608	CHL	O2D-CGD-O1D	-2.45	119.06	123.84
25	S	607	CHL	C4-C3-C5	2.45	119.39	115.27
25	s	607	CHL	C4-C3-C5	2.45	119.39	115.27
27	y	1621	LUT	C21-C26-C27	-2.45	109.61	112.70
30	C	2630	LHG	C11-C10-C9	-2.44	102.01	114.42
26	b	608	CLA	CMC-C2C-C1C	-2.44	121.32	125.04
30	c	2630	LHG	C11-C10-C9	-2.44	102.02	114.42
26	7	611	CLA	O2D-CGD-O1D	-2.44	119.06	123.84
31	C	515	BCR	C11-C12-C13	-2.44	119.55	126.42
26	y	603	CLA	C1-C2-C3	-2.44	121.82	126.04
27	G	1621	LUT	C21-C26-C27	-2.44	109.62	112.70
25	R	614	CHL	CAA-C2A-C3A	-2.44	110.40	116.10
29	S	1623	NEX	C39-C29-C30	-2.44	119.50	122.92
25	R	608	CHL	CHB-C4A-NA	2.44	127.88	124.51
27	6	1621	LUT	C16-C1-C6	-2.44	106.34	110.30
26	Y	610	CLA	O2A-CGA-O1A	-2.44	117.44	123.59
26	y	602	CLA	CAC-C3C-C4C	2.44	127.97	124.81

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	8	604	CLA	CHD-C1D-ND	-2.44	122.22	124.45
27	3	1621	LUT	C31-C30-C29	-2.44	123.83	127.31
30	D	408	LHG	C11-C10-C9	-2.44	102.06	114.42
25	2	601	CHL	CHB-C4A-NA	2.44	127.88	124.51
26	R	612	CLA	CHB-C4A-NA	2.44	127.88	124.51
29	s	1623	NEX	C39-C29-C30	-2.44	119.51	122.92
25	S	606	CHL	C3B-C4B-NB	2.43	112.36	109.21
27	1	1621	LUT	C30-C31-C32	-2.43	115.62	123.22
25	3	609	CHL	O2D-CGD-O1D	-2.43	119.08	123.84
30	d	408	LHG	C11-C10-C9	-2.43	102.07	114.42
26	B	615	CLA	CHB-C4A-NA	2.43	127.88	124.51
26	b	615	CLA	CHB-C4A-NA	2.43	127.88	124.51
26	7	612	CLA	C4A-NA-C1A	2.43	107.80	106.71
36	A	418	SQD	O5-C5-C4	2.43	114.11	109.69
26	a	405	CLA	C6-C7-C8	-2.43	108.06	115.92
26	3	611	CLA	C2A-C1A-CHA	2.43	128.11	123.86
26	7	611	CLA	C2A-C1A-CHA	2.43	128.11	123.86
27	5	1620	LUT	C39-C29-C28	2.43	121.91	118.08
26	y	610	CLA	O2A-CGA-O1A	-2.43	117.45	123.59
27	Y	1620	LUT	C28-C29-C30	-2.43	115.21	118.94
25	3	601	CHL	CMB-C2B-C3B	2.43	129.23	124.68
27	g	1621	LUT	C21-C26-C27	-2.43	109.63	112.70
26	g	602	CLA	CHB-C4A-NA	2.43	127.87	124.51
25	G	608	CHL	O2D-CGD-O1D	-2.43	119.09	123.84
27	N	1620	LUT	C39-C29-C28	2.43	121.91	118.08
26	N	603	CLA	CHD-C1D-ND	-2.43	122.22	124.45
26	A	405	CLA	C6-C7-C8	-2.43	108.06	115.92
26	R	601	CLA	CAC-C3C-C2C	-2.43	123.37	127.53
25	r	614	CHL	CAA-C2A-C3A	-2.43	110.43	116.10
28	7	1622	XAT	C19-C9-C8	2.43	121.90	118.08
31	4	623	BCR	C20-C19-C18	-2.43	119.59	126.42
27	r	620	LUT	C15-C35-C34	-2.43	118.50	123.47
31	8	623	BCR	C20-C19-C18	-2.43	119.60	126.42
31	D	404	BCR	C33-C5-C6	-2.43	121.80	124.53
26	r	610	CLA	O1D-CGD-CBD	2.43	129.45	124.48
28	3	1622	XAT	C19-C9-C8	2.43	121.90	118.08
27	7	1621	LUT	C31-C30-C29	-2.43	123.85	127.31
25	2	609	CHL	O2A-CGA-CBA	2.42	119.52	111.91
25	g	607	CHL	CED-O2D-CGD	2.42	121.42	115.94
26	b	608	CLA	CHC-C1C-NC	2.42	127.88	124.20
25	6	609	CHL	O2A-CGA-CBA	2.42	119.51	111.91
28	N	1622	XAT	C39-C29-C30	-2.42	119.53	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	r	601	CLA	CAC-C3C-C2C	-2.42	123.39	127.53
26	1	610	CLA	CHB-C4A-NA	2.42	127.86	124.51
25	7	609	CHL	O2D-CGD-O1D	-2.42	119.10	123.84
26	B	611	CLA	CHD-C1D-ND	-2.42	122.23	124.45
26	3	614	CLA	CHB-C4A-NA	2.42	127.86	124.51
27	Y	1621	LUT	C21-C26-C27	-2.42	109.64	112.70
25	Y	609	CHL	CMD-C2D-C3D	-2.42	122.04	127.61
25	y	609	CHL	CMD-C2D-C3D	-2.42	122.04	127.61
25	g	605	CHL	CHB-C4A-NA	2.42	127.86	124.51
27	2	1621	LUT	C16-C1-C6	-2.42	106.37	110.30
26	a	407	CLA	O2D-CGD-CBD	2.42	115.57	111.27
27	y	1620	LUT	C28-C29-C30	-2.42	115.23	118.94
25	G	607	CHL	C11-C10-C8	-2.42	108.10	115.92
26	5	610	CLA	CHB-C4A-NA	2.42	127.86	124.51
27	n	1620	LUT	C39-C29-C28	2.42	121.89	118.08
26	s	604	CLA	C2A-C1A-CHA	2.42	128.09	123.86
30	Y	2630	LHG	C11-C10-C9	-2.42	102.16	114.42
36	a	418	SQD	O5-C5-C4	2.42	114.08	109.69
30	y	2630	LHG	C11-C10-C9	-2.42	102.16	114.42
37	D	411	LMG	O1-C7-C8	-2.42	105.07	110.90
26	B	617	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
26	g	604	CLA	CHD-C1D-ND	-2.41	122.23	124.45
26	R	610	CLA	O1D-CGD-CBD	2.41	129.42	124.48
26	b	617	CLA	CAA-C2A-C3A	-2.41	106.17	112.78
25	y	607	CHL	C1-O2A-CGA	2.41	122.78	116.44
25	g	607	CHL	C11-C10-C8	-2.41	108.12	115.92
26	d	403	CLA	C7-C6-C5	-2.41	106.81	113.36
27	1	1620	LUT	C39-C29-C28	2.41	121.88	118.08
26	D	403	CLA	C7-C6-C5	-2.41	106.81	113.36
31	d	404	BCR	C33-C5-C6	-2.41	121.82	124.53
25	G	606	CHL	O2D-CGD-O1D	-2.41	119.13	123.84
37	B	622	LMG	C38-C37-C36	-2.41	102.19	114.42
25	6	607	CHL	O1D-CGD-CBD	-2.41	119.55	124.48
30	c	2630	LHG	O8-C23-C24	2.41	119.47	111.91
25	r	608	CHL	CHB-C4A-NA	2.41	127.84	124.51
30	C	2630	LHG	O8-C23-C24	2.41	119.47	111.91
37	d	411	LMG	O1-C7-C8	-2.41	105.09	110.90
26	c	501	CLA	CHB-C4A-NA	2.41	127.84	124.51
26	r	610	CLA	CHD-C1D-ND	-2.41	122.24	124.45
30	1	2630	LHG	C20-C19-C18	-2.41	102.20	114.42
28	n	1622	XAT	C39-C29-C30	-2.41	119.55	122.92
26	Y	603	CLA	C1-C2-C3	-2.41	121.88	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
30	R	2630	LHG	C20-C19-C18	-2.41	102.21	114.42
26	2	604	CLA	CHB-C4A-NA	2.41	127.84	124.51
30	r	2630	LHG	C20-C19-C18	-2.41	102.21	114.42
37	b	622	LMG	C38-C37-C36	-2.40	102.22	114.42
31	8	623	BCR	C27-C26-C25	-2.40	119.24	122.73
27	N	1621	LUT	C19-C9-C8	2.40	121.86	118.08
25	1	606	CHL	C1C-C2C-C3C	-2.40	105.21	107.11
26	7	614	CLA	CHB-C4A-NA	2.40	127.83	124.51
25	2	607	CHL	O1D-CGD-CBD	-2.40	119.57	124.48
25	G	607	CHL	CED-O2D-CGD	2.40	121.37	115.94
31	t	101	BCR	C39-C30-C25	-2.40	106.40	110.30
27	s	1621	LUT	C15-C14-C13	-2.40	123.88	127.31
26	C	501	CLA	CHB-C4A-NA	2.40	127.83	124.51
26	A	407	CLA	O2D-CGD-CBD	2.40	115.53	111.27
27	R	620	LUT	C15-C35-C34	-2.40	118.56	123.47
30	5	2630	LHG	C20-C19-C18	-2.40	102.24	114.42
26	N	602	CLA	C2D-C1D-ND	-2.40	108.33	110.10
25	Y	607	CHL	C1-O2A-CGA	2.40	122.74	116.44
25	2	609	CHL	O2D-CGD-O1D	-2.40	119.15	123.84
25	6	609	CHL	O2D-CGD-O1D	-2.40	119.15	123.84
25	s	606	CHL	C3B-C4B-NB	2.40	112.31	109.21
31	T	101	BCR	C39-C30-C25	-2.40	106.41	110.30
31	H	101	BCR	C31-C1-C6	-2.40	106.41	110.30
26	1	612	CLA	C2A-C1A-CHA	2.40	128.05	123.86
26	5	612	CLA	C2A-C1A-CHA	2.40	128.05	123.86
26	n	603	CLA	CHD-C1D-ND	-2.40	122.25	124.45
25	2	609	CHL	O1D-CGD-CBD	-2.40	119.58	124.48
25	s	606	CHL	C4D-CHA-C1A	-2.40	118.33	121.25
25	5	606	CHL	C1C-C2C-C3C	-2.40	105.21	107.11
30	D	409	LHG	C18-C17-C16	-2.40	102.26	114.42
26	c	501	CLA	C7-C6-C5	-2.40	106.85	113.36
25	6	601	CHL	CHB-C4A-NA	2.40	127.83	124.51
25	7	605	CHL	O2D-CGD-O1D	-2.40	119.16	123.84
27	2	1620	LUT	C28-C29-C30	-2.39	115.27	118.94
29	3	1623	NEX	C28-C29-C30	2.39	122.62	118.94
25	3	605	CHL	O2D-CGD-O1D	-2.39	119.16	123.84
26	y	613	CLA	O2D-CGD-O1D	-2.39	119.16	123.84
25	4	606	CHL	C1B-CHB-C4A	-2.39	125.37	130.12
25	6	609	CHL	O1D-CGD-CBD	-2.39	119.58	124.48
26	C	501	CLA	C7-C6-C5	-2.39	106.86	113.36
26	B	606	CLA	C2D-C1D-ND	-2.39	108.34	110.10
26	b	606	CLA	C2D-C1D-ND	-2.39	108.34	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	D	402	CLA	CAC-C3C-C4C	2.39	127.92	124.81
29	Y	1623	NEX	C15-C35-C34	-2.39	118.57	123.47
26	S	614	CLA	CHB-C4A-NA	2.39	127.82	124.51
28	r	622	XAT	C24-C23-C22	-2.39	106.15	110.77
29	y	1623	NEX	C15-C35-C34	-2.39	118.57	123.47
26	4	604	CLA	CHB-C4A-NA	2.39	127.82	124.51
30	7	2630	LHG	O8-C23-C24	2.39	119.41	111.91
39	c	519	DGD	C3G-C2G-C1G	-2.39	106.13	111.79
30	d	409	LHG	C18-C17-C16	-2.39	102.29	114.42
30	1	2630	LHG	O8-C23-C24	2.39	119.41	111.91
26	y	613	CLA	CHB-C4A-NA	2.39	127.82	124.51
37	a	415	LMG	O6-C1-O1	-2.39	104.31	109.97
25	Y	605	CHL	O2A-CGA-CBA	2.39	119.41	111.91
25	g	606	CHL	O2D-CGD-O1D	-2.39	119.17	123.84
27	S	1621	LUT	C38-C25-C24	-2.39	118.45	123.56
26	B	605	CLA	C6-C5-C3	-2.39	107.19	113.45
25	3	606	CHL	C4A-NA-C1A	-2.39	105.63	106.71
25	5	606	CHL	CED-O2D-CGD	2.39	121.34	115.94
28	N	1622	XAT	C18-C5-C4	2.39	116.97	114.28
25	y	605	CHL	O2A-CGA-CBA	2.39	119.40	111.91
30	5	2630	LHG	O8-C23-C24	2.39	119.40	111.91
25	8	609	CHL	C1C-C2C-C3C	-2.39	105.22	107.11
26	D	403	CLA	CHD-C1D-ND	-2.39	122.26	124.45
25	n	608	CHL	O2D-CGD-O1D	-2.39	119.17	123.84
31	B	619	BCR	C21-C20-C19	-2.39	115.77	123.22
26	S	604	CLA	C2A-C1A-CHA	2.39	128.03	123.86
25	8	606	CHL	CMB-C2B-C3B	2.39	129.14	124.68
27	S	1621	LUT	C15-C14-C13	-2.39	123.91	127.31
28	4	622	XAT	C30-C31-C32	-2.39	115.77	123.22
31	b	619	BCR	C21-C20-C19	-2.39	115.77	123.22
25	g	601	CHL	O2A-CGA-CBA	2.39	119.39	111.91
26	N	611	CLA	CMB-C2B-C3B	2.39	129.14	124.68
26	n	611	CLA	CMB-C2B-C3B	2.39	129.14	124.68
26	s	613	CLA	CHD-C1D-ND	-2.39	122.26	124.45
26	g	614	CLA	CHB-C4A-NA	2.38	127.81	124.51
30	b	2631	LHG	O8-C23-C24	2.38	119.39	111.91
25	N	607	CHL	CAA-C2A-C3A	-2.38	106.25	112.78
26	2	603	CLA	CAA-C2A-C3A	-2.38	106.25	112.78
26	6	603	CLA	CAA-C2A-C3A	-2.38	106.25	112.78
26	R	611	CLA	O2A-CGA-O1A	-2.38	117.58	123.59
26	N	611	CLA	CHB-C4A-NA	2.38	127.81	124.51
26	n	611	CLA	CHB-C4A-NA	2.38	127.81	124.51

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	4	606	CHL	CMB-C2B-C3B	2.38	129.14	124.68
25	3	607	CHL	CHD-C4C-C3C	-2.38	121.34	124.84
28	8	622	XAT	C30-C31-C32	-2.38	115.78	123.22
26	R	610	CLA	CHD-C1D-ND	-2.38	122.26	124.45
26	d	402	CLA	CAC-C3C-C4C	2.38	127.90	124.81
25	y	607	CHL	CMD-C2D-C3D	-2.38	122.13	127.61
28	5	1622	XAT	C24-C23-C22	-2.38	106.17	110.77
27	6	1620	LUT	C28-C29-C30	-2.38	115.29	118.94
25	6	606	CHL	CHB-C4A-NA	2.38	127.81	124.51
26	S	603	CLA	O2A-CGA-O1A	-2.38	117.36	123.30
37	a	413	LMG	C40-C39-C38	-2.38	102.34	114.42
25	G	601	CHL	O2A-CGA-CBA	2.38	119.38	111.91
36	B	621	SQD	C45-O47-C7	2.38	123.65	117.79
37	A	413	LMG	C40-C39-C38	-2.38	102.34	114.42
30	3	2630	LHG	O8-C23-C24	2.38	119.38	111.91
36	b	621	SQD	C45-O47-C7	2.38	123.65	117.79
25	1	607	CHL	C4-C3-C5	2.38	119.27	115.27
26	6	604	CLA	CHB-C4A-NA	2.38	127.80	124.51
25	N	607	CHL	O2A-CGA-CBA	2.38	119.37	111.91
26	n	602	CLA	C2D-C1D-ND	-2.38	108.35	110.10
31	h	101	BCR	C31-C1-C6	-2.38	106.44	110.30
26	Y	613	CLA	CHB-C4A-NA	2.38	127.80	124.51
37	A	413	LMG	C6-C5-C4	-2.38	107.44	113.00
39	C	519	DGD	C3G-C2G-C1G	-2.38	106.17	111.79
37	A	415	LMG	O6-C1-O1	-2.38	104.34	109.97
30	b	2631	LHG	C20-C19-C18	-2.38	102.36	114.42
27	3	1620	LUT	C39-C29-C28	2.38	121.82	118.08
25	N	608	CHL	O2D-CGD-O1D	-2.38	119.19	123.84
26	r	602	CLA	CHD-C1D-ND	-2.38	122.27	124.45
25	n	607	CHL	O2A-CGA-CBA	2.38	119.36	111.91
29	7	1623	NEX	C28-C29-C30	2.38	122.59	118.94
26	4	610	CLA	C4A-NA-C1A	2.38	107.77	106.71
26	8	610	CLA	C4A-NA-C1A	2.38	107.77	106.71
25	S	606	CHL	C4D-CHA-C1A	-2.38	118.36	121.25
25	8	606	CHL	C1B-CHB-C4A	-2.38	125.41	130.12
25	4	609	CHL	C1C-C2C-C3C	-2.38	105.23	107.11
30	B	2631	LHG	O8-C23-C24	2.38	119.36	111.91
25	5	607	CHL	C4-C3-C5	2.37	119.27	115.27
31	4	623	BCR	C27-C26-C25	-2.37	119.28	122.73
26	b	605	CLA	C6-C5-C3	-2.37	107.23	113.45
30	B	2631	LHG	C20-C19-C18	-2.37	102.37	114.42
25	R	608	CHL	C1C-C2C-C3C	-2.37	105.23	107.11

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
35	A	409	PHO	C1-C2-C3	-2.37	121.94	126.04
25	S	606	CHL	CMA-C3A-C2A	-2.37	104.25	113.83
25	7	606	CHL	C4A-NA-C1A	-2.37	105.64	106.71
26	r	611	CLA	O2A-CGA-O1A	-2.37	117.60	123.59
26	b	617	CLA	C1B-CHB-C4A	-2.37	125.42	130.12
27	n	1621	LUT	C19-C9-C8	2.37	121.81	118.08
26	B	610	CLA	CMD-C2D-C3D	2.37	133.07	127.61
37	a	413	LMG	C6-C5-C4	-2.37	107.45	113.00
26	7	603	CLA	CHA-C1A-NA	-2.37	120.97	126.40
30	G	2630	LHG	O8-C23-C24	2.37	119.35	111.91
28	n	1622	XAT	C18-C5-C4	2.37	116.95	114.28
27	Y	1621	LUT	C7-C8-C9	-2.37	122.65	126.23
30	D	409	LHG	C11-C10-C9	-2.37	102.39	114.42
26	b	610	CLA	CMD-C2D-C3D	2.37	133.07	127.61
39	C	518	DGD	CAB-C9B-C8B	-2.37	102.39	114.42
38	D	405	PL9	C8-C7-C3	2.37	118.68	111.98
27	7	1620	LUT	C39-C29-C28	2.37	121.81	118.08
27	Y	1620	LUT	C31-C30-C29	-2.37	123.93	127.31
27	6	1621	LUT	C38-C25-C24	-2.37	118.49	123.56
29	r	623	NEX	C11-C12-C13	-2.37	119.76	126.42
26	Y	610	CLA	C1-C2-C3	-2.37	121.95	126.04
25	Y	607	CHL	CMD-C2D-C3D	-2.37	122.17	127.61
31	t	101	BCR	C7-C6-C5	-2.37	115.72	121.46
26	Y	613	CLA	O2D-CGD-O1D	-2.37	119.21	123.84
31	C	516	BCR	C32-C1-C6	2.37	114.14	110.30
31	c	516	BCR	C32-C1-C6	2.37	114.14	110.30
27	s	1621	LUT	C38-C25-C24	-2.37	118.49	123.56
25	l	606	CHL	CED-O2D-CGD	2.37	121.29	115.94
30	d	409	LHG	C11-C10-C9	-2.37	102.40	114.42
26	G	614	CLA	CHB-C4A-NA	2.37	127.79	124.51
28	y	1622	XAT	O4-C5-C6	-2.37	57.00	58.96
25	n	607	CHL	CAA-C2A-C3A	-2.37	106.30	112.78
27	y	1621	LUT	C7-C8-C9	-2.37	122.66	126.23
25	7	606	CHL	O2D-CGD-O1D	-2.37	119.21	123.84
30	N	2630	LHG	C27-C26-C25	-2.37	102.41	114.42
26	B	610	CLA	CHB-C4A-NA	2.37	127.78	124.51
26	s	604	CLA	C3A-C2A-C1A	2.37	104.88	101.34
26	R	610	CLA	CAA-CBA-CGA	-2.37	106.34	113.25
29	R	623	NEX	C11-C12-C13	-2.37	119.77	126.42
28	l	1622	XAT	C24-C23-C22	-2.36	106.21	110.77
29	7	1623	NEX	C26-C27-C28	-2.36	120.99	125.99
26	3	603	CLA	CHA-C1A-NA	-2.36	120.98	126.40

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	3	606	CHL	O2D-CGD-O1D	-2.36	119.22	123.84
26	b	607	CLA	CAC-C3C-C4C	2.36	127.88	124.81
39	c	518	DGD	CAB-C9B-C8B	-2.36	102.42	114.42
30	g	2630	LHG	O8-C23-C24	2.36	119.33	111.91
31	T	101	BCR	C7-C6-C5	-2.36	115.74	121.46
26	s	614	CLA	CHB-C4A-NA	2.36	127.78	124.51
27	s	1621	LUT	C11-C10-C9	-2.36	123.94	127.31
26	C	501	CLA	CMB-C2B-C3B	2.36	129.10	124.68
25	7	607	CHL	CHD-C4C-C3C	-2.36	121.37	124.84
25	s	606	CHL	CMA-C3A-C2A	-2.36	104.30	113.83
28	R	622	XAT	C24-C23-C22	-2.36	106.21	110.77
31	a	411	BCR	C37-C22-C23	2.36	121.80	118.08
38	d	405	PL9	C8-C7-C3	2.36	118.65	111.98
27	2	1621	LUT	C38-C25-C24	-2.36	118.51	123.56
26	3	602	CLA	CHB-C4A-NA	2.36	127.78	124.51
26	7	602	CLA	CHB-C4A-NA	2.36	127.78	124.51
35	a	408	PHO	O2D-CGD-O1D	-2.36	119.22	123.84
26	r	610	CLA	CAA-CBA-CGA	-2.36	106.36	113.25
30	n	2630	LHG	C27-C26-C25	-2.36	102.44	114.42
39	H	102	DGD	C3G-C2G-C1G	-2.36	106.21	111.79
26	y	610	CLA	C1-C2-C3	-2.36	121.97	126.04
30	d	409	LHG	C27-C26-C25	-2.36	102.45	114.42
25	r	608	CHL	C1C-C2C-C3C	-2.36	105.24	107.11
26	Y	610	CLA	CHB-C4A-NA	2.36	127.77	124.51
26	8	604	CLA	CHB-C4A-NA	2.36	127.77	124.51
26	y	610	CLA	CHB-C4A-NA	2.36	127.77	124.51
27	y	1620	LUT	C31-C30-C29	-2.36	123.95	127.31
27	y	1620	LUT	C8-C9-C10	-2.36	115.32	118.94
36	b	621	SQD	C1-O5-C5	2.36	118.31	113.69
26	b	610	CLA	CHB-C4A-NA	2.36	127.77	124.51
26	B	605	CLA	CHA-C4D-ND	2.36	137.43	132.50
26	b	605	CLA	CHA-C4D-ND	2.36	137.43	132.50
27	4	620	LUT	C39-C29-C28	2.36	121.79	118.08
25	Y	605	CHL	O2D-CGD-O1D	-2.36	119.23	123.84
30	R	2630	LHG	O8-C23-C24	2.36	119.30	111.91
26	7	610	CLA	O2A-CGA-O1A	-2.36	117.65	123.59
27	Y	1620	LUT	C8-C9-C10	-2.36	115.33	118.94
30	D	409	LHG	C27-C26-C25	-2.36	102.47	114.42
26	3	612	CLA	C4A-NA-C1A	2.36	107.77	106.71
26	d	403	CLA	CHD-C1D-ND	-2.35	122.29	124.45
26	s	603	CLA	O2A-CGA-O1A	-2.35	117.43	123.30
30	N	2630	LHG	C18-C17-C16	-2.35	102.47	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	r	612	CLA	CAA-C2A-C3A	-2.35	106.33	112.78
27	G	1621	LUT	C39-C29-C28	2.35	121.79	118.08
26	G	604	CLA	CHD-C1D-ND	-2.35	122.29	124.45
27	g	1621	LUT	C39-C29-C28	2.35	121.78	118.08
25	5	605	CHL	C4A-NA-C1A	-2.35	105.65	106.71
39	c	519	DGD	CBB-CAB-C9B	-2.35	102.48	114.42
36	B	621	SQD	C1-O5-C5	2.35	118.31	113.69
29	3	1623	NEX	C26-C27-C28	-2.35	121.02	125.99
26	S	613	CLA	CHD-C1D-ND	-2.35	122.29	124.45
25	2	606	CHL	CHB-C4A-NA	2.35	127.76	124.51
26	s	611	CLA	O2A-CGA-O1A	-2.35	117.66	123.59
26	B	607	CLA	CAC-C3C-C4C	2.35	127.86	124.81
26	A	406	CLA	C11-C12-C13	-2.35	108.32	115.92
30	Y	2630	LHG	C20-C19-C18	-2.35	102.50	114.42
26	R	602	CLA	CHD-C1D-ND	-2.35	122.30	124.45
39	h	102	DGD	C3G-C2G-C1G	-2.35	106.23	111.79
26	S	602	CLA	CHB-C4A-NA	2.35	127.76	124.51
29	3	1623	NEX	C35-C34-C33	-2.35	123.96	127.31
29	7	1623	NEX	C35-C34-C33	-2.35	123.96	127.31
27	8	620	LUT	C39-C29-C28	2.35	121.78	118.08
35	a	409	PHO	C1-C2-C3	-2.35	121.98	126.04
29	r	623	NEX	O24-C25-C26	-2.35	57.02	58.96
26	c	503	CLA	O2D-CGD-O1D	-2.35	119.25	123.84
27	6	1620	LUT	C21-C26-C27	-2.35	109.73	112.70
26	r	603	CLA	CAA-C2A-C3A	-2.35	106.35	112.78
28	Y	1622	XAT	C31-C32-C33	-2.35	119.82	126.42
39	C	518	DGD	O3D-C3D-C4D	-2.35	104.92	110.35
26	S	611	CLA	O2A-CGA-O1A	-2.35	117.67	123.59
39	C	519	DGD	CBB-CAB-C9B	-2.35	102.52	114.42
25	y	605	CHL	O2D-CGD-O1D	-2.35	119.25	123.84
30	y	2630	LHG	C20-C19-C18	-2.35	102.52	114.42
26	B	609	CLA	CHD-C1D-ND	-2.34	122.30	124.45
26	b	609	CLA	CHD-C1D-ND	-2.34	122.30	124.45
30	n	2630	LHG	C18-C17-C16	-2.34	102.52	114.42
26	R	603	CLA	CAA-C2A-C3A	-2.34	106.36	112.78
26	B	617	CLA	C1B-CHB-C4A	-2.34	125.47	130.12
39	B	626	DGD	O3G-C3G-C2G	-2.34	105.24	110.90
26	R	613	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
28	y	1622	XAT	C31-C32-C33	-2.34	119.83	126.42
25	r	606	CHL	O2A-CGA-O1A	-2.34	117.68	123.59
25	5	606	CHL	C4D-CHA-C1A	-2.34	118.40	121.25
30	r	2630	LHG	O8-C23-C24	2.34	119.26	111.91

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	a	406	CLA	C11-C12-C13	-2.34	108.35	115.92
35	A	408	PHO	O2D-CGD-O1D	-2.34	119.26	123.84
26	3	610	CLA	O2A-CGA-O1A	-2.34	117.68	123.59
28	2	1622	XAT	C31-C32-C33	-2.34	119.84	126.42
39	b	626	DGD	O3G-C3G-C2G	-2.34	105.25	110.90
27	G	1620	LUT	C7-C8-C9	-2.34	122.70	126.23
39	c	518	DGD	O3D-C3D-C4D	-2.34	104.94	110.35
27	2	1620	LUT	C21-C26-C27	-2.34	109.74	112.70
26	c	507	CLA	CBC-CAC-C3C	-2.34	105.98	112.43
27	6	1620	LUT	C12-C13-C14	-2.34	115.35	118.94
26	c	501	CLA	CMB-C2B-C3B	2.34	129.06	124.68
27	S	1621	LUT	C11-C10-C9	-2.34	123.97	127.31
31	8	623	BCR	C37-C22-C23	2.34	121.76	118.08
25	2	608	CHL	CHB-C4A-NA	2.34	127.75	124.51
25	n	606	CHL	CMD-C2D-C3D	-2.34	122.24	127.61
26	C	507	CLA	CBC-CAC-C3C	-2.34	105.99	112.43
26	R	612	CLA	CAA-C2A-C3A	-2.34	106.38	112.78
26	1	603	CLA	CHD-C1D-ND	-2.34	122.31	124.45
26	5	603	CLA	CHD-C1D-ND	-2.34	122.31	124.45
27	2	1620	LUT	C12-C13-C14	-2.34	115.36	118.94
27	3	1620	LUT	C20-C13-C12	2.34	121.76	118.08
26	C	503	CLA	O2D-CGD-O1D	-2.34	119.27	123.84
25	r	606	CHL	CAC-C3C-C4C	2.34	127.84	124.81
35	a	409	PHO	C1B-NB-C4B	2.33	111.89	107.09
26	s	610	CLA	C1-C2-C3	-2.33	122.00	126.04
26	S	604	CLA	C3A-C2A-C1A	2.33	104.84	101.34
30	B	2630	LHG	C20-C19-C18	-2.33	102.57	114.42
31	A	411	BCR	C37-C22-C23	2.33	121.75	118.08
28	Y	1622	XAT	O4-C5-C6	-2.33	57.03	58.96
26	7	602	CLA	O2D-CGD-CBD	2.33	115.41	111.27
26	r	613	CLA	O2A-CGA-O1A	-2.33	117.71	123.59
26	C	512	CLA	CHB-C4A-NA	2.33	127.74	124.51
26	B	606	CLA	CHC-C1C-NC	2.33	127.74	124.20
26	b	606	CLA	CHC-C1C-NC	2.33	127.74	124.20
25	R	606	CHL	O2A-CGA-O1A	-2.33	117.71	123.59
37	a	415	LMG	C40-C39-C38	-2.33	102.59	114.42
26	b	605	CLA	C2A-C3A-C4A	2.33	105.63	101.87
30	b	2630	LHG	C20-C19-C18	-2.33	102.59	114.42
37	A	415	LMG	C40-C39-C38	-2.33	102.59	114.42
25	2	607	CHL	C1B-CHB-C4A	-2.33	125.50	130.12
41	f	101	HEM	C4D-ND-C1D	2.33	107.48	105.07
38	D	405	PL9	C22-C23-C24	-2.33	122.05	127.66

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
38	d	405	PL9	C22-C23-C24	-2.33	122.05	127.66
27	g	1620	LUT	C7-C8-C9	-2.33	122.72	126.23
26	2	610	CLA	C1-C2-C3	-2.33	122.98	126.75
25	N	606	CHL	CMD-C2D-C3D	-2.33	122.26	127.61
30	l	101	LHG	C20-C19-C18	-2.33	102.61	114.42
25	6	607	CHL	C1B-CHB-C4A	-2.33	125.51	130.12
28	6	1622	XAT	C31-C32-C33	-2.33	119.88	126.42
26	5	602	CLA	CAC-C3C-C4C	2.33	127.83	124.81
26	s	602	CLA	CHB-C4A-NA	2.33	127.73	124.51
26	s	602	CLA	C1-C2-C3	-2.33	122.02	126.04
27	1	1620	LUT	C19-C9-C8	2.33	121.74	118.08
25	R	606	CHL	CHB-C4A-NA	2.32	127.73	124.51
26	R	603	CLA	C2D-C1D-ND	-2.32	108.39	110.10
27	2	1621	LUT	C18-C5-C6	-2.32	121.92	124.53
27	Y	1621	LUT	C31-C30-C29	-2.32	123.99	127.31
35	A	408	PHO	C6-C7-C8	-2.32	108.41	115.92
25	1	609	CHL	CMB-C2B-C3B	2.32	129.03	124.68
26	B	611	CLA	C3A-C2A-C1A	2.32	104.82	101.34
30	s	2630	LHG	C11-C10-C9	-2.32	102.63	114.42
39	c	520	DGD	C3G-C2G-C1G	-2.32	106.29	111.79
26	R	613	CLA	CHD-C1D-ND	-2.32	122.32	124.45
26	r	613	CLA	CHD-C1D-ND	-2.32	122.32	124.45
26	b	615	CLA	C1B-CHB-C4A	-2.32	125.52	130.12
25	2	608	CHL	C2A-C1A-CHA	-2.32	119.80	123.86
25	g	601	CHL	CMB-C2B-C3B	2.32	129.02	124.68
28	g	1622	XAT	C39-C29-C30	-2.32	119.67	122.92
30	L	101	LHG	C20-C19-C18	-2.32	102.64	114.42
25	r	606	CHL	CHB-C4A-NA	2.32	127.72	124.51
25	G	601	CHL	CMB-C2B-C3B	2.32	129.02	124.68
25	s	608	CHL	C2A-C3A-C4A	-2.32	98.12	101.87
25	8	607	CHL	CMB-C2B-C3B	2.32	129.02	124.68
27	5	1620	LUT	C19-C9-C8	2.32	121.73	118.08
25	6	608	CHL	C2A-C1A-CHA	-2.32	119.80	123.86
35	a	408	PHO	C6-C7-C8	-2.32	108.42	115.92
35	a	409	PHO	CMC-C2C-C3C	2.32	129.32	124.94
25	1	606	CHL	C4D-CHA-C1A	-2.32	118.42	121.25
30	g	2630	LHG	C27-C26-C25	-2.32	102.65	114.42
31	4	623	BCR	C37-C22-C23	2.32	121.73	118.08
30	S	2630	LHG	C11-C10-C9	-2.32	102.65	114.42
26	c	512	CLA	CHB-C4A-NA	2.32	127.72	124.51
29	R	623	NEX	O24-C25-C26	-2.32	57.04	58.96
26	b	611	CLA	C3A-C2A-C1A	2.32	104.81	101.34

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	S	610	CLA	C1-C2-C3	-2.32	122.03	126.04
26	B	615	CLA	O2A-CGA-O1A	-2.32	117.74	123.59
27	n	1621	LUT	C35-C15-C14	-2.32	118.73	123.47
30	G	2630	LHG	C27-C26-C25	-2.32	102.66	114.42
26	R	613	CLA	O2D-CGD-O1D	-2.32	119.31	123.84
28	n	1622	XAT	C7-C8-C9	-2.32	121.94	125.53
35	A	409	PHO	C1B-NB-C4B	2.32	111.85	107.09
27	Y	1620	LUT	C15-C35-C34	-2.32	118.73	123.47
26	B	615	CLA	C1B-CHB-C4A	-2.32	125.53	130.12
26	3	602	CLA	O2D-CGD-CBD	2.32	115.38	111.27
29	r	623	NEX	C28-C29-C30	2.31	122.49	118.94
25	R	607	CHL	CED-O2D-CGD	2.31	121.17	115.94
26	a	406	CLA	C1C-C2C-C3C	-2.31	104.52	106.96
27	S	1621	LUT	C16-C1-C6	-2.31	106.55	110.30
25	y	605	CHL	CMD-C2D-C3D	-2.31	122.29	127.61
27	8	620	LUT	C1-C6-C5	-2.31	119.35	122.61
26	r	603	CLA	C2D-C1D-ND	-2.31	108.40	110.10
29	7	1623	NEX	C12-C13-C14	2.31	122.49	118.94
41	F	101	HEM	C4D-ND-C1D	2.31	107.46	105.07
26	C	505	CLA	C1-C2-C3	-2.31	122.04	126.04
26	r	612	CLA	C1B-CHB-C4A	-2.31	125.54	130.12
25	1	601	CHL	C2A-C1A-CHA	-2.31	119.82	123.86
27	4	620	LUT	C1-C6-C5	-2.31	119.36	122.61
39	C	520	DGD	C3G-C2G-C1G	-2.31	106.32	111.79
35	A	409	PHO	CMC-C2C-C3C	2.31	129.30	124.94
27	y	1620	LUT	C15-C35-C34	-2.31	118.74	123.47
25	5	601	CHL	C2A-C1A-CHA	-2.31	119.82	123.86
29	S	1623	NEX	O24-C25-C26	-2.31	57.05	58.96
26	S	602	CLA	C1-C2-C3	-2.31	122.05	126.04
25	G	606	CHL	C2A-C1A-CHA	-2.31	119.82	123.86
39	c	519	DGD	C5B-C4B-C3B	-2.31	102.70	114.42
31	C	515	BCR	C36-C18-C19	2.31	121.71	118.08
31	c	515	BCR	C36-C18-C19	2.31	121.71	118.08
25	6	608	CHL	CHB-C4A-NA	2.31	127.70	124.51
27	6	1621	LUT	C18-C5-C6	-2.31	121.94	124.53
26	7	602	CLA	CHD-C1D-ND	-2.31	122.33	124.45
27	G	1621	LUT	C15-C35-C34	-2.31	118.75	123.47
25	3	607	CHL	C1-O2A-CGA	2.31	122.50	116.44
25	5	609	CHL	CMB-C2B-C3B	2.31	128.99	124.68
26	B	605	CLA	C2A-C3A-C4A	2.31	105.59	101.87
25	7	608	CHL	CMD-C2D-C3D	-2.31	122.31	127.61
25	G	605	CHL	OMC-CMC-C2C	-2.31	120.47	125.69

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	7	1620	LUT	C20-C13-C12	2.31	121.71	118.08
25	s	601	CHL	C4D-CHA-C1A	-2.31	118.44	121.25
27	y	1621	LUT	C31-C30-C29	-2.31	124.02	127.31
28	8	622	XAT	C19-C9-C8	2.30	121.71	118.08
37	b	622	LMG	C40-C39-C38	-2.30	102.73	114.42
26	b	615	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
26	r	602	CLA	O2A-CGA-O1A	-2.30	117.78	123.59
26	6	610	CLA	C1-C2-C3	-2.30	123.02	126.75
25	s	607	CHL	CMD-C2D-C3D	-2.30	122.31	127.61
39	C	519	DGD	C5B-C4B-C3B	-2.30	102.73	114.42
26	c	513	CLA	CAA-CBA-CGA	-2.30	106.52	113.25
28	G	1622	XAT	C39-C29-C30	-2.30	119.70	122.92
25	5	609	CHL	O1D-CGD-CBD	-2.30	119.77	124.48
26	B	603	CLA	CHD-C1D-ND	-2.30	122.34	124.45
26	R	603	CLA	C3C-C4C-NC	-2.30	107.99	110.57
26	r	613	CLA	O2D-CGD-O1D	-2.30	119.34	123.84
37	C	521	LMG	C40-C39-C38	-2.30	102.74	114.42
26	1	612	CLA	CHA-C1A-NA	-2.30	121.13	126.40
25	7	607	CHL	C1-O2A-CGA	2.30	122.48	116.44
27	s	1621	LUT	C16-C1-C6	-2.30	106.57	110.30
39	B	626	DGD	O2G-C1B-O1B	-2.30	118.14	123.70
25	S	608	CHL	C2A-C3A-C4A	-2.30	98.15	101.87
27	N	1621	LUT	C35-C15-C14	-2.30	118.76	123.47
25	Y	605	CHL	CMD-C2D-C3D	-2.30	122.32	127.61
27	g	1621	LUT	C15-C35-C34	-2.30	118.76	123.47
28	4	622	XAT	C19-C9-C8	2.30	121.70	118.08
25	R	606	CHL	CAC-C3C-C4C	2.30	127.80	124.81
25	g	606	CHL	C2A-C1A-CHA	-2.30	119.84	123.86
26	g	611	CLA	O2D-CGD-CBD	2.30	115.35	111.27
26	b	612	CLA	CMC-C2C-C1C	-2.30	121.54	125.04
25	S	607	CHL	CMD-C2D-C3D	-2.30	122.33	127.61
25	4	607	CHL	CMB-C2B-C3B	2.30	128.98	124.68
26	c	505	CLA	CHB-C4A-NA	2.30	127.69	124.51
29	3	1623	NEX	C12-C13-C14	2.30	122.47	118.94
26	B	612	CLA	CMC-C2C-C1C	-2.30	121.54	125.04
37	c	521	LMG	C40-C39-C38	-2.30	102.76	114.42
26	1	602	CLA	CAC-C3C-C4C	2.30	127.79	124.81
37	B	622	LMG	C40-C39-C38	-2.30	102.76	114.42
29	R	623	NEX	C28-C29-C30	2.30	122.47	118.94
39	c	520	DGD	O3E-C3E-C2E	-2.30	105.04	110.35
37	A	413	LMG	C38-C37-C36	-2.30	102.77	114.42
37	A	415	LMG	O3-C3-C2	-2.30	105.04	110.35

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	a	415	LMG	O3-C3-C2	-2.30	105.04	110.35
30	d	409	LHG	C20-C19-C18	-2.30	102.77	114.42
26	b	603	CLA	CHD-C1D-ND	-2.30	122.34	124.45
26	c	505	CLA	C1-C2-C3	-2.30	122.07	126.04
29	s	1623	NEX	O24-C25-C26	-2.30	57.06	58.96
39	C	520	DGD	O3E-C3E-C2E	-2.30	105.04	110.35
37	B	2633	LMG	C40-C39-C38	-2.29	102.78	114.42
26	y	611	CLA	CMB-C2B-C3B	2.29	128.97	124.68
26	3	602	CLA	CHD-C1D-ND	-2.29	122.35	124.45
25	r	607	CHL	CED-O2D-CGD	2.29	121.12	115.94
28	N	1622	XAT	C7-C8-C9	-2.29	121.97	125.53
26	b	605	CLA	O2D-CGD-O1D	-2.29	119.36	123.84
26	5	612	CLA	CHA-C1A-NA	-2.29	121.15	126.40
39	b	626	DGD	O2G-C1B-O1B	-2.29	118.16	123.70
31	D	404	BCR	C35-C13-C12	2.29	121.69	118.08
31	d	404	BCR	C35-C13-C12	2.29	121.69	118.08
30	D	409	LHG	C20-C19-C18	-2.29	102.79	114.42
25	s	601	CHL	O2D-CGD-O1D	-2.29	119.36	123.84
37	a	413	LMG	C38-C37-C36	-2.29	102.80	114.42
26	R	602	CLA	O2A-CGA-O1A	-2.29	117.81	123.59
25	g	605	CHL	OMC-CMC-C2C	-2.29	120.51	125.69
27	Y	1621	LUT	C38-C25-C24	-2.29	118.66	123.56
25	3	608	CHL	CMD-C2D-C3D	-2.29	122.35	127.61
26	N	610	CLA	CHB-C4A-NA	2.29	127.68	124.51
37	b	2633	LMG	C40-C39-C38	-2.29	102.81	114.42
25	R	607	CHL	CAA-CBA-CGA	-2.29	106.57	113.25
25	g	608	CHL	CMB-C2B-C3B	2.29	128.96	124.68
26	S	602	CLA	O2A-CGA-O1A	-2.29	117.82	123.59
37	B	2633	LMG	C38-C37-C36	-2.28	102.83	114.42
37	b	2633	LMG	C38-C37-C36	-2.28	102.83	114.42
26	R	612	CLA	C1B-CHB-C4A	-2.28	125.59	130.12
27	G	1621	LUT	C38-C25-C24	-2.28	118.67	123.56
26	3	614	CLA	CMB-C2B-C3B	2.28	128.95	124.68
26	G	611	CLA	O2D-CGD-CBD	2.28	115.33	111.27
27	6	1621	LUT	C8-C9-C10	-2.28	115.44	118.94
31	b	618	BCR	C23-C22-C21	-2.28	115.44	118.94
26	r	603	CLA	C3C-C4C-NC	-2.28	108.01	110.57
26	s	602	CLA	O2A-CGA-O1A	-2.28	117.83	123.59
30	S	2630	LHG	O8-C23-C24	2.28	119.07	111.91
26	G	610	CLA	CHB-C4A-NA	2.28	127.67	124.51
26	C	513	CLA	CAA-CBA-CGA	-2.28	106.58	113.25
25	r	606	CHL	C1-C2-C3	-2.28	122.10	126.04

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	2	1621	LUT	C30-C31-C32	-2.28	116.10	123.22
26	B	605	CLA	O2D-CGD-O1D	-2.28	119.38	123.84
25	G	608	CHL	CMB-C2B-C3B	2.28	128.94	124.68
26	A	406	CLA	C1C-C2C-C3C	-2.28	104.56	106.96
25	1	609	CHL	O1D-CGD-CBD	-2.28	119.82	124.48
25	G	601	CHL	C2A-C1A-CHA	-2.28	119.87	123.86
25	g	601	CHL	C2A-C1A-CHA	-2.28	119.87	123.86
27	N	1620	LUT	C19-C9-C8	2.28	121.67	118.08
27	n	1620	LUT	C19-C9-C8	2.28	121.67	118.08
26	C	513	CLA	O2A-CGA-O1A	-2.28	117.84	123.59
31	C	516	BCR	C33-C5-C4	2.28	117.99	113.62
27	2	1621	LUT	C8-C9-C10	-2.28	115.44	118.94
26	Y	611	CLA	CMB-C2B-C3B	2.28	128.94	124.68
29	R	623	NEX	C4-C3-C2	-2.28	106.37	110.77
30	s	2630	LHG	O8-C23-C24	2.28	119.06	111.91
26	y	611	CLA	O2D-CGD-CBD	2.28	115.31	111.27
26	B	604	CLA	O2A-CGA-O1A	-2.28	117.85	123.59
26	C	505	CLA	CHB-C4A-NA	2.28	127.66	124.51
30	2	2630	LHG	C11-C10-C9	-2.28	102.87	114.42
31	C	516	BCR	C8-C9-C10	-2.28	115.45	118.94
27	6	1621	LUT	C30-C31-C32	-2.28	116.12	123.22
26	Y	611	CLA	O2D-CGD-CBD	2.28	115.31	111.27
30	6	2630	LHG	C11-C10-C9	-2.27	102.88	114.42
25	r	607	CHL	CAA-CBA-CGA	-2.27	106.61	113.25
28	g	1622	XAT	C18-C5-C4	2.27	116.84	114.28
30	D	410	LHG	C11-C10-C9	-2.27	102.88	114.42
25	S	601	CHL	C4D-CHA-C1A	-2.27	118.48	121.25
38	D	405	PL9	C20-C19-C21	2.27	119.09	115.27
26	C	504	CLA	CHD-C1D-ND	-2.27	122.36	124.45
25	S	601	CHL	O2D-CGD-O1D	-2.27	119.39	123.84
26	B	616	CLA	CAA-C2A-C3A	-2.27	106.55	112.78
27	g	1621	LUT	C19-C9-C8	2.27	121.66	118.08
31	B	618	BCR	C23-C22-C21	-2.27	115.45	118.94
25	R	606	CHL	C1-C2-C3	-2.27	122.11	126.04
26	b	616	CLA	CAA-C2A-C3A	-2.27	106.56	112.78
37	c	521	LMG	O3-C3-C2	-2.27	105.10	110.35
26	B	617	CLA	CAC-C3C-C4C	2.27	127.75	124.81
38	d	405	PL9	C20-C19-C21	2.27	119.09	115.27
26	n	610	CLA	CHB-C4A-NA	2.27	127.65	124.51
29	n	1623	NEX	C4-C3-C2	-2.27	106.39	110.77
26	B	617	CLA	O2A-C1-C2	-2.27	102.67	108.64
26	S	614	CLA	C2D-C1D-ND	-2.27	108.43	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	y	1620	LUT	C8-C7-C6	-2.27	120.83	127.20
31	c	516	BCR	C33-C5-C4	2.27	117.97	113.62
26	d	402	CLA	C1B-CHB-C4A	-2.27	125.62	130.12
25	N	609	CHL	CAA-C2A-C3A	-2.27	106.57	112.78
26	S	610	CLA	CHD-C1D-ND	-2.27	122.37	124.45
26	c	513	CLA	O2A-CGA-O1A	-2.27	117.87	123.59
30	d	410	LHG	C11-C10-C9	-2.27	102.91	114.42
37	C	521	LMG	O3-C3-C2	-2.27	105.11	110.35
25	n	609	CHL	CAA-C2A-C3A	-2.27	106.57	112.78
27	2	1621	LUT	C21-C26-C27	-2.27	109.83	112.70
27	G	1621	LUT	C19-C9-C8	2.27	121.65	118.08
27	g	1621	LUT	C38-C25-C24	-2.27	118.71	123.56
27	s	1621	LUT	C15-C35-C34	-2.27	118.83	123.47
26	S	603	CLA	CHC-C1C-NC	2.27	127.64	124.20
26	s	603	CLA	CHC-C1C-NC	2.27	127.64	124.20
27	S	1621	LUT	C15-C35-C34	-2.27	118.83	123.47
25	4	601	CHL	O2D-CGD-O1D	-2.26	118.95	124.09
25	8	601	CHL	O2D-CGD-O1D	-2.26	118.95	124.09
28	n	1622	XAT	C5-C4-C3	-2.26	108.27	112.75
26	G	604	CLA	O1D-CGD-CBD	2.26	129.12	124.48
26	b	611	CLA	O2D-CGD-CBD	2.26	115.29	111.27
29	r	623	NEX	C4-C3-C2	-2.26	106.40	110.77
25	3	608	CHL	O2D-CGD-O1D	-2.26	119.41	123.84
26	b	609	CLA	C1-C2-C3	-2.26	122.13	126.04
27	y	1621	LUT	C38-C25-C24	-2.26	118.72	123.56
25	4	608	CHL	CHB-C4A-NA	2.26	127.64	124.51
26	B	607	CLA	CHC-C1C-NC	2.26	127.64	124.20
26	b	604	CLA	O2A-CGA-O1A	-2.26	117.88	123.59
37	b	2633	LMG	C1-O6-C5	-2.26	109.25	113.69
31	c	516	BCR	C8-C9-C10	-2.26	115.47	118.94
30	r	2630	LHG	C11-C10-C9	-2.26	102.94	114.42
29	N	1623	NEX	C4-C3-C2	-2.26	106.41	110.77
27	6	1621	LUT	C21-C26-C27	-2.26	109.84	112.70
38	D	405	PL9	C31-C32-C33	-2.26	104.45	111.88
27	1	1621	LUT	C19-C9-C8	2.26	121.64	118.08
26	c	504	CLA	CHD-C1D-ND	-2.26	122.38	124.45
26	G	604	CLA	C2D-C1D-ND	-2.26	108.44	110.10
31	4	623	BCR	C20-C21-C22	-2.26	124.08	127.31
38	d	405	PL9	C31-C32-C33	-2.26	104.45	111.88
28	N	1622	XAT	C5-C4-C3	-2.26	108.28	112.75
26	B	611	CLA	O2D-CGD-CBD	2.26	115.28	111.27
26	c	511	CLA	CHD-C1D-ND	-2.26	122.38	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	7	614	CLA	CMB-C2B-C3B	2.26	128.90	124.68
27	Y	1620	LUT	C8-C7-C6	-2.26	120.87	127.20
30	R	2630	LHG	C11-C10-C9	-2.26	102.98	114.42
25	1	606	CHL	CBA-CAA-C2A	-2.25	107.21	113.86
26	g	604	CLA	C2D-C1D-ND	-2.25	108.44	110.10
25	3	606	CHL	CHB-C4A-NA	2.25	127.63	124.51
27	G	1621	LUT	C35-C15-C14	-2.25	118.86	123.47
25	3	609	CHL	C1-C2-C3	-2.25	122.15	126.04
26	g	610	CLA	CHB-C4A-NA	2.25	127.63	124.51
30	g	2630	LHG	C18-C17-C16	-2.25	102.99	114.42
30	Y	2630	LHG	O8-C23-C24	2.25	118.97	111.91
30	y	2630	LHG	O8-C23-C24	2.25	118.97	111.91
26	b	617	CLA	CAC-C3C-C4C	2.25	127.73	124.81
26	b	617	CLA	O2A-C1-C2	-2.25	102.72	108.64
26	s	609	CLA	CHD-C1D-ND	-2.25	122.39	124.45
26	G	614	CLA	O2D-CGD-CBD	2.25	115.27	111.27
26	B	616	CLA	C6-C7-C8	-2.25	108.65	115.92
25	8	608	CHL	CHB-C4A-NA	2.25	127.62	124.51
25	7	608	CHL	O2D-CGD-O1D	-2.25	119.44	123.84
37	B	2633	LMG	C1-O6-C5	-2.25	109.27	113.69
28	G	1622	XAT	C18-C5-C4	2.25	116.81	114.28
26	D	402	CLA	C1B-CHB-C4A	-2.25	125.66	130.12
26	s	614	CLA	C2D-C1D-ND	-2.25	108.45	110.10
30	5	2630	LHG	C27-C26-C25	-2.25	103.01	114.42
28	1	1622	XAT	C19-C9-C8	2.25	121.62	118.08
25	S	607	CHL	CMB-C2B-C3B	2.25	128.88	124.68
25	s	607	CHL	CMB-C2B-C3B	2.25	128.88	124.68
26	r	616	CLA	CMB-C2B-C3B	2.25	128.88	124.68
26	N	603	CLA	CHD-C1D-C2D	2.25	130.19	125.48
26	D	402	CLA	CMA-C3A-C2A	-2.25	104.76	113.83
26	d	402	CLA	CMA-C3A-C2A	-2.25	104.76	113.83
25	5	606	CHL	CBA-CAA-C2A	-2.25	107.23	113.86
27	g	1621	LUT	C35-C15-C14	-2.25	118.87	123.47
25	N	605	CHL	CMB-C2B-C3B	2.25	128.88	124.68
26	g	604	CLA	O1D-CGD-CBD	2.25	129.08	124.48
26	g	612	CLA	O2A-CGA-O1A	-2.25	117.92	123.59
27	1	1621	LUT	C8-C7-C6	-2.25	120.89	127.20
31	A	411	BCR	C10-C11-C12	-2.25	116.21	123.22
26	a	406	CLA	CHD-C4C-NC	2.24	127.74	124.20
27	r	620	LUT	C2-C3-C4	2.24	113.38	110.30
26	B	609	CLA	C1-C2-C3	-2.24	122.16	126.04
26	3	610	CLA	CHD-C1D-ND	-2.24	122.39	124.45

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	7	610	CLA	CHD-C1D-ND	-2.24	122.39	124.45
30	1	2630	LHG	C18-C17-C16	-2.24	103.04	114.42
30	1	2630	LHG	C27-C26-C25	-2.24	103.04	114.42
25	5	601	CHL	O2D-CGD-O1D	-2.24	119.45	123.84
26	c	506	CLA	C1-C2-C3	-2.24	122.17	126.04
26	n	603	CLA	CHD-C1D-C2D	2.24	130.18	125.48
26	G	613	CLA	O2D-CGD-O1D	-2.24	119.46	123.84
26	N	612	CLA	CAA-C2A-C3A	-2.24	106.64	112.78
30	C	523	LHG	C20-C19-C18	-2.24	103.05	114.42
37	z	101	LMG	C1-O6-C5	-2.24	109.29	113.69
38	D	405	PL9	C27-C28-C29	-2.24	122.27	127.66
38	d	405	PL9	C27-C28-C29	-2.24	122.27	127.66
26	b	607	CLA	CHC-C1C-NC	2.24	127.60	124.20
30	G	2630	LHG	C18-C17-C16	-2.24	103.06	114.42
26	b	616	CLA	C6-C7-C8	-2.24	108.68	115.92
31	a	411	BCR	C10-C11-C12	-2.24	116.23	123.22
25	n	609	CHL	CBC-CAC-C3C	-2.24	106.26	112.43
26	b	614	CLA	C1B-CHB-C4A	-2.24	125.68	130.12
26	s	610	CLA	CHD-C1D-ND	-2.24	122.40	124.45
30	c	523	LHG	C20-C19-C18	-2.24	103.07	114.42
29	y	1623	NEX	C11-C12-C13	-2.24	120.13	126.42
25	Y	601	CHL	CHD-C4C-C3C	-2.24	121.55	124.84
25	5	607	CHL	OMC-CMC-C2C	-2.24	120.63	125.69
25	7	607	CHL	CMB-C2B-C3B	2.24	128.86	124.68
25	n	605	CHL	CMB-C2B-C3B	2.24	128.86	124.68
27	5	1621	LUT	C19-C9-C8	2.24	121.60	118.08
28	2	1622	XAT	C10-C11-C12	-2.24	116.24	123.22
41	F	101	HEM	C4B-CHC-C1C	2.24	125.51	122.56
41	f	101	HEM	C4B-CHC-C1C	2.24	125.51	122.56
26	g	614	CLA	O2D-CGD-CBD	2.24	115.24	111.27
30	5	2630	LHG	C18-C17-C16	-2.24	103.08	114.42
28	4	622	XAT	C20-C13-C12	2.23	121.60	118.08
29	Y	1623	NEX	C11-C12-C13	-2.23	120.14	126.42
27	5	1621	LUT	C8-C7-C6	-2.23	120.93	127.20
25	5	607	CHL	C1-C2-C3	-2.23	122.18	126.04
28	6	1622	XAT	C10-C11-C12	-2.23	116.25	123.22
27	1	1621	LUT	C39-C29-C28	2.23	121.60	118.08
25	r	608	CHL	C4-C3-C5	2.23	119.03	115.27
30	d	410	LHG	C27-C26-C25	-2.23	103.09	114.42
26	B	614	CLA	C1B-CHB-C4A	-2.23	125.69	130.12
26	Y	613	CLA	C2D-C1D-ND	-2.23	108.46	110.10
26	s	610	CLA	C2D-C1D-ND	-2.23	108.46	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	y	607	CHL	O2A-CGA-CBA	2.23	118.91	111.91
26	a	405	CLA	CHC-C1C-NC	2.23	127.59	124.20
26	G	612	CLA	O2A-CGA-O1A	-2.23	117.96	123.59
26	Y	603	CLA	C2A-C1A-CHA	2.23	127.76	123.86
25	g	601	CHL	CED-O2D-CGD	2.23	120.98	115.94
30	2	2630	LHG	C27-C26-C25	-2.23	103.10	114.42
26	n	612	CLA	C2A-C1A-CHA	2.23	127.76	123.86
26	y	613	CLA	C2D-C1D-ND	-2.23	108.46	110.10
31	8	623	BCR	C20-C21-C22	-2.23	124.13	127.31
26	C	509	CLA	CGD-CBD-CAD	2.23	117.96	110.73
25	3	608	CHL	O2A-CGA-CBA	2.23	121.19	114.03
30	D	410	LHG	C27-C26-C25	-2.23	103.11	114.42
39	C	519	DGD	O2D-C2D-C1D	-2.23	104.63	110.05
39	c	519	DGD	O2D-C2D-C1D	-2.23	104.63	110.05
25	Y	607	CHL	O2A-CGA-CBA	2.23	118.90	111.91
26	c	503	CLA	C7-C6-C5	-2.23	107.30	113.36
27	Y	1621	LUT	C8-C9-C10	-2.23	115.52	118.94
26	c	509	CLA	CGD-CBD-CAD	2.23	117.95	110.73
26	y	603	CLA	C2A-C1A-CHA	2.23	127.76	123.86
26	B	616	CLA	O2D-CGD-CBD	2.23	115.23	111.27
26	C	503	CLA	C7-C6-C5	-2.23	107.31	113.36
28	N	1622	XAT	C28-C29-C30	2.23	122.36	118.94
36	a	412	SQD	O7-S-C6	2.23	109.59	106.94
25	g	607	CHL	C1B-CHB-C4A	-2.23	125.70	130.12
30	6	2630	LHG	C27-C26-C25	-2.23	103.12	114.42
25	7	609	CHL	C1-C2-C3	-2.23	122.19	126.04
27	G	1620	LUT	C16-C1-C6	-2.23	106.69	110.30
25	n	601	CHL	C2A-C1A-CHA	-2.23	119.97	123.86
26	C	506	CLA	C1-C2-C3	-2.23	122.19	126.04
27	R	620	LUT	C2-C3-C4	2.23	113.35	110.30
25	N	609	CHL	CBC-CAC-C3C	-2.23	106.30	112.43
28	5	1622	XAT	C19-C9-C8	2.22	121.58	118.08
25	G	607	CHL	C1B-CHB-C4A	-2.22	125.71	130.12
25	7	606	CHL	CHB-C4A-NA	2.22	127.59	124.51
26	n	612	CLA	CAA-C2A-C3A	-2.22	106.69	112.78
25	3	607	CHL	CMB-C2B-C3B	2.22	128.84	124.68
36	B	623	SQD	O5-C5-C4	2.22	113.73	109.69
36	b	623	SQD	O5-C5-C4	2.22	113.73	109.69
27	y	1621	LUT	C8-C9-C10	-2.22	115.53	118.94
25	7	608	CHL	O2A-CGA-CBA	2.22	121.17	114.03
26	S	609	CLA	O2A-CGA-O1A	-2.22	117.76	123.30
26	s	609	CLA	O2A-CGA-O1A	-2.22	117.76	123.30

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	R	616	CLA	CMB-C2B-C3B	2.22	128.84	124.68
25	l	607	CHL	OMC-CMC-C2C	-2.22	120.66	125.69
25	r	614	CHL	CBC-CAC-C3C	-2.22	106.31	112.43
27	r	620	LUT	C12-C13-C14	-2.22	115.53	118.94
30	b	2631	LHG	C11-C10-C9	-2.22	103.15	114.42
25	l	601	CHL	O2D-CGD-O1D	-2.22	119.50	123.84
26	B	608	CLA	CMC-C2C-C3C	2.22	132.15	126.12
26	B	607	CLA	O2A-CGA-O1A	-2.22	117.99	123.59
26	C	513	CLA	O2D-CGD-CBD	2.22	115.22	111.27
26	6	610	CLA	CHD-C1D-ND	-2.22	122.41	124.45
28	8	622	XAT	C20-C13-C12	2.22	121.58	118.08
26	S	610	CLA	C2D-C1D-ND	-2.22	108.47	110.10
25	3	607	CHL	O2D-CGD-O1D	-2.22	119.50	123.84
25	7	607	CHL	O2D-CGD-O1D	-2.22	119.50	123.84
26	b	616	CLA	O2D-CGD-CBD	2.22	115.21	111.27
25	y	609	CHL	O2A-CGA-CBA	2.22	118.87	111.91
25	1	607	CHL	C1-C2-C3	-2.22	122.20	126.04
30	B	2631	LHG	C11-C10-C9	-2.22	103.16	114.42
30	d	408	LHG	O8-C23-O10	-2.22	117.99	123.59
26	7	610	CLA	CHB-C4A-NA	2.22	127.58	124.51
25	Y	608	CHL	O2A-CGA-O1A	-2.22	118.00	123.59
27	n	1621	LUT	C31-C30-C29	-2.22	124.14	127.31
27	5	1621	LUT	C39-C29-C28	2.22	121.57	118.08
39	C	518	DGD	O3G-C1D-C2D	-2.22	104.84	108.30
26	B	616	CLA	O2A-CGA-O1A	-2.22	118.00	123.59
27	2	1621	LUT	C8-C7-C6	-2.22	120.98	127.20
25	R	608	CHL	C4-C3-C5	2.22	119.00	115.27
30	r	2630	LHG	C18-C17-C16	-2.22	103.17	114.42
26	A	406	CLA	CHD-C4C-NC	2.22	127.70	124.20
30	b	2630	LHG	C18-C17-C16	-2.22	103.17	114.42
37	Z	101	LMG	C1-O6-C5	-2.22	109.34	113.69
26	Y	602	CLA	CHB-C4A-NA	2.22	127.58	124.51
26	y	602	CLA	CHB-C4A-NA	2.22	127.58	124.51
26	N	612	CLA	C2A-C1A-CHA	2.21	127.73	123.86
26	C	503	CLA	O2A-C1-C2	-2.21	102.82	108.64
25	Y	607	CHL	CAA-C2A-C3A	-2.21	106.72	112.78
31	B	619	BCR	C10-C11-C12	-2.21	116.31	123.22
26	g	613	CLA	O2D-CGD-O1D	-2.21	119.51	123.84
25	n	609	CHL	O2A-CGA-CBA	2.21	118.85	111.91
28	8	622	XAT	C25-C24-C23	-2.21	108.37	112.75
27	7	1620	LUT	C18-C5-C6	-2.21	122.04	124.53
30	B	2630	LHG	C18-C17-C16	-2.21	103.19	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	513	CLA	O2D-CGD-CBD	2.21	115.20	111.27
27	N	1620	LUT	C17-C1-C6	2.21	113.89	110.30
26	A	406	CLA	C16-C15-C13	-2.21	108.77	115.92
25	G	601	CHL	CED-O2D-CGD	2.21	120.94	115.94
27	n	1620	LUT	C17-C1-C6	2.21	113.89	110.30
30	R	2630	LHG	C18-C17-C16	-2.21	103.20	114.42
27	N	1621	LUT	C31-C30-C29	-2.21	124.16	127.31
26	c	508	CLA	CMC-C2C-C3C	2.21	132.12	126.12
25	N	609	CHL	O2A-CGA-CBA	2.21	118.84	111.91
28	N	1622	XAT	C40-C33-C32	2.21	121.56	118.08
27	R	620	LUT	C12-C13-C14	-2.21	115.55	118.94
26	y	604	CLA	C2D-C1D-ND	-2.21	108.48	110.10
30	D	409	LHG	O8-C23-O10	-2.21	118.02	123.59
26	C	511	CLA	CHD-C1D-ND	-2.21	122.42	124.45
26	A	405	CLA	CHC-C1C-NC	2.21	127.55	124.20
31	C	516	BCR	C34-C9-C8	2.21	121.56	118.08
25	R	614	CHL	CBC-CAC-C3C	-2.21	106.34	112.43
25	N	601	CHL	C2A-C1A-CHA	-2.21	120.00	123.86
28	4	622	XAT	C25-C24-C23	-2.21	108.38	112.75
31	b	619	BCR	C10-C11-C12	-2.21	116.33	123.22
25	y	607	CHL	CAA-C2A-C3A	-2.21	106.73	112.78
26	a	406	CLA	C16-C15-C13	-2.21	108.78	115.92
25	y	608	CHL	O2A-CGA-O1A	-2.21	118.02	123.59
26	3	611	CLA	CHA-C1A-NA	-2.21	121.34	126.40
26	C	508	CLA	CMC-C2C-C3C	2.21	132.11	126.12
26	c	503	CLA	O2A-C1-C2	-2.21	102.83	108.64
28	1	1622	XAT	C5-C4-C3	-2.21	108.38	112.75
26	b	608	CLA	CMC-C2C-C3C	2.21	132.11	126.12
25	N	609	CHL	CMD-C2D-C3D	-2.21	122.54	127.61
26	Y	603	CLA	O2A-CGA-O1A	-2.21	118.02	123.59
25	Y	609	CHL	O2A-CGA-CBA	2.21	118.83	111.91
36	A	412	SQD	O7-S-C6	2.21	109.56	106.94
26	y	611	CLA	C2A-C1A-CHA	2.20	127.71	123.86
26	n	602	CLA	C6-C7-C8	-2.20	108.80	115.92
28	n	1622	XAT	C28-C29-C30	2.20	122.32	118.94
30	D	408	LHG	O8-C23-O10	-2.20	118.03	123.59
27	5	1620	LUT	C28-C29-C30	-2.20	115.56	118.94
26	3	611	CLA	CMB-C2B-C1B	-2.20	125.08	128.46
27	Y	1621	LUT	C35-C15-C14	-2.20	118.96	123.47
25	y	601	CHL	CHD-C4C-C3C	-2.20	121.60	124.84
27	3	1620	LUT	C18-C5-C6	-2.20	122.06	124.53
26	b	616	CLA	O2A-CGA-O1A	-2.20	118.04	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	C	520	DGD	O6E-C1E-O5D	-2.20	104.76	109.97
25	y	606	CHL	CHB-C4A-NA	2.20	127.56	124.51
30	c	2630	LHG	C27-C26-C25	-2.20	103.26	114.42
31	4	623	BCR	C2-C3-C4	-2.20	106.46	111.38
25	Y	606	CHL	CHB-C4A-NA	2.20	127.55	124.51
28	8	622	XAT	C39-C29-C28	2.20	121.54	118.08
29	S	1623	NEX	C15-C35-C34	-2.20	118.97	123.47
29	s	1623	NEX	C15-C35-C34	-2.20	118.97	123.47
26	Y	604	CLA	C2D-C1D-ND	-2.20	108.48	110.10
30	N	2630	LHG	O8-C23-C24	2.20	118.81	111.91
26	b	607	CLA	O2A-CGA-O1A	-2.20	118.04	123.59
27	N	1620	LUT	C28-C29-C30	-2.20	115.57	118.94
26	b	605	CLA	C11-C10-C8	-2.20	108.81	115.92
27	g	1620	LUT	C16-C1-C6	-2.20	106.73	110.30
26	S	609	CLA	CHD-C1D-ND	-2.20	122.43	124.45
26	Y	611	CLA	C2A-C1A-CHA	2.20	127.70	123.86
30	R	2630	LHG	C27-C26-C25	-2.20	103.27	114.42
27	6	1621	LUT	C8-C7-C6	-2.20	121.03	127.20
26	7	603	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
26	y	603	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
30	C	2630	LHG	C27-C26-C25	-2.20	103.27	114.42
25	n	609	CHL	CMD-C2D-C3D	-2.20	122.56	127.61
30	d	409	LHG	O8-C23-O10	-2.20	118.05	123.59
39	c	518	DGD	O6D-C5D-C6D	-2.20	102.23	106.67
26	B	605	CLA	C11-C10-C8	-2.20	108.82	115.92
26	7	611	CLA	CHA-C1A-NA	-2.20	121.37	126.40
25	6	601	CHL	C4D-C3D-CAD	2.20	110.68	108.10
25	1	605	CHL	CAA-C2A-C3A	-2.20	106.77	112.78
25	5	605	CHL	CAA-C2A-C3A	-2.20	106.77	112.78
26	a	405	CLA	CBC-CAC-C3C	2.20	118.48	112.43
26	C	507	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
39	c	520	DGD	O6E-C1E-O5D	-2.20	104.78	109.97
25	3	607	CHL	C1C-C2C-C3C	-2.20	105.37	107.11
26	7	611	CLA	CMB-C2B-C1B	-2.20	125.09	128.46
26	Y	611	CLA	O2A-CGA-O1A	-2.20	118.05	123.59
31	c	516	BCR	C34-C9-C8	2.19	121.53	118.08
26	6	603	CLA	O2A-CGA-O1A	-2.19	118.05	123.59
27	G	1620	LUT	C8-C9-C10	-2.19	115.57	118.94
26	3	610	CLA	CHB-C4A-NA	2.19	127.55	124.51
39	C	518	DGD	O6D-C5D-C6D	-2.19	102.24	106.67
30	r	2630	LHG	C27-C26-C25	-2.19	103.29	114.42
26	A	405	CLA	CBC-CAC-C3C	2.19	118.48	112.43

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	Y	609	CHL	O1D-CGD-CBD	-2.19	120.00	124.48
36	A	418	SQD	O47-C7-O49	-2.19	118.40	123.70
39	c	518	DGD	O3G-C1D-C2D	-2.19	104.88	108.30
36	a	418	SQD	O47-C7-O49	-2.19	118.40	123.70
27	l	1620	LUT	C28-C29-C30	-2.19	115.58	118.94
27	g	1620	LUT	C8-C9-C10	-2.19	115.58	118.94
25	7	607	CHL	C1C-C2C-C3C	-2.19	105.38	107.11
30	n	2630	LHG	O8-C23-C24	2.19	118.78	111.91
28	5	1622	XAT	C5-C4-C3	-2.19	108.41	112.75
26	b	602	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
26	c	507	CLA	O2A-CGA-O1A	-2.19	118.06	123.59
30	C	2630	LHG	O8-C6-C5	-2.19	102.06	108.43
25	7	609	CHL	O1D-CGD-CBD	-2.19	120.00	124.48
25	8	607	CHL	O1D-CGD-CBD	-2.19	120.00	124.48
26	y	603	CLA	CBC-CAC-C3C	-2.19	106.39	112.43
26	l	612	CLA	CAA-C2A-C3A	-2.19	106.78	112.78
26	C	508	CLA	CHC-C1C-NC	2.19	127.52	124.20
26	c	501	CLA	CHD-C1D-ND	-2.19	122.44	124.45
26	S	603	CLA	O1A-CGA-CBA	2.19	130.11	123.08
26	2	610	CLA	CHD-C1D-ND	-2.19	122.44	124.45
27	y	1621	LUT	C35-C15-C14	-2.19	118.99	123.47
25	4	607	CHL	O1D-CGD-CBD	-2.19	120.01	124.48
25	R	607	CHL	O2D-CGD-O1D	-2.19	119.56	123.84
27	n	1620	LUT	C28-C29-C30	-2.19	115.59	118.94
26	Y	603	CLA	CBC-CAC-C3C	-2.19	106.40	112.43
26	N	602	CLA	C6-C7-C8	-2.19	108.85	115.92
25	2	601	CHL	C4D-C3D-CAD	2.19	110.67	108.10
39	H	102	DGD	O6E-C5E-C4E	2.18	113.66	109.69
26	5	612	CLA	CAA-C2A-C3A	-2.18	106.80	112.78
26	y	611	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
31	d	404	BCR	C3-C4-C5	-2.18	110.18	114.08
28	n	1622	XAT	C40-C33-C32	2.18	121.52	118.08
26	2	603	CLA	O2A-CGA-O1A	-2.18	118.08	123.59
29	l	1623	NEX	C11-C12-C13	-2.18	120.28	126.42
26	N	610	CLA	C1-C2-C3	-2.18	122.27	126.04
27	6	1621	LUT	C35-C15-C14	-2.18	119.00	123.47
25	N	607	CHL	C4A-NA-C1A	2.18	107.69	106.71
25	n	607	CHL	C4A-NA-C1A	2.18	107.69	106.71
26	A	405	CLA	O2D-CGD-CBD	2.18	115.14	111.27
25	5	606	CHL	C2A-C1A-CHA	-2.18	120.04	123.86
39	h	102	DGD	O6E-C5E-C4E	2.18	113.66	109.69
26	3	603	CLA	O2A-CGA-O1A	-2.18	118.09	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
28	4	622	XAT	C39-C29-C28	2.18	121.51	118.08
26	b	604	CLA	C2D-C1D-ND	-2.18	108.50	110.10
26	g	602	CLA	C2D-C1D-ND	-2.18	108.50	110.10
25	r	606	CHL	C2A-C1A-CHA	-2.18	120.05	123.86
36	B	621	SQD	O47-C7-O49	-2.18	118.43	123.70
35	a	409	PHO	OBD-CAD-CBD	-2.18	122.62	125.82
31	8	623	BCR	C2-C3-C4	-2.18	106.51	111.38
37	C	521	LMG	C38-C37-C36	-2.18	103.36	114.42
30	c	2630	LHG	O8-C6-C5	-2.18	102.09	108.43
26	G	602	CLA	C6-C7-C8	-2.18	108.88	115.92
25	2	606	CHL	O2D-CGD-O1D	-2.18	119.58	123.84
37	A	415	LMG	C38-C37-C36	-2.18	103.37	114.42
37	a	415	LMG	C38-C37-C36	-2.18	103.37	114.42
26	C	501	CLA	O2A-CGA-O1A	-2.18	118.10	123.59
25	r	607	CHL	O2D-CGD-O1D	-2.18	119.58	123.84
27	2	1621	LUT	C35-C15-C14	-2.18	119.02	123.47
26	Y	614	CLA	C2D-C1D-ND	-2.18	108.50	110.10
25	6	606	CHL	O2D-CGD-O1D	-2.18	119.58	123.84
26	g	602	CLA	C6-C7-C8	-2.18	108.89	115.92
26	A	405	CLA	C1C-C2C-C3C	2.18	109.24	106.96
25	R	606	CHL	C2A-C1A-CHA	-2.18	120.06	123.86
26	1	611	CLA	CHB-C4A-NA	2.18	127.52	124.51
26	5	611	CLA	CHB-C4A-NA	2.18	127.52	124.51
25	3	609	CHL	C4-C3-C5	2.18	118.93	115.27
25	7	609	CHL	C4-C3-C5	2.18	118.93	115.27
31	B	620	BCR	C37-C22-C23	2.17	121.50	118.08
25	y	609	CHL	O1D-CGD-CBD	-2.17	120.03	124.48
26	s	610	CLA	O2D-CGD-CBD	2.17	115.13	111.27
26	n	610	CLA	C1-C2-C3	-2.17	122.28	126.04
39	C	520	DGD	C1E-O6E-C5E	2.17	117.95	113.69
39	c	520	DGD	C1E-O6E-C5E	2.17	117.95	113.69
26	d	403	CLA	CAA-CBA-CGA	-2.17	106.91	113.25
39	B	626	DGD	O2D-C2D-C3D	-2.17	105.33	110.35
25	n	606	CHL	C4D-CHA-C1A	-2.17	118.61	121.25
26	1	604	CLA	CHB-C4A-NA	2.17	127.51	124.51
26	a	405	CLA	O2D-CGD-CBD	2.17	115.12	111.27
39	b	626	DGD	O2D-C2D-C3D	-2.17	105.33	110.35
31	d	404	BCR	C15-C16-C17	-2.17	119.03	123.47
29	5	1623	NEX	C11-C12-C13	-2.17	120.32	126.42
26	S	610	CLA	O2D-CGD-CBD	2.17	115.12	111.27
37	c	521	LMG	C38-C37-C36	-2.17	103.41	114.42
35	A	409	PHO	OBD-CAD-CBD	-2.17	122.64	125.82

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	s	603	CLA	O1A-CGA-CBA	2.17	130.05	123.08
25	3	609	CHL	O1D-CGD-CBD	-2.17	120.05	124.48
26	n	603	CLA	O2D-CGD-CBD	2.17	115.12	111.27
31	b	619	BCR	C33-C5-C6	-2.17	122.09	124.53
36	b	621	SQD	O47-C7-O49	-2.17	118.47	123.70
31	B	619	BCR	C16-C15-C14	-2.17	119.04	123.47
26	B	616	CLA	CMB-C2B-C3B	2.17	128.73	124.68
25	N	601	CHL	O2A-CGA-CBA	2.17	118.70	111.91
26	B	604	CLA	C2D-C1D-ND	-2.17	108.51	110.10
26	G	602	CLA	C2D-C1D-ND	-2.17	108.51	110.10
30	Y	2630	LHG	C27-C26-C25	-2.17	103.43	114.42
26	B	602	CLA	O2A-CGA-O1A	-2.16	118.13	123.59
26	N	610	CLA	CHA-C1A-NA	-2.16	121.44	126.40
31	D	404	BCR	C3-C4-C5	-2.16	110.21	114.08
28	g	1622	XAT	O4-C5-C6	-2.16	57.17	58.96
26	c	508	CLA	CHC-C1C-NC	2.16	127.48	124.20
26	a	405	CLA	C1C-C2C-C3C	2.16	109.23	106.96
26	B	610	CLA	O2A-CGA-O1A	-2.16	118.14	123.59
30	y	2630	LHG	C27-C26-C25	-2.16	103.45	114.42
26	y	614	CLA	C2D-C1D-ND	-2.16	108.51	110.10
31	D	404	BCR	C15-C16-C17	-2.16	119.05	123.47
26	C	513	CLA	O2A-CGA-CBA	2.16	118.69	111.91
28	r	622	XAT	C38-C25-C24	2.16	116.71	114.28
25	n	601	CHL	O2A-CGA-CBA	2.16	118.69	111.91
25	5	608	CHL	CMB-C2B-C3B	2.16	128.72	124.68
26	D	403	CLA	CAA-CBA-CGA	-2.16	106.94	113.25
25	7	607	CHL	CAA-C2A-C3A	-2.16	106.87	112.78
30	b	2631	LHG	C18-C17-C16	-2.16	103.47	114.42
30	c	522	LHG	C27-C26-C25	-2.16	103.47	114.42
26	b	605	CLA	O2D-CGD-CBD	2.16	115.10	111.27
26	c	501	CLA	O2A-CGA-O1A	-2.16	118.15	123.59
31	b	620	BCR	C37-C22-C23	2.16	121.48	118.08
30	s	2630	LHG	C27-C26-C25	-2.16	103.48	114.42
26	n	610	CLA	CHA-C1A-NA	-2.16	121.46	126.40
30	S	2630	LHG	C27-C26-C25	-2.16	103.48	114.42
25	1	606	CHL	C2A-C1A-CHA	-2.16	120.09	123.86
26	C	502	CLA	O2D-CGD-CBD	2.15	115.09	111.27
26	c	502	CLA	O2D-CGD-CBD	2.15	115.09	111.27
25	4	608	CHL	C1C-C2C-C3C	-2.15	105.41	107.11
30	C	522	LHG	C27-C26-C25	-2.15	103.50	114.42
25	6	607	CHL	CHB-C4A-NA	2.15	127.49	124.51
25	Y	601	CHL	C2A-C1A-CHA	-2.15	120.10	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	B	605	CLA	O2D-CGD-CBD	2.15	115.09	111.27
26	C	501	CLA	CHD-C1D-ND	-2.15	122.48	124.45
26	b	610	CLA	O2A-CGA-O1A	-2.15	118.16	123.59
30	B	2631	LHG	C18-C17-C16	-2.15	103.51	114.42
31	b	619	BCR	C16-C15-C14	-2.15	119.07	123.47
25	8	608	CHL	C1C-C2C-C3C	-2.15	105.41	107.11
25	1	608	CHL	CMB-C2B-C3B	2.15	128.70	124.68
26	6	602	CLA	CHD-C1D-ND	-2.15	122.48	124.45
26	c	513	CLA	O2A-CGA-CBA	2.15	118.65	111.91
27	1	1620	LUT	C8-C7-C6	-2.15	121.17	127.20
28	R	622	XAT	C31-C30-C29	-2.15	124.24	127.31
29	Y	1623	NEX	C28-C29-C30	2.15	122.24	118.94
25	3	607	CHL	CAA-C2A-C3A	-2.15	106.90	112.78
26	6	603	CLA	C3C-C4C-NC	-2.15	108.16	110.57
39	c	519	DGD	CAB-C9B-C8B	-2.15	103.53	114.42
27	5	1621	LUT	C15-C35-C34	-2.15	119.08	123.47
26	5	604	CLA	CHB-C4A-NA	2.15	127.48	124.51
25	Y	601	CHL	C1-C2-C3	-2.15	122.33	126.04
27	Y	1621	LUT	C15-C35-C34	-2.15	119.08	123.47
26	C	508	CLA	CGD-CBD-CAD	2.15	117.68	110.73
26	g	603	CLA	O2D-CGD-CBD	2.15	115.08	111.27
25	S	601	CHL	C1C-C2C-C3C	-2.14	105.41	107.11
27	5	1621	LUT	C21-C26-C27	-2.14	109.99	112.70
25	s	601	CHL	C1C-C2C-C3C	-2.14	105.41	107.11
26	6	612	CLA	C2A-C1A-CHA	2.14	127.61	123.86
26	2	612	CLA	C2A-C1A-CHA	2.14	127.61	123.86
25	G	609	CHL	CBC-CAC-C3C	-2.14	106.52	112.43
30	C	522	LHG	C18-C17-C16	-2.14	103.55	114.42
26	R	609	CLA	C1D-ND-C4D	-2.14	104.81	106.33
30	c	522	LHG	C18-C17-C16	-2.14	103.55	114.42
39	b	626	DGD	O1G-C1A-O1A	-2.14	118.19	123.59
25	N	608	CHL	O1D-CGD-CBD	-2.14	120.10	124.48
27	1	1621	LUT	C15-C35-C34	-2.14	119.09	123.47
28	R	622	XAT	C38-C25-C24	2.14	116.69	114.28
26	c	503	CLA	O2A-CGA-O1A	-2.14	118.19	123.59
29	y	1623	NEX	C28-C29-C30	2.14	122.22	118.94
25	3	607	CHL	OMC-CMC-C2C	-2.14	120.85	125.69
35	a	408	PHO	CMD-C2D-C3D	2.14	128.68	124.68
39	C	519	DGD	CAB-C9B-C8B	-2.14	103.56	114.42
26	N	603	CLA	O2D-CGD-CBD	2.14	115.07	111.27
26	7	612	CLA	CMD-C2D-C3D	2.14	132.53	127.61
26	2	603	CLA	C3C-C4C-NC	-2.14	108.17	110.57

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	S	1621	LUT	C31-C30-C29	-2.14	124.26	127.31
31	c	514	BCR	C40-C30-C25	-2.14	106.83	110.30
26	b	616	CLA	CMB-C2B-C3B	2.14	128.68	124.68
26	d	403	CLA	O2A-CGA-O1A	-2.14	118.20	123.59
25	N	606	CHL	C4D-CHA-C1A	-2.14	118.65	121.25
35	a	408	PHO	CMA-C3A-C4A	-2.14	109.70	114.38
31	c	517	BCR	C11-C12-C13	-2.14	120.42	126.42
26	S	603	CLA	CHA-C1A-NA	-2.14	121.51	126.40
26	s	603	CLA	CHA-C1A-NA	-2.14	121.51	126.40
26	4	610	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
26	8	610	CLA	O2D-CGD-O1D	-2.14	119.66	123.84
26	c	508	CLA	CGD-CBD-CAD	2.14	117.65	110.73
25	Y	606	CHL	CMD-C2D-C3D	-2.14	122.70	127.61
25	y	606	CHL	CMD-C2D-C3D	-2.14	122.70	127.61
25	7	607	CHL	OMC-CMC-C2C	-2.14	120.86	125.69
36	b	621	SQD	O8-S-C6	2.14	109.14	105.74
27	5	1620	LUT	C8-C7-C6	-2.14	121.20	127.20
26	1	614	CLA	CHD-C1D-ND	-2.13	122.49	124.45
27	s	1621	LUT	C28-C29-C30	-2.13	115.67	118.94
25	S	607	CHL	O2D-CGD-O1D	-2.13	119.66	123.84
31	C	517	BCR	C11-C12-C13	-2.13	120.42	126.42
31	C	514	BCR	C40-C30-C25	-2.13	106.84	110.30
35	A	408	PHO	CMD-C2D-C3D	2.13	128.67	124.68
25	N	606	CHL	OMC-CMC-C2C	-2.13	120.86	125.69
25	n	605	CHL	OMC-CMC-C2C	-2.13	120.86	125.69
39	c	520	DGD	CAB-C9B-C8B	-2.13	103.59	114.42
25	4	606	CHL	C4D-CHA-C1A	-2.13	118.65	121.25
25	8	606	CHL	C4D-CHA-C1A	-2.13	118.65	121.25
26	8	612	CLA	O2A-CGA-O1A	-2.13	117.98	123.30
39	C	520	DGD	CAB-C9B-C8B	-2.13	103.60	114.42
28	R	622	XAT	C20-C13-C12	2.13	121.44	118.08
28	r	622	XAT	C20-C13-C12	2.13	121.44	118.08
26	b	611	CLA	O2A-CGA-O1A	-2.13	118.21	123.59
27	5	1620	LUT	C8-C9-C10	-2.13	115.67	118.94
25	y	601	CHL	C2A-C1A-CHA	-2.13	120.13	123.86
26	G	604	CLA	CHB-C4A-NA	2.13	127.46	124.51
25	n	608	CHL	C11-C12-C13	-2.13	109.03	115.92
27	G	1621	LUT	C37-C21-C22	-2.13	105.40	109.44
30	C	522	LHG	C20-C19-C18	-2.13	103.61	114.42
28	r	622	XAT	C31-C30-C29	-2.13	124.27	127.31
26	7	611	CLA	C2C-C1C-NC	2.13	111.97	109.97
30	c	522	LHG	C20-C19-C18	-2.13	103.62	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	S	1620	LUT	C8-C7-C6	-2.13	121.23	127.20
27	s	1620	LUT	C8-C7-C6	-2.13	121.23	127.20
25	g	609	CHL	CBC-CAC-C3C	-2.13	106.57	112.43
31	C	515	BCR	C4-C5-C6	-2.13	119.64	122.73
25	n	606	CHL	OMC-CMC-C2C	-2.13	120.88	125.69
35	A	408	PHO	CMA-C3A-C4A	-2.13	109.72	114.38
39	C	520	DGD	C7B-C6B-C5B	-2.13	103.63	114.42
25	4	608	CHL	O2A-CGA-CBA	2.13	120.86	114.03
26	b	605	CLA	CMB-C2B-C3B	2.13	128.66	124.68
25	N	605	CHL	OMC-CMC-C2C	-2.13	120.88	125.69
31	8	623	BCR	C38-C26-C27	2.13	117.70	113.62
26	B	611	CLA	O2A-CGA-O1A	-2.13	118.23	123.59
27	s	1621	LUT	C31-C30-C29	-2.13	124.28	127.31
25	6	601	CHL	O2D-CGD-O1D	-2.13	119.68	123.84
25	5	605	CHL	C2A-C1A-CHA	-2.13	120.14	123.86
27	7	1620	LUT	C8-C9-C10	-2.13	115.68	118.94
26	G	603	CLA	O2D-CGD-CBD	2.12	115.04	111.27
39	c	520	DGD	C7B-C6B-C5B	-2.12	103.64	114.42
26	C	503	CLA	O2A-CGA-O1A	-2.12	118.23	123.59
26	3	611	CLA	C2C-C1C-NC	2.12	111.96	109.97
26	b	607	CLA	C2D-C1D-ND	-2.12	108.54	110.10
39	c	520	DGD	CBB-CAB-C9B	-2.12	103.64	114.42
36	B	621	SQD	O8-S-C6	2.12	109.12	105.74
25	n	608	CHL	O1D-CGD-CBD	-2.12	120.14	124.48
25	2	607	CHL	CHB-C4A-NA	2.12	127.45	124.51
25	y	601	CHL	C1-C2-C3	-2.12	122.37	126.04
26	A	405	CLA	O2D-CGD-O1D	-2.12	119.69	123.84
27	S	1621	LUT	C28-C29-C30	-2.12	115.68	118.94
28	6	1622	XAT	C39-C29-C30	-2.12	119.95	122.92
39	B	626	DGD	O1G-C1A-O1A	-2.12	118.24	123.59
31	B	619	BCR	C33-C5-C6	-2.12	122.14	124.53
25	7	606	CHL	O1D-CGD-CBD	-2.12	120.14	124.48
26	1	604	CLA	CHD-C1D-ND	-2.12	122.50	124.45
25	2	607	CHL	C4-C3-C5	2.12	118.84	115.27
37	B	622	LMG	O3-C3-C2	-2.12	105.44	110.35
29	G	1623	NEX	C30-C31-C32	-2.12	116.60	123.22
26	7	613	CLA	CHD-C1D-ND	-2.12	122.50	124.45
26	b	614	CLA	O1D-CGD-CBD	2.12	128.82	124.48
25	s	607	CHL	O2D-CGD-O1D	-2.12	119.69	123.84
39	C	520	DGD	CBB-CAB-C9B	-2.12	103.66	114.42
27	6	1621	LUT	C3-C4-C5	-2.12	107.63	111.85
26	D	403	CLA	O2A-CGA-O1A	-2.12	118.24	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	y	1621	LUT	C15-C35-C34	-2.12	119.13	123.47
25	N	608	CHL	C11-C12-C13	-2.12	109.07	115.92
30	s	2630	LHG	C18-C17-C16	-2.12	103.66	114.42
30	S	2630	LHG	C18-C17-C16	-2.12	103.67	114.42
25	6	607	CHL	C4-C3-C5	2.12	118.84	115.27
39	c	520	DGD	C5B-C4B-C3B	-2.12	103.67	114.42
25	2	601	CHL	O2D-CGD-O1D	-2.12	119.70	123.84
27	4	620	LUT	C3-C4-C5	-2.12	107.63	111.85
26	G	602	CLA	O2A-CGA-O1A	-2.12	118.25	123.59
27	3	1620	LUT	C8-C9-C10	-2.12	115.69	118.94
39	C	520	DGD	C5B-C4B-C3B	-2.12	103.68	114.42
31	B	619	BCR	C11-C12-C13	-2.12	120.47	126.42
27	1	1621	LUT	C21-C26-C27	-2.12	110.03	112.70
29	g	1623	NEX	C30-C31-C32	-2.12	116.61	123.22
26	4	612	CLA	O2A-CGA-O1A	-2.12	118.03	123.30
26	c	502	CLA	CMC-C2C-C3C	2.12	131.86	126.12
25	6	601	CHL	CED-O2D-CGD	2.12	120.72	115.94
26	3	612	CLA	CMD-C2D-C3D	2.12	132.48	127.61
26	Y	603	CLA	CAA-C2A-C3A	-2.11	106.99	112.78
37	b	2633	LMG	C3-C4-C5	-2.11	106.47	110.24
25	g	608	CHL	C2A-C1A-CHA	-2.11	120.16	123.86
25	8	608	CHL	O2A-CGA-CBA	2.11	120.82	114.03
26	N	604	CLA	CHB-C4A-NA	2.11	127.43	124.51
31	c	515	BCR	C4-C5-C6	-2.11	119.66	122.73
26	C	506	CLA	CMC-C2C-C1C	-2.11	121.82	125.04
31	c	516	BCR	C31-C1-C6	-2.11	106.87	110.30
26	3	613	CLA	CHD-C1D-ND	-2.11	122.51	124.45
37	B	2633	LMG	C3-C4-C5	-2.11	106.47	110.24
30	s	2630	LHG	O8-C23-O10	-2.11	118.26	123.59
27	g	1621	LUT	C37-C21-C22	-2.11	105.44	109.44
26	B	605	CLA	CMB-C2B-C3B	2.11	128.63	124.68
31	b	619	BCR	C11-C12-C13	-2.11	120.49	126.42
26	c	506	CLA	CMC-C2C-C1C	-2.11	121.83	125.04
25	3	606	CHL	O1D-CGD-CBD	-2.11	120.17	124.48
26	B	612	CLA	CHC-C1C-NC	2.11	127.40	124.20
26	b	612	CLA	CHC-C1C-NC	2.11	127.40	124.20
31	T	101	BCR	C1-C6-C5	-2.11	119.64	122.61
27	6	1620	LUT	C19-C9-C8	2.11	121.40	118.08
30	S	2630	LHG	O8-C23-O10	-2.11	118.27	123.59
26	3	612	CLA	CHA-C1A-NA	-2.11	121.57	126.40
26	7	612	CLA	CHA-C1A-NA	-2.11	121.57	126.40
29	S	1623	NEX	C11-C12-C13	-2.11	120.49	126.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	N	601	CHL	CBC-CAC-C3C	-2.11	106.62	112.43
28	g	1622	XAT	C26-C27-C28	-2.11	121.53	125.99
27	R	620	LUT	C18-C5-C6	-2.11	122.16	124.53
27	r	620	LUT	C18-C5-C6	-2.11	122.16	124.53
39	b	626	DGD	C1E-O6E-C5E	2.11	117.83	113.69
25	N	609	CHL	C2A-C1A-CHA	-2.11	120.17	123.86
25	l	601	CHL	C4D-C3D-CAD	2.11	110.58	108.10
25	y	601	CHL	O2A-CGA-CBA	2.11	118.52	111.91
29	s	1623	NEX	C11-C12-C13	-2.11	120.50	126.42
26	a	407	CLA	O2A-CGA-O1A	-2.11	118.27	123.59
36	A	418	SQD	O48-C23-C24	2.11	118.52	111.91
25	8	607	CHL	OMC-CMC-C2C	-2.11	120.92	125.69
26	g	610	CLA	CAA-C2A-C1A	2.11	118.88	111.97
36	a	418	SQD	O48-C23-C24	2.11	118.52	111.91
26	g	602	CLA	O2A-CGA-O1A	-2.11	118.28	123.59
26	2	602	CLA	CHD-C1D-ND	-2.11	122.52	124.45
26	B	616	CLA	C2A-C1A-CHA	2.11	127.54	123.86
25	1	605	CHL	C2A-C1A-CHA	-2.11	120.18	123.86
27	1	1620	LUT	C8-C9-C10	-2.11	115.71	118.94
31	4	623	BCR	C38-C26-C27	2.11	117.66	113.62
28	G	1622	XAT	C26-C27-C28	-2.11	121.54	125.99
26	6	602	CLA	CHB-C4A-NA	2.11	127.42	124.51
26	a	405	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
26	C	506	CLA	C2A-C1A-CHA	2.11	127.54	123.86
25	1	601	CHL	C1B-CHB-C4A	-2.11	125.95	130.12
25	2	605	CHL	O2D-CGD-O1D	-2.11	119.72	123.84
26	S	609	CLA	O2D-CGD-O1D	-2.11	119.72	123.84
26	5	614	CLA	CHD-C1D-ND	-2.10	122.52	124.45
37	b	622	LMG	O3-C3-C2	-2.10	105.48	110.35
25	g	606	CHL	CED-O2D-CGD	2.10	120.70	115.94
26	y	602	CLA	CAA-CBA-CGA	-2.10	107.11	113.25
28	R	622	XAT	O24-C25-C26	-2.10	57.22	58.96
28	r	622	XAT	O24-C25-C26	-2.10	57.22	58.96
27	N	1620	LUT	C7-C8-C9	-2.10	123.06	126.23
30	3	2630	LHG	C18-C17-C16	-2.10	103.75	114.42
30	7	2630	LHG	C18-C17-C16	-2.10	103.75	114.42
37	Z	101	LMG	C38-C37-C36	-2.10	103.75	114.42
25	n	601	CHL	CBC-CAC-C3C	-2.10	106.63	112.43
39	C	519	DGD	C7B-C6B-C5B	-2.10	103.75	114.42
26	2	611	CLA	O2D-CGD-CBD	2.10	115.00	111.27
26	C	502	CLA	CMC-C2C-C3C	2.10	131.82	126.12
26	C	513	CLA	C2A-C1A-CHA	2.10	127.53	123.86

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	513	CLA	C2A-C1A-CHA	2.10	127.53	123.86
26	r	609	CLA	C1D-ND-C4D	-2.10	104.84	106.33
26	Y	602	CLA	CAA-CBA-CGA	-2.10	107.11	113.25
25	4	608	CHL	C2A-C1A-CHA	-2.10	120.19	123.86
25	8	608	CHL	C2A-C1A-CHA	-2.10	120.19	123.86
27	2	1621	LUT	C3-C4-C5	-2.10	107.67	111.85
26	S	609	CLA	O1A-CGA-CBA	2.10	129.83	123.08
25	n	609	CHL	C2A-C1A-CHA	-2.10	120.19	123.86
25	2	601	CHL	CED-O2D-CGD	2.10	120.69	115.94
26	b	617	CLA	C3A-C2A-C1A	2.10	104.48	101.34
26	B	605	CLA	CAC-C3C-C2C	-2.10	123.94	127.53
25	8	609	CHL	O1D-CGD-CBD	-2.10	120.19	124.48
26	B	614	CLA	O1D-CGD-CBD	2.10	128.78	124.48
25	s	601	CHL	CED-O2D-CGD	2.10	120.69	115.94
26	N	602	CLA	O2D-CGD-CBD	2.10	115.00	111.27
25	G	608	CHL	C2A-C1A-CHA	-2.10	120.19	123.86
26	C	511	CLA	C2A-C1A-CHA	2.10	127.53	123.86
39	c	519	DGD	C7B-C6B-C5B	-2.10	103.77	114.42
25	Y	609	CHL	C2A-C1A-CHA	-2.10	120.19	123.86
25	y	609	CHL	C2A-C1A-CHA	-2.10	120.19	123.86
37	z	101	LMG	C38-C37-C36	-2.10	103.78	114.42
26	A	407	CLA	O2A-CGA-O1A	-2.10	118.30	123.59
27	6	1621	LUT	C28-C29-C30	-2.10	115.72	118.94
26	y	603	CLA	CAA-C2A-C3A	-2.10	107.04	112.78
26	3	611	CLA	C2D-C1D-ND	-2.10	108.56	110.10
26	c	506	CLA	C2A-C1A-CHA	2.10	127.52	123.86
27	8	620	LUT	C3-C4-C5	-2.10	107.68	111.85
25	4	607	CHL	OMC-CMC-C2C	-2.10	120.95	125.69
31	C	514	BCR	C16-C15-C14	-2.10	119.18	123.47
26	g	604	CLA	CHB-C4A-NA	2.10	127.41	124.51
26	n	604	CLA	O1D-CGD-CBD	2.10	128.77	124.48
25	3	605	CHL	O1D-CGD-CBD	-2.10	120.20	124.48
27	1	1620	LUT	C20-C13-C12	2.10	121.38	118.08
25	R	614	CHL	CMB-C2B-C1B	2.09	131.68	128.46
25	r	614	CHL	CMB-C2B-C1B	2.09	131.68	128.46
25	6	605	CHL	O2D-CGD-O1D	-2.09	119.74	123.84
26	G	610	CLA	CAA-C2A-C1A	2.09	118.84	111.97
30	Y	2630	LHG	C18-C17-C16	-2.09	103.80	114.42
26	s	609	CLA	O1A-CGA-CBA	2.09	129.81	123.08
26	6	611	CLA	O2D-CGD-CBD	2.09	114.99	111.27
37	z	101	LMG	O2-C2-C1	-2.09	104.96	110.05
28	2	1622	XAT	C39-C29-C30	-2.09	119.99	122.92

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
39	B	626	DGD	C1E-O6E-C5E	2.09	117.80	113.69
28	G	1622	XAT	O4-C5-C6	-2.09	57.23	58.96
25	n	606	CHL	C2A-C1A-CHA	-2.09	120.20	123.86
25	R	606	CHL	CMB-C2B-C3B	2.09	128.59	124.68
27	2	1620	LUT	C19-C9-C8	2.09	121.37	118.08
26	b	613	CLA	C2A-C3A-C4A	2.09	105.25	101.87
31	C	516	BCR	C31-C1-C6	-2.09	106.91	110.30
26	N	604	CLA	O1D-CGD-CBD	2.09	128.76	124.48
27	G	1621	LUT	C1-C2-C3	2.09	118.37	113.64
27	5	1621	LUT	C31-C30-C29	-2.09	124.33	127.31
26	n	604	CLA	CHB-C4A-NA	2.09	127.40	124.51
30	y	2630	LHG	C18-C17-C16	-2.09	103.81	114.42
31	t	101	BCR	C1-C6-C5	-2.09	119.67	122.61
26	R	601	CLA	C1B-CHB-C4A	-2.09	125.97	130.12
26	s	609	CLA	O2D-CGD-O1D	-2.09	119.75	123.84
25	Y	601	CHL	O2A-CGA-CBA	2.09	118.47	111.91
25	4	606	CHL	O1D-CGD-CBD	-2.09	120.21	124.48
26	S	603	CLA	C3C-C4C-NC	-2.09	108.23	110.57
31	c	514	BCR	C16-C15-C14	-2.09	119.19	123.47
26	B	617	CLA	C3A-C2A-C1A	2.09	104.47	101.34
25	G	606	CHL	CED-O2D-CGD	2.09	120.66	115.94
27	S	1621	LUT	C20-C13-C12	2.09	121.37	118.08
27	4	620	LUT	C19-C9-C8	2.09	121.37	118.08
26	b	616	CLA	C2A-C1A-CHA	2.09	127.51	123.86
27	n	1620	LUT	C7-C8-C9	-2.09	123.08	126.23
35	A	408	PHO	C1B-NB-C4B	2.09	111.38	107.09
35	a	408	PHO	C1B-NB-C4B	2.09	111.38	107.09
27	6	1620	LUT	C8-C7-C6	-2.09	121.34	127.20
26	n	602	CLA	O2D-CGD-CBD	2.09	114.98	111.27
26	R	603	CLA	O1D-CGD-CBD	2.09	128.75	124.48
26	r	603	CLA	O1D-CGD-CBD	2.09	128.75	124.48
27	2	1620	LUT	C8-C7-C6	-2.09	121.34	127.20
26	3	610	CLA	C4A-NA-C1A	2.09	107.64	106.71
26	7	610	CLA	C4A-NA-C1A	2.09	107.64	106.71
29	1	1623	NEX	C10-C11-C12	-2.09	116.71	123.22
26	b	611	CLA	C2A-C1A-CHA	2.09	127.51	123.86
25	n	608	CHL	C2A-C1A-CHA	-2.09	120.21	123.86
26	B	604	CLA	C1D-ND-C4D	2.09	107.82	106.33
26	A	405	CLA	C11-C10-C8	-2.09	109.18	115.92
26	3	614	CLA	O2A-CGA-O1A	-2.09	118.33	123.59
26	s	603	CLA	C3C-C4C-NC	-2.09	108.23	110.57
41	F	101	HEM	C4C-CHD-C1D	2.09	125.31	122.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
37	B	2633	LMG	C42-C41-C40	-2.09	103.84	114.42
26	b	605	CLA	CAC-C3C-C2C	-2.08	123.96	127.53
25	n	607	CHL	C11-C10-C8	-2.08	109.18	115.92
27	g	1621	LUT	C1-C2-C3	2.08	118.35	113.64
25	S	601	CHL	CED-O2D-CGD	2.08	120.65	115.94
26	Y	612	CLA	O2A-C1-C2	-2.08	103.16	108.64
25	8	606	CHL	O1D-CGD-CBD	-2.08	120.22	124.48
26	b	604	CLA	C1D-ND-C4D	2.08	107.81	106.33
26	7	611	CLA	C2D-C1D-ND	-2.08	108.57	110.10
25	3	601	CHL	O2D-CGD-O1D	-2.08	119.77	123.84
37	Z	101	LMG	O2-C2-C1	-2.08	104.99	110.05
26	7	614	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
25	5	601	CHL	C1B-CHB-C4A	-2.08	125.99	130.12
27	s	1621	LUT	C20-C13-C12	2.08	121.36	118.08
39	C	518	DGD	C5B-C4B-C3B	-2.08	103.86	114.42
25	7	601	CHL	O2D-CGD-O1D	-2.08	119.77	123.84
25	4	609	CHL	O1D-CGD-CBD	-2.08	120.23	124.48
26	1	604	CLA	O2A-CGA-O1A	-2.08	118.34	123.59
27	1	1621	LUT	C31-C30-C29	-2.08	124.34	127.31
25	2	605	CHL	CAA-C2A-C3A	-2.08	107.08	112.78
41	F	101	HEM	C1B-NB-C4B	2.08	107.22	105.07
30	D	408	LHG	C27-C26-C25	-2.08	103.87	114.42
26	2	602	CLA	CHB-C4A-NA	2.08	127.39	124.51
27	2	1621	LUT	C28-C29-C30	-2.08	115.75	118.94
25	r	606	CHL	CMB-C2B-C3B	2.08	128.57	124.68
27	5	1620	LUT	C11-C10-C9	-2.08	124.34	127.31
25	g	606	CHL	C4D-C3D-CAD	2.08	110.55	108.10
26	1	610	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
25	6	605	CHL	CAA-C2A-C3A	-2.08	107.09	112.78
26	a	405	CLA	C11-C10-C8	-2.08	109.20	115.92
39	c	518	DGD	C5B-C4B-C3B	-2.08	103.88	114.42
26	5	610	CLA	O2A-CGA-O1A	-2.08	118.35	123.59
27	g	1620	LUT	C21-C26-C27	-2.08	110.08	112.70
30	S	2630	LHG	C5-O7-C7	-2.08	112.68	117.79
30	s	2630	LHG	C5-O7-C7	-2.08	112.68	117.79
37	b	2633	LMG	C42-C41-C40	-2.08	103.88	114.42
25	Y	608	CHL	C2A-C1A-CHA	-2.08	120.23	123.86
26	S	614	CLA	C3C-C4C-NC	-2.08	108.24	110.57
26	c	513	CLA	CHD-C1D-ND	-2.08	122.55	124.45
26	4	611	CLA	O2A-CGA-O1A	-2.08	118.13	123.30
25	r	606	CHL	C6-C7-C8	-2.07	109.21	115.92
26	y	612	CLA	O2A-C1-C2	-2.07	103.18	108.64

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	c	511	CLA	C2A-C1A-CHA	2.07	127.49	123.86
28	g	1622	XAT	C7-C8-C9	-2.07	122.31	125.53
30	d	408	LHG	C27-C26-C25	-2.07	103.89	114.42
25	R	606	CHL	C6-C7-C8	-2.07	109.22	115.92
25	n	607	CHL	O2D-CGD-O1D	-2.07	119.78	123.84
29	5	1623	NEX	C10-C11-C12	-2.07	116.75	123.22
31	t	101	BCR	C4-C5-C6	-2.07	119.72	122.73
25	G	606	CHL	C4D-C3D-CAD	2.07	110.54	108.10
28	G	1622	XAT	C7-C8-C9	-2.07	122.31	125.53
25	y	608	CHL	C2A-C1A-CHA	-2.07	120.23	123.86
25	5	601	CHL	C4D-C3D-CAD	2.07	110.54	108.10
26	C	513	CLA	CHD-C1D-ND	-2.07	122.55	124.45
25	7	605	CHL	O1D-CGD-CBD	-2.07	120.25	124.48
26	5	604	CLA	O2A-CGA-O1A	-2.07	118.36	123.59
25	N	607	CHL	C11-C10-C8	-2.07	109.22	115.92
26	r	601	CLA	C1B-CHB-C4A	-2.07	126.02	130.12
25	N	608	CHL	C2A-C1A-CHA	-2.07	120.24	123.86
27	8	620	LUT	C19-C9-C8	2.07	121.34	118.08
25	N	606	CHL	C2A-C1A-CHA	-2.07	120.24	123.86
26	c	510	CLA	CAA-C2A-C3A	-2.07	107.11	112.78
27	G	1620	LUT	C21-C26-C27	-2.07	110.08	112.70
27	N	1621	LUT	C28-C29-C30	-2.07	115.77	118.94
27	n	1621	LUT	C28-C29-C30	-2.07	115.77	118.94
26	B	613	CLA	C2A-C3A-C4A	2.07	105.21	101.87
38	d	405	PL9	C36-C37-C38	-2.07	105.08	111.88
31	B	620	BCR	C3-C4-C5	-2.07	110.38	114.08
26	8	612	CLA	CHA-C1A-NA	-2.07	121.66	126.40
30	C	523	LHG	C18-C17-C16	-2.07	103.93	114.42
30	c	523	LHG	C18-C17-C16	-2.07	103.93	114.42
25	N	608	CHL	OBD-CAD-C3D	-2.07	123.54	128.52
25	n	608	CHL	OBD-CAD-C3D	-2.07	123.54	128.52
26	5	604	CLA	CHD-C1D-ND	-2.07	122.55	124.45
26	c	510	CLA	C11-C10-C8	-2.07	109.24	115.92
26	c	509	CLA	C2A-C3A-C4A	2.07	105.21	101.87
25	r	606	CHL	C4-C3-C5	2.07	118.75	115.27
26	B	611	CLA	C2A-C1A-CHA	2.07	127.47	123.86
27	5	1620	LUT	C7-C8-C9	-2.07	123.11	126.23
38	D	405	PL9	C36-C37-C38	-2.07	105.09	111.88
31	b	620	BCR	C3-C4-C5	-2.06	110.39	114.08
27	1	1620	LUT	C7-C8-C9	-2.06	123.11	126.23
25	Y	608	CHL	C2A-C3A-C4A	-2.06	98.53	101.87
26	g	603	CLA	C2D-C1D-ND	-2.06	108.58	110.10

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1	604	CLA	C1-C2-C3	-2.06	123.41	126.75
25	3	601	CHL	C4D-C3D-CAD	2.06	110.53	108.10
36	B	621	SQD	O48-C23-C24	2.06	118.38	111.91
31	T	101	BCR	C29-C30-C25	2.06	113.66	110.48
25	G	608	CHL	C4D-CHA-C1A	-2.06	118.74	121.25
39	C	520	DGD	C3D-C4D-C5D	-2.06	106.56	110.24
39	c	520	DGD	C3D-C4D-C5D	-2.06	106.56	110.24
26	n	614	CLA	C2D-C1D-ND	-2.06	108.58	110.10
25	1	605	CHL	O2A-CGA-CBA	2.06	120.65	114.03
27	7	1621	LUT	C30-C31-C32	-2.06	116.78	123.22
26	C	510	CLA	C11-C10-C8	-2.06	109.26	115.92
41	f	101	HEM	C4C-CHD-C1D	2.06	125.28	122.56
27	5	1620	LUT	C20-C13-C12	2.06	121.32	118.08
39	C	519	DGD	C3D-C4D-C5D	-2.06	106.56	110.24
29	n	1623	NEX	O24-C25-C26	-2.06	57.25	58.96
25	G	607	CHL	C1-O2A-CGA	2.06	121.85	116.44
36	b	621	SQD	O48-C23-C24	2.06	118.37	111.91
26	B	616	CLA	C3A-C2A-C1A	2.06	104.42	101.34
26	b	616	CLA	C3A-C2A-C1A	2.06	104.42	101.34
26	s	614	CLA	C3C-C4C-NC	-2.06	108.26	110.57
26	4	612	CLA	CHA-C1A-NA	-2.06	121.68	126.40
26	5	604	CLA	C1-C2-C3	-2.06	123.42	126.75
27	3	1621	LUT	C30-C31-C32	-2.06	116.79	123.22
26	C	510	CLA	CAA-C2A-C3A	-2.06	107.14	112.78
39	c	519	DGD	C3D-C4D-C5D	-2.06	106.57	110.24
26	B	609	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
28	3	1622	XAT	O24-C25-C26	-2.06	57.26	58.96
31	4	623	BCR	C35-C13-C14	-2.06	120.04	122.92
27	S	1621	LUT	C21-C26-C27	-2.06	110.10	112.70
26	6	610	CLA	O2A-CGA-O1A	-2.06	118.40	123.59
31	c	516	BCR	C35-C13-C12	2.06	121.31	118.08
25	Y	607	CHL	O2A-C1-C2	2.06	114.04	108.64
25	R	606	CHL	C4-C3-C5	2.06	118.73	115.27
30	L	101	LHG	C27-C26-C25	-2.05	103.99	114.42
30	l	101	LHG	C27-C26-C25	-2.05	103.99	114.42
26	C	509	CLA	C2A-C3A-C4A	2.05	105.19	101.87
26	8	611	CLA	O2A-CGA-O1A	-2.05	118.18	123.30
26	R	601	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
26	r	603	CLA	O2A-CGA-O1A	-2.05	118.41	123.59
31	B	619	BCR	C34-C9-C8	2.05	121.31	118.08
26	b	608	CLA	CHD-C1D-ND	-2.05	122.57	124.45
25	y	608	CHL	C2A-C3A-C4A	-2.05	98.55	101.87

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
25	S	606	CHL	O2A-CGA-CBA	2.05	120.62	114.03
26	R	611	CLA	O1D-CGD-CBD	2.05	128.68	124.48
25	s	606	CHL	O2A-CGA-CBA	2.05	120.62	114.03
26	r	611	CLA	O1D-CGD-CBD	2.05	128.68	124.48
25	g	608	CHL	C4D-CHA-C1A	-2.05	118.75	121.25
31	b	619	BCR	C37-C22-C23	2.05	121.31	118.08
41	f	101	HEM	C1B-NB-C4B	2.05	107.19	105.07
27	s	1621	LUT	C21-C26-C27	-2.05	110.11	112.70
29	6	1623	NEX	C19-C9-C10	-2.05	120.05	122.92
25	G	601	CHL	C1-O2A-CGA	2.05	121.82	116.44
26	B	607	CLA	C2D-C1D-ND	-2.05	108.59	110.10
26	R	611	CLA	CAC-C3C-C4C	2.05	127.47	124.81
31	T	101	BCR	C4-C5-C6	-2.05	119.76	122.73
31	8	623	BCR	C2-C1-C6	2.05	113.63	110.48
31	c	515	BCR	C2-C1-C6	2.05	113.63	110.48
27	1	1620	LUT	C11-C10-C9	-2.05	124.39	127.31
25	R	608	CHL	CAA-C2A-C1A	2.05	118.69	111.97
28	N	1622	XAT	O24-C25-C26	-2.05	57.26	58.96
25	2	607	CHL	O2D-CGD-O1D	-2.05	119.83	123.84
30	B	2630	LHG	C27-C26-C25	-2.05	104.03	114.42
26	d	402	CLA	O2D-CGD-CBD	2.05	114.91	111.27
26	B	608	CLA	CHD-C1D-ND	-2.05	122.57	124.45
31	B	619	BCR	C37-C22-C23	2.05	121.30	118.08
31	C	516	BCR	C35-C13-C12	2.05	121.30	118.08
26	N	604	CLA	O2D-CGD-CBD	2.05	114.90	111.27
26	R	603	CLA	O2A-CGA-O1A	-2.05	118.43	123.59
25	n	608	CHL	C4D-CHA-C1A	-2.05	118.76	121.25
31	B	618	BCR	C16-C15-C14	-2.05	119.28	123.47
26	b	605	CLA	CHA-C1A-NA	-2.05	121.71	126.40
25	5	605	CHL	O2A-CGA-CBA	2.05	120.60	114.03
26	Y	614	CLA	O2A-CGA-O1A	-2.04	118.43	123.59
26	b	604	CLA	C4-C3-C5	2.04	118.71	115.27
29	2	1623	NEX	C19-C9-C10	-2.04	120.06	122.92
27	8	620	LUT	C40-C33-C32	2.04	121.30	118.08
30	b	2630	LHG	C27-C26-C25	-2.04	104.05	114.42
28	N	1622	XAT	C26-C27-C28	-2.04	121.67	125.99
26	B	604	CLA	C4-C3-C5	2.04	118.71	115.27
30	L	101	LHG	C18-C17-C16	-2.04	104.05	114.42
26	C	506	CLA	CMC-C2C-C3C	2.04	131.66	126.12
26	A	406	CLA	C1-C2-C3	-2.04	122.51	126.04
25	g	607	CHL	C1-O2A-CGA	2.04	121.80	116.44
31	B	620	BCR	C15-C16-C17	-2.04	119.29	123.47

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	1	1623	NEX	O24-C25-C26	-2.04	57.27	58.96
29	5	1623	NEX	O24-C25-C26	-2.04	57.27	58.96
26	a	406	CLA	C1-C2-C3	-2.04	122.51	126.04
26	r	601	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
26	4	610	CLA	O2A-CGA-O1A	-2.04	118.21	123.30
25	N	607	CHL	O2D-CGD-O1D	-2.04	119.85	123.84
30	8	2630	LHG	C5-O7-C7	-2.04	114.09	117.90
26	B	605	CLA	CHA-C1A-NA	-2.04	121.72	126.40
26	N	604	CLA	C1-C2-C3	-2.04	123.45	126.75
28	n	1622	XAT	O24-C25-C26	-2.04	57.27	58.96
25	r	608	CHL	CAA-C2A-C1A	2.04	118.66	111.97
26	y	610	CLA	O2D-CGD-O1D	-2.04	119.85	123.84
26	b	609	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
26	y	614	CLA	O2A-CGA-O1A	-2.04	118.44	123.59
29	N	1623	NEX	O24-C25-C26	-2.04	57.27	58.96
36	A	418	SQD	C44-O6-C1	2.04	117.72	113.74
36	a	418	SQD	C44-O6-C1	2.04	117.72	113.74
31	b	618	BCR	C16-C15-C14	-2.04	119.30	123.47
26	B	612	CLA	C2D-C1D-ND	-2.04	108.60	110.10
30	C	523	LHG	C11-C10-C9	-2.04	104.07	114.42
26	c	507	CLA	CHA-C1A-NA	-2.04	121.73	126.40
30	l	101	LHG	C18-C17-C16	-2.04	104.07	114.42
30	4	2630	LHG	C5-O7-C7	-2.04	114.10	117.90
26	7	613	CLA	O2A-C1-C2	-2.04	103.28	108.64
28	6	1622	XAT	C24-C23-C22	-2.04	106.84	110.77
26	B	609	CLA	C11-C10-C8	-2.04	109.33	115.92
26	b	609	CLA	C11-C10-C8	-2.04	109.33	115.92
25	R	608	CHL	O2D-CGD-O1D	-2.04	119.85	123.84
26	8	610	CLA	O2A-CGA-O1A	-2.04	118.22	123.30
25	7	605	CHL	OMC-CMC-C2C	-2.04	121.08	125.69
26	r	603	CLA	C1D-ND-C4D	2.04	107.78	106.33
28	3	1622	XAT	C38-C25-C24	2.04	116.57	114.28
39	B	626	DGD	O6E-C5E-C6E	-2.04	101.37	106.44
38	D	405	PL9	C36-C34-C33	-2.04	117.00	121.12
30	b	2631	LHG	C29-C28-C27	-2.04	104.09	114.42
30	c	523	LHG	C11-C10-C9	-2.04	104.09	114.42
25	3	605	CHL	OMC-CMC-C2C	-2.04	121.08	125.69
36	A	418	SQD	O49-C7-C8	-2.04	115.79	123.73
28	2	1622	XAT	C24-C23-C22	-2.04	106.84	110.77
38	D	405	PL9	C11-C12-C13	-2.03	105.19	111.88
31	b	620	BCR	C15-C16-C17	-2.03	119.31	123.47
27	5	1620	LUT	C38-C25-C24	-2.03	119.21	123.56

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
26	1	602	CLA	CHB-C4A-NA	2.03	127.33	124.51
25	g	601	CHL	C1-O2A-CGA	2.03	121.78	116.44
30	l	101	LHG	O8-C23-C24	2.03	118.29	111.91
36	a	418	SQD	O49-C7-C8	-2.03	115.80	123.73
30	3	2630	LHG	C27-C26-C25	-2.03	104.10	114.42
30	B	2631	LHG	C29-C28-C27	-2.03	104.10	114.42
25	y	606	CHL	C1C-C2C-C3C	-2.03	105.50	107.11
26	N	614	CLA	C2D-C1D-ND	-2.03	108.61	110.10
26	S	602	CLA	C6-C5-C3	-2.03	108.13	113.45
25	y	607	CHL	O2A-C1-C2	2.03	113.98	108.64
26	2	610	CLA	O2A-CGA-O1A	-2.03	118.46	123.59
28	n	1622	XAT	C26-C27-C28	-2.03	121.70	125.99
25	y	606	CHL	OMC-CMC-C2C	-2.03	121.09	125.69
31	C	515	BCR	C2-C1-C6	2.03	113.61	110.48
25	G	609	CHL	O2A-CGA-CBA	2.03	118.28	111.91
25	6	605	CHL	C4D-CHA-C1A	-2.03	118.78	121.25
25	3	601	CHL	CGD-CBD-CAD	-2.03	104.16	110.73
25	7	601	CHL	CGD-CBD-CAD	-2.03	104.16	110.73
26	S	609	CLA	CHB-C4A-NA	2.03	127.32	124.51
38	d	405	PL9	C36-C34-C33	-2.03	117.01	121.12
25	6	607	CHL	O2D-CGD-O1D	-2.03	119.87	123.84
26	3	613	CLA	O2A-C1-C2	-2.03	103.30	108.64
27	s	1620	LUT	C40-C33-C32	2.03	121.28	118.08
25	G	607	CHL	O2D-CGD-O1D	-2.03	119.87	123.84
26	c	506	CLA	CMC-C2C-C3C	2.03	131.62	126.12
25	2	605	CHL	C4D-CHA-C1A	-2.03	118.78	121.25
25	Y	606	CHL	OMC-CMC-C2C	-2.03	121.10	125.69
26	C	506	CLA	CHB-C4A-NA	2.03	127.32	124.51
31	C	514	BCR	C36-C18-C19	2.03	121.27	118.08
26	N	614	CLA	CHD-C1D-ND	-2.03	122.59	124.45
26	1	602	CLA	CHA-C1A-NA	-2.03	121.75	126.40
31	t	101	BCR	C29-C30-C25	2.03	113.60	110.48
25	g	607	CHL	O2D-CGD-O1D	-2.03	119.87	123.84
25	Y	606	CHL	C1C-C2C-C3C	-2.03	105.50	107.11
30	7	2630	LHG	C27-C26-C25	-2.03	104.13	114.42
26	C	512	CLA	CAA-C2A-C3A	-2.03	107.23	112.78
25	N	608	CHL	C4D-CHA-C1A	-2.03	118.78	121.25
26	R	603	CLA	C1D-ND-C4D	2.03	107.78	106.33
26	r	611	CLA	CHA-C1A-NA	-2.03	121.76	126.40
31	4	623	BCR	C2-C1-C6	2.03	113.60	110.48
27	5	1620	LUT	C21-C26-C27	-2.03	110.14	112.70
31	C	514	BCR	C7-C8-C9	-2.03	123.17	126.23

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
29	Y	1623	NEX	C4-C3-C2	-2.03	106.86	110.77
26	C	507	CLA	CHA-C1A-NA	-2.03	121.76	126.40
26	R	611	CLA	CHA-C1A-NA	-2.03	121.76	126.40
31	A	411	BCR	C15-C16-C17	-2.03	119.32	123.47
27	S	1620	LUT	C39-C29-C28	2.03	121.27	118.08
25	g	609	CHL	O2A-CGA-CBA	2.03	118.27	111.91
26	3	612	CLA	CMD-C2D-C1D	-2.03	121.14	124.71
26	7	612	CLA	CMD-C2D-C1D	-2.03	121.14	124.71
26	R	604	CLA	CHD-C1D-ND	-2.03	122.59	124.45
26	n	614	CLA	CHD-C1D-ND	-2.03	122.59	124.45
26	r	604	CLA	CHD-C1D-ND	-2.03	122.59	124.45
27	3	1621	LUT	C8-C7-C6	-2.02	121.52	127.20
26	c	512	CLA	CAA-C2A-C3A	-2.02	107.23	112.78
28	5	1622	XAT	O24-C25-C26	-2.02	57.28	58.96
26	n	604	CLA	C1-C2-C3	-2.02	123.48	126.75
38	d	405	PL9	C11-C12-C13	-2.02	105.23	111.88
39	b	626	DGD	O6E-C5E-C6E	-2.02	101.40	106.44
26	5	602	CLA	CHB-C4A-NA	2.02	127.31	124.51
27	y	1620	LUT	C19-C9-C8	2.02	121.27	118.08
26	G	603	CLA	C2D-C1D-ND	-2.02	108.61	110.10
28	G	1622	XAT	O24-C25-C26	-2.02	57.28	58.96
26	b	607	CLA	CMC-C2C-C1C	-2.02	121.96	125.04
31	8	623	BCR	C35-C13-C14	-2.02	120.09	122.92
26	s	602	CLA	C6-C5-C3	-2.02	108.15	113.45
29	r	623	NEX	C40-C33-C32	2.02	121.26	118.08
28	4	622	XAT	C15-C35-C34	-2.02	119.33	123.47
26	A	406	CLA	CMC-C2C-C3C	2.02	131.60	126.12
26	n	604	CLA	O2D-CGD-CBD	2.02	114.86	111.27
25	4	606	CHL	O2A-CGA-O1A	-2.02	118.26	123.30
25	7	601	CHL	C4D-C3D-CAD	2.02	110.48	108.10
31	b	619	BCR	C34-C9-C8	2.02	121.26	118.08
31	c	514	BCR	C7-C8-C9	-2.02	123.18	126.23
25	R	608	CHL	OBD-CAD-C3D	-2.02	123.66	128.52
26	D	402	CLA	O2D-CGD-CBD	2.02	114.86	111.27
31	a	411	BCR	C15-C16-C17	-2.02	119.34	123.47
27	7	1621	LUT	C8-C7-C6	-2.02	121.53	127.20
25	r	608	CHL	O2D-CGD-O1D	-2.02	119.89	123.84
25	3	605	CHL	C4D-CHA-C1A	-2.02	118.79	121.25
26	s	609	CLA	CHB-C4A-NA	2.02	127.30	124.51
27	s	1620	LUT	C39-C29-C28	2.02	121.26	118.08
31	C	516	BCR	C37-C22-C21	-2.02	120.09	122.92
37	B	2633	LMG	C24-C23-C22	-2.02	104.18	114.42

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	1	1620	LUT	C38-C25-C24	-2.02	119.24	123.56
30	L	101	LHG	O8-C23-C24	2.02	118.24	111.91
28	7	1622	XAT	O24-C25-C26	-2.02	57.29	58.96
37	a	415	LMG	O2-C2-C1	-2.02	105.14	110.05
31	b	618	BCR	C29-C28-C27	-2.02	106.87	111.38
25	2	606	CHL	C2A-C1A-CHA	-2.02	120.33	123.86
31	C	514	BCR	C37-C22-C23	2.02	121.25	118.08
31	c	514	BCR	C37-C22-C23	2.02	121.25	118.08
39	b	626	DGD	O6E-C1E-O5D	-2.02	105.20	109.97
26	B	605	CLA	C3D-C2D-C1D	2.02	108.58	105.83
26	b	605	CLA	C3D-C2D-C1D	2.02	108.58	105.83
26	a	406	CLA	CMC-C2C-C3C	2.02	131.59	126.12
25	7	608	CHL	C2A-C1A-CHA	-2.01	120.34	123.86
26	r	611	CLA	CAC-C3C-C4C	2.01	127.42	124.81
31	B	618	BCR	C29-C28-C27	-2.01	106.88	111.38
39	B	626	DGD	O6E-C1E-O5D	-2.01	105.20	109.97
26	y	612	CLA	O2A-CGA-O1A	-2.01	118.51	123.59
26	3	611	CLA	CAA-C2A-C1A	2.01	118.58	111.97
26	7	611	CLA	CAA-C2A-C1A	2.01	118.58	111.97
28	8	622	XAT	C15-C35-C34	-2.01	119.35	123.47
26	Y	610	CLA	O2D-CGD-O1D	-2.01	119.90	123.84
26	B	609	CLA	C16-C15-C13	-2.01	109.41	115.92
26	B	613	CLA	C11-C12-C13	-2.01	109.41	115.92
37	a	413	LMG	O7-C10-O9	-2.01	118.84	123.70
27	4	620	LUT	C40-C33-C32	2.01	121.25	118.08
26	C	503	CLA	CHD-C1D-ND	-2.01	122.60	124.45
26	8	603	CLA	C2A-C1A-CHA	2.01	127.38	123.86
37	A	413	LMG	O7-C10-O9	-2.01	118.84	123.70
26	C	502	CLA	CAA-C2A-C3A	-2.01	107.27	112.78
37	b	2633	LMG	C24-C23-C22	-2.01	104.21	114.42
26	A	407	CLA	C3C-C4C-NC	-2.01	108.31	110.57
26	a	407	CLA	C3C-C4C-NC	-2.01	108.31	110.57
31	c	514	BCR	C36-C18-C19	2.01	121.25	118.08
35	A	408	PHO	C1-C2-C3	-2.01	122.56	126.04
39	C	518	DGD	C1D-C2D-C3D	-2.01	105.81	110.00
26	N	603	CLA	C1D-ND-C4D	2.01	107.76	106.33
37	A	415	LMG	O2-C2-C1	-2.01	105.16	110.05
31	c	516	BCR	C37-C22-C21	-2.01	120.11	122.92
26	b	613	CLA	C16-C15-C13	-2.01	109.42	115.92
26	b	613	CLA	C11-C12-C13	-2.01	109.42	115.92
39	H	102	DGD	CBB-CAB-C9B	-2.01	104.23	114.42
36	b	621	SQD	O48-C23-O10	-2.01	118.52	123.59

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Mol	Chain	Res	Type	Atoms	Z	Observed(°)	Ideal(°)
27	S	1620	LUT	C40-C33-C32	2.01	121.24	118.08
26	n	603	CLA	C1D-ND-C4D	2.01	107.76	106.33
26	B	613	CLA	C16-C15-C13	-2.01	109.43	115.92
29	5	1623	NEX	C35-C15-C14	-2.01	119.36	123.47
26	B	608	CLA	CHC-C1C-C2C	-2.01	121.17	126.72
26	C	506	CLA	CHA-C1A-NA	-2.01	121.80	126.40
28	Y	1622	XAT	O24-C25-C26	-2.01	57.30	58.96
28	1	1622	XAT	O24-C25-C26	-2.01	57.30	58.96
29	y	1623	NEX	C4-C3-C2	-2.01	106.90	110.77
26	b	609	CLA	C16-C15-C13	-2.01	109.43	115.92
26	2	614	CLA	CHD-C1D-ND	-2.01	122.61	124.45
26	7	604	CLA	CHD-C1D-ND	-2.01	122.61	124.45
26	c	506	CLA	CHB-C4A-NA	2.01	127.29	124.51
28	y	1622	XAT	O24-C25-C26	-2.01	57.30	58.96
25	r	608	CHL	OBD-CAD-C3D	-2.01	123.69	128.52
25	Y	608	CHL	C6-C7-C8	-2.01	109.44	115.92
27	Y	1620	LUT	C19-C9-C8	2.01	121.24	118.08
28	7	1622	XAT	C38-C25-C24	2.01	116.54	114.28
27	3	1620	LUT	C21-C26-C27	-2.01	110.17	112.70
36	B	621	SQD	O48-C23-O10	-2.01	118.53	123.59
26	b	608	CLA	CHC-C1C-C2C	-2.00	121.18	126.72
39	h	102	DGD	CBB-CAB-C9B	-2.00	104.25	114.42
26	s	604	CLA	C1-C2-C3	-2.00	123.51	126.75
26	5	602	CLA	CHA-C1A-NA	-2.00	121.81	126.40
39	H	102	DGD	O5D-C6D-C5D	-2.00	105.34	109.05
39	h	102	DGD	O5D-C6D-C5D	-2.00	105.34	109.05
26	5	614	CLA	O2A-CGA-O1A	-2.00	118.31	123.30
25	G	607	CHL	O2A-CGA-O1A	-2.00	118.54	123.59
25	8	606	CHL	O2A-CGA-O1A	-2.00	118.31	123.30
26	4	603	CLA	C2A-C1A-CHA	2.00	127.36	123.86
25	R	608	CHL	CAA-C2A-C3A	-2.00	107.30	112.78
25	7	605	CHL	C4D-CHA-C1A	-2.00	118.81	121.25
30	l	101	LHG	C15-C14-C13	-2.00	104.27	114.42
29	R	623	NEX	C40-C33-C32	2.00	121.23	118.08
25	y	608	CHL	C6-C7-C8	-2.00	109.45	115.92
26	c	508	CLA	C11-C12-C13	-2.00	109.45	115.92
26	C	512	CLA	C1B-CHB-C4A	-2.00	126.15	130.12
25	4	606	CHL	O2A-CGA-CBA	2.00	120.46	114.03

All (532) chirality outliers are listed below:

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Mol	Chain	Res	Type	Atom
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Mol	Chain	Res	Type	Atom
25	1	601	CHL	ND
25	1	601	CHL	NA
25	1	601	CHL	NC
25	1	605	CHL	ND
25	1	605	CHL	NA
25	1	605	CHL	NC
25	1	606	CHL	ND
25	1	606	CHL	NA
25	1	606	CHL	NC
25	1	607	CHL	ND
25	1	607	CHL	C8
25	1	607	CHL	NA
25	1	607	CHL	NC
25	1	608	CHL	ND
25	1	608	CHL	NA
25	1	608	CHL	NC
25	1	609	CHL	ND
25	1	609	CHL	C8
25	1	609	CHL	NA
25	1	609	CHL	NC
25	2	601	CHL	ND
25	2	601	CHL	NA
25	2	601	CHL	NC
25	2	605	CHL	ND
25	2	605	CHL	NA
25	2	605	CHL	NC
25	2	606	CHL	ND
25	2	606	CHL	NA
25	2	606	CHL	NC
25	2	607	CHL	ND
25	2	607	CHL	C8
25	2	607	CHL	NA
25	2	607	CHL	NC
25	2	608	CHL	ND
25	2	608	CHL	NA
25	2	608	CHL	NC
25	2	609	CHL	ND
25	2	609	CHL	C8
25	2	609	CHL	NA
25	2	609	CHL	NC
25	3	601	CHL	ND

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Mol	Chain	Res	Type	Atom
25	3	601	CHL	C8
25	3	601	CHL	NA
25	3	601	CHL	NC
25	3	605	CHL	ND
25	3	605	CHL	NA
25	3	605	CHL	NC
25	3	606	CHL	ND
25	3	606	CHL	NA
25	3	606	CHL	NC
25	3	607	CHL	ND
25	3	607	CHL	NA
25	3	607	CHL	NC
25	3	608	CHL	ND
25	3	608	CHL	NA
25	3	608	CHL	NC
25	3	609	CHL	ND
25	3	609	CHL	C8
25	3	609	CHL	NA
25	3	609	CHL	NC
25	4	601	CHL	ND
25	4	601	CHL	NA
25	4	601	CHL	NC
25	4	606	CHL	ND
25	4	606	CHL	NA
25	4	606	CHL	NC
25	4	607	CHL	ND
25	4	607	CHL	NA
25	4	607	CHL	NC
25	4	608	CHL	ND
25	4	608	CHL	NA
25	4	608	CHL	NC
25	4	609	CHL	ND
25	4	609	CHL	NA
25	4	609	CHL	NC
25	G	601	CHL	ND
25	G	601	CHL	C8
25	G	601	CHL	NA
25	G	601	CHL	NC
25	G	605	CHL	ND
25	G	605	CHL	NA
25	G	605	CHL	NC
25	G	606	CHL	ND

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Mol	Chain	Res	Type	Atom
25	G	606	CHL	NA
25	G	606	CHL	NC
25	G	607	CHL	ND
25	G	607	CHL	C8
25	G	607	CHL	NA
25	G	607	CHL	NC
25	G	608	CHL	ND
25	G	608	CHL	C8
25	G	608	CHL	NA
25	G	608	CHL	NC
25	G	609	CHL	ND
25	G	609	CHL	C8
25	G	609	CHL	NA
25	G	609	CHL	NC
25	N	601	CHL	ND
25	N	601	CHL	C8
25	N	601	CHL	NA
25	N	601	CHL	NC
25	N	605	CHL	ND
25	N	605	CHL	NA
25	N	605	CHL	NC
25	N	606	CHL	ND
25	N	606	CHL	NA
25	N	606	CHL	NC
25	N	607	CHL	ND
25	N	607	CHL	C8
25	N	607	CHL	NA
25	N	607	CHL	NC
25	N	608	CHL	ND
25	N	608	CHL	C8
25	N	608	CHL	NA
25	N	608	CHL	NC
25	N	609	CHL	ND
25	N	609	CHL	C8
25	N	609	CHL	NA
25	N	609	CHL	NC
25	R	606	CHL	ND
25	R	606	CHL	C8
25	R	606	CHL	NA
25	R	606	CHL	NC
25	R	607	CHL	ND
25	R	607	CHL	C8

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

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Mol	Chain	Res	Type	Atom
25	Y	609	CHL	NA
25	Y	609	CHL	NC
25	5	601	CHL	ND
25	5	601	CHL	NA
25	5	601	CHL	NC
25	5	605	CHL	ND
25	5	605	CHL	NA
25	5	605	CHL	NC
25	5	606	CHL	ND
25	5	606	CHL	NA
25	5	606	CHL	NC
25	5	607	CHL	ND
25	5	607	CHL	C8
25	5	607	CHL	NA
25	5	607	CHL	NC
25	5	608	CHL	ND
25	5	608	CHL	NA
25	5	608	CHL	NC
25	5	609	CHL	ND
25	5	609	CHL	C8
25	5	609	CHL	NA
25	5	609	CHL	NC
25	6	601	CHL	ND
25	6	601	CHL	NA
25	6	601	CHL	NC
25	6	605	CHL	ND
25	6	605	CHL	NA
25	6	605	CHL	NC
25	6	606	CHL	ND
25	6	606	CHL	NA
25	6	606	CHL	NC
25	6	607	CHL	ND
25	6	607	CHL	C8
25	6	607	CHL	NA
25	6	607	CHL	NC
25	6	608	CHL	ND
25	6	608	CHL	NA
25	6	608	CHL	NC
25	6	609	CHL	ND
25	6	609	CHL	C8
25	6	609	CHL	NA
25	6	609	CHL	NC

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Mol	Chain	Res	Type	Atom
25	7	601	CHL	ND
25	7	601	CHL	C8
25	7	601	CHL	NA
25	7	601	CHL	NC
25	7	605	CHL	ND
25	7	605	CHL	NA
25	7	605	CHL	NC
25	7	606	CHL	ND
25	7	606	CHL	NA
25	7	606	CHL	NC
25	7	607	CHL	ND
25	7	607	CHL	NA
25	7	607	CHL	NC
25	7	608	CHL	ND
25	7	608	CHL	NA
25	7	608	CHL	NC
25	7	609	CHL	ND
25	7	609	CHL	C8
25	7	609	CHL	NA
25	7	609	CHL	NC
25	8	601	CHL	ND
25	8	601	CHL	NA
25	8	601	CHL	NC
25	8	606	CHL	ND
25	8	606	CHL	NA
25	8	606	CHL	NC
25	8	607	CHL	ND
25	8	607	CHL	NA
25	8	607	CHL	NC
25	8	608	CHL	ND
25	8	608	CHL	NA
25	8	608	CHL	NC
25	8	609	CHL	ND
25	8	609	CHL	NA
25	8	609	CHL	NC
25	g	601	CHL	ND
25	g	601	CHL	C8
25	g	601	CHL	NA
25	g	601	CHL	NC
25	g	605	CHL	ND
25	g	605	CHL	NA
25	g	605	CHL	NC

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

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

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Mol	Chain	Res	Type	Atom
25	y	609	CHL	C8
25	y	609	CHL	NA
25	y	609	CHL	NC
26	1	602	CLA	ND
26	1	603	CLA	ND
26	1	610	CLA	ND
26	1	611	CLA	ND
26	1	612	CLA	ND
26	1	614	CLA	ND
26	2	602	CLA	ND
26	2	603	CLA	ND
26	2	604	CLA	ND
26	2	610	CLA	ND
26	2	612	CLA	ND
26	2	614	CLA	ND
26	3	602	CLA	ND
26	3	603	CLA	ND
26	3	604	CLA	ND
26	3	610	CLA	ND
26	3	611	CLA	ND
26	3	612	CLA	ND
26	3	613	CLA	ND
26	3	614	CLA	ND
26	4	602	CLA	ND
26	4	603	CLA	ND
26	4	610	CLA	ND
26	4	611	CLA	ND
26	4	612	CLA	ND
26	A	405	CLA	ND
26	A	406	CLA	ND
26	A	410	CLA	ND
26	B	602	CLA	ND
26	B	603	CLA	ND
26	B	604	CLA	ND
26	B	605	CLA	ND
26	B	606	CLA	ND
26	B	607	CLA	ND
26	B	608	CLA	ND
26	B	611	CLA	ND
26	B	612	CLA	ND
26	B	613	CLA	ND
26	B	614	CLA	ND

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Mol	Chain	Res	Type	Atom
26	B	615	CLA	ND
26	B	616	CLA	ND
26	B	617	CLA	ND
26	C	501	CLA	ND
26	C	502	CLA	ND
26	C	503	CLA	ND
26	C	504	CLA	ND
26	C	505	CLA	ND
26	C	506	CLA	ND
26	C	507	CLA	ND
26	C	508	CLA	ND
26	C	509	CLA	ND
26	C	510	CLA	ND
26	C	511	CLA	ND
26	C	512	CLA	ND
26	D	402	CLA	ND
26	G	602	CLA	ND
26	G	603	CLA	ND
26	G	604	CLA	ND
26	G	610	CLA	ND
26	G	611	CLA	ND
26	G	612	CLA	ND
26	G	613	CLA	ND
26	G	614	CLA	ND
26	N	602	CLA	ND
26	N	603	CLA	ND
26	N	604	CLA	ND
26	N	610	CLA	ND
26	N	611	CLA	ND
26	N	612	CLA	ND
26	N	613	CLA	ND
26	N	614	CLA	ND
26	R	601	CLA	ND
26	R	602	CLA	ND
26	R	603	CLA	ND
26	R	604	CLA	ND
26	R	609	CLA	ND
26	R	610	CLA	ND
26	R	611	CLA	ND
26	R	612	CLA	ND
26	R	613	CLA	ND
26	S	602	CLA	ND

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Mol	Chain	Res	Type	Atom
26	S	603	CLA	ND
26	S	604	CLA	ND
26	S	609	CLA	ND
26	S	610	CLA	ND
26	S	611	CLA	ND
26	S	612	CLA	ND
26	S	613	CLA	ND
26	S	614	CLA	ND
26	Y	602	CLA	ND
26	Y	603	CLA	ND
26	Y	604	CLA	ND
26	Y	610	CLA	ND
26	Y	611	CLA	ND
26	Y	612	CLA	ND
26	Y	613	CLA	ND
26	Y	614	CLA	ND
26	5	602	CLA	ND
26	5	603	CLA	ND
26	5	610	CLA	ND
26	5	611	CLA	ND
26	5	612	CLA	ND
26	5	614	CLA	ND
26	6	602	CLA	ND
26	6	603	CLA	ND
26	6	604	CLA	ND
26	6	610	CLA	ND
26	6	612	CLA	ND
26	6	614	CLA	ND
26	7	602	CLA	ND
26	7	603	CLA	ND
26	7	604	CLA	ND
26	7	610	CLA	ND
26	7	611	CLA	ND
26	7	612	CLA	ND
26	7	613	CLA	ND
26	7	614	CLA	ND
26	8	602	CLA	ND
26	8	603	CLA	ND
26	8	610	CLA	ND
26	8	611	CLA	ND
26	8	612	CLA	ND
26	a	405	CLA	ND

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Mol	Chain	Res	Type	Atom
26	a	406	CLA	ND
26	a	410	CLA	ND
26	b	602	CLA	ND
26	b	603	CLA	ND
26	b	604	CLA	ND
26	b	605	CLA	ND
26	b	606	CLA	ND
26	b	607	CLA	ND
26	b	608	CLA	ND
26	b	611	CLA	ND
26	b	612	CLA	ND
26	b	613	CLA	ND
26	b	614	CLA	ND
26	b	615	CLA	ND
26	b	616	CLA	ND
26	b	617	CLA	ND
26	c	501	CLA	ND
26	c	502	CLA	ND
26	c	503	CLA	ND
26	c	504	CLA	ND
26	c	505	CLA	ND
26	c	506	CLA	ND
26	c	507	CLA	ND
26	c	508	CLA	ND
26	c	509	CLA	ND
26	c	510	CLA	ND
26	c	511	CLA	ND
26	c	512	CLA	ND
26	d	402	CLA	ND
26	g	602	CLA	ND
26	g	603	CLA	ND
26	g	604	CLA	ND
26	g	610	CLA	ND
26	g	611	CLA	ND
26	g	612	CLA	ND
26	g	613	CLA	ND
26	g	614	CLA	ND
26	n	602	CLA	ND
26	n	603	CLA	ND
26	n	604	CLA	ND
26	n	610	CLA	ND
26	n	611	CLA	ND

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Mol	Chain	Res	Type	Atom
26	n	612	CLA	ND
26	n	613	CLA	ND
26	n	614	CLA	ND
26	r	601	CLA	ND
26	r	602	CLA	ND
26	r	603	CLA	ND
26	r	604	CLA	ND
26	r	609	CLA	ND
26	r	610	CLA	ND
26	r	611	CLA	ND
26	r	612	CLA	ND
26	r	613	CLA	ND
26	s	602	CLA	ND
26	s	603	CLA	ND
26	s	604	CLA	ND
26	s	609	CLA	ND
26	s	610	CLA	ND
26	s	611	CLA	ND
26	s	612	CLA	ND
26	s	613	CLA	ND
26	s	614	CLA	ND
26	y	602	CLA	ND
26	y	603	CLA	ND
26	y	604	CLA	ND
26	y	610	CLA	ND
26	y	611	CLA	ND
26	y	612	CLA	ND
26	y	613	CLA	ND
26	y	614	CLA	ND

All (4969) torsion outliers are listed below:

Mol	Chain	Res	Type	Atoms
25	1	601	CHL	C1C-C2C-CMC-OMC
25	1	601	CHL	C3C-C2C-CMC-OMC
25	1	601	CHL	CHA-CBD-CGD-O1D
25	1	601	CHL	CHA-CBD-CGD-O2D
25	1	605	CHL	C1C-C2C-CMC-OMC
25	1	605	CHL	C3C-C2C-CMC-OMC
25	1	606	CHL	C1C-C2C-CMC-OMC
25	1	607	CHL	C1C-C2C-CMC-OMC
25	1	607	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
25	1	608	CHL	C1A-C2A-CAA-CBA
25	1	608	CHL	C1C-C2C-CMC-OMC
25	1	608	CHL	C3C-C2C-CMC-OMC
25	1	608	CHL	CBD-CGD-O2D-CED
25	1	609	CHL	C1C-C2C-CMC-OMC
25	1	609	CHL	C3C-C2C-CMC-OMC
25	2	601	CHL	C1A-C2A-CAA-CBA
25	2	601	CHL	CHA-CBD-CGD-O1D
25	2	601	CHL	CHA-CBD-CGD-O2D
25	2	605	CHL	C3C-C2C-CMC-OMC
25	2	607	CHL	C1C-C2C-CMC-OMC
25	2	607	CHL	C3C-C2C-CMC-OMC
25	2	608	CHL	C3C-C2C-CMC-OMC
25	2	608	CHL	CBD-CGD-O2D-CED
25	2	609	CHL	C1C-C2C-CMC-OMC
25	2	609	CHL	C3C-C2C-CMC-OMC
25	3	605	CHL	C1C-C2C-CMC-OMC
25	3	605	CHL	C3C-C2C-CMC-OMC
25	3	606	CHL	C1C-C2C-CMC-OMC
25	3	606	CHL	C3C-C2C-CMC-OMC
25	3	607	CHL	C1C-C2C-CMC-OMC
25	3	607	CHL	C3C-C2C-CMC-OMC
25	3	608	CHL	CBD-CGD-O2D-CED
25	3	609	CHL	C1C-C2C-CMC-OMC
25	3	609	CHL	C3C-C2C-CMC-OMC
25	4	601	CHL	C1C-C2C-CMC-OMC
25	4	601	CHL	C3C-C2C-CMC-OMC
25	4	606	CHL	C1A-C2A-CAA-CBA
25	4	606	CHL	C1C-C2C-CMC-OMC
25	4	606	CHL	C3C-C2C-CMC-OMC
25	4	607	CHL	C1C-C2C-CMC-OMC
25	4	607	CHL	C3C-C2C-CMC-OMC
25	4	608	CHL	C1C-C2C-CMC-OMC
25	4	608	CHL	C3C-C2C-CMC-OMC
25	4	608	CHL	CBD-CGD-O2D-CED
25	4	609	CHL	C1C-C2C-CMC-OMC
25	4	609	CHL	C3C-C2C-CMC-OMC
25	G	601	CHL	C2-C3-C5-C6
25	G	601	CHL	C4-C3-C5-C6
25	G	605	CHL	C1C-C2C-CMC-OMC
25	G	605	CHL	C3C-C2C-CMC-OMC
25	G	605	CHL	CAD-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	G	605	CHL	CAD-CBD-CGD-O2D
25	G	605	CHL	CBD-CGD-O2D-CED
25	G	606	CHL	C1C-C2C-CMC-OMC
25	G	609	CHL	CBD-CGD-O2D-CED
25	N	605	CHL	C1C-C2C-CMC-OMC
25	N	605	CHL	C3C-C2C-CMC-OMC
25	N	605	CHL	CAD-CBD-CGD-O1D
25	N	605	CHL	CAD-CBD-CGD-O2D
25	N	606	CHL	C1C-C2C-CMC-OMC
25	N	607	CHL	C1C-C2C-CMC-OMC
25	N	607	CHL	C3C-C2C-CMC-OMC
25	N	609	CHL	C1C-C2C-CMC-OMC
25	N	609	CHL	C3C-C2C-CMC-OMC
25	R	606	CHL	C11-C10-C8-C9
25	R	608	CHL	C1A-C2A-CAA-CBA
25	R	608	CHL	CBD-CGD-O2D-CED
25	R	614	CHL	CHA-CBD-CGD-O1D
25	R	614	CHL	CHA-CBD-CGD-O2D
25	R	614	CHL	CAD-CBD-CGD-O1D
25	R	614	CHL	CAD-CBD-CGD-O2D
25	R	614	CHL	CBD-CGD-O2D-CED
25	S	601	CHL	CHA-CBD-CGD-O1D
25	S	601	CHL	CHA-CBD-CGD-O2D
25	S	606	CHL	C1C-C2C-CMC-OMC
25	S	606	CHL	C3C-C2C-CMC-OMC
25	S	606	CHL	CHA-CBD-CGD-O1D
25	S	606	CHL	CHA-CBD-CGD-O2D
25	S	606	CHL	CAD-CBD-CGD-O1D
25	S	606	CHL	CAD-CBD-CGD-O2D
25	S	607	CHL	C3C-C2C-CMC-OMC
25	S	608	CHL	C1A-C2A-CAA-CBA
25	Y	601	CHL	C4-C3-C5-C6
25	Y	605	CHL	C1A-C2A-CAA-CBA
25	Y	605	CHL	C1C-C2C-CMC-OMC
25	Y	605	CHL	C3C-C2C-CMC-OMC
25	Y	606	CHL	C1C-C2C-CMC-OMC
25	Y	607	CHL	C1C-C2C-CMC-OMC
25	Y	607	CHL	C3C-C2C-CMC-OMC
25	Y	608	CHL	C1A-C2A-CAA-CBA
25	Y	608	CHL	C3C-C2C-CMC-OMC
25	5	601	CHL	C1C-C2C-CMC-OMC
25	5	601	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
25	5	601	CHL	CHA-CBD-CGD-O1D
25	5	601	CHL	CHA-CBD-CGD-O2D
25	5	605	CHL	C1C-C2C-CMC-OMC
25	5	605	CHL	C3C-C2C-CMC-OMC
25	5	606	CHL	C1C-C2C-CMC-OMC
25	5	607	CHL	C1C-C2C-CMC-OMC
25	5	607	CHL	C3C-C2C-CMC-OMC
25	5	608	CHL	C1A-C2A-CAA-CBA
25	5	608	CHL	C1C-C2C-CMC-OMC
25	5	608	CHL	C3C-C2C-CMC-OMC
25	5	608	CHL	CBD-CGD-O2D-CED
25	5	609	CHL	C1C-C2C-CMC-OMC
25	5	609	CHL	C3C-C2C-CMC-OMC
25	6	601	CHL	C1A-C2A-CAA-CBA
25	6	601	CHL	CHA-CBD-CGD-O1D
25	6	601	CHL	CHA-CBD-CGD-O2D
25	6	605	CHL	C3C-C2C-CMC-OMC
25	6	607	CHL	C1C-C2C-CMC-OMC
25	6	607	CHL	C3C-C2C-CMC-OMC
25	6	608	CHL	C3C-C2C-CMC-OMC
25	6	608	CHL	CBD-CGD-O2D-CED
25	6	609	CHL	C1C-C2C-CMC-OMC
25	6	609	CHL	C3C-C2C-CMC-OMC
25	7	605	CHL	C1C-C2C-CMC-OMC
25	7	605	CHL	C3C-C2C-CMC-OMC
25	7	606	CHL	C1C-C2C-CMC-OMC
25	7	606	CHL	C3C-C2C-CMC-OMC
25	7	607	CHL	C1C-C2C-CMC-OMC
25	7	607	CHL	C3C-C2C-CMC-OMC
25	7	608	CHL	CBD-CGD-O2D-CED
25	7	609	CHL	C1C-C2C-CMC-OMC
25	7	609	CHL	C3C-C2C-CMC-OMC
25	8	601	CHL	C1C-C2C-CMC-OMC
25	8	601	CHL	C3C-C2C-CMC-OMC
25	8	606	CHL	C1A-C2A-CAA-CBA
25	8	606	CHL	C1C-C2C-CMC-OMC
25	8	606	CHL	C3C-C2C-CMC-OMC
25	8	607	CHL	C1C-C2C-CMC-OMC
25	8	607	CHL	C3C-C2C-CMC-OMC
25	8	608	CHL	C1C-C2C-CMC-OMC
25	8	608	CHL	C3C-C2C-CMC-OMC
25	8	608	CHL	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	8	609	CHL	C1C-C2C-CMC-OMC
25	8	609	CHL	C3C-C2C-CMC-OMC
25	g	601	CHL	C2-C3-C5-C6
25	g	601	CHL	C4-C3-C5-C6
25	g	605	CHL	C1C-C2C-CMC-OMC
25	g	605	CHL	C3C-C2C-CMC-OMC
25	g	605	CHL	CAD-CBD-CGD-O1D
25	g	605	CHL	CAD-CBD-CGD-O2D
25	g	605	CHL	CBD-CGD-O2D-CED
25	g	606	CHL	C1C-C2C-CMC-OMC
25	g	609	CHL	CBD-CGD-O2D-CED
25	n	605	CHL	C1C-C2C-CMC-OMC
25	n	605	CHL	C3C-C2C-CMC-OMC
25	n	605	CHL	CAD-CBD-CGD-O1D
25	n	605	CHL	CAD-CBD-CGD-O2D
25	n	606	CHL	C1C-C2C-CMC-OMC
25	n	607	CHL	C1C-C2C-CMC-OMC
25	n	607	CHL	C3C-C2C-CMC-OMC
25	n	609	CHL	C1C-C2C-CMC-OMC
25	n	609	CHL	C3C-C2C-CMC-OMC
25	r	606	CHL	C11-C10-C8-C9
25	r	608	CHL	C1A-C2A-CAA-CBA
25	r	608	CHL	CBD-CGD-O2D-CED
25	r	614	CHL	CHA-CBD-CGD-O1D
25	r	614	CHL	CHA-CBD-CGD-O2D
25	r	614	CHL	CAD-CBD-CGD-O1D
25	r	614	CHL	CAD-CBD-CGD-O2D
25	r	614	CHL	CBD-CGD-O2D-CED
25	s	601	CHL	CHA-CBD-CGD-O1D
25	s	601	CHL	CHA-CBD-CGD-O2D
25	s	606	CHL	C1C-C2C-CMC-OMC
25	s	606	CHL	C3C-C2C-CMC-OMC
25	s	606	CHL	CHA-CBD-CGD-O1D
25	s	606	CHL	CHA-CBD-CGD-O2D
25	s	606	CHL	CAD-CBD-CGD-O1D
25	s	606	CHL	CAD-CBD-CGD-O2D
25	s	607	CHL	C3C-C2C-CMC-OMC
25	s	608	CHL	C1A-C2A-CAA-CBA
25	y	601	CHL	C4-C3-C5-C6
25	y	605	CHL	C1A-C2A-CAA-CBA
25	y	605	CHL	C1C-C2C-CMC-OMC
25	y	605	CHL	C3C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
25	y	606	CHL	C1C-C2C-CMC-OMC
25	y	607	CHL	C1C-C2C-CMC-OMC
25	y	607	CHL	C3C-C2C-CMC-OMC
25	y	608	CHL	C1A-C2A-CAA-CBA
25	y	608	CHL	C3C-C2C-CMC-OMC
26	1	603	CLA	CHA-CBD-CGD-O1D
26	1	603	CLA	CBD-CGD-O2D-CED
26	1	604	CLA	CHA-CBD-CGD-O1D
26	1	604	CLA	CHA-CBD-CGD-O2D
26	1	604	CLA	CAD-CBD-CGD-O1D
26	1	604	CLA	CAD-CBD-CGD-O2D
26	1	611	CLA	C2A-CAA-CBA-CGA
26	2	603	CLA	CBD-CGD-O2D-CED
26	2	604	CLA	C1A-C2A-CAA-CBA
26	2	604	CLA	CBD-CGD-O2D-CED
26	2	613	CLA	CHA-CBD-CGD-O1D
26	2	613	CLA	CHA-CBD-CGD-O2D
26	2	614	CLA	C1A-C2A-CAA-CBA
26	2	614	CLA	C3A-C2A-CAA-CBA
26	2	614	CLA	CBD-CGD-O2D-CED
26	3	603	CLA	CHA-CBD-CGD-O1D
26	3	603	CLA	CHA-CBD-CGD-O2D
26	3	604	CLA	C2A-CAA-CBA-CGA
26	3	604	CLA	CHA-CBD-CGD-O1D
26	3	611	CLA	C1A-C2A-CAA-CBA
26	3	612	CLA	CHA-CBD-CGD-O1D
26	3	612	CLA	CHA-CBD-CGD-O2D
26	3	612	CLA	CAD-CBD-CGD-O1D
26	3	613	CLA	CHA-CBD-CGD-O1D
26	3	613	CLA	CHA-CBD-CGD-O2D
26	3	613	CLA	CBD-CGD-O2D-CED
26	3	614	CLA	CHA-CBD-CGD-O1D
26	3	614	CLA	CHA-CBD-CGD-O2D
26	4	602	CLA	CBD-CGD-O2D-CED
26	4	603	CLA	CBD-CGD-O2D-CED
26	4	604	CLA	C2A-CAA-CBA-CGA
26	4	604	CLA	CHA-CBD-CGD-O1D
26	4	604	CLA	CHA-CBD-CGD-O2D
26	4	604	CLA	CBD-CGD-O2D-CED
26	A	406	CLA	C1A-C2A-CAA-CBA
26	A	406	CLA	CHA-CBD-CGD-O1D
26	A	406	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
26	A	407	CLA	CHA-CBD-CGD-O1D
26	A	407	CLA	CHA-CBD-CGD-O2D
26	B	602	CLA	C2A-CAA-CBA-CGA
26	B	602	CLA	CHA-CBD-CGD-O1D
26	B	602	CLA	CHA-CBD-CGD-O2D
26	B	605	CLA	CHA-CBD-CGD-O2D
26	B	613	CLA	C1A-C2A-CAA-CBA
26	B	613	CLA	C3A-C2A-CAA-CBA
26	B	615	CLA	CBD-CGD-O2D-CED
26	C	502	CLA	CHA-CBD-CGD-O1D
26	C	502	CLA	CHA-CBD-CGD-O2D
26	C	502	CLA	CAD-CBD-CGD-O1D
26	C	504	CLA	C2-C3-C5-C6
26	C	504	CLA	C4-C3-C5-C6
26	C	506	CLA	C4-C3-C5-C6
26	C	507	CLA	C1A-C2A-CAA-CBA
26	C	507	CLA	C3A-C2A-CAA-CBA
26	C	507	CLA	C11-C10-C8-C9
26	D	403	CLA	CBD-CGD-O2D-CED
26	G	610	CLA	C1A-C2A-CAA-CBA
26	G	610	CLA	C4-C3-C5-C6
26	G	611	CLA	C1A-C2A-CAA-CBA
26	G	611	CLA	C3A-C2A-CAA-CBA
26	N	610	CLA	C1A-C2A-CAA-CBA
26	N	610	CLA	C3A-C2A-CAA-CBA
26	R	601	CLA	C1A-C2A-CAA-CBA
26	R	601	CLA	C3A-C2A-CAA-CBA
26	R	601	CLA	CBD-CGD-O2D-CED
26	R	611	CLA	C1A-C2A-CAA-CBA
26	R	611	CLA	C3A-C2A-CAA-CBA
26	R	611	CLA	CBA-CGA-O2A-C1
26	R	612	CLA	CBD-CGD-O2D-CED
26	R	613	CLA	CHA-CBD-CGD-O1D
26	R	613	CLA	CHA-CBD-CGD-O2D
26	R	616	CLA	C1A-C2A-CAA-CBA
26	R	616	CLA	C3A-C2A-CAA-CBA
26	R	616	CLA	CHA-CBD-CGD-O1D
26	R	616	CLA	CHA-CBD-CGD-O2D
26	S	602	CLA	C1A-C2A-CAA-CBA
26	S	602	CLA	C3A-C2A-CAA-CBA
26	S	604	CLA	C1A-C2A-CAA-CBA
26	S	609	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	S	610	CLA	C2-C3-C5-C6
26	S	610	CLA	C4-C3-C5-C6
26	S	612	CLA	CBD-CGD-O2D-CED
26	5	603	CLA	CHA-CBD-CGD-O1D
26	5	603	CLA	CBD-CGD-O2D-CED
26	5	604	CLA	CHA-CBD-CGD-O1D
26	5	604	CLA	CHA-CBD-CGD-O2D
26	5	604	CLA	CAD-CBD-CGD-O1D
26	5	604	CLA	CAD-CBD-CGD-O2D
26	5	611	CLA	C2A-CAA-CBA-CGA
26	6	603	CLA	CBD-CGD-O2D-CED
26	6	604	CLA	C1A-C2A-CAA-CBA
26	6	604	CLA	CBD-CGD-O2D-CED
26	6	613	CLA	CHA-CBD-CGD-O1D
26	6	613	CLA	CHA-CBD-CGD-O2D
26	6	614	CLA	C1A-C2A-CAA-CBA
26	6	614	CLA	C3A-C2A-CAA-CBA
26	6	614	CLA	CBD-CGD-O2D-CED
26	7	603	CLA	CHA-CBD-CGD-O1D
26	7	603	CLA	CHA-CBD-CGD-O2D
26	7	604	CLA	C2A-CAA-CBA-CGA
26	7	604	CLA	CHA-CBD-CGD-O1D
26	7	611	CLA	C1A-C2A-CAA-CBA
26	7	612	CLA	CHA-CBD-CGD-O1D
26	7	612	CLA	CHA-CBD-CGD-O2D
26	7	612	CLA	CAD-CBD-CGD-O1D
26	7	613	CLA	CHA-CBD-CGD-O1D
26	7	613	CLA	CHA-CBD-CGD-O2D
26	7	613	CLA	CBD-CGD-O2D-CED
26	7	614	CLA	CHA-CBD-CGD-O1D
26	7	614	CLA	CHA-CBD-CGD-O2D
26	8	602	CLA	CBD-CGD-O2D-CED
26	8	603	CLA	CBD-CGD-O2D-CED
26	8	604	CLA	C2A-CAA-CBA-CGA
26	8	604	CLA	CHA-CBD-CGD-O1D
26	8	604	CLA	CHA-CBD-CGD-O2D
26	8	604	CLA	CBD-CGD-O2D-CED
26	a	406	CLA	C1A-C2A-CAA-CBA
26	a	406	CLA	CHA-CBD-CGD-O1D
26	a	406	CLA	CHA-CBD-CGD-O2D
26	a	407	CLA	CHA-CBD-CGD-O1D
26	a	407	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
26	b	602	CLA	C2A-CAA-CBA-CGA
26	b	602	CLA	CHA-CBD-CGD-O1D
26	b	602	CLA	CHA-CBD-CGD-O2D
26	b	605	CLA	CHA-CBD-CGD-O2D
26	b	613	CLA	C1A-C2A-CAA-CBA
26	b	613	CLA	C3A-C2A-CAA-CBA
26	b	615	CLA	CBD-CGD-O2D-CED
26	c	502	CLA	CHA-CBD-CGD-O1D
26	c	502	CLA	CHA-CBD-CGD-O2D
26	c	502	CLA	CAD-CBD-CGD-O1D
26	c	504	CLA	C2-C3-C5-C6
26	c	504	CLA	C4-C3-C5-C6
26	c	506	CLA	C4-C3-C5-C6
26	c	506	CLA	C11-C12-C13-C14
26	c	507	CLA	C1A-C2A-CAA-CBA
26	c	507	CLA	C3A-C2A-CAA-CBA
26	c	507	CLA	C11-C10-C8-C9
26	d	403	CLA	CBD-CGD-O2D-CED
26	g	610	CLA	C1A-C2A-CAA-CBA
26	g	610	CLA	C4-C3-C5-C6
26	g	611	CLA	C1A-C2A-CAA-CBA
26	g	611	CLA	C3A-C2A-CAA-CBA
26	n	610	CLA	C1A-C2A-CAA-CBA
26	n	610	CLA	C3A-C2A-CAA-CBA
26	r	601	CLA	C1A-C2A-CAA-CBA
26	r	601	CLA	C3A-C2A-CAA-CBA
26	r	601	CLA	CBD-CGD-O2D-CED
26	r	611	CLA	C1A-C2A-CAA-CBA
26	r	611	CLA	C3A-C2A-CAA-CBA
26	r	611	CLA	CBA-CGA-O2A-C1
26	r	612	CLA	CBD-CGD-O2D-CED
26	r	613	CLA	CHA-CBD-CGD-O1D
26	r	613	CLA	CHA-CBD-CGD-O2D
26	r	616	CLA	C1A-C2A-CAA-CBA
26	r	616	CLA	C3A-C2A-CAA-CBA
26	r	616	CLA	CHA-CBD-CGD-O1D
26	r	616	CLA	CHA-CBD-CGD-O2D
26	s	602	CLA	C1A-C2A-CAA-CBA
26	s	602	CLA	C3A-C2A-CAA-CBA
26	s	604	CLA	C1A-C2A-CAA-CBA
26	s	609	CLA	C1A-C2A-CAA-CBA
26	s	610	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
26	s	610	CLA	C4-C3-C5-C6
26	s	612	CLA	CBD-CGD-O2D-CED
27	1	1620	LUT	C1-C6-C7-C8
27	2	1620	LUT	C1-C6-C7-C8
27	5	1620	LUT	C1-C6-C7-C8
27	6	1620	LUT	C1-C6-C7-C8
28	1	1622	XAT	C31-C32-C33-C34
28	1	1622	XAT	C31-C32-C33-C40
28	2	1622	XAT	O4-C6-C7-C8
28	2	1622	XAT	C31-C32-C33-C34
28	2	1622	XAT	C31-C32-C33-C40
28	G	1622	XAT	C11-C12-C13-C14
28	G	1622	XAT	C11-C12-C13-C20
28	N	1622	XAT	C11-C12-C13-C14
28	N	1622	XAT	C11-C12-C13-C20
28	Y	1622	XAT	C11-C12-C13-C14
28	Y	1622	XAT	C11-C12-C13-C20
28	5	1622	XAT	C31-C32-C33-C34
28	5	1622	XAT	C31-C32-C33-C40
28	6	1622	XAT	O4-C6-C7-C8
28	6	1622	XAT	C31-C32-C33-C34
28	6	1622	XAT	C31-C32-C33-C40
28	g	1622	XAT	C11-C12-C13-C14
28	g	1622	XAT	C11-C12-C13-C20
28	n	1622	XAT	C11-C12-C13-C14
28	n	1622	XAT	C11-C12-C13-C20
28	y	1622	XAT	C11-C12-C13-C14
28	y	1622	XAT	C11-C12-C13-C20
29	1	1623	NEX	C11-C12-C13-C14
29	1	1623	NEX	C11-C12-C13-C20
29	G	1623	NEX	C11-C12-C13-C14
29	G	1623	NEX	C11-C12-C13-C20
29	5	1623	NEX	C11-C12-C13-C14
29	5	1623	NEX	C11-C12-C13-C20
29	6	1623	NEX	C31-C32-C33-C40
29	g	1623	NEX	C11-C12-C13-C14
29	g	1623	NEX	C11-C12-C13-C20
30	1	2630	LHG	C4-O6-P-O5
30	1	2630	LHG	O7-C5-C6-O8
30	2	2630	LHG	C4-O6-P-O5
30	3	2630	LHG	C4-O6-P-O3
30	3	2630	LHG	C4-O6-P-O4

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Mol	Chain	Res	Type	Atoms
30	3	2630	LHG	C4-O6-P-O5
30	4	2630	LHG	C3-O3-P-O5
30	B	2630	LHG	C1-C2-C3-O3
30	B	2630	LHG	C3-O3-P-O5
30	B	2631	LHG	O1-C1-C2-O2
30	B	2631	LHG	O1-C1-C2-C3
30	C	2630	LHG	O1-C1-C2-O2
30	C	2630	LHG	O1-C1-C2-C3
30	C	522	LHG	C3-O3-P-O4
30	C	522	LHG	C3-O3-P-O6
30	C	523	LHG	C3-O3-P-O5
30	C	523	LHG	C4-O6-P-O4
30	C	523	LHG	C8-C7-O7-C5
30	D	408	LHG	C4-O6-P-O5
30	D	409	LHG	C4-O6-P-O4
30	D	409	LHG	C4-O6-P-O5
30	G	2630	LHG	C4-O6-P-O5
30	L	101	LHG	C3-O3-P-O4
30	L	101	LHG	C4-O6-P-O4
30	N	2630	LHG	C4-O6-P-O5
30	S	2630	LHG	O1-C1-C2-C3
30	S	2630	LHG	C4-O6-P-O5
30	Y	2630	LHG	C4-O6-P-O5
30	5	2630	LHG	C4-O6-P-O5
30	5	2630	LHG	O7-C5-C6-O8
30	6	2630	LHG	C4-O6-P-O5
30	7	2630	LHG	C4-O6-P-O3
30	7	2630	LHG	C4-O6-P-O4
30	7	2630	LHG	C4-O6-P-O5
30	8	2630	LHG	C3-O3-P-O5
30	b	2630	LHG	C1-C2-C3-O3
30	b	2630	LHG	C3-O3-P-O5
30	b	2631	LHG	O1-C1-C2-O2
30	b	2631	LHG	O1-C1-C2-C3
30	c	2630	LHG	O1-C1-C2-O2
30	c	2630	LHG	O1-C1-C2-C3
30	c	522	LHG	C3-O3-P-O4
30	c	522	LHG	C3-O3-P-O6
30	c	523	LHG	C3-O3-P-O5
30	c	523	LHG	C4-O6-P-O4
30	c	523	LHG	C8-C7-O7-C5
30	d	408	LHG	C4-O6-P-O5

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Mol	Chain	Res	Type	Atoms
30	d	409	LHG	C4-O6-P-O4
30	d	409	LHG	C4-O6-P-O5
30	g	2630	LHG	C4-O6-P-O5
30	l	101	LHG	C3-O3-P-O4
30	l	101	LHG	C4-O6-P-O4
30	n	2630	LHG	C4-O6-P-O5
30	s	2630	LHG	O1-C1-C2-C3
30	s	2630	LHG	C4-O6-P-O5
30	y	2630	LHG	C4-O6-P-O5
31	4	623	BCR	C7-C8-C9-C10
31	4	623	BCR	C7-C8-C9-C34
31	4	623	BCR	C21-C22-C23-C24
31	4	623	BCR	C37-C22-C23-C24
31	B	618	BCR	C5-C6-C7-C8
31	B	619	BCR	C7-C8-C9-C10
31	B	619	BCR	C7-C8-C9-C34
31	B	620	BCR	C7-C8-C9-C10
31	B	620	BCR	C7-C8-C9-C34
31	B	620	BCR	C37-C22-C23-C24
31	B	620	BCR	C23-C24-C25-C30
31	C	516	BCR	C7-C8-C9-C10
31	C	516	BCR	C7-C8-C9-C34
31	C	517	BCR	C7-C8-C9-C10
31	C	517	BCR	C7-C8-C9-C34
31	D	404	BCR	C1-C6-C7-C8
31	D	404	BCR	C7-C8-C9-C10
31	D	404	BCR	C7-C8-C9-C34
31	D	404	BCR	C37-C22-C23-C24
31	H	101	BCR	C7-C8-C9-C10
31	H	101	BCR	C7-C8-C9-C34
31	T	101	BCR	C1-C6-C7-C8
31	T	101	BCR	C5-C6-C7-C8
31	T	101	BCR	C7-C8-C9-C10
31	T	101	BCR	C7-C8-C9-C34
31	T	101	BCR	C17-C18-C19-C20
31	T	101	BCR	C36-C18-C19-C20
31	T	101	BCR	C21-C22-C23-C24
31	T	101	BCR	C37-C22-C23-C24
31	8	623	BCR	C7-C8-C9-C10
31	8	623	BCR	C7-C8-C9-C34
31	8	623	BCR	C21-C22-C23-C24
31	8	623	BCR	C37-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
31	b	618	BCR	C5-C6-C7-C8
31	b	619	BCR	C7-C8-C9-C10
31	b	619	BCR	C7-C8-C9-C34
31	b	620	BCR	C7-C8-C9-C10
31	b	620	BCR	C7-C8-C9-C34
31	b	620	BCR	C37-C22-C23-C24
31	b	620	BCR	C23-C24-C25-C30
31	c	516	BCR	C7-C8-C9-C10
31	c	516	BCR	C7-C8-C9-C34
31	c	517	BCR	C7-C8-C9-C10
31	c	517	BCR	C7-C8-C9-C34
31	d	404	BCR	C1-C6-C7-C8
31	d	404	BCR	C7-C8-C9-C10
31	d	404	BCR	C7-C8-C9-C34
31	d	404	BCR	C37-C22-C23-C24
31	h	101	BCR	C7-C8-C9-C10
31	h	101	BCR	C7-C8-C9-C34
31	t	101	BCR	C1-C6-C7-C8
31	t	101	BCR	C5-C6-C7-C8
31	t	101	BCR	C7-C8-C9-C10
31	t	101	BCR	C7-C8-C9-C34
31	t	101	BCR	C17-C18-C19-C20
31	t	101	BCR	C36-C18-C19-C20
31	t	101	BCR	C21-C22-C23-C24
31	t	101	BCR	C37-C22-C23-C24
35	A	408	PHO	CBA-CGA-O2A-C1
35	A	408	PHO	O1A-CGA-O2A-C1
35	a	408	PHO	CBA-CGA-O2A-C1
35	a	408	PHO	O1A-CGA-O2A-C1
36	A	412	SQD	O49-C7-O47-C45
36	A	412	SQD	O5-C5-C6-S
36	A	418	SQD	C2-C1-O6-C44
36	A	418	SQD	O5-C1-O6-C44
36	A	418	SQD	O5-C5-C6-S
36	B	621	SQD	O5-C1-O6-C44
36	B	621	SQD	O49-C7-O47-C45
36	B	621	SQD	C8-C7-O47-C45
36	B	621	SQD	C5-C6-S-O7
36	B	623	SQD	C8-C7-O47-C45
36	B	623	SQD	C5-C6-S-O7
36	a	412	SQD	O49-C7-O47-C45
36	a	412	SQD	O5-C5-C6-S

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Mol	Chain	Res	Type	Atoms
36	a	418	SQD	C2-C1-O6-C44
36	a	418	SQD	O5-C1-O6-C44
36	a	418	SQD	O5-C5-C6-S
36	b	621	SQD	O5-C1-O6-C44
36	b	621	SQD	O49-C7-O47-C45
36	b	621	SQD	C8-C7-O47-C45
36	b	621	SQD	C5-C6-S-O7
36	b	623	SQD	C8-C7-O47-C45
36	b	623	SQD	C5-C6-S-O7
37	A	413	LMG	C2-C1-O1-C7
37	A	413	LMG	O6-C1-O1-C7
37	B	2633	LMG	O9-C10-O7-C8
37	C	521	LMG	C2-C1-O1-C7
37	C	521	LMG	O6-C1-O1-C7
37	Z	101	LMG	O10-C28-O8-C9
37	Z	101	LMG	C29-C28-O8-C9
37	a	413	LMG	C2-C1-O1-C7
37	a	413	LMG	O6-C1-O1-C7
37	b	2633	LMG	O9-C10-O7-C8
37	c	521	LMG	C2-C1-O1-C7
37	c	521	LMG	O6-C1-O1-C7
37	z	101	LMG	O10-C28-O8-C9
37	z	101	LMG	C29-C28-O8-C9
39	B	626	DGD	O1A-C1A-O1G-C1G
39	B	626	DGD	C2D-C1D-O3G-C3G
39	B	626	DGD	O6D-C1D-O3G-C3G
39	C	519	DGD	O1G-C1G-C2G-O2G
39	b	626	DGD	O1A-C1A-O1G-C1G
39	b	626	DGD	C2D-C1D-O3G-C3G
39	b	626	DGD	O6D-C1D-O3G-C3G
39	c	519	DGD	O1G-C1G-C2G-O2G
26	R	601	CLA	C2C-C3C-CAC-CBC
26	r	601	CLA	C2C-C3C-CAC-CBC
25	Y	608	CHL	O1D-CGD-O2D-CED
25	y	608	CHL	O1D-CGD-O2D-CED
26	2	612	CLA	O1D-CGD-O2D-CED
26	2	613	CLA	O1D-CGD-O2D-CED
26	A	405	CLA	O1D-CGD-O2D-CED
26	B	606	CLA	O1D-CGD-O2D-CED
26	6	612	CLA	O1D-CGD-O2D-CED
26	6	613	CLA	O1D-CGD-O2D-CED
26	a	405	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	b	606	CLA	O1D-CGD-O2D-CED
25	G	606	CHL	O1D-CGD-O2D-CED
25	S	608	CHL	O1D-CGD-O2D-CED
25	g	606	CHL	O1D-CGD-O2D-CED
25	s	608	CHL	O1D-CGD-O2D-CED
26	1	614	CLA	O1D-CGD-O2D-CED
26	4	604	CLA	O1D-CGD-O2D-CED
26	R	601	CLA	O1D-CGD-O2D-CED
26	R	612	CLA	O1D-CGD-O2D-CED
26	5	614	CLA	O1D-CGD-O2D-CED
26	8	604	CLA	O1D-CGD-O2D-CED
26	r	601	CLA	O1D-CGD-O2D-CED
26	r	612	CLA	O1D-CGD-O2D-CED
25	2	605	CHL	CBD-CGD-O2D-CED
25	G	601	CHL	CBD-CGD-O2D-CED
25	G	606	CHL	CBD-CGD-O2D-CED
25	G	608	CHL	CBD-CGD-O2D-CED
25	N	601	CHL	CBD-CGD-O2D-CED
25	N	605	CHL	CBD-CGD-O2D-CED
25	N	608	CHL	CBD-CGD-O2D-CED
25	R	607	CHL	CBD-CGD-O2D-CED
25	S	608	CHL	CBD-CGD-O2D-CED
25	Y	608	CHL	CBD-CGD-O2D-CED
25	6	605	CHL	CBD-CGD-O2D-CED
25	g	601	CHL	CBD-CGD-O2D-CED
25	g	606	CHL	CBD-CGD-O2D-CED
25	g	608	CHL	CBD-CGD-O2D-CED
25	n	601	CHL	CBD-CGD-O2D-CED
25	n	605	CHL	CBD-CGD-O2D-CED
25	n	608	CHL	CBD-CGD-O2D-CED
25	r	607	CHL	CBD-CGD-O2D-CED
25	s	608	CHL	CBD-CGD-O2D-CED
25	y	608	CHL	CBD-CGD-O2D-CED
26	1	614	CLA	CBD-CGD-O2D-CED
26	2	612	CLA	CBD-CGD-O2D-CED
26	2	613	CLA	CBD-CGD-O2D-CED
26	3	603	CLA	CBD-CGD-O2D-CED
26	3	614	CLA	CBD-CGD-O2D-CED
26	4	611	CLA	CBD-CGD-O2D-CED
26	4	612	CLA	CBD-CGD-O2D-CED
26	A	405	CLA	CBD-CGD-O2D-CED
26	B	606	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	B	608	CLA	CBD-CGD-O2D-CED
26	C	502	CLA	CBD-CGD-O2D-CED
26	C	503	CLA	CBD-CGD-O2D-CED
26	C	506	CLA	CBD-CGD-O2D-CED
26	C	513	CLA	CBD-CGD-O2D-CED
26	G	612	CLA	CBD-CGD-O2D-CED
26	G	613	CLA	CBD-CGD-O2D-CED
26	N	604	CLA	CBD-CGD-O2D-CED
26	N	612	CLA	CBD-CGD-O2D-CED
26	N	614	CLA	CBD-CGD-O2D-CED
26	R	603	CLA	CBD-CGD-O2D-CED
26	S	602	CLA	CBD-CGD-O2D-CED
26	S	603	CLA	CBD-CGD-O2D-CED
26	Y	604	CLA	CBD-CGD-O2D-CED
26	5	614	CLA	CBD-CGD-O2D-CED
26	6	612	CLA	CBD-CGD-O2D-CED
26	6	613	CLA	CBD-CGD-O2D-CED
26	7	603	CLA	CBD-CGD-O2D-CED
26	7	614	CLA	CBD-CGD-O2D-CED
26	8	611	CLA	CBD-CGD-O2D-CED
26	8	612	CLA	CBD-CGD-O2D-CED
26	a	405	CLA	CBD-CGD-O2D-CED
26	b	606	CLA	CBD-CGD-O2D-CED
26	b	608	CLA	CBD-CGD-O2D-CED
26	c	502	CLA	CBD-CGD-O2D-CED
26	c	503	CLA	CBD-CGD-O2D-CED
26	c	506	CLA	CBD-CGD-O2D-CED
26	c	513	CLA	CBD-CGD-O2D-CED
26	g	612	CLA	CBD-CGD-O2D-CED
26	g	613	CLA	CBD-CGD-O2D-CED
26	n	604	CLA	CBD-CGD-O2D-CED
26	n	612	CLA	CBD-CGD-O2D-CED
26	n	614	CLA	CBD-CGD-O2D-CED
26	r	603	CLA	CBD-CGD-O2D-CED
26	s	602	CLA	CBD-CGD-O2D-CED
26	s	603	CLA	CBD-CGD-O2D-CED
26	y	604	CLA	CBD-CGD-O2D-CED
26	C	510	CLA	O1A-CGA-O2A-C1
26	N	611	CLA	O1A-CGA-O2A-C1
26	R	611	CLA	O1A-CGA-O2A-C1
26	Y	611	CLA	O1A-CGA-O2A-C1
26	c	510	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	n	611	CLA	O1A-CGA-O2A-C1
26	r	611	CLA	O1A-CGA-O2A-C1
26	y	611	CLA	O1A-CGA-O2A-C1
25	G	608	CHL	O1D-CGD-O2D-CED
25	N	608	CHL	O1D-CGD-O2D-CED
25	g	608	CHL	O1D-CGD-O2D-CED
25	n	608	CHL	O1D-CGD-O2D-CED
26	3	603	CLA	O1D-CGD-O2D-CED
26	4	611	CLA	O1D-CGD-O2D-CED
26	C	503	CLA	O1D-CGD-O2D-CED
26	G	613	CLA	O1D-CGD-O2D-CED
26	N	612	CLA	O1D-CGD-O2D-CED
26	7	603	CLA	O1D-CGD-O2D-CED
26	8	611	CLA	O1D-CGD-O2D-CED
26	c	503	CLA	O1D-CGD-O2D-CED
26	g	613	CLA	O1D-CGD-O2D-CED
26	n	612	CLA	O1D-CGD-O2D-CED
25	2	608	CHL	O1D-CGD-O2D-CED
25	3	608	CHL	O1D-CGD-O2D-CED
25	6	608	CHL	O1D-CGD-O2D-CED
25	7	608	CHL	O1D-CGD-O2D-CED
26	1	603	CLA	O1D-CGD-O2D-CED
26	2	603	CLA	O1D-CGD-O2D-CED
26	2	614	CLA	O1D-CGD-O2D-CED
26	3	613	CLA	O1D-CGD-O2D-CED
26	4	603	CLA	O1D-CGD-O2D-CED
26	D	403	CLA	O1D-CGD-O2D-CED
26	S	612	CLA	O1D-CGD-O2D-CED
26	5	603	CLA	O1D-CGD-O2D-CED
26	6	603	CLA	O1D-CGD-O2D-CED
26	6	614	CLA	O1D-CGD-O2D-CED
26	7	613	CLA	O1D-CGD-O2D-CED
26	8	603	CLA	O1D-CGD-O2D-CED
26	d	403	CLA	O1D-CGD-O2D-CED
26	s	612	CLA	O1D-CGD-O2D-CED
26	C	510	CLA	CBA-CGA-O2A-C1
26	N	611	CLA	CBA-CGA-O2A-C1
26	Y	611	CLA	CBA-CGA-O2A-C1
26	c	510	CLA	CBA-CGA-O2A-C1
26	n	611	CLA	CBA-CGA-O2A-C1
26	y	611	CLA	CBA-CGA-O2A-C1
39	B	626	DGD	C2A-C1A-O1G-C1G

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Mol	Chain	Res	Type	Atoms
39	b	626	DGD	C2A-C1A-O1G-C1G
25	1	606	CHL	CBD-CGD-O2D-CED
25	S	606	CHL	CBD-CGD-O2D-CED
25	Y	609	CHL	CBD-CGD-O2D-CED
25	5	606	CHL	CBD-CGD-O2D-CED
25	s	606	CHL	CBD-CGD-O2D-CED
25	y	609	CHL	CBD-CGD-O2D-CED
26	1	602	CLA	CBD-CGD-O2D-CED
26	2	602	CLA	CBD-CGD-O2D-CED
26	2	610	CLA	CBD-CGD-O2D-CED
26	3	612	CLA	CBD-CGD-O2D-CED
26	B	610	CLA	CBD-CGD-O2D-CED
26	C	508	CLA	CBD-CGD-O2D-CED
26	C	512	CLA	CBD-CGD-O2D-CED
26	Y	612	CLA	CBD-CGD-O2D-CED
26	Y	614	CLA	CBD-CGD-O2D-CED
26	5	602	CLA	CBD-CGD-O2D-CED
26	6	602	CLA	CBD-CGD-O2D-CED
26	6	610	CLA	CBD-CGD-O2D-CED
26	7	612	CLA	CBD-CGD-O2D-CED
26	b	610	CLA	CBD-CGD-O2D-CED
26	c	508	CLA	CBD-CGD-O2D-CED
26	c	512	CLA	CBD-CGD-O2D-CED
26	y	612	CLA	CBD-CGD-O2D-CED
26	y	614	CLA	CBD-CGD-O2D-CED
26	R	601	CLA	C4C-C3C-CAC-CBC
26	r	601	CLA	C4C-C3C-CAC-CBC
26	3	603	CLA	O1A-CGA-O2A-C1
26	7	603	CLA	O1A-CGA-O2A-C1
30	S	2630	LHG	O10-C23-O8-C6
30	s	2630	LHG	O10-C23-O8-C6
25	1	608	CHL	O1D-CGD-O2D-CED
25	4	608	CHL	O1D-CGD-O2D-CED
25	5	608	CHL	O1D-CGD-O2D-CED
25	8	608	CHL	O1D-CGD-O2D-CED
26	2	604	CLA	O1D-CGD-O2D-CED
26	B	615	CLA	O1D-CGD-O2D-CED
26	6	604	CLA	O1D-CGD-O2D-CED
26	b	615	CLA	O1D-CGD-O2D-CED
25	G	605	CHL	O1D-CGD-O2D-CED
25	G	609	CHL	O1D-CGD-O2D-CED
25	R	608	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	R	614	CHL	O1D-CGD-O2D-CED
25	g	605	CHL	O1D-CGD-O2D-CED
25	g	609	CHL	O1D-CGD-O2D-CED
25	r	608	CHL	O1D-CGD-O2D-CED
25	r	614	CHL	O1D-CGD-O2D-CED
26	4	602	CLA	O1D-CGD-O2D-CED
26	N	614	CLA	O1D-CGD-O2D-CED
26	8	602	CLA	O1D-CGD-O2D-CED
26	n	614	CLA	O1D-CGD-O2D-CED
25	S	607	CHL	CBD-CGD-O2D-CED
25	s	607	CHL	CBD-CGD-O2D-CED
26	1	604	CLA	CBD-CGD-O2D-CED
26	C	501	CLA	CBD-CGD-O2D-CED
26	G	604	CLA	CBD-CGD-O2D-CED
26	R	602	CLA	CBD-CGD-O2D-CED
26	5	604	CLA	CBD-CGD-O2D-CED
26	c	501	CLA	CBD-CGD-O2D-CED
26	g	604	CLA	CBD-CGD-O2D-CED
26	r	602	CLA	CBD-CGD-O2D-CED
25	R	607	CHL	O1D-CGD-O2D-CED
25	r	607	CHL	O1D-CGD-O2D-CED
30	C	523	LHG	O9-C7-O7-C5
30	c	523	LHG	O9-C7-O7-C5
36	B	623	SQD	O49-C7-O47-C45
36	b	623	SQD	O49-C7-O47-C45
26	S	611	CLA	O1A-CGA-O2A-C1
26	s	611	CLA	O1A-CGA-O2A-C1
25	2	607	CHL	C3-C5-C6-C7
25	G	607	CHL	C3-C5-C6-C7
25	R	606	CHL	C3-C5-C6-C7
25	6	607	CHL	C3-C5-C6-C7
25	g	607	CHL	C3-C5-C6-C7
25	r	606	CHL	C3-C5-C6-C7
26	3	611	CLA	C3-C5-C6-C7
26	B	615	CLA	C3-C5-C6-C7
26	B	617	CLA	C3-C5-C6-C7
26	C	512	CLA	C3-C5-C6-C7
26	G	613	CLA	C3-C5-C6-C7
26	R	603	CLA	C3-C5-C6-C7
26	R	613	CLA	C3-C5-C6-C7
26	5	613	CLA	C3-C5-C6-C7
26	7	611	CLA	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
26	b	615	CLA	C3-C5-C6-C7
26	b	617	CLA	C3-C5-C6-C7
26	c	512	CLA	C3-C5-C6-C7
26	g	613	CLA	C3-C5-C6-C7
26	r	603	CLA	C3-C5-C6-C7
26	r	613	CLA	C3-C5-C6-C7
26	1	603	CLA	CBA-CGA-O2A-C1
26	3	603	CLA	CBA-CGA-O2A-C1
26	N	603	CLA	CBA-CGA-O2A-C1
26	5	603	CLA	CBA-CGA-O2A-C1
26	7	603	CLA	CBA-CGA-O2A-C1
26	n	603	CLA	CBA-CGA-O2A-C1
36	A	412	SQD	C8-C7-O47-C45
36	a	412	SQD	C8-C7-O47-C45
37	B	2633	LMG	C11-C10-O7-C8
37	b	2633	LMG	C11-C10-O7-C8
39	B	626	DGD	C2B-C1B-O2G-C2G
39	b	626	DGD	C2B-C1B-O2G-C2G
26	B	608	CLA	O1D-CGD-O2D-CED
26	b	608	CLA	O1D-CGD-O2D-CED
26	B	617	CLA	CBD-CGD-O2D-CED
26	C	510	CLA	CBD-CGD-O2D-CED
26	b	617	CLA	CBD-CGD-O2D-CED
26	c	510	CLA	CBD-CGD-O2D-CED
26	B	604	CLA	C4-C3-C5-C6
26	B	615	CLA	C4-C3-C5-C6
26	G	611	CLA	C4-C3-C5-C6
26	b	604	CLA	C4-C3-C5-C6
26	b	615	CLA	C4-C3-C5-C6
26	g	611	CLA	C4-C3-C5-C6
39	B	626	DGD	C4E-C5E-C6E-O5E
39	b	626	DGD	C4E-C5E-C6E-O5E
26	B	604	CLA	C2-C3-C5-C6
26	B	615	CLA	C2-C3-C5-C6
26	C	506	CLA	C2-C3-C5-C6
26	G	610	CLA	C2-C3-C5-C6
26	b	604	CLA	C2-C3-C5-C6
26	b	615	CLA	C2-C3-C5-C6
26	c	506	CLA	C2-C3-C5-C6
26	g	610	CLA	C2-C3-C5-C6
26	3	604	CLA	CBD-CGD-O2D-CED
26	7	604	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	y	603	CLA	CBD-CGD-O2D-CED
25	3	605	CHL	C2A-CAA-CBA-CGA
25	N	601	CHL	C2A-CAA-CBA-CGA
25	N	607	CHL	C2A-CAA-CBA-CGA
25	R	608	CHL	C2A-CAA-CBA-CGA
25	S	607	CHL	C2A-CAA-CBA-CGA
25	Y	607	CHL	C2A-CAA-CBA-CGA
25	7	605	CHL	C2A-CAA-CBA-CGA
25	n	601	CHL	C2A-CAA-CBA-CGA
25	n	607	CHL	C2A-CAA-CBA-CGA
25	r	608	CHL	C2A-CAA-CBA-CGA
25	s	607	CHL	C2A-CAA-CBA-CGA
25	y	607	CHL	C2A-CAA-CBA-CGA
26	2	604	CLA	C2A-CAA-CBA-CGA
26	3	603	CLA	C2A-CAA-CBA-CGA
26	B	607	CLA	C2A-CAA-CBA-CGA
26	B	611	CLA	C2A-CAA-CBA-CGA
26	C	507	CLA	C2A-CAA-CBA-CGA
26	R	604	CLA	C2A-CAA-CBA-CGA
26	R	611	CLA	C2A-CAA-CBA-CGA
26	6	604	CLA	C2A-CAA-CBA-CGA
26	7	603	CLA	C2A-CAA-CBA-CGA
26	b	607	CLA	C2A-CAA-CBA-CGA
26	b	611	CLA	C2A-CAA-CBA-CGA
26	c	507	CLA	C2A-CAA-CBA-CGA
26	r	604	CLA	C2A-CAA-CBA-CGA
26	r	611	CLA	C2A-CAA-CBA-CGA
25	N	607	CHL	C3-C5-C6-C7
25	Y	607	CHL	C3-C5-C6-C7
25	n	607	CHL	C3-C5-C6-C7
25	y	607	CHL	C3-C5-C6-C7
26	1	613	CLA	C3-C5-C6-C7
26	2	602	CLA	C3-C5-C6-C7
26	N	613	CLA	C3-C5-C6-C7
26	S	611	CLA	C3-C5-C6-C7
26	S	613	CLA	C3-C5-C6-C7
26	6	602	CLA	C3-C5-C6-C7
26	n	613	CLA	C3-C5-C6-C7
26	s	611	CLA	C3-C5-C6-C7
26	s	613	CLA	C3-C5-C6-C7
35	A	408	PHO	C3-C5-C6-C7
35	a	408	PHO	C3-C5-C6-C7

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Mol	Chain	Res	Type	Atoms
25	G	601	CHL	CBA-CGA-O2A-C1
25	Y	601	CHL	CBA-CGA-O2A-C1
25	g	601	CHL	CBA-CGA-O2A-C1
25	y	601	CHL	CBA-CGA-O2A-C1
26	2	603	CLA	CBA-CGA-O2A-C1
26	G	603	CLA	CBA-CGA-O2A-C1
26	S	611	CLA	CBA-CGA-O2A-C1
26	6	603	CLA	CBA-CGA-O2A-C1
26	g	603	CLA	CBA-CGA-O2A-C1
26	s	611	CLA	CBA-CGA-O2A-C1
39	C	520	DGD	C2A-C1A-O1G-C1G
39	c	520	DGD	C2A-C1A-O1G-C1G
30	4	2630	LHG	C24-C23-O8-C6
30	8	2630	LHG	C24-C23-O8-C6
25	G	601	CHL	O1D-CGD-O2D-CED
25	N	605	CHL	O1D-CGD-O2D-CED
25	g	601	CHL	O1D-CGD-O2D-CED
25	n	605	CHL	O1D-CGD-O2D-CED
26	4	612	CLA	O1D-CGD-O2D-CED
26	C	506	CLA	O1D-CGD-O2D-CED
26	8	612	CLA	O1D-CGD-O2D-CED
26	c	506	CLA	O1D-CGD-O2D-CED
26	B	611	CLA	CBD-CGD-O2D-CED
26	Y	603	CLA	CBD-CGD-O2D-CED
26	b	611	CLA	CBD-CGD-O2D-CED
25	N	601	CHL	O1D-CGD-O2D-CED
25	n	601	CHL	O1D-CGD-O2D-CED
26	C	502	CLA	O1D-CGD-O2D-CED
26	R	603	CLA	O1D-CGD-O2D-CED
26	S	603	CLA	O1D-CGD-O2D-CED
26	c	502	CLA	O1D-CGD-O2D-CED
26	r	603	CLA	O1D-CGD-O2D-CED
26	s	603	CLA	O1D-CGD-O2D-CED
36	A	418	SQD	O49-C7-O47-C45
36	a	418	SQD	O49-C7-O47-C45
26	2	603	CLA	O1A-CGA-O2A-C1
26	G	603	CLA	O1A-CGA-O2A-C1
26	N	603	CLA	O1A-CGA-O2A-C1
26	6	603	CLA	O1A-CGA-O2A-C1
26	g	603	CLA	O1A-CGA-O2A-C1
26	n	603	CLA	O1A-CGA-O2A-C1
25	2	605	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	6	605	CHL	O1D-CGD-O2D-CED
31	C	516	BCR	C19-C20-C21-C22
31	c	516	BCR	C19-C20-C21-C22
39	h	102	DGD	O6E-C5E-C6E-O5E
25	3	605	CHL	CBD-CGD-O2D-CED
25	R	606	CHL	CBD-CGD-O2D-CED
25	S	601	CHL	CBD-CGD-O2D-CED
25	7	605	CHL	CBD-CGD-O2D-CED
25	r	606	CHL	CBD-CGD-O2D-CED
25	s	601	CHL	CBD-CGD-O2D-CED
26	3	602	CLA	CBD-CGD-O2D-CED
26	B	604	CLA	CBD-CGD-O2D-CED
26	B	612	CLA	CBD-CGD-O2D-CED
26	G	602	CLA	CBD-CGD-O2D-CED
26	7	602	CLA	CBD-CGD-O2D-CED
26	b	604	CLA	CBD-CGD-O2D-CED
26	b	612	CLA	CBD-CGD-O2D-CED
26	g	602	CLA	CBD-CGD-O2D-CED
26	Y	604	CLA	O1D-CGD-O2D-CED
26	y	604	CLA	O1D-CGD-O2D-CED
30	B	2630	LHG	O2-C2-C3-O3
30	B	2631	LHG	O2-C2-C3-O3
30	b	2630	LHG	O2-C2-C3-O3
30	b	2631	LHG	O2-C2-C3-O3
25	R	608	CHL	C3-C5-C6-C7
25	r	608	CHL	C3-C5-C6-C7
26	B	608	CLA	C3-C5-C6-C7
26	b	608	CLA	C3-C5-C6-C7
25	S	607	CHL	CBA-CGA-O2A-C1
25	s	607	CHL	CBA-CGA-O2A-C1
26	b	617	CLA	CBA-CGA-O2A-C1
30	B	2631	LHG	C24-C23-O8-C6
30	S	2630	LHG	C24-C23-O8-C6
30	b	2631	LHG	C24-C23-O8-C6
30	s	2630	LHG	C24-C23-O8-C6
36	B	623	SQD	C24-C23-O48-C46
36	b	623	SQD	C24-C23-O48-C46
25	Y	601	CHL	O1A-CGA-O2A-C1
25	y	601	CHL	O1A-CGA-O2A-C1
26	1	603	CLA	O1A-CGA-O2A-C1
26	B	617	CLA	O1A-CGA-O2A-C1
26	5	603	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	b	617	CLA	O1A-CGA-O2A-C1
30	3	2630	LHG	O10-C23-O8-C6
30	7	2630	LHG	O10-C23-O8-C6
37	Z	101	LMG	O6-C5-C6-O5
37	z	101	LMG	O6-C5-C6-O5
39	H	102	DGD	O6E-C5E-C6E-O5E
26	S	602	CLA	O1D-CGD-O2D-CED
26	s	602	CLA	O1D-CGD-O2D-CED
25	3	609	CHL	CBD-CGD-O2D-CED
25	Y	601	CHL	CBD-CGD-O2D-CED
25	7	609	CHL	CBD-CGD-O2D-CED
25	y	601	CHL	CBD-CGD-O2D-CED
26	C	507	CLA	CBD-CGD-O2D-CED
26	N	613	CLA	CBD-CGD-O2D-CED
26	c	507	CLA	CBD-CGD-O2D-CED
26	n	613	CLA	CBD-CGD-O2D-CED
26	3	614	CLA	O1D-CGD-O2D-CED
26	G	612	CLA	O1D-CGD-O2D-CED
26	7	614	CLA	O1D-CGD-O2D-CED
25	Y	605	CHL	CBD-CGD-O2D-CED
26	C	513	CLA	C3-C5-C6-C7
26	Y	613	CLA	C3-C5-C6-C7
26	c	513	CLA	C3-C5-C6-C7
26	y	613	CLA	C3-C5-C6-C7
26	B	617	CLA	CBA-CGA-O2A-C1
36	B	621	SQD	C24-C23-O48-C46
36	b	621	SQD	C24-C23-O48-C46
26	g	612	CLA	O1D-CGD-O2D-CED
37	Z	101	LMG	C4-C5-C6-O5
37	z	101	LMG	C4-C5-C6-O5
25	G	601	CHL	O1A-CGA-O2A-C1
25	g	601	CHL	O1A-CGA-O2A-C1
26	B	614	CLA	C4-C3-C5-C6
26	b	614	CLA	C4-C3-C5-C6
25	Y	601	CHL	C2-C3-C5-C6
25	y	601	CHL	C2-C3-C5-C6
26	B	614	CLA	C2-C3-C5-C6
26	b	614	CLA	C2-C3-C5-C6
25	3	606	CHL	CBD-CGD-O2D-CED
25	7	606	CHL	CBD-CGD-O2D-CED
25	y	605	CHL	CBD-CGD-O2D-CED
30	4	2630	LHG	O10-C23-O8-C6

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Mol	Chain	Res	Type	Atoms
30	8	2630	LHG	O10-C23-O8-C6
25	1	606	CHL	C2A-CAA-CBA-CGA
25	G	607	CHL	C2A-CAA-CBA-CGA
25	R	607	CHL	C2A-CAA-CBA-CGA
25	5	606	CHL	C2A-CAA-CBA-CGA
25	g	607	CHL	C2A-CAA-CBA-CGA
25	r	607	CHL	C2A-CAA-CBA-CGA
26	3	611	CLA	C2A-CAA-CBA-CGA
26	B	605	CLA	C2A-CAA-CBA-CGA
26	7	611	CLA	C2A-CAA-CBA-CGA
26	b	605	CLA	C2A-CAA-CBA-CGA
26	C	513	CLA	O1D-CGD-O2D-CED
26	c	513	CLA	O1D-CGD-O2D-CED
39	B	626	DGD	O6E-C5E-C6E-O5E
39	b	626	DGD	O6E-C5E-C6E-O5E
25	S	607	CHL	O1A-CGA-O2A-C1
25	s	607	CHL	O1A-CGA-O2A-C1
30	B	2631	LHG	O10-C23-O8-C6
30	b	2631	LHG	O10-C23-O8-C6
25	R	608	CHL	CBA-CGA-O2A-C1
25	r	608	CHL	CBA-CGA-O2A-C1
26	N	604	CLA	O1D-CGD-O2D-CED
26	Y	612	CLA	O1D-CGD-O2D-CED
26	n	604	CLA	O1D-CGD-O2D-CED
26	y	612	CLA	O1D-CGD-O2D-CED
37	a	415	LMG	O6-C5-C6-O5
25	Y	609	CHL	O1D-CGD-O2D-CED
25	y	609	CHL	O1D-CGD-O2D-CED
26	6	610	CLA	O1D-CGD-O2D-CED
30	D	409	LHG	C23-C24-C25-C26
30	d	409	LHG	C23-C24-C25-C26
26	2	610	CLA	O1D-CGD-O2D-CED
30	B	2631	LHG	C1-C2-C3-O3
30	b	2631	LHG	C1-C2-C3-O3
37	A	415	LMG	O6-C5-C6-O5
37	A	413	LMG	C4-C5-C6-O5
37	a	413	LMG	C4-C5-C6-O5
25	R	608	CHL	O1A-CGA-O2A-C1
25	r	608	CHL	O1A-CGA-O2A-C1
25	3	601	CHL	C3-C5-C6-C7
25	7	601	CHL	C3-C5-C6-C7
25	S	606	CHL	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
25	s	606	CHL	O1D-CGD-O2D-CED
26	3	612	CLA	O1D-CGD-O2D-CED
26	Y	614	CLA	O1D-CGD-O2D-CED
26	7	612	CLA	O1D-CGD-O2D-CED
26	y	614	CLA	O1D-CGD-O2D-CED
26	3	613	CLA	CBA-CGA-O2A-C1
26	D	403	CLA	CBA-CGA-O2A-C1
26	R	612	CLA	CBA-CGA-O2A-C1
26	S	604	CLA	CBA-CGA-O2A-C1
26	Y	612	CLA	CBA-CGA-O2A-C1
26	7	613	CLA	CBA-CGA-O2A-C1
26	d	403	CLA	CBA-CGA-O2A-C1
26	r	612	CLA	CBA-CGA-O2A-C1
26	s	604	CLA	CBA-CGA-O2A-C1
26	y	612	CLA	CBA-CGA-O2A-C1
30	3	2630	LHG	C24-C23-O8-C6
30	7	2630	LHG	C24-C23-O8-C6
37	B	622	LMG	C29-C28-O8-C9
37	b	622	LMG	C29-C28-O8-C9
26	B	616	CLA	CBD-CGD-O2D-CED
26	b	616	CLA	CBD-CGD-O2D-CED
30	B	2630	LHG	C23-C24-C25-C26
30	b	2630	LHG	C23-C24-C25-C26
26	B	609	CLA	C8-C10-C11-C12
26	N	602	CLA	C10-C11-C12-C13
26	b	609	CLA	C8-C10-C11-C12
26	c	503	CLA	C5-C6-C7-C8
26	n	602	CLA	C10-C11-C12-C13
26	B	615	CLA	C15-C16-C17-C18
26	B	617	CLA	C13-C15-C16-C17
26	C	503	CLA	C5-C6-C7-C8
26	b	615	CLA	C15-C16-C17-C18
26	b	617	CLA	C13-C15-C16-C17
30	R	2630	LHG	O2-C2-C3-O3
30	r	2630	LHG	O2-C2-C3-O3
26	3	614	CLA	O2A-C1-C2-C3
26	7	614	CLA	O2A-C1-C2-C3
30	3	2630	LHG	O7-C5-C6-O8
30	B	2631	LHG	O7-C5-C6-O8
30	7	2630	LHG	O7-C5-C6-O8
30	b	2631	LHG	O7-C5-C6-O8
36	B	623	SQD	O6-C44-C45-O47

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Mol	Chain	Res	Type	Atoms
36	b	623	SQD	O6-C44-C45-O47
26	N	610	CLA	C4-C3-C5-C6
26	n	610	CLA	C4-C3-C5-C6
37	A	415	LMG	C4-C5-C6-O5
37	a	415	LMG	C4-C5-C6-O5
26	G	611	CLA	C2-C3-C5-C6
26	g	611	CLA	C2-C3-C5-C6
25	1	607	CHL	C11-C10-C8-C9
25	3	601	CHL	C6-C7-C8-C9
25	3	601	CHL	C14-C13-C15-C16
25	G	608	CHL	C14-C13-C15-C16
25	N	601	CHL	C11-C10-C8-C9
25	N	608	CHL	C14-C13-C15-C16
25	Y	608	CHL	C14-C13-C15-C16
25	Y	609	CHL	C14-C13-C15-C16
25	5	607	CHL	C11-C10-C8-C9
25	7	601	CHL	C6-C7-C8-C9
25	7	601	CHL	C14-C13-C15-C16
25	g	608	CHL	C14-C13-C15-C16
25	n	601	CHL	C11-C10-C8-C9
25	n	608	CHL	C14-C13-C15-C16
25	y	608	CHL	C14-C13-C15-C16
25	y	609	CHL	C14-C13-C15-C16
26	B	602	CLA	C14-C13-C15-C16
26	B	606	CLA	C6-C7-C8-C9
26	B	611	CLA	C14-C13-C15-C16
26	B	615	CLA	C6-C7-C8-C9
26	B	616	CLA	C11-C10-C8-C9
26	C	502	CLA	C6-C7-C8-C9
26	C	504	CLA	C11-C12-C13-C14
26	C	506	CLA	C11-C12-C13-C14
26	C	507	CLA	C11-C12-C13-C14
26	C	509	CLA	C6-C7-C8-C9
26	C	511	CLA	C11-C10-C8-C9
26	N	612	CLA	C6-C7-C8-C9
26	R	610	CLA	C11-C12-C13-C14
26	Y	611	CLA	C6-C7-C8-C9
26	b	602	CLA	C14-C13-C15-C16
26	b	606	CLA	C6-C7-C8-C9
26	b	611	CLA	C14-C13-C15-C16
26	b	615	CLA	C6-C7-C8-C9
26	b	616	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
26	c	502	CLA	C6-C7-C8-C9
26	c	504	CLA	C11-C12-C13-C14
26	c	507	CLA	C11-C12-C13-C14
26	c	509	CLA	C6-C7-C8-C9
26	c	511	CLA	C11-C10-C8-C9
26	n	612	CLA	C6-C7-C8-C9
26	r	610	CLA	C11-C12-C13-C14
26	y	611	CLA	C6-C7-C8-C9
35	A	408	PHO	C14-C13-C15-C16
35	a	408	PHO	C14-C13-C15-C16
26	C	512	CLA	O1D-CGD-O2D-CED
26	c	512	CLA	O1D-CGD-O2D-CED
30	Y	2630	LHG	C26-C27-C28-C29
30	y	2630	LHG	C26-C27-C28-C29
26	N	612	CLA	C10-C11-C12-C13
26	n	612	CLA	C10-C11-C12-C13
25	2	605	CHL	C2A-CAA-CBA-CGA
25	2	607	CHL	C2A-CAA-CBA-CGA
25	6	605	CHL	C2A-CAA-CBA-CGA
25	6	607	CHL	C2A-CAA-CBA-CGA
26	N	610	CLA	C2A-CAA-CBA-CGA
26	n	610	CLA	C2A-CAA-CBA-CGA
27	4	620	LUT	C27-C28-C29-C39
27	8	620	LUT	C27-C28-C29-C39
28	3	1622	XAT	C31-C32-C33-C40
28	R	622	XAT	C27-C28-C29-C39
28	7	1622	XAT	C31-C32-C33-C40
28	r	622	XAT	C27-C28-C29-C39
29	2	1623	NEX	C31-C32-C33-C40
29	Y	1623	NEX	C11-C12-C13-C20
29	y	1623	NEX	C11-C12-C13-C20
31	C	516	BCR	C37-C22-C23-C24
31	T	101	BCR	C11-C12-C13-C35
31	c	516	BCR	C37-C22-C23-C24
31	t	101	BCR	C11-C12-C13-C35
31	C	516	BCR	C21-C22-C23-C24
31	T	101	BCR	C11-C12-C13-C14
31	c	516	BCR	C21-C22-C23-C24
31	t	101	BCR	C11-C12-C13-C14
30	D	408	LHG	C23-C24-C25-C26
30	G	2630	LHG	C23-C24-C25-C26
30	d	408	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
30	g	2630	LHG	C23-C24-C25-C26
36	A	418	SQD	C7-C8-C9-C10
36	a	418	SQD	C7-C8-C9-C10
39	C	520	DGD	C1B-C2B-C3B-C4B
39	c	520	DGD	C1B-C2B-C3B-C4B
25	3	601	CHL	C5-C6-C7-C8
25	Y	601	CHL	C5-C6-C7-C8
25	7	601	CHL	C5-C6-C7-C8
25	y	601	CHL	C5-C6-C7-C8
26	A	410	CLA	C10-C11-C12-C13
26	B	611	CLA	C13-C15-C16-C17
26	B	614	CLA	C8-C10-C11-C12
26	B	614	CLA	C13-C15-C16-C17
26	B	616	CLA	C8-C10-C11-C12
26	G	603	CLA	C15-C16-C17-C18
26	a	410	CLA	C10-C11-C12-C13
26	b	611	CLA	C13-C15-C16-C17
26	b	614	CLA	C8-C10-C11-C12
26	b	614	CLA	C13-C15-C16-C17
26	b	616	CLA	C8-C10-C11-C12
26	g	603	CLA	C15-C16-C17-C18
25	1	606	CHL	O1D-CGD-O2D-CED
25	5	606	CHL	O1D-CGD-O2D-CED
26	1	602	CLA	O1D-CGD-O2D-CED
26	5	602	CLA	O1D-CGD-O2D-CED
26	A	410	CLA	C3-C5-C6-C7
26	C	506	CLA	C3-C5-C6-C7
26	a	410	CLA	C3-C5-C6-C7
26	c	506	CLA	C3-C5-C6-C7
25	3	601	CHL	C10-C11-C12-C13
25	R	606	CHL	C15-C16-C17-C18
25	S	607	CHL	C5-C6-C7-C8
25	Y	608	CHL	C15-C16-C17-C18
25	7	601	CHL	C10-C11-C12-C13
25	r	606	CHL	C15-C16-C17-C18
25	s	607	CHL	C5-C6-C7-C8
25	y	608	CHL	C15-C16-C17-C18
26	B	603	CLA	C5-C6-C7-C8
26	B	607	CLA	C13-C15-C16-C17
26	C	507	CLA	C13-C15-C16-C17
26	C	510	CLA	C15-C16-C17-C18
26	G	602	CLA	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
26	Y	602	CLA	C10-C11-C12-C13
26	b	603	CLA	C5-C6-C7-C8
26	b	607	CLA	C13-C15-C16-C17
26	c	507	CLA	C13-C15-C16-C17
26	c	510	CLA	C15-C16-C17-C18
26	y	602	CLA	C10-C11-C12-C13
30	N	2630	LHG	C23-C24-C25-C26
30	n	2630	LHG	C23-C24-C25-C26
37	B	2633	LMG	C10-C11-C12-C13
37	b	2633	LMG	C10-C11-C12-C13
25	1	609	CHL	C8-C10-C11-C12
25	3	601	CHL	C8-C10-C11-C12
25	N	609	CHL	C15-C16-C17-C18
25	Y	601	CHL	C8-C10-C11-C12
25	Y	601	CHL	C13-C15-C16-C17
25	5	609	CHL	C8-C10-C11-C12
25	7	601	CHL	C8-C10-C11-C12
25	n	609	CHL	C15-C16-C17-C18
25	y	601	CHL	C8-C10-C11-C12
25	y	601	CHL	C13-C15-C16-C17
26	A	406	CLA	C15-C16-C17-C18
26	B	608	CLA	C5-C6-C7-C8
26	B	615	CLA	C13-C15-C16-C17
26	B	617	CLA	C5-C6-C7-C8
26	C	504	CLA	C13-C15-C16-C17
26	D	402	CLA	C15-C16-C17-C18
26	N	603	CLA	C5-C6-C7-C8
26	a	406	CLA	C15-C16-C17-C18
26	b	608	CLA	C5-C6-C7-C8
26	b	615	CLA	C13-C15-C16-C17
26	b	617	CLA	C5-C6-C7-C8
26	c	504	CLA	C13-C15-C16-C17
26	d	402	CLA	C15-C16-C17-C18
26	g	602	CLA	C10-C11-C12-C13
26	n	603	CLA	C5-C6-C7-C8
26	2	602	CLA	O1D-CGD-O2D-CED
26	6	602	CLA	O1D-CGD-O2D-CED
30	2	2630	LHG	O1-C1-C2-O2
30	6	2630	LHG	O1-C1-C2-O2
38	D	405	PL9	C7-C8-C9-C10
38	d	405	PL9	C7-C8-C9-C10
30	1	2630	LHG	C23-C24-C25-C26

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Mol	Chain	Res	Type	Atoms
30	5	2630	LHG	C23-C24-C25-C26
37	C	521	LMG	C28-C29-C30-C31
37	c	521	LMG	C28-C29-C30-C31
39	C	519	DGD	O6E-C5E-C6E-O5E
39	c	519	DGD	O6E-C5E-C6E-O5E
26	R	609	CLA	CBD-CGD-O2D-CED
26	r	609	CLA	CBD-CGD-O2D-CED
25	3	609	CHL	C10-C11-C12-C13
25	G	608	CHL	C15-C16-C17-C18
25	7	609	CHL	C10-C11-C12-C13
25	g	608	CHL	C15-C16-C17-C18
26	B	604	CLA	C5-C6-C7-C8
26	C	512	CLA	C8-C10-C11-C12
26	G	602	CLA	C8-C10-C11-C12
26	G	603	CLA	C13-C15-C16-C17
26	b	604	CLA	C5-C6-C7-C8
26	c	512	CLA	C8-C10-C11-C12
26	g	602	CLA	C8-C10-C11-C12
26	g	603	CLA	C13-C15-C16-C17
25	N	609	CHL	CBA-CGA-O2A-C1
25	n	609	CHL	CBA-CGA-O2A-C1
26	B	602	CLA	CBA-CGA-O2A-C1
26	b	602	CLA	CBA-CGA-O2A-C1
39	C	519	DGD	C2A-C1A-O1G-C1G
39	c	519	DGD	C2A-C1A-O1G-C1G
26	G	604	CLA	O1D-CGD-O2D-CED
26	g	604	CLA	O1D-CGD-O2D-CED
37	B	2633	LMG	O6-C5-C6-O5
37	b	2633	LMG	O6-C5-C6-O5
39	C	518	DGD	O6E-C5E-C6E-O5E
39	c	518	DGD	O6E-C5E-C6E-O5E
25	R	606	CHL	C8-C10-C11-C12
25	Y	607	CHL	C15-C16-C17-C18
25	Y	609	CHL	C13-C15-C16-C17
25	r	606	CHL	C8-C10-C11-C12
25	y	607	CHL	C15-C16-C17-C18
25	y	609	CHL	C13-C15-C16-C17
26	3	602	CLA	C10-C11-C12-C13
26	B	608	CLA	C13-C15-C16-C17
26	C	503	CLA	C15-C16-C17-C18
26	b	608	CLA	C13-C15-C16-C17
26	c	503	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
30	D	408	LHG	C7-C8-C9-C10
30	d	408	LHG	C7-C8-C9-C10
36	B	621	SQD	C7-C8-C9-C10
36	b	621	SQD	C7-C8-C9-C10
37	Z	101	LMG	C10-C11-C12-C13
37	z	101	LMG	C10-C11-C12-C13
39	H	102	DGD	C1A-C2A-C3A-C4A
39	h	102	DGD	C1A-C2A-C3A-C4A
26	1	612	CLA	CBD-CGD-O2D-CED
26	5	612	CLA	CBD-CGD-O2D-CED
25	1	607	CHL	C13-C15-C16-C17
25	S	607	CHL	C8-C10-C11-C12
25	5	607	CHL	C13-C15-C16-C17
25	s	607	CHL	C8-C10-C11-C12
41	F	101	HEM	C3D-CAD-CBD-CGD
41	f	101	HEM	C3D-CAD-CBD-CGD
25	Y	609	CHL	C15-C16-C17-C18
25	y	609	CHL	C15-C16-C17-C18
26	7	602	CLA	C10-C11-C12-C13
26	c	508	CLA	O1D-CGD-O2D-CED
25	G	601	CHL	C6-C7-C8-C10
25	R	606	CHL	C11-C10-C8-C7
25	Y	601	CHL	C6-C7-C8-C10
25	g	601	CHL	C6-C7-C8-C10
25	r	606	CHL	C11-C10-C8-C7
25	y	601	CHL	C6-C7-C8-C10
26	3	613	CLA	C6-C7-C8-C10
26	A	406	CLA	C11-C12-C13-C15
26	B	612	CLA	C11-C10-C8-C7
26	B	612	CLA	C12-C13-C15-C16
26	C	504	CLA	C11-C12-C13-C15
26	N	603	CLA	C11-C10-C8-C7
26	7	613	CLA	C6-C7-C8-C10
26	a	406	CLA	C11-C12-C13-C15
26	b	612	CLA	C11-C10-C8-C7
26	b	612	CLA	C12-C13-C15-C16
26	c	504	CLA	C11-C12-C13-C15
26	n	603	CLA	C11-C10-C8-C7
25	N	608	CHL	C3-C5-C6-C7
25	n	608	CHL	C3-C5-C6-C7
26	3	613	CLA	O1A-CGA-O2A-C1
26	7	613	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	r	612	CLA	O1A-CGA-O2A-C1
37	Z	101	LMG	C28-C29-C30-C31
37	z	101	LMG	C28-C29-C30-C31
26	G	614	CLA	CBA-CGA-O2A-C1
26	g	614	CLA	CBA-CGA-O2A-C1
25	1	607	CHL	C2A-CAA-CBA-CGA
25	5	607	CHL	C2A-CAA-CBA-CGA
26	G	611	CLA	C2A-CAA-CBA-CGA
26	g	611	CLA	C2A-CAA-CBA-CGA
26	B	610	CLA	O1D-CGD-O2D-CED
26	C	508	CLA	O1D-CGD-O2D-CED
26	b	610	CLA	O1D-CGD-O2D-CED
25	2	609	CHL	C8-C10-C11-C12
25	3	601	CHL	C13-C15-C16-C17
25	6	609	CHL	C8-C10-C11-C12
25	7	601	CHL	C13-C15-C16-C17
26	D	403	CLA	C8-C10-C11-C12
26	d	403	CLA	C8-C10-C11-C12
26	D	403	CLA	O1A-CGA-O2A-C1
26	R	612	CLA	O1A-CGA-O2A-C1
26	Y	612	CLA	O1A-CGA-O2A-C1
26	d	403	CLA	O1A-CGA-O2A-C1
26	y	612	CLA	O1A-CGA-O2A-C1
37	B	2633	LMG	O6-C1-O1-C7
37	Z	101	LMG	O6-C1-O1-C7
37	b	2633	LMG	O6-C1-O1-C7
37	z	101	LMG	O6-C1-O1-C7
39	C	519	DGD	O6E-C1E-O5D-C6D
39	c	519	DGD	O6E-C1E-O5D-C6D
26	Y	610	CLA	C5-C6-C7-C8
26	g	610	CLA	C5-C6-C7-C8
26	y	610	CLA	C5-C6-C7-C8
37	A	413	LMG	O6-C5-C6-O5
37	a	413	LMG	O6-C5-C6-O5
30	C	2630	LHG	O2-C2-C3-O3
30	D	408	LHG	O2-C2-C3-O3
30	N	2630	LHG	O2-C2-C3-O3
30	c	2630	LHG	O2-C2-C3-O3
30	d	408	LHG	O2-C2-C3-O3
30	n	2630	LHG	O2-C2-C3-O3
25	2	607	CHL	C5-C6-C7-C8
25	G	607	CHL	C10-C11-C12-C13

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Mol	Chain	Res	Type	Atoms
25	6	607	CHL	C5-C6-C7-C8
25	g	607	CHL	C10-C11-C12-C13
26	A	406	CLA	C13-C15-C16-C17
26	C	508	CLA	C5-C6-C7-C8
26	C	511	CLA	C8-C10-C11-C12
26	G	610	CLA	C5-C6-C7-C8
26	N	602	CLA	C8-C10-C11-C12
26	Y	602	CLA	C8-C10-C11-C12
26	a	406	CLA	C13-C15-C16-C17
26	c	508	CLA	C5-C6-C7-C8
26	c	511	CLA	C8-C10-C11-C12
26	n	602	CLA	C8-C10-C11-C12
26	y	602	CLA	C8-C10-C11-C12
26	C	511	CLA	CBA-CGA-O2A-C1
26	c	511	CLA	CBA-CGA-O2A-C1
30	C	522	LHG	C24-C23-O8-C6
30	c	522	LHG	C24-C23-O8-C6
26	S	604	CLA	O1A-CGA-O2A-C1
26	s	604	CLA	O1A-CGA-O2A-C1
37	B	622	LMG	O10-C28-O8-C9
37	b	622	LMG	O10-C28-O8-C9
39	C	520	DGD	O1A-C1A-O1G-C1G
39	c	520	DGD	O1A-C1A-O1G-C1G
30	D	409	LHG	C7-C8-C9-C10
30	d	409	LHG	C7-C8-C9-C10
25	N	601	CHL	C13-C15-C16-C17
25	R	608	CHL	C10-C11-C12-C13
25	n	601	CHL	C13-C15-C16-C17
25	r	608	CHL	C10-C11-C12-C13
26	B	606	CLA	C15-C16-C17-C18
26	B	607	CLA	C8-C10-C11-C12
26	B	608	CLA	C8-C10-C11-C12
26	R	603	CLA	C10-C11-C12-C13
26	Y	613	CLA	C8-C10-C11-C12
26	b	606	CLA	C15-C16-C17-C18
26	b	607	CLA	C8-C10-C11-C12
26	b	608	CLA	C8-C10-C11-C12
26	r	603	CLA	C10-C11-C12-C13
26	y	613	CLA	C8-C10-C11-C12
30	D	409	LHG	C32-C33-C34-C35
26	C	501	CLA	O1D-CGD-O2D-CED
26	c	501	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
39	H	102	DGD	C4E-C5E-C6E-O5E
39	h	102	DGD	C4E-C5E-C6E-O5E
25	n	609	CHL	O1A-CGA-O2A-C1
30	d	409	LHG	C32-C33-C34-C35
26	b	617	CLA	O1D-CGD-O2D-CED
25	N	607	CHL	C5-C6-C7-C8
25	N	607	CHL	C13-C15-C16-C17
25	n	607	CHL	C5-C6-C7-C8
25	n	607	CHL	C13-C15-C16-C17
26	B	617	CLA	C15-C16-C17-C18
26	N	612	CLA	C5-C6-C7-C8
26	b	617	CLA	C15-C16-C17-C18
26	n	612	CLA	C5-C6-C7-C8
30	4	2630	LHG	C3-O3-P-O6
30	B	2630	LHG	C4-O6-P-O3
30	D	409	LHG	C4-O6-P-O3
30	D	410	LHG	C4-O6-P-O3
30	G	2630	LHG	C4-O6-P-O3
30	N	2630	LHG	C3-O3-P-O6
30	Y	2630	LHG	C4-O6-P-O3
30	8	2630	LHG	C3-O3-P-O6
30	b	2630	LHG	C4-O6-P-O3
30	d	409	LHG	C4-O6-P-O3
30	d	410	LHG	C4-O6-P-O3
30	g	2630	LHG	C4-O6-P-O3
30	n	2630	LHG	C3-O3-P-O6
30	y	2630	LHG	C4-O6-P-O3
37	A	413	LMG	C28-C29-C30-C31
37	a	413	LMG	C28-C29-C30-C31
25	N	601	CHL	CBA-CGA-O2A-C1
25	n	601	CHL	CBA-CGA-O2A-C1
26	C	502	CLA	CBA-CGA-O2A-C1
26	c	502	CLA	CBA-CGA-O2A-C1
26	B	617	CLA	O1D-CGD-O2D-CED
25	N	609	CHL	O1A-CGA-O2A-C1
26	5	604	CLA	O1D-CGD-O2D-CED
25	S	607	CHL	O1D-CGD-O2D-CED
25	s	607	CHL	O1D-CGD-O2D-CED
26	1	604	CLA	O1D-CGD-O2D-CED
26	C	510	CLA	O1D-CGD-O2D-CED
26	R	602	CLA	O1D-CGD-O2D-CED
26	c	510	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	r	602	CLA	O1D-CGD-O2D-CED
30	C	2630	LHG	C1-C2-C3-O3
30	D	408	LHG	C1-C2-C3-O3
30	N	2630	LHG	C1-C2-C3-O3
30	c	2630	LHG	C1-C2-C3-O3
30	d	408	LHG	C1-C2-C3-O3
30	n	2630	LHG	C1-C2-C3-O3
30	B	2630	LHG	O9-C7-O7-C5
30	S	2630	LHG	O9-C7-O7-C5
30	b	2630	LHG	O9-C7-O7-C5
30	s	2630	LHG	O9-C7-O7-C5
35	A	408	PHO	C4-C3-C5-C6
35	a	408	PHO	C4-C3-C5-C6
25	N	608	CHL	C15-C16-C17-C18
25	n	608	CHL	C15-C16-C17-C18
26	C	501	CLA	C2A-CAA-CBA-CGA
26	G	610	CLA	C2A-CAA-CBA-CGA
26	S	602	CLA	C2A-CAA-CBA-CGA
26	c	501	CLA	C2A-CAA-CBA-CGA
26	g	610	CLA	C2A-CAA-CBA-CGA
26	s	602	CLA	C2A-CAA-CBA-CGA
26	B	614	CLA	C3-C5-C6-C7
26	b	614	CLA	C3-C5-C6-C7
26	3	614	CLA	CBA-CGA-O2A-C1
26	B	613	CLA	CBA-CGA-O2A-C1
26	N	614	CLA	CBA-CGA-O2A-C1
26	R	603	CLA	CBA-CGA-O2A-C1
26	7	614	CLA	CBA-CGA-O2A-C1
26	b	613	CLA	CBA-CGA-O2A-C1
26	n	614	CLA	CBA-CGA-O2A-C1
26	r	603	CLA	CBA-CGA-O2A-C1
30	1	2630	LHG	C24-C23-O8-C6
30	5	2630	LHG	C24-C23-O8-C6
26	N	613	CLA	C8-C10-C11-C12
26	n	613	CLA	C8-C10-C11-C12
26	b	602	CLA	O1A-CGA-O2A-C1
31	T	101	BCR	C19-C20-C21-C22
31	t	101	BCR	C19-C20-C21-C22
30	2	2630	LHG	C23-C24-C25-C26
30	6	2630	LHG	C23-C24-C25-C26
26	3	604	CLA	O1D-CGD-O2D-CED
26	7	604	CLA	O1D-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
36	A	418	SQD	C8-C7-O47-C45
36	a	418	SQD	C8-C7-O47-C45
25	2	607	CHL	C8-C10-C11-C12
25	6	607	CHL	C8-C10-C11-C12
26	B	614	CLA	C10-C11-C12-C13
26	C	504	CLA	C10-C11-C12-C13
26	b	614	CLA	C10-C11-C12-C13
26	c	504	CLA	C10-C11-C12-C13
25	S	607	CHL	C3-C5-C6-C7
25	s	607	CHL	C3-C5-C6-C7
30	B	2630	LHG	C25-C26-C27-C28
30	C	2630	LHG	C31-C32-C33-C34
30	D	408	LHG	C26-C27-C28-C29
30	N	2630	LHG	C25-C26-C27-C28
30	b	2630	LHG	C25-C26-C27-C28
30	d	408	LHG	C26-C27-C28-C29
37	C	521	LMG	C11-C12-C13-C14
37	C	521	LMG	C12-C13-C14-C15
37	C	521	LMG	C32-C33-C34-C35
37	D	411	LMG	C19-C20-C21-C22
37	c	521	LMG	C11-C12-C13-C14
37	c	521	LMG	C12-C13-C14-C15
37	c	521	LMG	C32-C33-C34-C35
37	d	411	LMG	C19-C20-C21-C22
39	B	626	DGD	CCB-CDB-CEB-CFB
39	b	626	DGD	CCB-CDB-CEB-CFB
26	B	602	CLA	O1A-CGA-O2A-C1
39	C	519	DGD	C4E-C5E-C6E-O5E
25	R	606	CHL	O1D-CGD-O2D-CED
25	r	606	CHL	O1D-CGD-O2D-CED
26	B	612	CLA	O1D-CGD-O2D-CED
26	b	612	CLA	O1D-CGD-O2D-CED
25	Y	607	CHL	C16-C17-C18-C19
25	y	607	CHL	C16-C17-C18-C19
26	1	613	CLA	C6-C7-C8-C10
26	B	605	CLA	C16-C17-C18-C20
26	C	502	CLA	C16-C17-C18-C19
26	5	613	CLA	C6-C7-C8-C10
26	b	605	CLA	C16-C17-C18-C20
26	c	502	CLA	C16-C17-C18-C19
30	B	2630	LHG	C11-C10-C9-C8
30	B	2631	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
30	L	101	LHG	C32-C33-C34-C35
30	b	2630	LHG	C11-C10-C9-C8
30	c	2630	LHG	C31-C32-C33-C34
30	l	101	LHG	C32-C33-C34-C35
30	n	2630	LHG	C25-C26-C27-C28
36	A	412	SQD	C13-C14-C15-C16
36	a	412	SQD	C13-C14-C15-C16
37	D	411	LMG	C17-C18-C19-C20
37	d	411	LMG	C17-C18-C19-C20
30	C	2630	LHG	O9-C7-O7-C5
30	c	2630	LHG	O9-C7-O7-C5
26	N	611	CLA	C8-C10-C11-C12
26	n	611	CLA	C8-C10-C11-C12
25	1	607	CHL	CBD-CGD-O2D-CED
25	5	607	CHL	CBD-CGD-O2D-CED
30	G	2630	LHG	C25-C26-C27-C28
30	b	2631	LHG	C27-C28-C29-C30
30	g	2630	LHG	C25-C26-C27-C28
39	C	519	DGD	C4A-C5A-C6A-C7A
39	c	519	DGD	C4A-C5A-C6A-C7A
26	Y	603	CLA	O1D-CGD-O2D-CED
26	y	603	CLA	O1D-CGD-O2D-CED
30	1	2630	LHG	C12-C13-C14-C15
30	D	410	LHG	C13-C14-C15-C16
30	5	2630	LHG	C12-C13-C14-C15
30	d	410	LHG	C13-C14-C15-C16
39	B	626	DGD	C5A-C6A-C7A-C8A
39	H	102	DGD	C6A-C7A-C8A-C9A
39	b	626	DGD	C5B-C6B-C7B-C8B
39	h	102	DGD	C6A-C7A-C8A-C9A
39	c	519	DGD	C4E-C5E-C6E-O5E
26	b	611	CLA	O1D-CGD-O2D-CED
26	B	613	CLA	C10-C11-C12-C13
26	b	613	CLA	C10-C11-C12-C13
26	b	615	CLA	C5-C6-C7-C8
30	C	2630	LHG	C32-C33-C34-C35
30	C	522	LHG	C27-C28-C29-C30
30	D	408	LHG	C25-C26-C27-C28
30	D	409	LHG	C34-C35-C36-C37
30	D	410	LHG	C15-C16-C17-C18
30	c	2630	LHG	C32-C33-C34-C35
30	c	522	LHG	C27-C28-C29-C30

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Mol	Chain	Res	Type	Atoms
30	d	408	LHG	C25-C26-C27-C28
30	d	409	LHG	C34-C35-C36-C37
30	d	410	LHG	C15-C16-C17-C18
36	A	412	SQD	C18-C19-C20-C21
36	a	412	SQD	C18-C19-C20-C21
37	A	415	LMG	C30-C31-C32-C33
37	C	521	LMG	C35-C36-C37-C38
37	a	415	LMG	C30-C31-C32-C33
39	B	626	DGD	C2A-C3A-C4A-C5A
39	B	626	DGD	C5B-C6B-C7B-C8B
39	C	518	DGD	C4B-C5B-C6B-C7B
39	b	626	DGD	C2A-C3A-C4A-C5A
39	b	626	DGD	C5A-C6A-C7A-C8A
39	c	518	DGD	C4B-C5B-C6B-C7B
26	1	603	CLA	C3-C5-C6-C7
26	5	603	CLA	C3-C5-C6-C7
37	D	411	LMG	O6-C5-C6-O5
37	d	411	LMG	O6-C5-C6-O5
30	2	2630	LHG	C7-C8-C9-C10
30	6	2630	LHG	C7-C8-C9-C10
26	B	611	CLA	O1D-CGD-O2D-CED
37	B	2633	LMG	C2-C1-O1-C7
37	b	2633	LMG	C2-C1-O1-C7
39	C	519	DGD	C2E-C1E-O5D-C6D
39	c	519	DGD	C2E-C1E-O5D-C6D
25	R	607	CHL	CBA-CGA-O2A-C1
25	r	607	CHL	CBA-CGA-O2A-C1
26	B	611	CLA	CBA-CGA-O2A-C1
26	b	611	CLA	CBA-CGA-O2A-C1
37	D	411	LMG	C29-C28-O8-C9
37	d	411	LMG	C29-C28-O8-C9
30	3	2630	LHG	C27-C28-C29-C30
30	7	2630	LHG	C27-C28-C29-C30
37	A	415	LMG	C37-C38-C39-C40
37	a	413	LMG	C30-C31-C32-C33
37	c	521	LMG	C35-C36-C37-C38
39	C	520	DGD	C8B-C9B-CAB-CBB
39	c	520	DGD	C8B-C9B-CAB-CBB
25	G	601	CHL	C13-C15-C16-C17
25	g	601	CHL	C13-C15-C16-C17
26	1	603	CLA	C5-C6-C7-C8
26	B	615	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	N	603	CLA	C10-C11-C12-C13
26	N	611	CLA	C5-C6-C7-C8
26	5	603	CLA	C5-C6-C7-C8
26	b	610	CLA	C15-C16-C17-C18
26	b	612	CLA	C8-C10-C11-C12
26	n	603	CLA	C10-C11-C12-C13
26	n	611	CLA	C5-C6-C7-C8
25	N	601	CHL	O1A-CGA-O2A-C1
25	n	601	CHL	O1A-CGA-O2A-C1
25	2	609	CHL	C11-C12-C13-C15
25	6	609	CHL	C11-C12-C13-C15
26	C	508	CLA	C16-C17-C18-C19
26	c	508	CLA	C16-C17-C18-C19
25	3	601	CHL	C4-C3-C5-C6
25	7	601	CHL	C4-C3-C5-C6
26	C	510	CLA	C4-C3-C5-C6
26	c	510	CLA	C4-C3-C5-C6
38	D	405	PL9	C30-C29-C31-C32
38	d	405	PL9	C30-C29-C31-C32
30	3	2630	LHG	C31-C32-C33-C34
30	S	2630	LHG	C32-C33-C34-C35
30	7	2630	LHG	C31-C32-C33-C34
30	s	2630	LHG	C32-C33-C34-C35
36	A	412	SQD	C12-C13-C14-C15
36	A	418	SQD	C25-C26-C27-C28
36	a	412	SQD	C12-C13-C14-C15
36	a	418	SQD	C25-C26-C27-C28
37	A	413	LMG	C30-C31-C32-C33
37	B	2633	LMG	C30-C31-C32-C33
37	D	411	LMG	C20-C21-C22-C23
37	a	415	LMG	C37-C38-C39-C40
37	b	2633	LMG	C30-C31-C32-C33
37	d	411	LMG	C20-C21-C22-C23
39	C	520	DGD	CCA-CDA-CEA-CFA
39	H	102	DGD	C9A-CAA-CBA-CCA
39	c	520	DGD	CCA-CDA-CEA-CFA
39	h	102	DGD	C9A-CAA-CBA-CCA
25	3	601	CHL	C2-C3-C5-C6
25	7	601	CHL	C2-C3-C5-C6
26	C	510	CLA	C2-C3-C5-C6
26	c	510	CLA	C2-C3-C5-C6
38	D	405	PL9	C13-C14-C16-C17

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Mol	Chain	Res	Type	Atoms
38	d	405	PL9	C13-C14-C16-C17
26	B	604	CLA	C6-C7-C8-C9
26	C	505	CLA	C14-C13-C15-C16
26	C	513	CLA	C11-C12-C13-C14
26	G	602	CLA	C6-C7-C8-C9
26	R	610	CLA	C14-C13-C15-C16
26	b	604	CLA	C6-C7-C8-C9
26	c	505	CLA	C14-C13-C15-C16
26	c	513	CLA	C11-C12-C13-C14
26	g	602	CLA	C6-C7-C8-C9
26	r	610	CLA	C14-C13-C15-C16
25	S	601	CHL	O1D-CGD-O2D-CED
25	s	601	CHL	O1D-CGD-O2D-CED
36	A	418	SQD	C23-C24-C25-C26
36	a	418	SQD	C23-C24-C25-C26
30	C	523	LHG	C15-C16-C17-C18
30	C	523	LHG	C24-C25-C26-C27
30	D	410	LHG	C14-C15-C16-C17
30	G	2630	LHG	C27-C28-C29-C30
30	N	2630	LHG	C11-C10-C9-C8
30	S	2630	LHG	C24-C25-C26-C27
30	c	523	LHG	C15-C16-C17-C18
30	c	523	LHG	C24-C25-C26-C27
30	d	410	LHG	C14-C15-C16-C17
30	g	2630	LHG	C27-C28-C29-C30
30	l	101	LHG	C29-C30-C31-C32
30	n	2630	LHG	C11-C10-C9-C8
30	s	2630	LHG	C24-C25-C26-C27
36	A	418	SQD	C11-C10-C9-C8
36	B	621	SQD	C24-C25-C26-C27
36	a	418	SQD	C11-C10-C9-C8
36	b	621	SQD	C24-C25-C26-C27
39	C	518	DGD	C4A-C5A-C6A-C7A
39	c	518	DGD	C4A-C5A-C6A-C7A
25	G	601	CHL	C10-C11-C12-C13
25	g	601	CHL	C10-C11-C12-C13
26	B	604	CLA	C15-C16-C17-C18
26	B	610	CLA	C15-C16-C17-C18
26	B	612	CLA	C8-C10-C11-C12
26	b	604	CLA	C15-C16-C17-C18
25	3	607	CHL	C2A-CAA-CBA-CGA
25	3	608	CHL	C2A-CAA-CBA-CGA

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Mol	Chain	Res	Type	Atoms
25	G	605	CHL	C2A-CAA-CBA-CGA
25	Y	601	CHL	C2A-CAA-CBA-CGA
25	7	607	CHL	C2A-CAA-CBA-CGA
25	7	608	CHL	C2A-CAA-CBA-CGA
25	g	605	CHL	C2A-CAA-CBA-CGA
25	y	601	CHL	C2A-CAA-CBA-CGA
26	B	613	CLA	C2A-CAA-CBA-CGA
26	S	611	CLA	C2A-CAA-CBA-CGA
26	b	613	CLA	C2A-CAA-CBA-CGA
26	s	611	CLA	C2A-CAA-CBA-CGA
26	C	502	CLA	O1A-CGA-O2A-C1
26	G	614	CLA	O1A-CGA-O2A-C1
26	c	502	CLA	O1A-CGA-O2A-C1
26	g	614	CLA	O1A-CGA-O2A-C1
28	4	622	XAT	C27-C28-C29-C39
28	8	622	XAT	C27-C28-C29-C39
30	L	101	LHG	C10-C11-C12-C13
30	L	101	LHG	C29-C30-C31-C32
30	c	522	LHG	C24-C25-C26-C27
30	l	101	LHG	C10-C11-C12-C13
36	A	418	SQD	C15-C16-C17-C18
36	a	418	SQD	C15-C16-C17-C18
39	C	519	DGD	C4B-C5B-C6B-C7B
39	C	520	DGD	C7A-C8A-C9A-CAA
39	c	519	DGD	C4B-C5B-C6B-C7B
39	c	520	DGD	C7A-C8A-C9A-CAA
30	2	2630	LHG	O1-C1-C2-C3
30	4	2630	LHG	O1-C1-C2-C3
30	D	408	LHG	O1-C1-C2-C3
30	D	410	LHG	O1-C1-C2-C3
30	R	2630	LHG	O1-C1-C2-C3
30	Y	2630	LHG	O1-C1-C2-C3
30	6	2630	LHG	O1-C1-C2-C3
30	8	2630	LHG	O1-C1-C2-C3
30	d	408	LHG	O1-C1-C2-C3
30	d	410	LHG	O1-C1-C2-C3
30	r	2630	LHG	O1-C1-C2-C3
30	y	2630	LHG	O1-C1-C2-C3
28	3	1622	XAT	C31-C32-C33-C34
28	7	1622	XAT	C31-C32-C33-C34
31	D	404	BCR	C21-C22-C23-C24
31	d	404	BCR	C21-C22-C23-C24

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Mol	Chain	Res	Type	Atoms
26	R	602	CLA	C3-C5-C6-C7
26	r	602	CLA	C3-C5-C6-C7
26	R	602	CLA	C8-C10-C11-C12
26	r	602	CLA	C8-C10-C11-C12
30	3	2630	LHG	C28-C29-C30-C31
30	C	522	LHG	C24-C25-C26-C27
30	D	408	LHG	C28-C29-C30-C31
30	D	408	LHG	C29-C30-C31-C32
30	L	101	LHG	C11-C12-C13-C14
30	7	2630	LHG	C28-C29-C30-C31
30	d	408	LHG	C28-C29-C30-C31
30	l	101	LHG	C11-C12-C13-C14
36	A	412	SQD	C9-C10-C11-C12
36	a	412	SQD	C9-C10-C11-C12
30	1	2630	LHG	C7-C8-C9-C10
30	C	2630	LHG	C23-C24-C25-C26
30	Y	2630	LHG	C23-C24-C25-C26
30	5	2630	LHG	C7-C8-C9-C10
30	c	2630	LHG	C23-C24-C25-C26
30	y	2630	LHG	C23-C24-C25-C26
26	3	602	CLA	O1D-CGD-O2D-CED
26	7	602	CLA	O1D-CGD-O2D-CED
30	3	2630	LHG	C15-C16-C17-C18
30	B	2630	LHG	C12-C13-C14-C15
30	D	409	LHG	C26-C27-C28-C29
30	L	101	LHG	C34-C35-C36-C37
30	Y	2630	LHG	C32-C33-C34-C35
30	6	2630	LHG	C24-C25-C26-C27
30	7	2630	LHG	C15-C16-C17-C18
30	b	2630	LHG	C12-C13-C14-C15
30	d	408	LHG	C29-C30-C31-C32
30	d	409	LHG	C26-C27-C28-C29
30	l	101	LHG	C34-C35-C36-C37
30	y	2630	LHG	C32-C33-C34-C35
36	A	418	SQD	C10-C11-C12-C13
36	B	621	SQD	C28-C29-C30-C31
36	b	623	SQD	C9-C10-C11-C12
37	B	2633	LMG	C15-C16-C17-C18
37	D	411	LMG	C33-C34-C35-C36
37	Z	101	LMG	C18-C19-C20-C21
37	b	2633	LMG	C15-C16-C17-C18
37	d	411	LMG	C33-C34-C35-C36

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Mol	Chain	Res	Type	Atoms
37	z	101	LMG	C18-C19-C20-C21
25	N	609	CHL	C16-C17-C18-C20
25	n	609	CHL	C16-C17-C18-C20
26	C	501	CLA	C16-C17-C18-C19
26	C	502	CLA	C16-C17-C18-C20
26	R	613	CLA	C11-C12-C13-C15
26	c	501	CLA	C16-C17-C18-C19
26	c	502	CLA	C16-C17-C18-C20
26	r	613	CLA	C11-C12-C13-C15
25	Y	608	CHL	C8-C10-C11-C12
25	y	608	CHL	C8-C10-C11-C12
26	C	506	CLA	C13-C15-C16-C17
26	Y	612	CLA	C10-C11-C12-C13
26	c	506	CLA	C13-C15-C16-C17
26	y	612	CLA	C10-C11-C12-C13
30	2	2630	LHG	C24-C25-C26-C27
36	B	623	SQD	C9-C10-C11-C12
36	a	418	SQD	C10-C11-C12-C13
36	b	621	SQD	C28-C29-C30-C31
37	B	622	LMG	C37-C38-C39-C40
37	b	622	LMG	C37-C38-C39-C40
39	C	519	DGD	C5B-C6B-C7B-C8B
39	c	519	DGD	C5B-C6B-C7B-C8B
30	C	2630	LHG	C24-C25-C26-C27
30	R	2630	LHG	C12-C13-C14-C15
30	c	2630	LHG	C24-C25-C26-C27
30	r	2630	LHG	C12-C13-C14-C15
36	A	412	SQD	C29-C30-C31-C32
36	B	621	SQD	C18-C19-C20-C21
36	a	412	SQD	C29-C30-C31-C32
36	b	621	SQD	C18-C19-C20-C21
37	B	622	LMG	C21-C22-C23-C24
37	B	2633	LMG	C16-C17-C18-C19
37	b	622	LMG	C21-C22-C23-C24
37	b	2633	LMG	C16-C17-C18-C19
30	L	101	LHG	C7-C8-C9-C10
30	l	101	LHG	C7-C8-C9-C10
36	B	623	SQD	C23-C24-C25-C26
36	b	623	SQD	C23-C24-C25-C26
26	G	613	CLA	C8-C10-C11-C12
26	g	613	CLA	C8-C10-C11-C12
26	3	614	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	B	613	CLA	O1A-CGA-O2A-C1
26	N	614	CLA	O1A-CGA-O2A-C1
26	7	614	CLA	O1A-CGA-O2A-C1
26	b	613	CLA	O1A-CGA-O2A-C1
26	n	614	CLA	O1A-CGA-O2A-C1
36	B	623	SQD	O10-C23-O48-C46
36	b	623	SQD	O10-C23-O48-C46
37	B	622	LMG	C13-C14-C15-C16
37	B	622	LMG	C29-C30-C31-C32
37	B	2633	LMG	C32-C33-C34-C35
37	C	521	LMG	C31-C32-C33-C34
37	D	411	LMG	C14-C15-C16-C17
37	b	622	LMG	C13-C14-C15-C16
37	b	622	LMG	C29-C30-C31-C32
37	b	2633	LMG	C32-C33-C34-C35
37	c	521	LMG	C31-C32-C33-C34
37	d	411	LMG	C14-C15-C16-C17
25	G	609	CHL	CBA-CGA-O2A-C1
25	g	609	CHL	CBA-CGA-O2A-C1
30	G	2630	LHG	C18-C19-C20-C21
30	N	2630	LHG	C24-C25-C26-C27
30	g	2630	LHG	C18-C19-C20-C21
30	n	2630	LHG	C24-C25-C26-C27
25	3	605	CHL	O1D-CGD-O2D-CED
25	Y	601	CHL	O1D-CGD-O2D-CED
25	7	605	CHL	O1D-CGD-O2D-CED
25	y	601	CHL	O1D-CGD-O2D-CED
26	g	602	CLA	O1D-CGD-O2D-CED
25	1	605	CHL	C3A-C2A-CAA-CBA
25	1	607	CHL	C3A-C2A-CAA-CBA
25	2	601	CHL	C3A-C2A-CAA-CBA
25	2	605	CHL	C3A-C2A-CAA-CBA
25	3	605	CHL	C3A-C2A-CAA-CBA
25	3	606	CHL	C3A-C2A-CAA-CBA
25	4	606	CHL	C3A-C2A-CAA-CBA
25	R	606	CHL	C3A-C2A-CAA-CBA
25	S	608	CHL	C3A-C2A-CAA-CBA
25	Y	605	CHL	C3A-C2A-CAA-CBA
25	Y	608	CHL	C3A-C2A-CAA-CBA
25	5	605	CHL	C3A-C2A-CAA-CBA
25	5	607	CHL	C3A-C2A-CAA-CBA
25	6	601	CHL	C3A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	6	605	CHL	C3A-C2A-CAA-CBA
25	7	605	CHL	C3A-C2A-CAA-CBA
25	7	606	CHL	C3A-C2A-CAA-CBA
25	8	606	CHL	C3A-C2A-CAA-CBA
25	r	606	CHL	C3A-C2A-CAA-CBA
25	s	608	CHL	C3A-C2A-CAA-CBA
25	y	605	CHL	C3A-C2A-CAA-CBA
25	y	608	CHL	C3A-C2A-CAA-CBA
26	1	611	CLA	C3A-C2A-CAA-CBA
26	3	611	CLA	C3A-C2A-CAA-CBA
26	G	610	CLA	C3A-C2A-CAA-CBA
26	R	604	CLA	C3A-C2A-CAA-CBA
26	S	609	CLA	C3A-C2A-CAA-CBA
26	5	611	CLA	C3A-C2A-CAA-CBA
26	7	611	CLA	C3A-C2A-CAA-CBA
26	g	610	CLA	C3A-C2A-CAA-CBA
26	r	604	CLA	C3A-C2A-CAA-CBA
26	s	609	CLA	C3A-C2A-CAA-CBA
25	N	607	CHL	C8-C10-C11-C12
25	N	608	CHL	C13-C15-C16-C17
25	n	607	CHL	C8-C10-C11-C12
25	n	608	CHL	C13-C15-C16-C17
26	2	602	CLA	C10-C11-C12-C13
26	6	602	CLA	C10-C11-C12-C13
30	2	2630	LHG	C12-C13-C14-C15
30	6	2630	LHG	C12-C13-C14-C15
36	B	621	SQD	C10-C11-C12-C13
36	b	621	SQD	C10-C11-C12-C13
39	C	519	DGD	C3A-C4A-C5A-C6A
39	C	519	DGD	C9A-CAA-CBA-CCA
39	c	519	DGD	C3A-C4A-C5A-C6A
39	c	519	DGD	C9A-CAA-CBA-CCA
26	B	604	CLA	O1D-CGD-O2D-CED
26	G	602	CLA	O1D-CGD-O2D-CED
26	b	604	CLA	O1D-CGD-O2D-CED
37	C	521	LMG	C4-C5-C6-O5
37	c	521	LMG	C4-C5-C6-O5
25	2	609	CHL	C11-C12-C13-C14
25	N	607	CHL	C16-C17-C18-C19
25	N	608	CHL	C16-C17-C18-C20
25	Y	607	CHL	C16-C17-C18-C20
25	6	609	CHL	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
25	n	607	CHL	C16-C17-C18-C19
25	n	608	CHL	C16-C17-C18-C20
25	y	607	CHL	C16-C17-C18-C20
26	C	505	CLA	C16-C17-C18-C20
26	R	613	CLA	C11-C12-C13-C14
26	c	505	CLA	C16-C17-C18-C20
26	r	613	CLA	C11-C12-C13-C14
30	B	2630	LHG	C26-C27-C28-C29
30	B	2630	LHG	C27-C28-C29-C30
30	D	408	LHG	C27-C28-C29-C30
30	D	410	LHG	C27-C28-C29-C30
30	N	2630	LHG	C30-C31-C32-C33
30	b	2630	LHG	C26-C27-C28-C29
30	d	410	LHG	C27-C28-C29-C30
30	l	101	LHG	C16-C17-C18-C19
30	n	2630	LHG	C30-C31-C32-C33
39	C	520	DGD	C4B-C5B-C6B-C7B
39	c	520	DGD	C4B-C5B-C6B-C7B
30	C	522	LHG	C28-C29-C30-C31
30	L	101	LHG	C16-C17-C18-C19
30	Y	2630	LHG	C12-C13-C14-C15
30	b	2630	LHG	C27-C28-C29-C30
30	c	522	LHG	C28-C29-C30-C31
30	d	408	LHG	C27-C28-C29-C30
30	y	2630	LHG	C12-C13-C14-C15
39	B	626	DGD	O6D-C5D-C6D-O5D
39	b	626	DGD	O6D-C5D-C6D-O5D
26	C	510	CLA	C3-C5-C6-C7
26	c	510	CLA	C3-C5-C6-C7
26	B	612	CLA	C4-C3-C5-C6
26	b	612	CLA	C4-C3-C5-C6
25	2	609	CHL	CBA-CGA-O2A-C1
25	6	609	CHL	CBA-CGA-O2A-C1
25	R	608	CHL	C2-C3-C5-C6
25	r	608	CHL	C2-C3-C5-C6
35	A	408	PHO	C2-C3-C5-C6
35	a	408	PHO	C2-C3-C5-C6
38	D	405	PL9	C43-C44-C46-C47
38	d	405	PL9	C43-C44-C46-C47
30	S	2630	LHG	C8-C7-O7-C5
30	s	2630	LHG	C8-C7-O7-C5
37	C	521	LMG	C11-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
37	c	521	LMG	C11-C10-O7-C8
30	N	2630	LHG	C27-C28-C29-C30
30	n	2630	LHG	C27-C28-C29-C30
38	A	414	PL9	C7-C8-C9-C10
38	a	414	PL9	C7-C8-C9-C10
25	3	601	CHL	C2A-CAA-CBA-CGA
25	7	601	CHL	C2A-CAA-CBA-CGA
30	D	410	LHG	O1-C1-C2-O2
30	R	2630	LHG	O1-C1-C2-O2
30	Y	2630	LHG	O1-C1-C2-O2
30	d	410	LHG	O1-C1-C2-O2
30	r	2630	LHG	O1-C1-C2-O2
30	y	2630	LHG	O1-C1-C2-O2
30	B	2630	LHG	C10-C11-C12-C13
30	C	522	LHG	C32-C33-C34-C35
30	G	2630	LHG	C29-C30-C31-C32
30	S	2630	LHG	C11-C12-C13-C14
30	S	2630	LHG	C29-C30-C31-C32
30	b	2630	LHG	C10-C11-C12-C13
30	c	522	LHG	C32-C33-C34-C35
30	g	2630	LHG	C29-C30-C31-C32
30	s	2630	LHG	C11-C12-C13-C14
37	A	413	LMG	C32-C33-C34-C35
37	A	413	LMG	C37-C38-C39-C40
37	A	415	LMG	C32-C33-C34-C35
37	a	413	LMG	C32-C33-C34-C35
37	a	413	LMG	C37-C38-C39-C40
37	a	415	LMG	C32-C33-C34-C35
39	C	519	DGD	C6B-C7B-C8B-C9B
39	c	519	DGD	C6B-C7B-C8B-C9B
26	C	511	CLA	O1A-CGA-O2A-C1
26	c	511	CLA	O1A-CGA-O2A-C1
25	R	606	CHL	C16-C17-C18-C19
25	r	606	CHL	C16-C17-C18-C19
30	B	2630	LHG	C32-C33-C34-C35
30	C	2630	LHG	C14-C15-C16-C17
30	b	2630	LHG	C32-C33-C34-C35
30	c	2630	LHG	C14-C15-C16-C17
30	s	2630	LHG	C29-C30-C31-C32
30	C	523	LHG	O2-C2-C3-O3
30	c	523	LHG	O2-C2-C3-O3
30	d	410	LHG	O2-C2-C3-O3

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Mol	Chain	Res	Type	Atoms
25	N	607	CHL	C15-C16-C17-C18
25	n	607	CHL	C15-C16-C17-C18
30	1	2630	LHG	C11-C12-C13-C14
30	5	2630	LHG	C11-C12-C13-C14
36	B	621	SQD	C33-C34-C35-C36
36	b	621	SQD	C33-C34-C35-C36
39	H	102	DGD	C7A-C8A-C9A-CAA
39	h	102	DGD	C7A-C8A-C9A-CAA
26	R	603	CLA	O1A-CGA-O2A-C1
26	r	603	CLA	O1A-CGA-O2A-C1
39	C	520	DGD	C1A-C2A-C3A-C4A
39	c	520	DGD	C1A-C2A-C3A-C4A
25	1	607	CHL	C5-C6-C7-C8
25	5	607	CHL	C5-C6-C7-C8
39	C	519	DGD	C3B-C4B-C5B-C6B
39	C	520	DGD	C2B-C3B-C4B-C5B
39	c	519	DGD	C3B-C4B-C5B-C6B
39	c	520	DGD	C2B-C3B-C4B-C5B
25	R	608	CHL	C2-C1-O2A-CGA
25	r	608	CHL	C2-C1-O2A-CGA
30	G	2630	LHG	C24-C25-C26-C27
30	L	101	LHG	C11-C10-C9-C8
30	g	2630	LHG	C24-C25-C26-C27
30	l	101	LHG	C11-C10-C9-C8
37	B	622	LMG	C19-C20-C21-C22
37	b	622	LMG	C19-C20-C21-C22
39	H	102	DGD	C3B-C4B-C5B-C6B
39	h	102	DGD	C3B-C4B-C5B-C6B
25	G	607	CHL	C15-C16-C17-C18
25	g	607	CHL	C15-C16-C17-C18
26	B	611	CLA	O1A-CGA-O2A-C1
26	b	611	CLA	O1A-CGA-O2A-C1
30	B	2630	LHG	C29-C30-C31-C32
30	b	2630	LHG	C29-C30-C31-C32
37	Z	101	LMG	C20-C21-C22-C23
37	z	101	LMG	C20-C21-C22-C23
39	H	102	DGD	C3A-C4A-C5A-C6A
39	h	102	DGD	C3A-C4A-C5A-C6A
27	1	1620	LUT	C5-C6-C7-C8
27	2	1620	LUT	C5-C6-C7-C8
27	3	1620	LUT	C1-C6-C7-C8
27	3	1620	LUT	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	R	620	LUT	C1-C6-C7-C8
27	R	620	LUT	C5-C6-C7-C8
27	Y	1620	LUT	C1-C6-C7-C8
27	Y	1620	LUT	C5-C6-C7-C8
27	5	1620	LUT	C5-C6-C7-C8
27	6	1620	LUT	C5-C6-C7-C8
27	7	1620	LUT	C1-C6-C7-C8
27	7	1620	LUT	C5-C6-C7-C8
27	r	620	LUT	C1-C6-C7-C8
27	r	620	LUT	C5-C6-C7-C8
27	y	1620	LUT	C1-C6-C7-C8
27	y	1620	LUT	C5-C6-C7-C8
31	A	411	BCR	C5-C6-C7-C8
31	A	411	BCR	C23-C24-C25-C26
31	A	411	BCR	C23-C24-C25-C30
31	B	618	BCR	C1-C6-C7-C8
31	B	620	BCR	C23-C24-C25-C26
31	C	514	BCR	C1-C6-C7-C8
31	C	514	BCR	C5-C6-C7-C8
31	C	515	BCR	C23-C24-C25-C26
31	C	515	BCR	C23-C24-C25-C30
31	C	516	BCR	C1-C6-C7-C8
31	C	516	BCR	C5-C6-C7-C8
31	D	404	BCR	C5-C6-C7-C8
31	T	101	BCR	C23-C24-C25-C26
31	a	411	BCR	C5-C6-C7-C8
31	a	411	BCR	C23-C24-C25-C26
31	a	411	BCR	C23-C24-C25-C30
31	b	618	BCR	C1-C6-C7-C8
31	b	620	BCR	C23-C24-C25-C26
31	c	514	BCR	C1-C6-C7-C8
31	c	514	BCR	C5-C6-C7-C8
31	c	515	BCR	C23-C24-C25-C26
31	c	515	BCR	C23-C24-C25-C30
31	c	516	BCR	C1-C6-C7-C8
31	c	516	BCR	C5-C6-C7-C8
31	d	404	BCR	C5-C6-C7-C8
31	t	101	BCR	C23-C24-C25-C26
30	G	2630	LHG	C17-C18-C19-C20
30	g	2630	LHG	C17-C18-C19-C20
36	A	412	SQD	C24-C23-O48-C46
36	a	412	SQD	C24-C23-O48-C46

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Mol	Chain	Res	Type	Atoms
26	3	610	CLA	C10-C11-C12-C13
26	C	505	CLA	C5-C6-C7-C8
26	7	610	CLA	C10-C11-C12-C13
26	c	505	CLA	C5-C6-C7-C8
30	S	2630	LHG	C34-C35-C36-C37
30	s	2630	LHG	C34-C35-C36-C37
37	A	415	LMG	C36-C37-C38-C39
37	B	2633	LMG	C17-C18-C19-C20
37	C	521	LMG	C17-C18-C19-C20
37	Z	101	LMG	C32-C33-C34-C35
37	a	415	LMG	C36-C37-C38-C39
37	b	2633	LMG	C17-C18-C19-C20
37	c	521	LMG	C17-C18-C19-C20
37	z	101	LMG	C32-C33-C34-C35
25	R	607	CHL	O1A-CGA-O2A-C1
30	C	522	LHG	O10-C23-O8-C6
30	c	522	LHG	O10-C23-O8-C6
36	B	621	SQD	O10-C23-O48-C46
36	b	621	SQD	O10-C23-O48-C46
25	1	607	CHL	C8-C10-C11-C12
25	Y	601	CHL	C10-C11-C12-C13
25	5	607	CHL	C8-C10-C11-C12
25	y	601	CHL	C10-C11-C12-C13
26	B	606	CLA	C5-C6-C7-C8
26	b	606	CLA	C5-C6-C7-C8
25	2	607	CHL	C4-C3-C5-C6
25	R	608	CHL	C4-C3-C5-C6
25	6	607	CHL	C4-C3-C5-C6
25	r	608	CHL	C4-C3-C5-C6
26	C	505	CLA	C4-C3-C5-C6
26	Y	603	CLA	C4-C3-C5-C6
26	c	505	CLA	C4-C3-C5-C6
26	y	603	CLA	C4-C3-C5-C6
38	D	405	PL9	C45-C44-C46-C47
38	d	405	PL9	C45-C44-C46-C47
25	3	606	CHL	O1D-CGD-O2D-CED
25	7	606	CHL	O1D-CGD-O2D-CED
25	3	601	CHL	C6-C7-C8-C10
25	N	608	CHL	C12-C13-C15-C16
25	Y	608	CHL	C12-C13-C15-C16
25	7	601	CHL	C6-C7-C8-C10
25	n	608	CHL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	y	608	CHL	C12-C13-C15-C16
26	B	604	CLA	C6-C7-C8-C10
26	B	611	CLA	C12-C13-C15-C16
26	B	612	CLA	C2-C3-C5-C6
26	C	501	CLA	C11-C10-C8-C7
26	C	502	CLA	C12-C13-C15-C16
26	C	504	CLA	C11-C10-C8-C7
26	C	505	CLA	C2-C3-C5-C6
26	G	602	CLA	C6-C7-C8-C10
26	Y	603	CLA	C2-C3-C5-C6
26	Y	612	CLA	C6-C7-C8-C10
26	Y	613	CLA	C11-C12-C13-C15
26	b	604	CLA	C6-C7-C8-C10
26	b	611	CLA	C12-C13-C15-C16
26	b	612	CLA	C2-C3-C5-C6
26	c	501	CLA	C11-C10-C8-C7
26	c	502	CLA	C12-C13-C15-C16
26	c	504	CLA	C11-C10-C8-C7
26	c	505	CLA	C2-C3-C5-C6
26	g	602	CLA	C6-C7-C8-C10
26	y	603	CLA	C2-C3-C5-C6
26	y	612	CLA	C6-C7-C8-C10
26	y	613	CLA	C11-C12-C13-C15
25	1	609	CHL	C3-C5-C6-C7
25	5	609	CHL	C3-C5-C6-C7
26	A	405	CLA	C3-C5-C6-C7
26	a	405	CLA	C3-C5-C6-C7
25	G	609	CHL	O1A-CGA-O2A-C1
25	g	609	CHL	O1A-CGA-O2A-C1
25	r	607	CHL	O1A-CGA-O2A-C1
30	3	2630	LHG	C30-C31-C32-C33
30	7	2630	LHG	C30-C31-C32-C33
25	Y	607	CHL	C13-C15-C16-C17
25	y	607	CHL	C13-C15-C16-C17
26	3	602	CLA	C8-C10-C11-C12
26	B	605	CLA	C8-C10-C11-C12
26	b	605	CLA	C8-C10-C11-C12
26	R	603	CLA	C11-C12-C13-C14
26	r	603	CLA	C11-C12-C13-C14
30	R	2630	LHG	C23-C24-C25-C26
30	r	2630	LHG	C23-C24-C25-C26
26	C	513	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	R	613	CLA	CBA-CGA-O2A-C1
26	Y	603	CLA	CBA-CGA-O2A-C1
26	c	513	CLA	CBA-CGA-O2A-C1
26	r	613	CLA	CBA-CGA-O2A-C1
26	y	603	CLA	CBA-CGA-O2A-C1
30	R	2630	LHG	C24-C23-O8-C6
30	r	2630	LHG	C24-C23-O8-C6
30	Y	2630	LHG	C28-C29-C30-C31
30	y	2630	LHG	C28-C29-C30-C31
37	A	415	LMG	C35-C36-C37-C38
37	a	415	LMG	C35-C36-C37-C38
25	2	606	CHL	C2A-CAA-CBA-CGA
25	N	606	CHL	C2A-CAA-CBA-CGA
25	6	606	CHL	C2A-CAA-CBA-CGA
25	n	606	CHL	C2A-CAA-CBA-CGA
26	1	602	CLA	C2A-CAA-CBA-CGA
26	3	602	CLA	C2A-CAA-CBA-CGA
26	3	613	CLA	C2A-CAA-CBA-CGA
26	4	602	CLA	C2A-CAA-CBA-CGA
26	5	602	CLA	C2A-CAA-CBA-CGA
26	7	602	CLA	C2A-CAA-CBA-CGA
26	7	613	CLA	C2A-CAA-CBA-CGA
26	8	602	CLA	C2A-CAA-CBA-CGA
25	N	601	CHL	C15-C16-C17-C18
25	R	608	CHL	C8-C10-C11-C12
25	n	601	CHL	C15-C16-C17-C18
25	r	608	CHL	C8-C10-C11-C12
26	C	506	CLA	C15-C16-C17-C18
26	7	602	CLA	C8-C10-C11-C12
26	c	506	CLA	C15-C16-C17-C18
30	C	2630	LHG	C12-C13-C14-C15
30	c	2630	LHG	C12-C13-C14-C15
30	Y	2630	LHG	C16-C17-C18-C19
30	y	2630	LHG	C16-C17-C18-C19
37	C	521	LMG	C29-C30-C31-C32
37	c	521	LMG	C29-C30-C31-C32
26	S	602	CLA	C12-C13-C15-C16
26	s	602	CLA	C12-C13-C15-C16
26	D	402	CLA	C8-C10-C11-C12
26	G	612	CLA	C8-C10-C11-C12
26	d	402	CLA	C8-C10-C11-C12
25	1	609	CHL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
30	B	2631	LHG	C33-C34-C35-C36
30	b	2631	LHG	C33-C34-C35-C36
25	5	609	CHL	C2C-C3C-CAC-CBC
30	B	2631	LHG	C31-C32-C33-C34
30	C	523	LHG	C26-C27-C28-C29
30	b	2631	LHG	C31-C32-C33-C34
30	c	523	LHG	C26-C27-C28-C29
36	A	412	SQD	C30-C31-C32-C33
25	2	609	CHL	O1A-CGA-O2A-C1
26	B	604	CLA	C16-C17-C18-C20
26	b	604	CLA	C16-C17-C18-C20
26	g	612	CLA	C8-C10-C11-C12
30	C	522	LHG	C11-C10-C9-C8
30	D	409	LHG	C17-C18-C19-C20
30	S	2630	LHG	C27-C28-C29-C30
30	c	522	LHG	C11-C10-C9-C8
30	d	409	LHG	C17-C18-C19-C20
30	s	2630	LHG	C27-C28-C29-C30
36	a	412	SQD	C30-C31-C32-C33
30	2	2630	LHG	C8-C7-O7-C5
30	B	2630	LHG	C8-C7-O7-C5
30	C	2630	LHG	C8-C7-O7-C5
30	6	2630	LHG	C8-C7-O7-C5
30	b	2630	LHG	C8-C7-O7-C5
30	c	2630	LHG	C8-C7-O7-C5
30	B	2631	LHG	C28-C29-C30-C31
30	b	2631	LHG	C28-C29-C30-C31
36	B	621	SQD	C34-C35-C36-C37
36	b	621	SQD	C34-C35-C36-C37
25	G	601	CHL	C15-C16-C17-C18
25	G	607	CHL	C8-C10-C11-C12
25	g	601	CHL	C15-C16-C17-C18
25	g	607	CHL	C8-C10-C11-C12
26	B	614	CLA	C15-C16-C17-C18
26	b	614	CLA	C15-C16-C17-C18
25	6	609	CHL	O1A-CGA-O2A-C1
39	H	102	DGD	CCA-CDA-CEA-CFA
39	h	102	DGD	CCA-CDA-CEA-CFA
30	D	410	LHG	O2-C2-C3-O3
30	C	522	LHG	O9-C7-O7-C5
30	G	2630	LHG	O9-C7-O7-C5
30	c	522	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
39	b	626	DGD	O1B-C1B-O2G-C2G
30	s	2630	LHG	C13-C14-C15-C16
37	C	521	LMG	C16-C17-C18-C19
37	c	521	LMG	C16-C17-C18-C19
30	S	2630	LHG	O7-C5-C6-O8
30	s	2630	LHG	O7-C5-C6-O8
25	Y	609	CHL	CBA-CGA-O2A-C1
25	y	609	CHL	CBA-CGA-O2A-C1
30	S	2630	LHG	C13-C14-C15-C16
30	b	2631	LHG	C14-C15-C16-C17
26	1	613	CLA	C6-C7-C8-C9
26	B	605	CLA	C16-C17-C18-C19
26	B	610	CLA	C16-C17-C18-C20
26	5	613	CLA	C6-C7-C8-C9
26	b	605	CLA	C16-C17-C18-C19
26	b	610	CLA	C16-C17-C18-C20
26	c	508	CLA	C16-C17-C18-C20
30	B	2631	LHG	C14-C15-C16-C17
26	6	602	CLA	C4-C3-C5-C6
38	D	405	PL9	C15-C14-C16-C17
38	d	405	PL9	C15-C14-C16-C17
25	2	607	CHL	C2-C3-C5-C6
25	6	607	CHL	C2-C3-C5-C6
26	N	610	CLA	C2-C3-C5-C6
26	n	610	CLA	C2-C3-C5-C6
39	C	520	DGD	C4A-C5A-C6A-C7A
39	c	520	DGD	C4A-C5A-C6A-C7A
25	G	607	CHL	C14-C13-C15-C16
25	g	607	CHL	C14-C13-C15-C16
26	1	602	CLA	C6-C7-C8-C9
26	3	613	CLA	C6-C7-C8-C9
26	A	406	CLA	C11-C12-C13-C14
26	C	501	CLA	C11-C10-C8-C9
26	C	504	CLA	C11-C10-C8-C9
26	C	510	CLA	C14-C13-C15-C16
26	C	511	CLA	C11-C12-C13-C14
26	N	603	CLA	C11-C10-C8-C9
26	S	602	CLA	C6-C7-C8-C9
26	Y	602	CLA	C6-C7-C8-C9
26	Y	611	CLA	C11-C10-C8-C9
26	Y	612	CLA	C11-C10-C8-C9
26	Y	613	CLA	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	5	602	CLA	C6-C7-C8-C9
26	7	613	CLA	C6-C7-C8-C9
26	a	406	CLA	C11-C12-C13-C14
26	c	501	CLA	C11-C10-C8-C9
26	c	504	CLA	C11-C10-C8-C9
26	c	510	CLA	C14-C13-C15-C16
26	c	511	CLA	C11-C12-C13-C14
26	n	603	CLA	C11-C10-C8-C9
26	s	602	CLA	C6-C7-C8-C9
26	y	602	CLA	C6-C7-C8-C9
26	y	611	CLA	C11-C10-C8-C9
26	y	612	CLA	C11-C10-C8-C9
26	y	613	CLA	C11-C12-C13-C14
25	3	609	CHL	O1D-CGD-O2D-CED
25	7	609	CHL	O1D-CGD-O2D-CED
25	3	606	CHL	C2A-CAA-CBA-CGA
25	Y	606	CHL	C2A-CAA-CBA-CGA
25	7	606	CHL	C2A-CAA-CBA-CGA
25	y	606	CHL	C2A-CAA-CBA-CGA
26	G	603	CLA	C2A-CAA-CBA-CGA
26	g	603	CLA	C2A-CAA-CBA-CGA
37	B	622	LMG	C18-C19-C20-C21
37	b	622	LMG	C18-C19-C20-C21
25	Y	609	CHL	C8-C10-C11-C12
25	y	609	CHL	C8-C10-C11-C12
30	R	2630	LHG	C18-C19-C20-C21
30	r	2630	LHG	C18-C19-C20-C21
36	b	623	SQD	C11-C10-C9-C8
37	B	622	LMG	C35-C36-C37-C38
37	D	411	LMG	C32-C33-C34-C35
37	b	622	LMG	C35-C36-C37-C38
37	d	411	LMG	C32-C33-C34-C35
39	C	520	DGD	C5A-C6A-C7A-C8A
39	c	520	DGD	C5A-C6A-C7A-C8A
31	B	620	BCR	C21-C22-C23-C24
31	b	620	BCR	C21-C22-C23-C24
25	1	605	CHL	C1A-C2A-CAA-CBA
25	2	605	CHL	C1A-C2A-CAA-CBA
25	2	608	CHL	C1A-C2A-CAA-CBA
25	3	605	CHL	C1A-C2A-CAA-CBA
25	3	606	CHL	C1A-C2A-CAA-CBA
25	4	607	CHL	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
25	4	608	CHL	C1A-C2A-CAA-CBA
25	G	608	CHL	C1A-C2A-CAA-CBA
25	N	605	CHL	C1A-C2A-CAA-CBA
25	N	608	CHL	C1A-C2A-CAA-CBA
25	R	606	CHL	C1A-C2A-CAA-CBA
25	5	605	CHL	C1A-C2A-CAA-CBA
25	6	605	CHL	C1A-C2A-CAA-CBA
25	6	608	CHL	C1A-C2A-CAA-CBA
25	7	605	CHL	C1A-C2A-CAA-CBA
25	7	606	CHL	C1A-C2A-CAA-CBA
25	8	607	CHL	C1A-C2A-CAA-CBA
25	8	608	CHL	C1A-C2A-CAA-CBA
25	g	608	CHL	C1A-C2A-CAA-CBA
25	n	605	CHL	C1A-C2A-CAA-CBA
25	n	608	CHL	C1A-C2A-CAA-CBA
25	r	606	CHL	C1A-C2A-CAA-CBA
26	1	602	CLA	C1A-C2A-CAA-CBA
26	1	604	CLA	C1A-C2A-CAA-CBA
26	1	610	CLA	C1A-C2A-CAA-CBA
26	1	611	CLA	C1A-C2A-CAA-CBA
26	3	604	CLA	C1A-C2A-CAA-CBA
26	3	614	CLA	C1A-C2A-CAA-CBA
26	4	604	CLA	C1A-C2A-CAA-CBA
26	4	610	CLA	C1A-C2A-CAA-CBA
26	A	407	CLA	C1A-C2A-CAA-CBA
26	A	410	CLA	C1A-C2A-CAA-CBA
26	B	610	CLA	C1A-C2A-CAA-CBA
26	B	612	CLA	C1A-C2A-CAA-CBA
26	C	501	CLA	C1A-C2A-CAA-CBA
26	C	506	CLA	C1A-C2A-CAA-CBA
26	C	508	CLA	C1A-C2A-CAA-CBA
26	C	511	CLA	C1A-C2A-CAA-CBA
26	G	602	CLA	C1A-C2A-CAA-CBA
26	N	602	CLA	C1A-C2A-CAA-CBA
26	R	604	CLA	C1A-C2A-CAA-CBA
26	R	610	CLA	C1A-C2A-CAA-CBA
26	Y	602	CLA	C1A-C2A-CAA-CBA
26	Y	610	CLA	C1A-C2A-CAA-CBA
26	Y	614	CLA	C1A-C2A-CAA-CBA
26	5	602	CLA	C1A-C2A-CAA-CBA
26	5	604	CLA	C1A-C2A-CAA-CBA
26	5	610	CLA	C1A-C2A-CAA-CBA

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Mol	Chain	Res	Type	Atoms
26	5	611	CLA	C1A-C2A-CAA-CBA
26	7	604	CLA	C1A-C2A-CAA-CBA
26	7	614	CLA	C1A-C2A-CAA-CBA
26	8	604	CLA	C1A-C2A-CAA-CBA
26	8	610	CLA	C1A-C2A-CAA-CBA
26	a	407	CLA	C1A-C2A-CAA-CBA
26	a	410	CLA	C1A-C2A-CAA-CBA
26	b	610	CLA	C1A-C2A-CAA-CBA
26	b	612	CLA	C1A-C2A-CAA-CBA
26	c	501	CLA	C1A-C2A-CAA-CBA
26	c	506	CLA	C1A-C2A-CAA-CBA
26	c	508	CLA	C1A-C2A-CAA-CBA
26	c	511	CLA	C1A-C2A-CAA-CBA
26	g	602	CLA	C1A-C2A-CAA-CBA
26	n	602	CLA	C1A-C2A-CAA-CBA
26	r	604	CLA	C1A-C2A-CAA-CBA
26	r	610	CLA	C1A-C2A-CAA-CBA
26	y	602	CLA	C1A-C2A-CAA-CBA
26	y	610	CLA	C1A-C2A-CAA-CBA
26	y	614	CLA	C1A-C2A-CAA-CBA
25	N	608	CHL	C16-C17-C18-C19
25	R	607	CHL	C6-C7-C8-C9
25	n	608	CHL	C16-C17-C18-C19
25	r	607	CHL	C6-C7-C8-C9
26	B	610	CLA	C16-C17-C18-C19
26	C	501	CLA	C16-C17-C18-C20
26	C	508	CLA	C16-C17-C18-C20
26	b	610	CLA	C16-C17-C18-C19
26	c	501	CLA	C16-C17-C18-C20
30	1	2630	LHG	O9-C7-O7-C5
30	Y	2630	LHG	O9-C7-O7-C5
30	5	2630	LHG	O9-C7-O7-C5
30	g	2630	LHG	O9-C7-O7-C5
30	y	2630	LHG	O9-C7-O7-C5
39	B	626	DGD	O1B-C1B-O2G-C2G
37	B	622	LMG	C11-C10-O7-C8
37	b	622	LMG	C11-C10-O7-C8
30	C	2630	LHG	C26-C27-C28-C29
30	C	2630	LHG	C28-C29-C30-C31
30	G	2630	LHG	C13-C14-C15-C16
30	b	2631	LHG	C32-C33-C34-C35
30	c	2630	LHG	C26-C27-C28-C29

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Mol	Chain	Res	Type	Atoms
30	c	2630	LHG	C28-C29-C30-C31
30	g	2630	LHG	C13-C14-C15-C16
36	B	623	SQD	C11-C10-C9-C8
37	B	622	LMG	C17-C18-C19-C20
39	B	626	DGD	C6A-C7A-C8A-C9A
39	b	626	DGD	C6A-C7A-C8A-C9A
26	N	613	CLA	O1D-CGD-O2D-CED
26	n	613	CLA	O1D-CGD-O2D-CED
30	3	2630	LHG	C3-O3-P-O6
30	L	101	LHG	C4-O6-P-O3
30	7	2630	LHG	C3-O3-P-O6
30	l	101	LHG	C4-O6-P-O3
30	B	2631	LHG	C32-C33-C34-C35
37	b	622	LMG	C17-C18-C19-C20
37	B	622	LMG	C28-C29-C30-C31
37	b	622	LMG	C28-C29-C30-C31
26	C	507	CLA	O1D-CGD-O2D-CED
26	c	507	CLA	O1D-CGD-O2D-CED
30	3	2630	LHG	C13-C14-C15-C16
30	3	2630	LHG	C24-C25-C26-C27
30	7	2630	LHG	C13-C14-C15-C16
30	7	2630	LHG	C24-C25-C26-C27
36	a	412	SQD	C10-C11-C12-C13
39	H	102	DGD	CBA-CCA-CDA-CEA
25	1	609	CHL	C10-C11-C12-C13
25	N	607	CHL	C10-C11-C12-C13
25	5	609	CHL	C10-C11-C12-C13
25	n	607	CHL	C10-C11-C12-C13
26	B	617	CLA	C10-C11-C12-C13
26	b	617	CLA	C10-C11-C12-C13
25	1	609	CHL	CBA-CGA-O2A-C1
25	5	609	CHL	CBA-CGA-O2A-C1
26	S	614	CLA	CBA-CGA-O2A-C1
26	s	614	CLA	CBA-CGA-O2A-C1
30	D	410	LHG	C10-C11-C12-C13
30	d	410	LHG	C10-C11-C12-C13
36	A	412	SQD	C10-C11-C12-C13
39	C	519	DGD	C2B-C3B-C4B-C5B
39	c	519	DGD	C2B-C3B-C4B-C5B
39	h	102	DGD	CBA-CCA-CDA-CEA
25	1	607	CHL	C2C-C3C-CAC-CBC
25	5	607	CHL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
39	h	102	DGD	CAB-CBB-CCB-CDB
30	Y	2630	LHG	C27-C28-C29-C30
30	y	2630	LHG	C27-C28-C29-C30
37	A	413	LMG	C29-C30-C31-C32
37	a	413	LMG	C29-C30-C31-C32
39	H	102	DGD	CAB-CBB-CCB-CDB
26	N	612	CLA	C8-C10-C11-C12
26	n	612	CLA	C8-C10-C11-C12
25	Y	605	CHL	CBA-CGA-O2A-C1
25	y	605	CHL	CBA-CGA-O2A-C1
37	A	413	LMG	C29-C28-O8-C9
37	a	413	LMG	C29-C28-O8-C9
30	D	409	LHG	O9-C7-O7-C5
26	2	602	CLA	C4-C3-C5-C6
30	D	409	LHG	C14-C15-C16-C17
30	D	410	LHG	C25-C26-C27-C28
30	d	410	LHG	C25-C26-C27-C28
37	A	413	LMG	C18-C19-C20-C21
37	a	413	LMG	C18-C19-C20-C21
25	Y	609	CHL	C10-C11-C12-C13
25	y	609	CHL	C10-C11-C12-C13
26	B	606	CLA	C8-C10-C11-C12
26	N	603	CLA	C15-C16-C17-C18
26	b	606	CLA	C8-C10-C11-C12
26	n	603	CLA	C15-C16-C17-C18
30	N	2630	LHG	C29-C30-C31-C32
30	d	409	LHG	C14-C15-C16-C17
30	n	2630	LHG	C29-C30-C31-C32
26	C	513	CLA	O1A-CGA-O2A-C1
26	c	513	CLA	O1A-CGA-O2A-C1
30	C	2630	LHG	O10-C23-O8-C6
30	c	2630	LHG	O10-C23-O8-C6
37	B	2633	LMG	O10-C28-O8-C9
37	b	2633	LMG	O10-C28-O8-C9
30	N	2630	LHG	C13-C14-C15-C16
30	n	2630	LHG	C13-C14-C15-C16
26	2	613	CLA	C2A-CAA-CBA-CGA
26	G	602	CLA	C2A-CAA-CBA-CGA
26	6	613	CLA	C2A-CAA-CBA-CGA
26	g	602	CLA	C2A-CAA-CBA-CGA
39	B	626	DGD	C4D-C5D-C6D-O5D
39	b	626	DGD	C4D-C5D-C6D-O5D

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Mol	Chain	Res	Type	Atoms
30	C	2630	LHG	C4-C5-C6-O8
30	R	2630	LHG	C4-C5-C6-O8
30	Y	2630	LHG	C4-C5-C6-O8
30	c	2630	LHG	C4-C5-C6-O8
30	r	2630	LHG	C4-C5-C6-O8
30	y	2630	LHG	C4-C5-C6-O8
36	B	623	SQD	O6-C44-C45-C46
36	b	623	SQD	O6-C44-C45-C46
37	A	413	LMG	C7-C8-C9-O8
37	Z	101	LMG	O1-C7-C8-C9
37	a	413	LMG	C7-C8-C9-O8
37	z	101	LMG	O1-C7-C8-C9
39	C	519	DGD	O1G-C1G-C2G-C3G
39	c	519	DGD	O1G-C1G-C2G-C3G
30	n	2630	LHG	C34-C35-C36-C37
37	Z	101	LMG	C8-C7-O1-C1
37	z	101	LMG	C8-C7-O1-C1
30	N	2630	LHG	C14-C15-C16-C17
30	N	2630	LHG	C34-C35-C36-C37
30	S	2630	LHG	C26-C27-C28-C29
30	n	2630	LHG	C14-C15-C16-C17
30	s	2630	LHG	C26-C27-C28-C29
37	B	2633	LMG	C31-C32-C33-C34
37	a	413	LMG	C19-C20-C21-C22
37	b	2633	LMG	C31-C32-C33-C34
26	b	616	CLA	O1D-CGD-O2D-CED
25	3	609	CHL	C8-C10-C11-C12
25	Y	607	CHL	C5-C6-C7-C8
25	y	607	CHL	C5-C6-C7-C8
26	B	612	CLA	C13-C15-C16-C17
26	b	612	CLA	C13-C15-C16-C17
26	S	602	CLA	C14-C13-C15-C16
26	s	602	CLA	C14-C13-C15-C16
30	3	2630	LHG	C35-C36-C37-C38
30	7	2630	LHG	C35-C36-C37-C38
37	A	413	LMG	C19-C20-C21-C22
37	Z	101	LMG	C30-C31-C32-C33
37	z	101	LMG	C30-C31-C32-C33
26	B	616	CLA	O1D-CGD-O2D-CED
26	Y	603	CLA	O1A-CGA-O2A-C1
26	y	603	CLA	O1A-CGA-O2A-C1
30	d	409	LHG	O9-C7-O7-C5

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Mol	Chain	Res	Type	Atoms
30	3	2630	LHG	C10-C11-C12-C13
30	7	2630	LHG	C10-C11-C12-C13
39	B	626	DGD	CDB-CEB-CFB-CGB
39	b	626	DGD	C4B-C5B-C6B-C7B
39	b	626	DGD	CDB-CEB-CFB-CGB
37	B	622	LMG	C16-C17-C18-C19
37	b	622	LMG	C16-C17-C18-C19
39	B	626	DGD	C4B-C5B-C6B-C7B
39	H	102	DGD	C5B-C6B-C7B-C8B
39	h	102	DGD	C5B-C6B-C7B-C8B
26	c	511	CLA	CBD-CGD-O2D-CED
30	S	2630	LHG	O1-C1-C2-O2
30	s	2630	LHG	O1-C1-C2-O2
30	Y	2630	LHG	C18-C19-C20-C21
30	y	2630	LHG	C18-C19-C20-C21
37	A	413	LMG	C12-C13-C14-C15
37	a	413	LMG	C12-C13-C14-C15
25	7	609	CHL	C8-C10-C11-C12
26	R	613	CLA	O1A-CGA-O2A-C1
26	r	613	CLA	O1A-CGA-O2A-C1
30	5	2630	LHG	C27-C28-C29-C30
25	G	601	CHL	C8-C10-C11-C12
25	g	601	CHL	C8-C10-C11-C12
25	1	607	CHL	C4-C3-C5-C6
25	1	609	CHL	C4-C3-C5-C6
25	5	607	CHL	C4-C3-C5-C6
25	5	609	CHL	C4-C3-C5-C6
26	1	603	CLA	C4-C3-C5-C6
26	N	612	CLA	C4-C3-C5-C6
26	5	603	CLA	C4-C3-C5-C6
30	1	2630	LHG	C27-C28-C29-C30
26	R	603	CLA	C11-C12-C13-C15
26	r	603	CLA	C11-C12-C13-C15
25	3	609	CHL	CBA-CGA-O2A-C1
25	7	609	CHL	CBA-CGA-O2A-C1
26	C	511	CLA	CBD-CGD-O2D-CED
25	G	608	CHL	C13-C15-C16-C17
25	g	608	CHL	C13-C15-C16-C17
26	B	602	CLA	C5-C6-C7-C8
26	B	614	CLA	C5-C6-C7-C8
26	b	602	CLA	C5-C6-C7-C8
26	b	614	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
30	g	2630	LHG	C28-C29-C30-C31
36	A	418	SQD	C44-C45-O47-C7
36	B	621	SQD	C46-C45-O47-C7
36	a	418	SQD	C44-C45-O47-C7
36	b	621	SQD	C46-C45-O47-C7
26	r	609	CLA	O1D-CGD-O2D-CED
30	3	2630	LHG	C29-C30-C31-C32
30	D	409	LHG	C19-C20-C21-C22
30	7	2630	LHG	C29-C30-C31-C32
30	d	409	LHG	C19-C20-C21-C22
37	B	622	LMG	C22-C23-C24-C25
37	b	622	LMG	C22-C23-C24-C25
26	R	609	CLA	O1D-CGD-O2D-CED
30	B	2630	LHG	C11-C12-C13-C14
30	D	408	LHG	C16-C17-C18-C19
30	G	2630	LHG	C28-C29-C30-C31
30	b	2631	LHG	C13-C14-C15-C16
30	d	408	LHG	C16-C17-C18-C19
30	B	2631	LHG	C13-C14-C15-C16
30	b	2630	LHG	C11-C12-C13-C14
36	A	418	SQD	C32-C33-C34-C35
36	B	623	SQD	C25-C26-C27-C28
36	a	418	SQD	C32-C33-C34-C35
36	b	623	SQD	C25-C26-C27-C28
37	A	413	LMG	C33-C34-C35-C36
37	a	413	LMG	C33-C34-C35-C36
30	D	410	LHG	O6-C4-C5-O7
30	d	410	LHG	O6-C4-C5-O7
30	B	2630	LHG	C19-C20-C21-C22
30	D	409	LHG	C25-C26-C27-C28
30	b	2630	LHG	C19-C20-C21-C22
30	d	409	LHG	C25-C26-C27-C28
26	1	612	CLA	O1D-CGD-O2D-CED
26	5	612	CLA	O1D-CGD-O2D-CED
26	S	614	CLA	O1A-CGA-O2A-C1
26	s	614	CLA	O1A-CGA-O2A-C1
30	3	2630	LHG	C17-C18-C19-C20
30	L	101	LHG	C35-C36-C37-C38
30	7	2630	LHG	C17-C18-C19-C20
26	A	405	CLA	C15-C16-C17-C18
26	D	402	CLA	C13-C15-C16-C17
26	a	405	CLA	C15-C16-C17-C18

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Mol	Chain	Res	Type	Atoms
26	d	402	CLA	C13-C15-C16-C17
30	G	2630	LHG	C14-C15-C16-C17
30	S	2630	LHG	C9-C10-C11-C12
30	g	2630	LHG	C14-C15-C16-C17
30	l	101	LHG	C35-C36-C37-C38
30	s	2630	LHG	C9-C10-C11-C12
25	Y	605	CHL	O1D-CGD-O2D-CED
30	D	408	LHG	C13-C14-C15-C16
30	N	2630	LHG	C28-C29-C30-C31
30	d	408	LHG	C13-C14-C15-C16
37	B	2633	LMG	C21-C22-C23-C24
37	b	622	LMG	C33-C34-C35-C36
30	D	410	LHG	O9-C7-O7-C5
30	d	410	LHG	O9-C7-O7-C5
39	C	520	DGD	O1B-C1B-O2G-C2G
39	c	520	DGD	O1B-C1B-O2G-C2G
26	B	607	CLA	C15-C16-C17-C18
26	B	613	CLA	C13-C15-C16-C17
26	b	607	CLA	C15-C16-C17-C18
26	b	613	CLA	C13-C15-C16-C17
25	R	606	CHL	C16-C17-C18-C20
25	r	606	CHL	C16-C17-C18-C20
26	N	603	CLA	C16-C17-C18-C19
26	n	603	CLA	C16-C17-C18-C19
30	C	2630	LHG	C30-C31-C32-C33
30	c	2630	LHG	C30-C31-C32-C33
30	n	2630	LHG	C28-C29-C30-C31
37	B	622	LMG	C33-C34-C35-C36
37	b	2633	LMG	C21-C22-C23-C24
26	2	603	CLA	C4-C3-C5-C6
26	6	603	CLA	C4-C3-C5-C6
26	n	612	CLA	C4-C3-C5-C6
30	C	523	LHG	C33-C34-C35-C36
30	c	523	LHG	C33-C34-C35-C36
25	y	605	CHL	O1D-CGD-O2D-CED
25	1	607	CHL	C6-C7-C8-C10
25	3	601	CHL	C11-C10-C8-C7
25	3	601	CHL	C12-C13-C15-C16
25	G	607	CHL	C11-C10-C8-C7
25	G	607	CHL	C12-C13-C15-C16
25	G	608	CHL	C12-C13-C15-C16
25	N	601	CHL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	Y	601	CHL	C12-C13-C15-C16
25	5	607	CHL	C6-C7-C8-C10
25	7	601	CHL	C11-C10-C8-C7
25	7	601	CHL	C12-C13-C15-C16
25	g	607	CHL	C11-C10-C8-C7
25	g	607	CHL	C12-C13-C15-C16
25	g	608	CHL	C12-C13-C15-C16
25	n	601	CHL	C12-C13-C15-C16
25	y	601	CHL	C12-C13-C15-C16
26	1	602	CLA	C6-C7-C8-C10
26	2	602	CLA	C11-C12-C13-C15
26	2	603	CLA	C2-C3-C5-C6
26	B	613	CLA	C11-C10-C8-C7
26	B	616	CLA	C12-C13-C15-C16
26	C	502	CLA	C6-C7-C8-C10
26	C	505	CLA	C12-C13-C15-C16
26	C	507	CLA	C11-C10-C8-C7
26	C	507	CLA	C12-C13-C15-C16
26	C	510	CLA	C12-C13-C15-C16
26	C	511	CLA	C11-C12-C13-C15
26	C	512	CLA	C12-C13-C15-C16
26	C	513	CLA	C11-C12-C13-C15
26	G	603	CLA	C11-C10-C8-C7
26	G	610	CLA	C11-C12-C13-C15
26	G	610	CLA	C12-C13-C15-C16
26	G	612	CLA	C11-C10-C8-C7
26	G	613	CLA	C11-C12-C13-C15
26	N	602	CLA	C6-C7-C8-C10
26	N	612	CLA	C2-C3-C5-C6
26	N	612	CLA	C6-C7-C8-C10
26	R	610	CLA	C11-C10-C8-C7
26	S	602	CLA	C6-C7-C8-C10
26	Y	602	CLA	C6-C7-C8-C10
26	Y	612	CLA	C11-C10-C8-C7
26	Y	613	CLA	C12-C13-C15-C16
26	5	602	CLA	C6-C7-C8-C10
26	6	602	CLA	C11-C12-C13-C15
26	6	603	CLA	C2-C3-C5-C6
26	b	613	CLA	C11-C10-C8-C7
26	b	616	CLA	C12-C13-C15-C16
26	c	502	CLA	C6-C7-C8-C10
26	c	505	CLA	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
26	c	507	CLA	C6-C7-C8-C10
26	c	507	CLA	C11-C10-C8-C7
26	c	507	CLA	C12-C13-C15-C16
26	c	510	CLA	C12-C13-C15-C16
26	c	511	CLA	C11-C12-C13-C15
26	c	512	CLA	C12-C13-C15-C16
26	c	513	CLA	C11-C12-C13-C15
26	g	603	CLA	C11-C10-C8-C7
26	g	610	CLA	C11-C12-C13-C15
26	g	610	CLA	C12-C13-C15-C16
26	g	612	CLA	C11-C10-C8-C7
26	g	613	CLA	C11-C12-C13-C15
26	n	602	CLA	C6-C7-C8-C10
26	n	612	CLA	C2-C3-C5-C6
26	n	612	CLA	C6-C7-C8-C10
26	r	610	CLA	C11-C10-C8-C7
26	s	602	CLA	C6-C7-C8-C10
26	y	602	CLA	C6-C7-C8-C10
26	y	612	CLA	C11-C10-C8-C7
26	y	613	CLA	C12-C13-C15-C16
25	N	601	CHL	C3-C5-C6-C7
25	n	601	CHL	C3-C5-C6-C7
25	1	607	CHL	C6-C7-C8-C9
25	3	601	CHL	C11-C10-C8-C9
25	N	607	CHL	C14-C13-C15-C16
25	5	607	CHL	C6-C7-C8-C9
25	7	601	CHL	C11-C10-C8-C9
25	n	607	CHL	C14-C13-C15-C16
26	3	602	CLA	C6-C7-C8-C9
26	B	609	CLA	C14-C13-C15-C16
26	B	612	CLA	C14-C13-C15-C16
26	B	616	CLA	C14-C13-C15-C16
26	C	502	CLA	C14-C13-C15-C16
26	C	507	CLA	C14-C13-C15-C16
26	C	509	CLA	C11-C12-C13-C14
26	C	512	CLA	C14-C13-C15-C16
26	G	603	CLA	C11-C10-C8-C9
26	G	610	CLA	C11-C12-C13-C14
26	G	610	CLA	C14-C13-C15-C16
26	G	613	CLA	C11-C12-C13-C14
26	N	602	CLA	C6-C7-C8-C9
26	R	610	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
26	7	602	CLA	C6-C7-C8-C9
26	b	609	CLA	C14-C13-C15-C16
26	b	612	CLA	C14-C13-C15-C16
26	b	616	CLA	C14-C13-C15-C16
26	c	502	CLA	C14-C13-C15-C16
26	c	507	CLA	C14-C13-C15-C16
26	c	509	CLA	C11-C12-C13-C14
26	c	512	CLA	C14-C13-C15-C16
26	g	603	CLA	C11-C10-C8-C9
26	g	610	CLA	C11-C12-C13-C14
26	g	610	CLA	C14-C13-C15-C16
26	g	613	CLA	C11-C12-C13-C14
26	n	602	CLA	C6-C7-C8-C9
26	r	610	CLA	C11-C10-C8-C9
28	R	622	XAT	C29-C30-C31-C32
28	r	622	XAT	C29-C30-C31-C32
36	b	621	SQD	C11-C12-C13-C14
26	C	506	CLA	CBA-CGA-O2A-C1
26	c	506	CLA	CBA-CGA-O2A-C1
26	Y	613	CLA	C2A-CAA-CBA-CGA
26	y	613	CLA	C2A-CAA-CBA-CGA
36	B	621	SQD	C11-C12-C13-C14
25	Y	605	CHL	O1A-CGA-O2A-C1
25	y	605	CHL	O1A-CGA-O2A-C1
39	c	519	DGD	C2A-C3A-C4A-C5A
29	Y	1623	NEX	C11-C12-C13-C14
29	y	1623	NEX	C11-C12-C13-C14
39	C	519	DGD	C2A-C3A-C4A-C5A
26	B	602	CLA	C13-C15-C16-C17
26	D	402	CLA	C10-C11-C12-C13
26	b	602	CLA	C13-C15-C16-C17
26	d	402	CLA	C10-C11-C12-C13
26	G	610	CLA	C15-C16-C17-C18
26	g	610	CLA	C15-C16-C17-C18
30	D	408	LHG	C11-C12-C13-C14
39	C	518	DGD	C6A-C7A-C8A-C9A
39	c	518	DGD	C6A-C7A-C8A-C9A
26	C	501	CLA	CBA-CGA-O2A-C1
26	G	604	CLA	CBA-CGA-O2A-C1
26	c	501	CLA	CBA-CGA-O2A-C1
26	g	604	CLA	CBA-CGA-O2A-C1
30	d	408	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
37	B	622	LMG	C40-C41-C42-C43
37	b	622	LMG	C40-C41-C42-C43
25	Y	608	CHL	C13-C15-C16-C17
25	y	608	CHL	C13-C15-C16-C17
26	N	610	CLA	C5-C6-C7-C8
26	Y	602	CLA	C13-C15-C16-C17
26	c	502	CLA	C8-C10-C11-C12
26	n	610	CLA	C5-C6-C7-C8
26	y	602	CLA	C13-C15-C16-C17
30	S	2630	LHG	C35-C36-C37-C38
30	s	2630	LHG	C35-C36-C37-C38
26	C	502	CLA	C8-C10-C11-C12
30	D	409	LHG	O6-C4-C5-C6
30	d	409	LHG	O6-C4-C5-C6
30	R	2630	LHG	C14-C15-C16-C17
30	r	2630	LHG	C14-C15-C16-C17
26	C	505	CLA	C15-C16-C17-C18
26	C	510	CLA	C13-C15-C16-C17
26	c	505	CLA	C15-C16-C17-C18
26	c	510	CLA	C13-C15-C16-C17
26	B	603	CLA	C4-C3-C5-C6
26	C	507	CLA	C4-C3-C5-C6
26	b	603	CLA	C4-C3-C5-C6
25	1	607	CHL	C2-C3-C5-C6
25	1	609	CHL	C2-C3-C5-C6
25	5	607	CHL	C2-C3-C5-C6
25	5	609	CHL	C2-C3-C5-C6
26	1	603	CLA	C2-C3-C5-C6
26	5	603	CLA	C2-C3-C5-C6
39	B	626	DGD	C1A-C2A-C3A-C4A
39	b	626	DGD	C1A-C2A-C3A-C4A
30	C	522	LHG	C33-C34-C35-C36
30	C	523	LHG	C12-C13-C14-C15
30	c	522	LHG	C33-C34-C35-C36
30	c	523	LHG	C12-C13-C14-C15
37	C	521	LMG	O9-C10-O7-C8
37	c	521	LMG	O9-C10-O7-C8
25	1	609	CHL	O1A-CGA-O2A-C1
39	C	518	DGD	CCB-CDB-CEB-CFB
39	H	102	DGD	CCB-CDB-CEB-CFB
39	c	518	DGD	CCB-CDB-CEB-CFB
39	h	102	DGD	CCB-CDB-CEB-CFB

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Mol	Chain	Res	Type	Atoms
26	N	602	CLA	C16-C17-C18-C20
26	Y	610	CLA	C11-C12-C13-C14
26	n	602	CLA	C16-C17-C18-C20
26	y	610	CLA	C11-C12-C13-C14
30	Y	2630	LHG	C25-C26-C27-C28
30	Y	2630	LHG	C34-C35-C36-C37
30	y	2630	LHG	C25-C26-C27-C28
30	y	2630	LHG	C34-C35-C36-C37
26	C	505	CLA	CBA-CGA-O2A-C1
26	G	613	CLA	CBA-CGA-O2A-C1
26	c	505	CLA	CBA-CGA-O2A-C1
26	g	613	CLA	CBA-CGA-O2A-C1
25	5	609	CHL	O1A-CGA-O2A-C1
25	4	601	CHL	C3A-C2A-CAA-CBA
25	R	608	CHL	C3A-C2A-CAA-CBA
25	8	601	CHL	C3A-C2A-CAA-CBA
25	r	608	CHL	C3A-C2A-CAA-CBA
26	2	604	CLA	C3A-C2A-CAA-CBA
26	6	604	CLA	C3A-C2A-CAA-CBA
30	C	2630	LHG	C34-C35-C36-C37
30	R	2630	LHG	C13-C14-C15-C16
30	S	2630	LHG	C31-C32-C33-C34
30	c	2630	LHG	C34-C35-C36-C37
30	r	2630	LHG	C13-C14-C15-C16
36	B	621	SQD	C9-C10-C11-C12
36	b	621	SQD	C9-C10-C11-C12
27	1	1621	LUT	C29-C30-C31-C32
27	2	1621	LUT	C29-C30-C31-C32
27	N	1621	LUT	C29-C30-C31-C32
27	5	1621	LUT	C29-C30-C31-C32
27	6	1621	LUT	C29-C30-C31-C32
27	n	1621	LUT	C29-C30-C31-C32
30	s	2630	LHG	C31-C32-C33-C34
30	l	101	LHG	C26-C27-C28-C29
39	C	518	DGD	O6D-C5D-C6D-O5D
39	c	518	DGD	O6D-C5D-C6D-O5D
26	G	612	CLA	CBA-CGA-O2A-C1
26	g	612	CLA	CBA-CGA-O2A-C1
30	1	2630	LHG	C18-C19-C20-C21
30	B	2630	LHG	C31-C32-C33-C34
30	L	101	LHG	C26-C27-C28-C29
30	5	2630	LHG	C18-C19-C20-C21

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Mol	Chain	Res	Type	Atoms
30	b	2630	LHG	C31-C32-C33-C34
26	1	602	CLA	C10-C11-C12-C13
26	5	602	CLA	C10-C11-C12-C13
30	3	2630	LHG	C4-C5-C6-O8
30	B	2630	LHG	C4-C5-C6-O8
30	B	2631	LHG	C4-C5-C6-O8
30	D	410	LHG	C4-C5-C6-O8
30	G	2630	LHG	C4-C5-C6-O8
30	7	2630	LHG	C4-C5-C6-O8
30	b	2630	LHG	C4-C5-C6-O8
30	b	2631	LHG	C4-C5-C6-O8
30	d	410	LHG	C4-C5-C6-O8
30	g	2630	LHG	C4-C5-C6-O8
36	A	418	SQD	C44-C45-C46-O48
36	a	418	SQD	C44-C45-C46-O48
37	A	415	LMG	C7-C8-C9-O8
37	B	2633	LMG	C7-C8-C9-O8
37	D	411	LMG	C7-C8-C9-O8
37	a	415	LMG	C7-C8-C9-O8
37	b	2633	LMG	C7-C8-C9-O8
37	d	411	LMG	C7-C8-C9-O8
39	C	520	DGD	O1G-C1G-C2G-C3G
39	c	520	DGD	O1G-C1G-C2G-C3G
26	r	610	CLA	CBD-CGD-O2D-CED
39	C	518	DGD	C4D-C5D-C6D-O5D
25	3	609	CHL	O1A-CGA-O2A-C1
25	7	609	CHL	O1A-CGA-O2A-C1
30	R	2630	LHG	C26-C27-C28-C29
30	r	2630	LHG	C26-C27-C28-C29
25	Y	607	CHL	O2A-C1-C2-C3
25	y	607	CHL	O2A-C1-C2-C3
30	D	409	LHG	C27-C28-C29-C30
30	d	409	LHG	C27-C28-C29-C30
26	c	507	CLA	C4-C3-C5-C6
26	A	406	CLA	C16-C17-C18-C20
26	C	505	CLA	C16-C17-C18-C19
26	N	602	CLA	C16-C17-C18-C19
26	a	406	CLA	C16-C17-C18-C20
26	c	505	CLA	C16-C17-C18-C19
26	n	602	CLA	C16-C17-C18-C19
39	c	518	DGD	C4D-C5D-C6D-O5D
26	C	504	CLA	CBD-CGD-O2D-CED

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Mol	Chain	Res	Type	Atoms
26	c	504	CLA	CBD-CGD-O2D-CED
25	l	606	CHL	C3C-C2C-CMC-OMC
25	G	606	CHL	C3C-C2C-CMC-OMC
25	N	606	CHL	C3C-C2C-CMC-OMC
25	R	608	CHL	C3C-C2C-CMC-OMC
25	Y	606	CHL	C3C-C2C-CMC-OMC
25	5	606	CHL	C3C-C2C-CMC-OMC
25	g	606	CHL	C3C-C2C-CMC-OMC
25	n	606	CHL	C3C-C2C-CMC-OMC
25	r	608	CHL	C3C-C2C-CMC-OMC
25	y	606	CHL	C3C-C2C-CMC-OMC
25	y	609	CHL	O1A-CGA-O2A-C1
26	C	503	CLA	C2A-CAA-CBA-CGA
26	R	601	CLA	C2A-CAA-CBA-CGA
26	c	503	CLA	C2A-CAA-CBA-CGA
26	r	601	CLA	C2A-CAA-CBA-CGA
26	A	410	CLA	C5-C6-C7-C8
26	a	410	CLA	C5-C6-C7-C8
30	D	408	LHG	C30-C31-C32-C33
30	d	408	LHG	C30-C31-C32-C33
30	s	2630	LHG	C16-C17-C18-C19
36	B	621	SQD	C12-C13-C14-C15
36	b	621	SQD	C12-C13-C14-C15
37	c	521	LMG	C40-C41-C42-C43
37	c	521	LMG	O6-C5-C6-O5
26	Y	613	CLA	CBA-CGA-O2A-C1
26	y	613	CLA	CBA-CGA-O2A-C1
37	C	521	LMG	C40-C41-C42-C43
25	Y	609	CHL	O1A-CGA-O2A-C1
26	Y	610	CLA	C11-C12-C13-C15
26	y	610	CLA	C11-C12-C13-C15
30	B	2630	LHG	C13-C14-C15-C16
30	S	2630	LHG	C16-C17-C18-C19
30	b	2630	LHG	C13-C14-C15-C16
25	G	607	CHL	C13-C15-C16-C17
25	g	607	CHL	C13-C15-C16-C17
26	G	614	CLA	O2A-C1-C2-C3
26	R	604	CLA	O2A-C1-C2-C3
26	g	614	CLA	O2A-C1-C2-C3
26	r	604	CLA	O2A-C1-C2-C3
30	4	2630	LHG	O7-C5-C6-O8
30	C	2630	LHG	O7-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
30	G	2630	LHG	O7-C5-C6-O8
30	R	2630	LHG	O7-C5-C6-O8
30	Y	2630	LHG	O7-C5-C6-O8
30	8	2630	LHG	O7-C5-C6-O8
30	c	2630	LHG	O7-C5-C6-O8
30	g	2630	LHG	O7-C5-C6-O8
30	r	2630	LHG	O7-C5-C6-O8
30	y	2630	LHG	O7-C5-C6-O8
36	B	623	SQD	O47-C45-C46-O48
36	b	623	SQD	O47-C45-C46-O48
37	C	521	LMG	O7-C8-C9-O8
37	D	411	LMG	O7-C8-C9-O8
37	c	521	LMG	O7-C8-C9-O8
37	d	411	LMG	O7-C8-C9-O8
39	C	520	DGD	O1G-C1G-C2G-O2G
39	c	520	DGD	O1G-C1G-C2G-O2G
26	R	610	CLA	CBD-CGD-O2D-CED
26	c	505	CLA	CBD-CGD-O2D-CED
26	R	601	CLA	CBA-CGA-O2A-C1
26	r	601	CLA	CBA-CGA-O2A-C1
30	L	101	LHG	C30-C31-C32-C33
30	l	101	LHG	C30-C31-C32-C33
37	C	521	LMG	O6-C5-C6-O5
26	Y	603	CLA	C16-C17-C18-C20
26	y	603	CLA	C16-C17-C18-C20
26	C	505	CLA	CBD-CGD-O2D-CED
30	Y	2630	LHG	C1-C2-C3-O3
30	y	2630	LHG	C1-C2-C3-O3
30	2	2630	LHG	O9-C7-O7-C5
30	6	2630	LHG	O9-C7-O7-C5
25	2	609	CHL	C2-C1-O2A-CGA
25	6	609	CHL	C2-C1-O2A-CGA
26	3	610	CLA	C2-C1-O2A-CGA
26	G	603	CLA	C2-C1-O2A-CGA
26	7	610	CLA	C2-C1-O2A-CGA
26	g	603	CLA	C2-C1-O2A-CGA
25	2	607	CHL	C6-C7-C8-C9
25	6	607	CHL	C6-C7-C8-C9
26	B	606	CLA	C14-C13-C15-C16
26	B	616	CLA	C11-C12-C13-C14
26	C	506	CLA	C11-C10-C8-C9
26	G	612	CLA	C11-C10-C8-C9

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Mol	Chain	Res	Type	Atoms
26	S	602	CLA	C11-C12-C13-C14
26	Y	613	CLA	C14-C13-C15-C16
26	b	606	CLA	C14-C13-C15-C16
26	b	616	CLA	C11-C12-C13-C14
26	c	506	CLA	C11-C10-C8-C9
26	g	612	CLA	C11-C10-C8-C9
26	s	602	CLA	C11-C12-C13-C14
26	y	613	CLA	C14-C13-C15-C16
30	1	2630	LHG	C24-C25-C26-C27
30	5	2630	LHG	C24-C25-C26-C27
36	b	621	SQD	C32-C33-C34-C35
39	C	520	DGD	CBB-CCB-CDB-CEB
39	c	520	DGD	CBB-CCB-CDB-CEB
36	B	621	SQD	C32-C33-C34-C35
37	A	413	LMG	C39-C40-C41-C42
37	a	413	LMG	C39-C40-C41-C42
26	A	405	CLA	C5-C6-C7-C8
26	C	501	CLA	C10-C11-C12-C13
26	a	405	CLA	C5-C6-C7-C8
26	c	501	CLA	C10-C11-C12-C13
30	C	522	LHG	C15-C16-C17-C18
30	D	410	LHG	C32-C33-C34-C35
30	S	2630	LHG	C19-C20-C21-C22
30	c	522	LHG	C15-C16-C17-C18
30	d	410	LHG	C32-C33-C34-C35
39	H	102	DGD	C4A-C5A-C6A-C7A
39	h	102	DGD	C4A-C5A-C6A-C7A
25	S	601	CHL	C2A-CAA-CBA-CGA
25	s	601	CHL	C2A-CAA-CBA-CGA
25	N	609	CHL	C16-C17-C18-C19
25	n	609	CHL	C16-C17-C18-C19
26	B	604	CLA	C16-C17-C18-C19
26	b	604	CLA	C16-C17-C18-C19
27	1	1621	LUT	C5-C6-C7-C8
27	3	1621	LUT	C1-C6-C7-C8
27	3	1621	LUT	C5-C6-C7-C8
27	G	1620	LUT	C1-C6-C7-C8
27	G	1620	LUT	C5-C6-C7-C8
27	N	1620	LUT	C1-C6-C7-C8
27	N	1620	LUT	C5-C6-C7-C8
27	N	1621	LUT	C5-C6-C7-C8
27	S	1620	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	S	1620	LUT	C5-C6-C7-C8
27	S	1621	LUT	C1-C6-C7-C8
27	S	1621	LUT	C5-C6-C7-C8
27	5	1621	LUT	C5-C6-C7-C8
27	7	1621	LUT	C1-C6-C7-C8
27	7	1621	LUT	C5-C6-C7-C8
27	g	1620	LUT	C1-C6-C7-C8
27	g	1620	LUT	C5-C6-C7-C8
27	n	1620	LUT	C1-C6-C7-C8
27	n	1620	LUT	C5-C6-C7-C8
27	n	1621	LUT	C5-C6-C7-C8
27	s	1620	LUT	C1-C6-C7-C8
27	s	1620	LUT	C5-C6-C7-C8
27	s	1621	LUT	C1-C6-C7-C8
27	s	1621	LUT	C5-C6-C7-C8
31	4	623	BCR	C5-C6-C7-C8
31	A	411	BCR	C1-C6-C7-C8
31	C	517	BCR	C23-C24-C25-C26
31	T	101	BCR	C23-C24-C25-C30
31	8	623	BCR	C5-C6-C7-C8
31	a	411	BCR	C1-C6-C7-C8
31	c	517	BCR	C23-C24-C25-C26
31	t	101	BCR	C23-C24-C25-C30
25	1	609	CHL	C5-C6-C7-C8
25	5	609	CHL	C5-C6-C7-C8
26	1	602	CLA	C8-C10-C11-C12
26	5	602	CLA	C8-C10-C11-C12
25	3	601	CHL	C15-C16-C17-C18
25	7	601	CHL	C15-C16-C17-C18
30	s	2630	LHG	C19-C20-C21-C22
36	B	621	SQD	C25-C26-C27-C28
36	b	621	SQD	C25-C26-C27-C28
39	C	520	DGD	C2A-C3A-C4A-C5A
39	c	520	DGD	C2A-C3A-C4A-C5A
39	H	102	DGD	O2G-C1B-C2B-C3B
39	h	102	DGD	O2G-C1B-C2B-C3B
27	4	620	LUT	C27-C28-C29-C30
27	8	620	LUT	C27-C28-C29-C30
29	2	1623	NEX	C31-C32-C33-C34
29	6	1623	NEX	C31-C32-C33-C34
37	Z	101	LMG	O9-C10-O7-C8
37	z	101	LMG	O9-C10-O7-C8

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Mol	Chain	Res	Type	Atoms
30	G	2630	LHG	C8-C7-O7-C5
30	g	2630	LHG	C8-C7-O7-C5
30	N	2630	LHG	C26-C27-C28-C29
30	n	2630	LHG	C26-C27-C28-C29
37	C	521	LMG	C39-C40-C41-C42
37	c	521	LMG	C39-C40-C41-C42
30	C	2630	LHG	C27-C28-C29-C30
30	c	2630	LHG	C27-C28-C29-C30
25	N	607	CHL	C16-C17-C18-C20
25	R	607	CHL	C6-C7-C8-C10
25	n	607	CHL	C16-C17-C18-C20
25	r	607	CHL	C6-C7-C8-C10
26	A	406	CLA	C16-C17-C18-C19
26	C	511	CLA	C16-C17-C18-C20
26	a	406	CLA	C16-C17-C18-C19
25	N	609	CHL	CBD-CGD-O2D-CED
25	1	609	CHL	C14-C13-C15-C16
25	5	609	CHL	C14-C13-C15-C16
35	A	408	PHO	C13-C15-C16-C17
35	a	408	PHO	C13-C15-C16-C17
30	B	2630	LHG	C28-C29-C30-C31
30	G	2630	LHG	C12-C13-C14-C15
30	b	2630	LHG	C28-C29-C30-C31
30	g	2630	LHG	C12-C13-C14-C15
37	B	622	LMG	C30-C31-C32-C33
37	b	622	LMG	C30-C31-C32-C33
25	N	608	CHL	C10-C11-C12-C13
25	n	608	CHL	C10-C11-C12-C13
30	B	2630	LHG	O6-C4-C5-C6
30	b	2630	LHG	O6-C4-C5-C6
25	2	607	CHL	C6-C7-C8-C10
25	N	601	CHL	C11-C10-C8-C7
25	N	607	CHL	C12-C13-C15-C16
25	R	606	CHL	C6-C7-C8-C10
25	R	606	CHL	C12-C13-C15-C16
25	Y	607	CHL	C12-C13-C15-C16
25	Y	609	CHL	C12-C13-C15-C16
25	6	607	CHL	C6-C7-C8-C10
25	n	601	CHL	C11-C10-C8-C7
25	n	607	CHL	C12-C13-C15-C16
25	r	606	CHL	C6-C7-C8-C10
25	r	606	CHL	C12-C13-C15-C16

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Mol	Chain	Res	Type	Atoms
25	y	607	CHL	C12-C13-C15-C16
25	y	609	CHL	C12-C13-C15-C16
26	3	602	CLA	C6-C7-C8-C10
26	A	406	CLA	C6-C7-C8-C10
26	B	608	CLA	C12-C13-C15-C16
26	B	609	CLA	C12-C13-C15-C16
26	B	616	CLA	C11-C10-C8-C7
26	C	502	CLA	C11-C10-C8-C7
26	C	506	CLA	C6-C7-C8-C10
26	C	506	CLA	C11-C12-C13-C15
26	C	507	CLA	C6-C7-C8-C10
26	C	507	CLA	C11-C12-C13-C15
26	C	509	CLA	C6-C7-C8-C10
26	C	509	CLA	C11-C12-C13-C15
26	D	403	CLA	C11-C12-C13-C15
26	R	610	CLA	C11-C12-C13-C15
26	S	611	CLA	C6-C7-C8-C10
26	Y	603	CLA	C12-C13-C15-C16
26	7	602	CLA	C6-C7-C8-C10
26	a	406	CLA	C6-C7-C8-C10
26	b	608	CLA	C12-C13-C15-C16
26	b	609	CLA	C12-C13-C15-C16
26	b	616	CLA	C11-C10-C8-C7
26	c	502	CLA	C11-C10-C8-C7
26	c	506	CLA	C6-C7-C8-C10
26	c	506	CLA	C11-C12-C13-C15
26	c	507	CLA	C11-C12-C13-C15
26	c	509	CLA	C6-C7-C8-C10
26	c	509	CLA	C11-C12-C13-C15
26	d	403	CLA	C11-C12-C13-C15
26	r	610	CLA	C11-C12-C13-C15
26	s	611	CLA	C6-C7-C8-C10
26	y	603	CLA	C12-C13-C15-C16
26	c	505	CLA	O1D-CGD-O2D-CED
26	G	604	CLA	O1A-CGA-O2A-C1
30	D	410	LHG	C31-C32-C33-C34
30	d	410	LHG	C31-C32-C33-C34
27	3	1621	LUT	C29-C30-C31-C32
27	G	1621	LUT	C29-C30-C31-C32
27	Y	1621	LUT	C29-C30-C31-C32
27	7	1621	LUT	C29-C30-C31-C32
27	g	1621	LUT	C29-C30-C31-C32

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Mol	Chain	Res	Type	Atoms
27	y	1621	LUT	C29-C30-C31-C32
28	N	1622	XAT	C29-C30-C31-C32
28	n	1622	XAT	C29-C30-C31-C32
29	1	1623	NEX	C29-C30-C31-C32
29	5	1623	NEX	C29-C30-C31-C32
31	4	623	BCR	C19-C20-C21-C22
31	D	404	BCR	C9-C10-C11-C12
31	8	623	BCR	C19-C20-C21-C22
31	d	404	BCR	C9-C10-C11-C12
26	b	613	CLA	C16-C17-C18-C19
26	c	511	CLA	C16-C17-C18-C20
30	3	2630	LHG	O9-C7-O7-C5
30	7	2630	LHG	O9-C7-O7-C5
26	C	503	CLA	CBA-CGA-O2A-C1
37	D	411	LMG	C16-C17-C18-C19
37	d	411	LMG	C16-C17-C18-C19
26	C	505	CLA	O1D-CGD-O2D-CED
35	A	409	PHO	C5-C6-C7-C8
35	a	409	PHO	C5-C6-C7-C8
26	g	604	CLA	O1A-CGA-O2A-C1
25	n	609	CHL	CBD-CGD-O2D-CED
30	L	101	LHG	C24-C25-C26-C27
30	l	101	LHG	C24-C25-C26-C27
26	y	611	CLA	C5-C6-C7-C8
30	3	2630	LHG	C26-C27-C28-C29
30	G	2630	LHG	C9-C10-C11-C12
39	B	626	DGD	C7B-C8B-C9B-CAB
39	b	626	DGD	C7B-C8B-C9B-CAB
26	B	613	CLA	C16-C17-C18-C19
25	G	608	CHL	C10-C11-C12-C13
25	g	608	CHL	C10-C11-C12-C13
26	C	507	CLA	C15-C16-C17-C18
26	Y	611	CLA	C5-C6-C7-C8
26	B	605	CLA	CBA-CGA-O2A-C1
26	C	512	CLA	CBA-CGA-O2A-C1
26	b	605	CLA	CBA-CGA-O2A-C1
26	c	503	CLA	CBA-CGA-O2A-C1
26	c	512	CLA	CBA-CGA-O2A-C1
30	7	2630	LHG	C26-C27-C28-C29
30	g	2630	LHG	C9-C10-C11-C12
26	c	507	CLA	C15-C16-C17-C18
26	C	506	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	c	506	CLA	O1A-CGA-O2A-C1
25	1	606	CHL	CAD-CBD-CGD-O2D
25	G	609	CHL	CAD-CBD-CGD-O2D
25	R	606	CHL	CAD-CBD-CGD-O2D
25	5	606	CHL	CAD-CBD-CGD-O2D
25	g	609	CHL	CAD-CBD-CGD-O2D
25	r	606	CHL	CAD-CBD-CGD-O2D
26	1	602	CLA	CAD-CBD-CGD-O2D
26	1	610	CLA	CAD-CBD-CGD-O2D
26	3	612	CLA	CAD-CBD-CGD-O2D
26	B	611	CLA	CAD-CBD-CGD-O2D
26	C	506	CLA	CAD-CBD-CGD-O2D
26	C	508	CLA	CAD-CBD-CGD-O2D
26	G	602	CLA	CAD-CBD-CGD-O2D
26	N	603	CLA	CAD-CBD-CGD-O2D
26	N	613	CLA	CAD-CBD-CGD-O2D
26	R	603	CLA	CAD-CBD-CGD-O2D
26	Y	603	CLA	CAD-CBD-CGD-O2D
26	Y	604	CLA	CAD-CBD-CGD-O2D
26	Y	612	CLA	CAD-CBD-CGD-O2D
26	5	602	CLA	CAD-CBD-CGD-O2D
26	5	610	CLA	CAD-CBD-CGD-O2D
26	7	612	CLA	CAD-CBD-CGD-O2D
26	b	611	CLA	CAD-CBD-CGD-O2D
26	c	506	CLA	CAD-CBD-CGD-O2D
26	c	508	CLA	CAD-CBD-CGD-O2D
26	g	602	CLA	CAD-CBD-CGD-O2D
26	n	603	CLA	CAD-CBD-CGD-O2D
26	n	613	CLA	CAD-CBD-CGD-O2D
26	r	603	CLA	CAD-CBD-CGD-O2D
26	y	603	CLA	CAD-CBD-CGD-O2D
26	y	604	CLA	CAD-CBD-CGD-O2D
26	y	612	CLA	CAD-CBD-CGD-O2D
29	S	1623	NEX	C7-C8-C9-C19
29	s	1623	NEX	C7-C8-C9-C19
35	A	408	PHO	CAD-CBD-CGD-O2D
35	a	408	PHO	CAD-CBD-CGD-O2D
26	C	508	CLA	C15-C16-C17-C18
26	c	508	CLA	C15-C16-C17-C18
37	B	622	LMG	C38-C39-C40-C41
37	b	622	LMG	C38-C39-C40-C41
30	1	2630	LHG	C4-C5-C6-O8

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Mol	Chain	Res	Type	Atoms
30	5	2630	LHG	C4-C5-C6-O8
36	B	621	SQD	O6-C44-C45-C46
36	b	621	SQD	O6-C44-C45-C46
37	A	413	LMG	O1-C7-C8-C9
37	a	413	LMG	O1-C7-C8-C9
30	1	2630	LHG	C8-C7-O7-C5
30	C	522	LHG	C8-C7-O7-C5
30	5	2630	LHG	C8-C7-O7-C5
30	c	522	LHG	C8-C7-O7-C5
30	B	2630	LHG	O6-C4-C5-O7
30	C	522	LHG	O6-C4-C5-O7
30	b	2630	LHG	O6-C4-C5-O7
30	c	522	LHG	O6-C4-C5-O7
25	G	609	CHL	C8-C10-C11-C12
25	g	609	CHL	C8-C10-C11-C12
26	3	611	CLA	C5-C6-C7-C8
26	7	611	CLA	C5-C6-C7-C8
26	y	610	CLA	C10-C11-C12-C13
26	G	613	CLA	C2A-CAA-CBA-CGA
26	Y	602	CLA	C2A-CAA-CBA-CGA
26	g	613	CLA	C2A-CAA-CBA-CGA
26	y	602	CLA	C2A-CAA-CBA-CGA
26	Y	610	CLA	C10-C11-C12-C13
26	G	613	CLA	O1A-CGA-O2A-C1
26	g	613	CLA	O1A-CGA-O2A-C1
26	3	610	CLA	C11-C12-C13-C14
26	B	602	CLA	C16-C17-C18-C20
26	B	616	CLA	C16-C17-C18-C20
26	N	603	CLA	C16-C17-C18-C20
26	7	610	CLA	C11-C12-C13-C14
26	b	602	CLA	C16-C17-C18-C20
26	b	616	CLA	C16-C17-C18-C20
26	n	603	CLA	C16-C17-C18-C20
25	G	605	CHL	CHA-CBD-CGD-O1D
25	g	605	CHL	CHA-CBD-CGD-O1D
26	1	603	CLA	CHA-CBD-CGD-O2D
26	2	603	CLA	CHA-CBD-CGD-O1D
26	2	603	CLA	CHA-CBD-CGD-O2D
26	3	604	CLA	CHA-CBD-CGD-O2D
26	B	605	CLA	CHA-CBD-CGD-O1D
26	B	606	CLA	CHA-CBD-CGD-O1D
26	B	606	CLA	CHA-CBD-CGD-O2D

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Mol	Chain	Res	Type	Atoms
26	B	613	CLA	CHA-CBD-CGD-O1D
26	B	613	CLA	CHA-CBD-CGD-O2D
26	C	504	CLA	CHA-CBD-CGD-O1D
26	C	504	CLA	CHA-CBD-CGD-O2D
26	C	505	CLA	CHA-CBD-CGD-O1D
26	C	505	CLA	CHA-CBD-CGD-O2D
26	R	601	CLA	CHA-CBD-CGD-O1D
26	R	604	CLA	CHA-CBD-CGD-O1D
26	R	604	CLA	CHA-CBD-CGD-O2D
26	5	603	CLA	CHA-CBD-CGD-O2D
26	6	603	CLA	CHA-CBD-CGD-O1D
26	6	603	CLA	CHA-CBD-CGD-O2D
26	7	604	CLA	CHA-CBD-CGD-O2D
26	b	605	CLA	CHA-CBD-CGD-O1D
26	b	606	CLA	CHA-CBD-CGD-O1D
26	b	606	CLA	CHA-CBD-CGD-O2D
26	b	613	CLA	CHA-CBD-CGD-O1D
26	b	613	CLA	CHA-CBD-CGD-O2D
26	c	504	CLA	CHA-CBD-CGD-O1D
26	c	504	CLA	CHA-CBD-CGD-O2D
26	c	505	CLA	CHA-CBD-CGD-O1D
26	c	505	CLA	CHA-CBD-CGD-O2D
26	r	601	CLA	CHA-CBD-CGD-O1D
26	r	604	CLA	CHA-CBD-CGD-O1D
26	r	604	CLA	CHA-CBD-CGD-O2D
26	C	501	CLA	O1A-CGA-O2A-C1
26	C	505	CLA	O1A-CGA-O2A-C1
26	c	501	CLA	O1A-CGA-O2A-C1
26	c	505	CLA	O1A-CGA-O2A-C1
26	r	601	CLA	O1A-CGA-O2A-C1
30	c	2630	LHG	C11-C10-C9-C8
30	B	2630	LHG	C33-C34-C35-C36
30	C	2630	LHG	C11-C10-C9-C8
30	B	2630	LHG	O7-C5-C6-O8
30	D	410	LHG	O7-C5-C6-O8
30	b	2630	LHG	O7-C5-C6-O8
30	d	410	LHG	O7-C5-C6-O8
36	B	621	SQD	O47-C45-C46-O48
36	b	621	SQD	O47-C45-C46-O48
37	A	413	LMG	O1-C7-C8-O7
37	A	415	LMG	O7-C8-C9-O8
37	B	2633	LMG	O7-C8-C9-O8

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Mol	Chain	Res	Type	Atoms
37	a	413	LMG	O1-C7-C8-O7
37	a	415	LMG	O7-C8-C9-O8
37	b	2633	LMG	O7-C8-C9-O8
30	N	2630	LHG	C31-C32-C33-C34
30	b	2630	LHG	C33-C34-C35-C36
30	n	2630	LHG	C31-C32-C33-C34
26	C	501	CLA	C15-C16-C17-C18
26	c	501	CLA	C15-C16-C17-C18
26	R	601	CLA	O1A-CGA-O2A-C1
30	D	409	LHG	C12-C13-C14-C15
26	B	612	CLA	C3-C5-C6-C7
26	b	612	CLA	C3-C5-C6-C7
30	D	410	LHG	C29-C30-C31-C32
30	d	409	LHG	C12-C13-C14-C15
30	d	410	LHG	C29-C30-C31-C32
26	G	612	CLA	O1A-CGA-O2A-C1
26	g	612	CLA	O1A-CGA-O2A-C1
25	8	606	CHL	O1D-CGD-O2D-CED
25	R	606	CHL	C6-C7-C8-C9
25	r	606	CHL	C6-C7-C8-C9
26	C	502	CLA	C11-C10-C8-C9
26	N	610	CLA	C11-C12-C13-C14
26	c	502	CLA	C11-C10-C8-C9
26	n	610	CLA	C11-C12-C13-C14
25	4	606	CHL	O1D-CGD-O2D-CED
26	C	504	CLA	O1D-CGD-O2D-CED
26	c	504	CLA	O1D-CGD-O2D-CED
37	B	2633	LMG	C8-C9-O8-C28
37	b	2633	LMG	C8-C9-O8-C28
30	D	409	LHG	C33-C34-C35-C36
30	d	409	LHG	C33-C34-C35-C36
26	C	512	CLA	O1A-CGA-O2A-C1
26	c	512	CLA	O1A-CGA-O2A-C1
26	y	613	CLA	O1A-CGA-O2A-C1
26	b	605	CLA	C13-C15-C16-C17
36	B	623	SQD	C5-C6-S-O8
36	b	623	SQD	C5-C6-S-O8
26	B	605	CLA	C13-C15-C16-C17
26	D	403	CLA	C10-C11-C12-C13
37	A	413	LMG	C36-C37-C38-C39
37	a	413	LMG	C36-C37-C38-C39
26	Y	613	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
29	S	1623	NEX	C11-C12-C13-C20
29	s	1623	NEX	C11-C12-C13-C20
25	N	601	CHL	C8-C10-C11-C12
25	n	601	CHL	C8-C10-C11-C12
26	d	403	CLA	C10-C11-C12-C13
26	G	603	CLA	CBD-CGD-O2D-CED
30	C	2630	LHG	C13-C14-C15-C16
30	c	2630	LHG	C13-C14-C15-C16
25	7	609	CHL	C2C-C3C-CAC-CBC
36	b	621	SQD	C13-C14-C15-C16
25	1	607	CHL	C1A-C2A-CAA-CBA
25	1	609	CHL	C1A-C2A-CAA-CBA
25	3	609	CHL	C1A-C2A-CAA-CBA
25	4	601	CHL	C1A-C2A-CAA-CBA
25	4	601	CHL	CHA-CBD-CGD-O2D
25	N	609	CHL	C1A-C2A-CAA-CBA
25	5	607	CHL	C1A-C2A-CAA-CBA
25	5	609	CHL	C1A-C2A-CAA-CBA
25	7	609	CHL	C1A-C2A-CAA-CBA
25	8	601	CHL	C1A-C2A-CAA-CBA
25	8	601	CHL	CHA-CBD-CGD-O2D
25	n	609	CHL	C1A-C2A-CAA-CBA
26	2	602	CLA	C1A-C2A-CAA-CBA
26	2	610	CLA	C1A-C2A-CAA-CBA
26	G	604	CLA	C1A-C2A-CAA-CBA
26	S	610	CLA	C1A-C2A-CAA-CBA
26	6	602	CLA	C1A-C2A-CAA-CBA
26	6	610	CLA	C1A-C2A-CAA-CBA
26	g	604	CLA	C1A-C2A-CAA-CBA
26	s	610	CLA	C1A-C2A-CAA-CBA
35	A	409	PHO	C16-C17-C18-C20
35	a	409	PHO	C16-C17-C18-C20
26	c	505	CLA	C10-C11-C12-C13
30	L	101	LHG	C25-C26-C27-C28
30	l	101	LHG	C25-C26-C27-C28
26	g	603	CLA	CBD-CGD-O2D-CED
25	G	606	CHL	CBA-CGA-O2A-C1
25	g	606	CHL	CBA-CGA-O2A-C1
25	3	609	CHL	C2C-C3C-CAC-CBC
30	B	2631	LHG	C12-C13-C14-C15
30	b	2631	LHG	C12-C13-C14-C15
36	B	621	SQD	C13-C14-C15-C16

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Mol	Chain	Res	Type	Atoms
39	C	519	DGD	C8B-C9B-CAB-CBB
39	c	519	DGD	C8B-C9B-CAB-CBB
39	C	519	DGD	O1A-C1A-O1G-C1G
26	C	505	CLA	C10-C11-C12-C13
30	2	2630	LHG	C4-O6-P-O3
30	B	2630	LHG	C3-O3-P-O6
30	S	2630	LHG	C4-O6-P-O3
30	6	2630	LHG	C4-O6-P-O3
30	b	2630	LHG	C3-O3-P-O6
30	s	2630	LHG	C4-O6-P-O3
30	S	2630	LHG	O2-C2-C3-O3
30	s	2630	LHG	O2-C2-C3-O3
25	4	606	CHL	CBD-CGD-O2D-CED
30	Y	2630	LHG	C5-C4-O6-P
30	y	2630	LHG	C5-C4-O6-P
26	B	605	CLA	O1A-CGA-O2A-C1
26	b	605	CLA	O1A-CGA-O2A-C1
26	g	611	CLA	O1A-CGA-O2A-C1
30	1	2630	LHG	O10-C23-O8-C6
30	5	2630	LHG	O10-C23-O8-C6
39	c	519	DGD	O1A-C1A-O1G-C1G
30	3	2630	LHG	C3-O3-P-O5
30	B	2630	LHG	C4-O6-P-O5
30	D	410	LHG	C3-O3-P-O4
30	D	410	LHG	C4-O6-P-O5
30	G	2630	LHG	C4-O6-P-O4
30	N	2630	LHG	C3-O3-P-O5
30	Y	2630	LHG	C4-O6-P-O4
30	7	2630	LHG	C3-O3-P-O5
30	b	2630	LHG	C4-O6-P-O5
30	d	410	LHG	C3-O3-P-O4
30	d	410	LHG	C4-O6-P-O5
30	g	2630	LHG	C4-O6-P-O4
30	n	2630	LHG	C3-O3-P-O5
30	y	2630	LHG	C4-O6-P-O4
39	h	102	DGD	C8A-C9A-CAA-CBA
37	B	622	LMG	O6-C1-O1-C7
37	b	622	LMG	O6-C1-O1-C7
25	R	607	CHL	C5-C6-C7-C8
25	8	606	CHL	CBD-CGD-O2D-CED
30	C	522	LHG	O6-C4-C5-C6
30	C	523	LHG	O6-C4-C5-C6

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Mol	Chain	Res	Type	Atoms
30	c	522	LHG	O6-C4-C5-C6
30	c	523	LHG	O6-C4-C5-C6
30	D	410	LHG	C28-C29-C30-C31
37	C	521	LMG	C14-C15-C16-C17
37	c	521	LMG	C14-C15-C16-C17
39	H	102	DGD	C8A-C9A-CAA-CBA
39	h	102	DGD	CDA-CEA-CFA-CGA
26	G	611	CLA	O1A-CGA-O2A-C1
39	H	102	DGD	CDA-CEA-CFA-CGA
25	r	607	CHL	C5-C6-C7-C8
26	c	511	CLA	O1D-CGD-O2D-CED
30	d	410	LHG	C28-C29-C30-C31
39	c	519	DGD	CBA-CCA-CDA-CEA
26	N	610	CLA	C16-C17-C18-C19
26	n	610	CLA	C16-C17-C18-C19
39	C	519	DGD	CBA-CCA-CDA-CEA
39	C	520	DGD	C3B-C4B-C5B-C6B
26	1	603	CLA	CAD-CBD-CGD-O1D
26	2	603	CLA	CAD-CBD-CGD-O1D
26	3	603	CLA	CAD-CBD-CGD-O1D
26	3	604	CLA	CAD-CBD-CGD-O1D
26	3	614	CLA	CAD-CBD-CGD-O1D
26	B	602	CLA	CAD-CBD-CGD-O1D
26	B	605	CLA	CAD-CBD-CGD-O1D
26	B	606	CLA	CAD-CBD-CGD-O1D
26	C	504	CLA	CAD-CBD-CGD-O1D
26	C	513	CLA	CAD-CBD-CGD-O1D
26	5	603	CLA	CAD-CBD-CGD-O1D
26	6	603	CLA	CAD-CBD-CGD-O1D
26	7	603	CLA	CAD-CBD-CGD-O1D
26	7	604	CLA	CAD-CBD-CGD-O1D
26	7	614	CLA	CAD-CBD-CGD-O1D
26	b	602	CLA	CAD-CBD-CGD-O1D
26	b	605	CLA	CAD-CBD-CGD-O1D
26	b	606	CLA	CAD-CBD-CGD-O1D
26	c	504	CLA	CAD-CBD-CGD-O1D
26	c	513	CLA	CAD-CBD-CGD-O1D
26	B	612	CLA	C15-C16-C17-C18
26	b	612	CLA	C15-C16-C17-C18
39	c	520	DGD	C3B-C4B-C5B-C6B
26	C	503	CLA	O1A-CGA-O2A-C1
26	c	503	CLA	O1A-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
25	R	606	CHL	C5-C6-C7-C8
25	r	606	CHL	C5-C6-C7-C8
26	R	602	CLA	CBA-CGA-O2A-C1
26	r	602	CLA	CBA-CGA-O2A-C1
30	D	409	LHG	C24-C23-O8-C6
30	d	409	LHG	C24-C23-O8-C6
26	C	511	CLA	O1D-CGD-O2D-CED
30	D	410	LHG	C1-C2-C3-O3
30	d	410	LHG	C1-C2-C3-O3
39	C	518	DGD	C5A-C6A-C7A-C8A
39	c	518	DGD	C5A-C6A-C7A-C8A
26	C	511	CLA	C16-C17-C18-C19
26	c	511	CLA	C16-C17-C18-C19
25	l	607	CHL	C11-C10-C8-C7
25	G	601	CHL	C12-C13-C15-C16
25	G	608	CHL	C11-C12-C13-C15
25	Y	608	CHL	C6-C7-C8-C10
25	Y	608	CHL	C11-C10-C8-C7
25	5	607	CHL	C11-C10-C8-C7
25	g	601	CHL	C12-C13-C15-C16
25	g	608	CHL	C11-C12-C13-C15
25	y	608	CHL	C6-C7-C8-C10
25	y	608	CHL	C11-C10-C8-C7
26	B	615	CLA	C6-C7-C8-C10
26	B	616	CLA	C11-C12-C13-C15
26	B	617	CLA	C6-C7-C8-C10
26	C	504	CLA	C12-C13-C15-C16
26	C	509	CLA	C11-C10-C8-C7
26	C	510	CLA	C11-C10-C8-C7
26	G	613	CLA	C12-C13-C15-C16
26	N	603	CLA	C12-C13-C15-C16
26	6	602	CLA	C2-C3-C5-C6
26	b	614	CLA	C11-C12-C13-C15
26	b	615	CLA	C6-C7-C8-C10
26	b	616	CLA	C11-C12-C13-C15
26	b	617	CLA	C6-C7-C8-C10
26	c	504	CLA	C12-C13-C15-C16
26	c	509	CLA	C11-C10-C8-C7
26	c	510	CLA	C11-C10-C8-C7
26	g	613	CLA	C12-C13-C15-C16
26	n	603	CLA	C12-C13-C15-C16
30	C	2630	LHG	C7-C8-C9-C10

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Mol	Chain	Res	Type	Atoms
30	C	523	LHG	O6-C4-C5-O7
30	D	409	LHG	O6-C4-C5-O7
30	c	2630	LHG	C7-C8-C9-C10
30	c	523	LHG	O6-C4-C5-O7
30	d	409	LHG	O6-C4-C5-O7
25	R	608	CHL	C5-C6-C7-C8
26	C	506	CLA	C10-C11-C12-C13
26	C	508	CLA	C10-C11-C12-C13
26	c	506	CLA	C10-C11-C12-C13
26	c	508	CLA	C10-C11-C12-C13
30	C	523	LHG	C11-C10-C9-C8
30	c	523	LHG	C11-C10-C9-C8
30	d	409	LHG	C16-C17-C18-C19
26	C	504	CLA	O1A-CGA-O2A-C1
26	c	504	CLA	O1A-CGA-O2A-C1
25	1	607	CHL	C4C-C3C-CAC-CBC
25	5	607	CHL	C4C-C3C-CAC-CBC
25	5	609	CHL	C4C-C3C-CAC-CBC
30	D	409	LHG	C16-C17-C18-C19
25	r	608	CHL	C5-C6-C7-C8
26	C	503	CLA	C10-C11-C12-C13
26	c	503	CLA	C10-C11-C12-C13
26	2	602	CLA	C2A-CAA-CBA-CGA
26	C	506	CLA	C2A-CAA-CBA-CGA
26	N	602	CLA	C2A-CAA-CBA-CGA
26	N	603	CLA	C2A-CAA-CBA-CGA
26	6	602	CLA	C2A-CAA-CBA-CGA
26	c	506	CLA	C2A-CAA-CBA-CGA
26	n	602	CLA	C2A-CAA-CBA-CGA
26	n	603	CLA	C2A-CAA-CBA-CGA
39	B	626	DGD	C1B-C2B-C3B-C4B
39	b	626	DGD	C1B-C2B-C3B-C4B
26	G	611	CLA	C5-C6-C7-C8
25	2	605	CHL	C1C-C2C-CMC-OMC
25	2	608	CHL	C1C-C2C-CMC-OMC
25	R	608	CHL	C1C-C2C-CMC-OMC
25	S	607	CHL	C1C-C2C-CMC-OMC
25	Y	608	CHL	C1C-C2C-CMC-OMC
25	6	605	CHL	C1C-C2C-CMC-OMC
25	6	608	CHL	C1C-C2C-CMC-OMC
25	r	608	CHL	C1C-C2C-CMC-OMC
25	s	607	CHL	C1C-C2C-CMC-OMC

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Mol	Chain	Res	Type	Atoms
25	y	608	CHL	C1C-C2C-CMC-OMC
36	B	621	SQD	C44-C45-C46-O48
36	B	623	SQD	C44-C45-C46-O48
36	b	621	SQD	C44-C45-C46-O48
36	b	623	SQD	C44-C45-C46-O48
37	C	521	LMG	C7-C8-C9-O8
37	c	521	LMG	C7-C8-C9-O8
36	A	418	SQD	O47-C45-C46-O48
36	B	621	SQD	O6-C44-C45-O47
36	a	418	SQD	O47-C45-C46-O48
36	b	621	SQD	O6-C44-C45-O47
37	A	413	LMG	O7-C8-C9-O8
37	Z	101	LMG	O1-C7-C8-O7
37	a	413	LMG	O7-C8-C9-O8
37	z	101	LMG	O1-C7-C8-O7
25	1	609	CHL	C4C-C3C-CAC-CBC
25	G	606	CHL	O1A-CGA-O2A-C1
25	g	606	CHL	O1A-CGA-O2A-C1
39	C	519	DGD	C5D-C6D-O5D-C1E
39	c	519	DGD	C5D-C6D-O5D-C1E
26	R	610	CLA	O1D-CGD-O2D-CED
26	r	610	CLA	O1D-CGD-O2D-CED
26	Y	603	CLA	C16-C17-C18-C19
26	y	603	CLA	C16-C17-C18-C19
26	g	611	CLA	C5-C6-C7-C8
30	D	409	LHG	C28-C29-C30-C31
30	d	409	LHG	C28-C29-C30-C31
30	G	2630	LHG	C5-C4-O6-P
30	g	2630	LHG	C5-C4-O6-P
37	A	413	LMG	O10-C28-O8-C9
37	a	413	LMG	O10-C28-O8-C9
26	Y	610	CLA	C8-C10-C11-C12
26	Y	612	CLA	C4-C3-C5-C6
26	y	612	CLA	C4-C3-C5-C6
26	G	611	CLA	CBA-CGA-O2A-C1
26	g	611	CLA	CBA-CGA-O2A-C1
30	B	2630	LHG	C17-C18-C19-C20
30	L	101	LHG	C28-C29-C30-C31
30	b	2630	LHG	C17-C18-C19-C20
30	l	101	LHG	C28-C29-C30-C31
37	b	622	LMG	C39-C40-C41-C42
26	2	602	CLA	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
35	A	409	PHO	CAA-CBA-CGA-O2A
35	a	409	PHO	CAA-CBA-CGA-O2A
37	B	622	LMG	C39-C40-C41-C42
39	h	102	DGD	CBB-CCB-CDB-CEB
26	y	610	CLA	C8-C10-C11-C12
25	G	601	CHL	C6-C7-C8-C9
25	G	607	CHL	C11-C10-C8-C9
25	N	601	CHL	C14-C13-C15-C16
25	R	606	CHL	C14-C13-C15-C16
25	Y	601	CHL	C14-C13-C15-C16
25	Y	607	CHL	C14-C13-C15-C16
25	g	601	CHL	C6-C7-C8-C9
25	g	607	CHL	C11-C10-C8-C9
25	n	601	CHL	C14-C13-C15-C16
25	r	606	CHL	C14-C13-C15-C16
25	y	601	CHL	C14-C13-C15-C16
25	y	607	CHL	C14-C13-C15-C16
26	A	406	CLA	C6-C7-C8-C9
26	B	608	CLA	C14-C13-C15-C16
26	B	613	CLA	C11-C10-C8-C9
26	B	617	CLA	C14-C13-C15-C16
26	C	506	CLA	C6-C7-C8-C9
26	S	611	CLA	C6-C7-C8-C9
26	Y	603	CLA	C14-C13-C15-C16
26	a	406	CLA	C6-C7-C8-C9
26	b	608	CLA	C14-C13-C15-C16
26	b	613	CLA	C11-C10-C8-C9
26	b	617	CLA	C14-C13-C15-C16
26	c	506	CLA	C6-C7-C8-C9
26	s	611	CLA	C6-C7-C8-C9
26	y	603	CLA	C14-C13-C15-C16
39	H	102	DGD	CBB-CCB-CDB-CEB
36	A	412	SQD	C17-C18-C19-C20
36	a	412	SQD	C17-C18-C19-C20
30	D	408	LHG	O1-C1-C2-O2
30	d	408	LHG	O1-C1-C2-O2
30	G	2630	LHG	C34-C35-C36-C37
25	N	609	CHL	O1D-CGD-O2D-CED
30	g	2630	LHG	C34-C35-C36-C37
31	4	623	BCR	C36-C18-C19-C20
31	C	515	BCR	C36-C18-C19-C20
31	8	623	BCR	C36-C18-C19-C20

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Mol	Chain	Res	Type	Atoms
31	c	515	BCR	C36-C18-C19-C20
26	3	610	CLA	C11-C12-C13-C15
26	7	610	CLA	C11-C12-C13-C15
30	R	2630	LHG	C15-C16-C17-C18
30	r	2630	LHG	C15-C16-C17-C18
37	A	415	LMG	C29-C30-C31-C32
37	a	415	LMG	C29-C30-C31-C32
26	8	610	CLA	O1D-CGD-O2D-CED
26	g	603	CLA	O1D-CGD-O2D-CED
26	C	509	CLA	C8-C10-C11-C12
26	N	610	CLA	C13-C15-C16-C17
26	c	509	CLA	C8-C10-C11-C12
26	n	610	CLA	C13-C15-C16-C17
30	G	2630	LHG	C30-C31-C32-C33
39	c	520	DGD	C9B-CAB-CBB-CCB
30	C	522	LHG	C29-C30-C31-C32
30	g	2630	LHG	C30-C31-C32-C33
39	C	520	DGD	C9B-CAB-CBB-CCB
25	G	607	CHL	C4-C3-C5-C6
25	g	607	CHL	C4-C3-C5-C6
30	c	522	LHG	C29-C30-C31-C32
30	l	101	LHG	C31-C32-C33-C34
25	n	609	CHL	O1D-CGD-O2D-CED
26	4	610	CLA	O1D-CGD-O2D-CED
30	L	101	LHG	C31-C32-C33-C34
30	N	2630	LHG	C11-C12-C13-C14
30	n	2630	LHG	C11-C12-C13-C14
39	H	102	DGD	C2A-C3A-C4A-C5A
39	h	102	DGD	C2A-C3A-C4A-C5A
25	G	606	CHL	C1-C2-C3-C4
25	N	606	CHL	C1-C2-C3-C4
25	Y	606	CHL	C1-C2-C3-C4
25	g	606	CHL	C1-C2-C3-C4
25	n	606	CHL	C1-C2-C3-C4
25	y	606	CHL	C1-C2-C3-C4
26	R	601	CLA	C1-C2-C3-C4
26	R	611	CLA	C1-C2-C3-C4
26	R	612	CLA	C1-C2-C3-C4
26	S	612	CLA	C1-C2-C3-C4
26	r	601	CLA	C1-C2-C3-C4
26	r	611	CLA	C1-C2-C3-C4
26	r	612	CLA	C1-C2-C3-C4

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Mol	Chain	Res	Type	Atoms
26	s	612	CLA	C1-C2-C3-C4
26	R	602	CLA	O1A-CGA-O2A-C1
26	r	602	CLA	O1A-CGA-O2A-C1
26	G	603	CLA	O1D-CGD-O2D-CED
35	A	408	PHO	C10-C11-C12-C13
35	a	408	PHO	C10-C11-C12-C13
30	R	2630	LHG	C1-C2-C3-O3
30	r	2630	LHG	C1-C2-C3-O3
26	1	603	CLA	C2A-CAA-CBA-CGA
26	4	612	CLA	C2A-CAA-CBA-CGA
26	C	513	CLA	C2A-CAA-CBA-CGA
26	N	613	CLA	C2A-CAA-CBA-CGA
26	R	602	CLA	C2A-CAA-CBA-CGA
26	Y	610	CLA	C2A-CAA-CBA-CGA
26	5	603	CLA	C2A-CAA-CBA-CGA
26	8	612	CLA	C2A-CAA-CBA-CGA
26	c	513	CLA	C2A-CAA-CBA-CGA
26	n	613	CLA	C2A-CAA-CBA-CGA
26	r	602	CLA	C2A-CAA-CBA-CGA
26	y	610	CLA	C2A-CAA-CBA-CGA
25	1	609	CHL	C2-C1-O2A-CGA
25	G	606	CHL	C2-C1-O2A-CGA
25	Y	606	CHL	C2-C1-O2A-CGA
25	Y	609	CHL	C2-C1-O2A-CGA
25	5	609	CHL	C2-C1-O2A-CGA
25	g	606	CHL	C2-C1-O2A-CGA
25	y	606	CHL	C2-C1-O2A-CGA
25	y	609	CHL	C2-C1-O2A-CGA
26	S	602	CLA	C2-C1-O2A-CGA
26	Y	603	CLA	C2-C1-O2A-CGA
26	s	602	CLA	C2-C1-O2A-CGA
26	y	603	CLA	C2-C1-O2A-CGA
36	a	418	SQD	C13-C14-C15-C16
36	A	418	SQD	C13-C14-C15-C16
30	d	408	LHG	C10-C11-C12-C13
30	2	2630	LHG	C5-C4-O6-P
30	6	2630	LHG	C5-C4-O6-P
30	D	408	LHG	C10-C11-C12-C13
26	1	604	CLA	CBA-CGA-O2A-C1
26	3	611	CLA	CBA-CGA-O2A-C1
26	5	604	CLA	CBA-CGA-O2A-C1
26	7	611	CLA	CBA-CGA-O2A-C1

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Mol	Chain	Res	Type	Atoms
26	B	608	CLA	C16-C17-C18-C20
26	b	608	CLA	C16-C17-C18-C20
26	Y	612	CLA	C8-C10-C11-C12
26	y	612	CLA	C8-C10-C11-C12
26	C	501	CLA	C4-C3-C5-C6
26	c	501	CLA	C4-C3-C5-C6
27	1	1621	LUT	C1-C6-C7-C8
27	2	1621	LUT	C1-C6-C7-C8
27	G	1621	LUT	C5-C6-C7-C8
27	N	1621	LUT	C1-C6-C7-C8
27	5	1621	LUT	C1-C6-C7-C8
27	6	1621	LUT	C1-C6-C7-C8
27	g	1621	LUT	C5-C6-C7-C8
27	n	1621	LUT	C1-C6-C7-C8
31	4	623	BCR	C1-C6-C7-C8
31	C	514	BCR	C23-C24-C25-C26
31	C	517	BCR	C23-C24-C25-C30
31	8	623	BCR	C1-C6-C7-C8
31	c	514	BCR	C23-C24-C25-C26
31	c	517	BCR	C23-C24-C25-C30
30	r	2630	LHG	O9-C7-O7-C5
30	G	2630	LHG	C26-C27-C28-C29
26	C	504	CLA	CBA-CGA-O2A-C1
26	c	504	CLA	CBA-CGA-O2A-C1
37	a	415	LMG	C29-C28-O8-C9
26	A	405	CLA	C4C-C3C-CAC-CBC
26	a	405	CLA	C4C-C3C-CAC-CBC
36	a	418	SQD	C18-C19-C20-C21
37	a	413	LMG	C15-C16-C17-C18
30	g	2630	LHG	C26-C27-C28-C29
36	A	418	SQD	C18-C19-C20-C21
37	A	413	LMG	C15-C16-C17-C18
26	B	607	CLA	C16-C17-C18-C20
26	B	613	CLA	C16-C17-C18-C20
26	b	607	CLA	C16-C17-C18-C20
26	b	613	CLA	C16-C17-C18-C20
39	C	519	DGD	C1B-C2B-C3B-C4B
30	Y	2630	LHG	C9-C10-C11-C12
37	A	415	LMG	C33-C34-C35-C36
37	a	415	LMG	C33-C34-C35-C36
37	A	415	LMG	C29-C28-O8-C9
30	2	2630	LHG	C3-O3-P-O6

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Mol	Chain	Res	Type	Atoms
30	B	2631	LHG	C4-O6-P-O3
30	C	523	LHG	C3-O3-P-O6
30	D	409	LHG	C3-O3-P-O6
30	D	410	LHG	C3-O3-P-O6
30	R	2630	LHG	C3-O3-P-O6
30	6	2630	LHG	C3-O3-P-O6
30	b	2631	LHG	C4-O6-P-O3
30	c	523	LHG	C3-O3-P-O6
30	d	409	LHG	C3-O3-P-O6
30	d	410	LHG	C3-O3-P-O6
30	r	2630	LHG	C3-O3-P-O6
39	c	519	DGD	C1B-C2B-C3B-C4B
30	y	2630	LHG	C9-C10-C11-C12
37	D	411	LMG	C31-C32-C33-C34
37	d	411	LMG	C31-C32-C33-C34
25	G	608	CHL	C8-C10-C11-C12
25	g	608	CHL	C8-C10-C11-C12
35	A	409	PHO	CHA-CBD-CGD-O2D
35	a	409	PHO	CHA-CBD-CGD-O2D
25	1	605	CHL	O1D-CGD-O2D-CED
25	1	607	CHL	O1D-CGD-O2D-CED
30	N	2630	LHG	C35-C36-C37-C38
30	d	410	LHG	C12-C13-C14-C15
30	n	2630	LHG	C35-C36-C37-C38
25	5	607	CHL	O1D-CGD-O2D-CED
30	S	2630	LHG	C4-C5-C6-O8
30	s	2630	LHG	C4-C5-C6-O8
30	D	410	LHG	C12-C13-C14-C15
25	N	601	CHL	C6-C7-C8-C10
25	n	601	CHL	C6-C7-C8-C10
26	B	614	CLA	C11-C12-C13-C15
26	C	502	CLA	C11-C12-C13-C15
26	C	506	CLA	C12-C13-C15-C16
26	N	610	CLA	C11-C12-C13-C15
26	S	602	CLA	C11-C12-C13-C15
26	c	506	CLA	C12-C13-C15-C16
26	n	610	CLA	C11-C12-C13-C15
26	s	602	CLA	C11-C12-C13-C15
35	A	408	PHO	C12-C13-C15-C16
35	a	408	PHO	C12-C13-C15-C16
38	D	405	PL9	C18-C19-C21-C22
38	D	405	PL9	C28-C29-C31-C32

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Mol	Chain	Res	Type	Atoms
38	d	405	PL9	C28-C29-C31-C32
37	A	413	LMG	C17-C18-C19-C20
37	a	413	LMG	C17-C18-C19-C20
39	b	626	DGD	C9B-CAB-CBB-CCB
25	Y	608	CHL	C6-C7-C8-C9
25	y	608	CHL	C6-C7-C8-C9
26	2	602	CLA	C11-C12-C13-C14
26	B	617	CLA	C6-C7-C8-C9
26	C	510	CLA	C11-C10-C8-C9
26	D	403	CLA	C11-C12-C13-C14
26	N	603	CLA	C14-C13-C15-C16
26	6	602	CLA	C11-C12-C13-C14
26	b	617	CLA	C6-C7-C8-C9
26	c	510	CLA	C11-C10-C8-C9
26	d	403	CLA	C11-C12-C13-C14
26	n	603	CLA	C14-C13-C15-C16
25	4	607	CHL	O1D-CGD-O2D-CED
25	5	605	CHL	O1D-CGD-O2D-CED
29	Y	1623	NEX	C33-C34-C35-C15
29	y	1623	NEX	C33-C34-C35-C15
26	B	602	CLA	C16-C17-C18-C19
26	b	602	CLA	C16-C17-C18-C19
37	B	2633	LMG	C35-C36-C37-C38
30	R	2630	LHG	O9-C7-O7-C5
26	R	613	CLA	C5-C6-C7-C8
26	r	613	CLA	C5-C6-C7-C8
37	b	2633	LMG	C35-C36-C37-C38
39	B	626	DGD	C9B-CAB-CBB-CCB
39	h	102	DGD	CAA-CBA-CCA-CDA
30	B	2631	LHG	C35-C36-C37-C38
30	b	2631	LHG	C35-C36-C37-C38
39	H	102	DGD	CAA-CBA-CCA-CDA
26	1	604	CLA	O1A-CGA-O2A-C1
26	5	604	CLA	O1A-CGA-O2A-C1
27	4	620	LUT	C7-C8-C9-C19
29	3	1623	NEX	C11-C12-C13-C20
29	7	1623	NEX	C11-C12-C13-C20
31	A	411	BCR	C7-C8-C9-C34
31	a	411	BCR	C7-C8-C9-C34
26	r	610	CLA	C10-C11-C12-C13
26	B	616	CLA	C16-C17-C18-C19
26	N	610	CLA	C16-C17-C18-C20

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Mol	Chain	Res	Type	Atoms
26	b	603	CLA	C16-C17-C18-C19
26	b	616	CLA	C16-C17-C18-C19
26	n	610	CLA	C16-C17-C18-C20
30	B	2630	LHG	O1-C1-C2-C3
30	b	2630	LHG	O1-C1-C2-C3
30	3	2630	LHG	C5-C4-O6-P
30	7	2630	LHG	C5-C4-O6-P
26	1	610	CLA	C5-C6-C7-C8
26	R	610	CLA	C10-C11-C12-C13
26	5	610	CLA	C5-C6-C7-C8
25	8	607	CHL	O1D-CGD-O2D-CED
39	c	518	DGD	C3B-C4B-C5B-C6B
37	Z	101	LMG	C29-C30-C31-C32
39	C	518	DGD	C3B-C4B-C5B-C6B
25	1	609	CHL	C12-C13-C15-C16
25	5	609	CHL	C12-C13-C15-C16
26	1	610	CLA	C11-C10-C8-C7
26	R	612	CLA	O2A-C1-C2-C3
26	5	610	CLA	C11-C10-C8-C7
26	r	612	CLA	O2A-C1-C2-C3
26	C	507	CLA	C5-C6-C7-C8
26	D	403	CLA	C5-C6-C7-C8
26	c	507	CLA	C5-C6-C7-C8
26	d	403	CLA	C5-C6-C7-C8
37	z	101	LMG	C29-C30-C31-C32
39	C	518	DGD	C5B-C6B-C7B-C8B
39	c	518	DGD	C5B-C6B-C7B-C8B
25	S	607	CHL	C4-C3-C5-C6
25	s	607	CHL	C4-C3-C5-C6
26	B	610	CLA	C4-C3-C5-C6
26	b	610	CLA	C4-C3-C5-C6
30	R	2630	LHG	O10-C23-O8-C6
30	4	2630	LHG	O1-C1-C2-O2
30	8	2630	LHG	O1-C1-C2-O2
25	G	607	CHL	C2-C3-C5-C6
25	g	607	CHL	C2-C3-C5-C6
26	B	610	CLA	C2-C3-C5-C6
26	C	507	CLA	C2-C3-C5-C6
26	b	610	CLA	C2-C3-C5-C6
26	c	507	CLA	C2-C3-C5-C6
38	d	405	PL9	C18-C19-C21-C22
30	D	409	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
30	C	523	LHG	C24-C23-O8-C6
30	c	523	LHG	C24-C23-O8-C6
30	r	2630	LHG	O10-C23-O8-C6
30	d	409	LHG	C11-C12-C13-C14
30	D	409	LHG	C29-C30-C31-C32
30	d	409	LHG	C29-C30-C31-C32
36	A	418	SQD	C24-C25-C26-C27
37	B	2633	LMG	C34-C35-C36-C37
37	b	2633	LMG	C34-C35-C36-C37
36	a	418	SQD	C24-C25-C26-C27
39	C	520	DGD	C6A-C7A-C8A-C9A
39	c	520	DGD	C6A-C7A-C8A-C9A
26	r	609	CLA	C8-C10-C11-C12
26	S	614	CLA	C2A-CAA-CBA-CGA
26	s	614	CLA	C2A-CAA-CBA-CGA
26	B	603	CLA	C16-C17-C18-C19
39	c	518	DGD	O6E-C1E-O5D-C6D
29	1	1623	NEX	C33-C34-C35-C15
29	N	1623	NEX	C33-C34-C35-C15
29	5	1623	NEX	C33-C34-C35-C15
29	n	1623	NEX	C33-C34-C35-C15
39	c	519	DGD	C7A-C8A-C9A-CAA
25	R	606	CHL	C13-C15-C16-C17
25	r	606	CHL	C13-C15-C16-C17
26	C	512	CLA	C10-C11-C12-C13
26	R	603	CLA	C5-C6-C7-C8
26	R	609	CLA	C8-C10-C11-C12
26	Y	602	CLA	C15-C16-C17-C18
26	r	603	CLA	C5-C6-C7-C8
26	y	602	CLA	C15-C16-C17-C18
39	C	519	DGD	C7A-C8A-C9A-CAA
26	7	611	CLA	O1A-CGA-O2A-C1
26	c	512	CLA	C10-C11-C12-C13
26	3	602	CLA	C4-C3-C5-C6
26	Y	611	CLA	C4-C3-C5-C6
26	7	602	CLA	C4-C3-C5-C6
26	y	611	CLA	C4-C3-C5-C6
26	3	611	CLA	O1A-CGA-O2A-C1
26	G	602	CLA	C15-C16-C17-C18
26	g	602	CLA	C15-C16-C17-C18
26	G	610	CLA	C16-C17-C18-C19
26	g	610	CLA	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
26	B	602	CLA	CAA-CBA-CGA-O2A
26	b	602	CLA	CAA-CBA-CGA-O2A
26	B	603	CLA	C2-C1-O2A-CGA
26	B	609	CLA	C2-C1-O2A-CGA
26	b	603	CLA	C2-C1-O2A-CGA
26	b	609	CLA	C2-C1-O2A-CGA
30	G	2630	LHG	C11-C12-C13-C14
30	g	2630	LHG	C11-C12-C13-C14
26	l	613	CLA	C2A-CAA-CBA-CGA
26	R	613	CLA	C2A-CAA-CBA-CGA
26	5	613	CLA	C2A-CAA-CBA-CGA
26	r	613	CLA	C2A-CAA-CBA-CGA
26	N	604	CLA	CBA-CGA-O2A-C1
26	n	604	CLA	CBA-CGA-O2A-C1
26	y	611	CLA	C8-C10-C11-C12
30	c	523	LHG	C30-C31-C32-C33
30	C	523	LHG	C30-C31-C32-C33
26	B	610	CLA	C3A-C2A-CAA-CBA
26	C	513	CLA	C3A-C2A-CAA-CBA
26	S	604	CLA	C3A-C2A-CAA-CBA
26	b	610	CLA	C3A-C2A-CAA-CBA
26	c	513	CLA	C3A-C2A-CAA-CBA
26	s	604	CLA	C3A-C2A-CAA-CBA
30	C	2630	LHG	C19-C20-C21-C22
26	S	612	CLA	O2A-C1-C2-C3
26	s	612	CLA	O2A-C1-C2-C3
30	c	2630	LHG	C19-C20-C21-C22
37	Z	101	LMG	C11-C12-C13-C14
37	z	101	LMG	C11-C12-C13-C14
31	C	515	BCR	C19-C20-C21-C22
31	c	515	BCR	C19-C20-C21-C22
26	B	606	CLA	CBA-CGA-O2A-C1
26	b	606	CLA	CBA-CGA-O2A-C1
25	G	601	CHL	C14-C13-C15-C16
25	G	607	CHL	C11-C12-C13-C14
25	Y	607	CHL	C11-C12-C13-C14
25	Y	608	CHL	C11-C10-C8-C9
25	g	601	CHL	C14-C13-C15-C16
25	g	607	CHL	C11-C12-C13-C14
25	y	607	CHL	C11-C12-C13-C14
25	y	608	CHL	C11-C10-C8-C9
26	B	602	CLA	C6-C7-C8-C9

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Mol	Chain	Res	Type	Atoms
26	B	603	CLA	C6-C7-C8-C9
26	B	617	CLA	C11-C10-C8-C9
26	G	611	CLA	C6-C7-C8-C9
26	R	610	CLA	C6-C7-C8-C9
26	Y	603	CLA	C6-C7-C8-C9
26	b	602	CLA	C6-C7-C8-C9
26	b	603	CLA	C6-C7-C8-C9
26	b	617	CLA	C11-C10-C8-C9
26	g	611	CLA	C6-C7-C8-C9
26	r	610	CLA	C6-C7-C8-C9
26	y	603	CLA	C6-C7-C8-C9
39	C	518	DGD	CAB-CBB-CCB-CDB
26	Y	611	CLA	C8-C10-C11-C12
30	N	2630	LHG	C24-C23-O8-C6
39	c	518	DGD	CAB-CBB-CCB-CDB
37	A	413	LMG	C14-C15-C16-C17
29	1	1623	NEX	C39-C29-C30-C31
29	2	1623	NEX	C39-C29-C30-C31
29	3	1623	NEX	C39-C29-C30-C31
29	G	1623	NEX	C39-C29-C30-C31
29	N	1623	NEX	C39-C29-C30-C31
29	R	623	NEX	C39-C29-C30-C31
29	S	1623	NEX	C39-C29-C30-C31
29	Y	1623	NEX	C39-C29-C30-C31
29	5	1623	NEX	C39-C29-C30-C31
29	6	1623	NEX	C39-C29-C30-C31
29	7	1623	NEX	C39-C29-C30-C31
29	g	1623	NEX	C39-C29-C30-C31
29	n	1623	NEX	C39-C29-C30-C31
29	r	623	NEX	C39-C29-C30-C31
29	s	1623	NEX	C39-C29-C30-C31
29	y	1623	NEX	C39-C29-C30-C31
30	2	2630	LHG	C4-C5-C6-O8
30	C	523	LHG	C1-C2-C3-O3
30	6	2630	LHG	C4-C5-C6-O8
30	c	523	LHG	C1-C2-C3-O3
37	D	411	LMG	O1-C7-C8-C9
37	d	411	LMG	O1-C7-C8-C9
37	z	101	LMG	C19-C20-C21-C22
26	3	604	CLA	CAA-CBA-CGA-O2A
26	4	603	CLA	CAA-CBA-CGA-O2A
26	7	604	CLA	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
26	8	603	CLA	CAA-CBA-CGA-O2A
25	1	608	CHL	C2A-CAA-CBA-CGA
25	5	608	CHL	C2A-CAA-CBA-CGA
26	S	603	CLA	C2A-CAA-CBA-CGA
26	s	603	CLA	C2A-CAA-CBA-CGA
37	Z	101	LMG	C19-C20-C21-C22
37	a	413	LMG	C14-C15-C16-C17
26	B	607	CLA	C16-C17-C18-C19
26	b	607	CLA	C16-C17-C18-C19
25	G	607	CHL	O2A-C1-C2-C3
25	g	607	CHL	O2A-C1-C2-C3
30	n	2630	LHG	C24-C23-O8-C6
39	B	626	DGD	O6E-C1E-O5D-C6D
39	C	518	DGD	O6E-C1E-O5D-C6D
39	b	626	DGD	O6E-C1E-O5D-C6D
27	8	620	LUT	C7-C8-C9-C19
30	R	2630	LHG	C24-C25-C26-C27
30	S	2630	LHG	C33-C34-C35-C36
30	r	2630	LHG	C24-C25-C26-C27
37	C	521	LMG	C36-C37-C38-C39
37	c	521	LMG	C36-C37-C38-C39
26	4	610	CLA	CBD-CGD-O2D-CED
30	s	2630	LHG	C33-C34-C35-C36
37	B	2633	LMG	C41-C42-C43-C44
26	4	603	CLA	CAA-CBA-CGA-O1A
26	8	603	CLA	CAA-CBA-CGA-O1A
37	B	2633	LMG	C7-C8-O7-C10
37	b	2633	LMG	C7-C8-O7-C10
25	2	607	CHL	C1A-C2A-CAA-CBA
25	6	607	CHL	C1A-C2A-CAA-CBA
26	3	602	CLA	C1A-C2A-CAA-CBA
26	3	610	CLA	C1A-C2A-CAA-CBA
26	7	602	CLA	C1A-C2A-CAA-CBA
26	7	610	CLA	C1A-C2A-CAA-CBA
30	C	523	LHG	C27-C28-C29-C30
30	b	2631	LHG	C11-C12-C13-C14
37	b	2633	LMG	C41-C42-C43-C44
26	8	610	CLA	CBD-CGD-O2D-CED
25	G	608	CHL	C11-C10-C8-C7
25	g	608	CHL	C11-C10-C8-C7
26	B	614	CLA	C6-C7-C8-C10
26	D	403	CLA	C11-C10-C8-C7

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Mol	Chain	Res	Type	Atoms
26	N	613	CLA	C11-C10-C8-C7
26	R	610	CLA	C12-C13-C15-C16
26	b	614	CLA	C6-C7-C8-C10
26	c	502	CLA	C11-C12-C13-C15
26	d	403	CLA	C11-C10-C8-C7
26	n	613	CLA	C11-C10-C8-C7
26	r	610	CLA	C12-C13-C15-C16
30	B	2631	LHG	C11-C12-C13-C14
36	B	621	SQD	C14-C15-C16-C17
36	b	621	SQD	C14-C15-C16-C17
26	s	602	CLA	O1A-CGA-O2A-C1
30	c	523	LHG	C27-C28-C29-C30
31	C	515	BCR	C9-C10-C11-C12
31	c	515	BCR	C9-C10-C11-C12
25	2	606	CHL	C3C-C2C-CMC-OMC
25	6	606	CHL	C3C-C2C-CMC-OMC
26	S	602	CLA	O1A-CGA-O2A-C1
26	n	604	CLA	O1A-CGA-O2A-C1
26	3	604	CLA	CAA-CBA-CGA-O1A
26	7	604	CLA	CAA-CBA-CGA-O1A
30	B	2630	LHG	C18-C19-C20-C21
30	b	2630	LHG	C18-C19-C20-C21
36	B	621	SQD	C29-C30-C31-C32
37	B	2633	LMG	C23-C24-C25-C26
37	b	2633	LMG	C23-C24-C25-C26
26	B	617	CLA	C2A-CAA-CBA-CGA
26	C	505	CLA	C2A-CAA-CBA-CGA
26	b	617	CLA	C2A-CAA-CBA-CGA
26	c	505	CLA	C2A-CAA-CBA-CGA
36	b	621	SQD	C29-C30-C31-C32
26	N	604	CLA	O1A-CGA-O2A-C1
39	C	518	DGD	CDB-CEB-CFB-CGB
39	c	518	DGD	CDB-CEB-CFB-CGB
25	2	605	CHL	CAA-CBA-CGA-O2A
25	6	605	CHL	CAA-CBA-CGA-O2A
37	B	622	LMG	C32-C33-C34-C35
25	2	609	CHL	C4-C3-C5-C6
25	3	609	CHL	C4-C3-C5-C6
25	G	608	CHL	C4-C3-C5-C6
25	6	609	CHL	C4-C3-C5-C6
25	7	609	CHL	C4-C3-C5-C6
25	g	608	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
37	b	622	LMG	C32-C33-C34-C35
26	Y	611	CLA	C2-C3-C5-C6
26	y	611	CLA	C2-C3-C5-C6
26	G	602	CLA	CBA-CGA-O2A-C1
26	S	602	CLA	CBA-CGA-O2A-C1
26	g	602	CLA	CBA-CGA-O2A-C1
37	z	101	LMG	C17-C18-C19-C20
37	Z	101	LMG	C17-C18-C19-C20
29	1	1623	NEX	C28-C29-C30-C31
29	2	1623	NEX	C28-C29-C30-C31
29	3	1623	NEX	C28-C29-C30-C31
29	G	1623	NEX	C28-C29-C30-C31
29	N	1623	NEX	C28-C29-C30-C31
29	R	623	NEX	C28-C29-C30-C31
29	S	1623	NEX	C28-C29-C30-C31
29	Y	1623	NEX	C28-C29-C30-C31
29	5	1623	NEX	C28-C29-C30-C31
29	6	1623	NEX	C28-C29-C30-C31
29	7	1623	NEX	C28-C29-C30-C31
29	g	1623	NEX	C28-C29-C30-C31
29	n	1623	NEX	C28-C29-C30-C31
29	r	623	NEX	C28-C29-C30-C31
29	s	1623	NEX	C28-C29-C30-C31
29	y	1623	NEX	C28-C29-C30-C31
25	4	606	CHL	CAA-CBA-CGA-O1A
25	4	606	CHL	CAA-CBA-CGA-O2A
25	4	607	CHL	CAA-CBA-CGA-O2A
25	8	606	CHL	CAA-CBA-CGA-O2A
25	8	607	CHL	CAA-CBA-CGA-O2A
26	s	602	CLA	CBA-CGA-O2A-C1
30	C	2630	LHG	C24-C23-O8-C6
30	c	2630	LHG	C24-C23-O8-C6
26	B	608	CLA	C2A-CAA-CBA-CGA
26	b	608	CLA	C2A-CAA-CBA-CGA
29	2	1623	NEX	C13-C14-C15-C35
29	6	1623	NEX	C13-C14-C15-C35
25	8	606	CHL	CAA-CBA-CGA-O1A
30	D	409	LHG	C24-C25-C26-C27
30	d	409	LHG	C24-C25-C26-C27
37	Z	101	LMG	C16-C17-C18-C19
37	z	101	LMG	C16-C17-C18-C19
25	7	607	CHL	C2C-C3C-CAC-CBC

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Mol	Chain	Res	Type	Atoms
39	C	518	DGD	CBB-CCB-CDB-CEB
39	c	518	DGD	CBB-CCB-CDB-CEB
25	Y	609	CHL	C4-C3-C5-C6
25	y	609	CHL	C4-C3-C5-C6
26	1	604	CLA	C2-C1-O2A-CGA
26	C	502	CLA	C2-C1-O2A-CGA
26	5	604	CLA	C2-C1-O2A-CGA
26	c	502	CLA	C2-C1-O2A-CGA
26	Y	612	CLA	C2-C3-C5-C6
26	y	612	CLA	C2-C3-C5-C6
25	3	607	CHL	C2C-C3C-CAC-CBC
25	S	607	CHL	C11-C10-C8-C9
25	s	607	CHL	C11-C10-C8-C9
26	B	605	CLA	C6-C7-C8-C9
26	B	612	CLA	C11-C10-C8-C9
26	C	507	CLA	C6-C7-C8-C9
26	R	603	CLA	C11-C10-C8-C9
26	b	605	CLA	C6-C7-C8-C9
26	b	612	CLA	C11-C10-C8-C9
26	r	603	CLA	C11-C10-C8-C9
26	G	612	CLA	C3-C5-C6-C7
26	g	612	CLA	C3-C5-C6-C7
26	4	602	CLA	CAA-CBA-CGA-O2A
26	8	602	CLA	CAA-CBA-CGA-O2A
35	A	409	PHO	C1A-C2A-CAA-CBA
35	a	409	PHO	C1A-C2A-CAA-CBA
26	B	606	CLA	C2A-CAA-CBA-CGA
26	R	603	CLA	C2A-CAA-CBA-CGA
26	R	610	CLA	C2A-CAA-CBA-CGA
26	S	613	CLA	C2A-CAA-CBA-CGA
26	b	606	CLA	C2A-CAA-CBA-CGA
26	r	603	CLA	C2A-CAA-CBA-CGA
26	r	610	CLA	C2A-CAA-CBA-CGA
26	s	613	CLA	C2A-CAA-CBA-CGA
26	B	603	CLA	C16-C17-C18-C20
26	b	603	CLA	C16-C17-C18-C20
25	4	601	CHL	CAA-CBA-CGA-O2A
25	8	601	CHL	CAA-CBA-CGA-O2A
26	B	606	CLA	O1A-CGA-O2A-C1
26	b	606	CLA	O1A-CGA-O2A-C1
27	2	1621	LUT	C5-C6-C7-C8
27	G	1621	LUT	C1-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
27	6	1621	LUT	C5-C6-C7-C8
27	g	1621	LUT	C1-C6-C7-C8
31	C	514	BCR	C23-C24-C25-C30
31	H	101	BCR	C23-C24-C25-C26
31	H	101	BCR	C23-C24-C25-C30
31	c	514	BCR	C23-C24-C25-C30
31	h	101	BCR	C23-C24-C25-C26
31	h	101	BCR	C23-C24-C25-C30
36	a	418	SQD	C16-C17-C18-C19
36	A	418	SQD	C16-C17-C18-C19
25	2	601	CHL	CAA-CBA-CGA-O1A
25	2	605	CHL	CAA-CBA-CGA-O1A
25	6	601	CHL	CAA-CBA-CGA-O1A
25	6	605	CHL	CAA-CBA-CGA-O1A
25	N	609	CHL	C10-C11-C12-C13
25	n	609	CHL	C10-C11-C12-C13
26	B	609	CLA	C5-C6-C7-C8
26	b	609	CLA	C5-C6-C7-C8
39	C	519	DGD	CDB-CEB-CFB-CGB
39	c	519	DGD	CDB-CEB-CFB-CGB
25	N	608	CHL	C4-C3-C5-C6
27	4	620	LUT	C7-C8-C9-C10
27	8	620	LUT	C7-C8-C9-C10
28	4	622	XAT	C27-C28-C29-C30
28	8	622	XAT	C27-C28-C29-C30
25	G	609	CHL	C10-C11-C12-C13
25	g	609	CHL	C10-C11-C12-C13
26	B	613	CLA	C15-C16-C17-C18
26	b	613	CLA	C15-C16-C17-C18
25	g	609	CHL	C2C-C3C-CAC-CBC
36	B	623	SQD	C27-C28-C29-C30
36	b	623	SQD	C27-C28-C29-C30
25	Y	607	CHL	C2-C3-C5-C6
25	y	607	CHL	C2-C3-C5-C6
26	B	616	CLA	C2-C3-C5-C6
26	S	613	CLA	C2-C3-C5-C6
26	b	616	CLA	C2-C3-C5-C6
26	s	613	CLA	C2-C3-C5-C6
25	4	607	CHL	CAA-CBA-CGA-O1A
25	8	607	CHL	CAA-CBA-CGA-O1A
26	S	609	CLA	CAA-CBA-CGA-O2A
39	C	518	DGD	C5D-C6D-O5D-C1E

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Mol	Chain	Res	Type	Atoms
39	c	518	DGD	C5D-C6D-O5D-C1E
30	D	410	LHG	C23-C24-C25-C26
25	3	609	CHL	C4C-C3C-CAC-CBC
25	4	609	CHL	CAA-CBA-CGA-O1A
25	8	609	CHL	CAA-CBA-CGA-O1A
26	s	609	CLA	CAA-CBA-CGA-O2A
25	7	609	CHL	C4C-C3C-CAC-CBC
26	B	609	CLA	C15-C16-C17-C18
26	b	609	CLA	C15-C16-C17-C18
26	1	610	CLA	C11-C10-C8-C9
26	5	610	CLA	C11-C10-C8-C9
30	d	410	LHG	C23-C24-C25-C26
25	4	601	CHL	CAA-CBA-CGA-O1A
25	8	601	CHL	CAA-CBA-CGA-O1A
26	4	602	CLA	CAA-CBA-CGA-O1A
26	8	602	CLA	CAA-CBA-CGA-O1A
25	4	607	CHL	C2A-CAA-CBA-CGA
25	8	607	CHL	C2A-CAA-CBA-CGA
26	G	612	CLA	C10-C11-C12-C13
26	g	612	CLA	C10-C11-C12-C13
25	G	609	CHL	C2C-C3C-CAC-CBC
30	1	2630	LHG	C13-C14-C15-C16
30	5	2630	LHG	C13-C14-C15-C16
37	B	622	LMG	C20-C21-C22-C23
37	b	622	LMG	C20-C21-C22-C23
25	3	605	CHL	CAA-CBA-CGA-O1A
26	4	612	CLA	CAA-CBA-CGA-O1A
26	8	612	CLA	CAA-CBA-CGA-O1A
25	n	608	CHL	C4-C3-C5-C6
26	R	613	CLA	C4-C3-C5-C6
26	r	613	CLA	C4-C3-C5-C6
38	D	405	PL9	C34-C36-C37-C38
38	d	405	PL9	C34-C36-C37-C38
25	S	607	CHL	C6-C7-C8-C10
25	s	607	CHL	C6-C7-C8-C10
26	B	617	CLA	C12-C13-C15-C16
26	C	503	CLA	C12-C13-C15-C16
26	b	617	CLA	C12-C13-C15-C16
26	c	503	CLA	C12-C13-C15-C16
25	S	601	CHL	CAA-CBA-CGA-O2A
25	7	605	CHL	CAA-CBA-CGA-O1A
25	s	601	CHL	CAA-CBA-CGA-O2A

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Mol	Chain	Res	Type	Atoms
26	4	611	CLA	CAA-CBA-CGA-O2A
26	8	611	CLA	CAA-CBA-CGA-O2A
30	C	522	LHG	C30-C31-C32-C33
30	c	522	LHG	C30-C31-C32-C33
39	c	520	DGD	C6B-C7B-C8B-C9B
26	B	614	CLA	CAA-CBA-CGA-O2A
26	b	614	CLA	CAA-CBA-CGA-O2A
39	B	626	DGD	C2E-C1E-O5D-C6D
39	b	626	DGD	C2E-C1E-O5D-C6D
39	C	520	DGD	C6B-C7B-C8B-C9B
26	4	612	CLA	CAA-CBA-CGA-O2A
26	8	612	CLA	CAA-CBA-CGA-O2A
30	2	2630	LHG	O7-C5-C6-O8
30	6	2630	LHG	O7-C5-C6-O8
26	G	602	CLA	O1A-CGA-O2A-C1
25	2	608	CHL	CAA-CBA-CGA-O2A
25	6	608	CHL	CAA-CBA-CGA-O2A
25	Y	606	CHL	O2A-C1-C2-C3
25	y	606	CHL	O2A-C1-C2-C3
26	g	602	CLA	O1A-CGA-O2A-C1
30	d	410	LHG	C8-C7-O7-C5
25	3	605	CHL	CAA-CBA-CGA-O2A
25	7	605	CHL	CAA-CBA-CGA-O2A
26	Y	612	CLA	CAA-CBA-CGA-O2A
26	y	612	CLA	CAA-CBA-CGA-O2A
26	1	602	CLA	C4-C3-C5-C6
26	3	603	CLA	C4-C3-C5-C6
26	B	607	CLA	C4-C3-C5-C6
26	R	602	CLA	C4-C3-C5-C6
26	5	602	CLA	C4-C3-C5-C6
26	7	603	CLA	C4-C3-C5-C6
26	b	607	CLA	C4-C3-C5-C6
26	r	602	CLA	C4-C3-C5-C6
26	s	613	CLA	C4-C3-C5-C6
25	N	609	CHL	C8-C10-C11-C12
25	n	609	CHL	C8-C10-C11-C12
26	1	611	CLA	CAA-CBA-CGA-O2A
26	5	611	CLA	CAA-CBA-CGA-O2A
25	3	609	CHL	C2-C3-C5-C6
25	S	607	CHL	C2-C3-C5-C6
25	Y	609	CHL	C2-C3-C5-C6
25	7	609	CHL	C2-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	s	607	CHL	C2-C3-C5-C6
25	y	609	CHL	C2-C3-C5-C6
26	B	603	CLA	C2-C3-C5-C6
26	b	603	CLA	C2-C3-C5-C6
26	C	506	CLA	C8-C10-C11-C12
30	d	409	LHG	O8-C23-C24-C25
25	G	608	CHL	C11-C10-C8-C9
25	N	609	CHL	C14-C13-C15-C16
25	Y	601	CHL	C6-C7-C8-C9
25	g	608	CHL	C11-C10-C8-C9
25	n	609	CHL	C14-C13-C15-C16
25	y	601	CHL	C6-C7-C8-C9
26	C	506	CLA	C14-C13-C15-C16
26	C	508	CLA	C11-C12-C13-C14
26	C	509	CLA	C11-C10-C8-C9
26	C	511	CLA	C6-C7-C8-C9
26	G	613	CLA	C14-C13-C15-C16
26	Y	612	CLA	C6-C7-C8-C9
26	c	503	CLA	C14-C13-C15-C16
26	c	506	CLA	C14-C13-C15-C16
26	c	507	CLA	C6-C7-C8-C9
26	c	508	CLA	C11-C12-C13-C14
26	c	509	CLA	C11-C10-C8-C9
26	c	511	CLA	C6-C7-C8-C9
26	g	613	CLA	C14-C13-C15-C16
26	y	612	CLA	C6-C7-C8-C9
25	6	606	CHL	CAA-CBA-CGA-O2A
26	2	604	CLA	CAA-CBA-CGA-O1A
26	6	604	CLA	CAA-CBA-CGA-O1A
26	c	506	CLA	C8-C10-C11-C12
39	H	102	DGD	CDB-CEB-CFB-CGB
39	h	102	DGD	CDB-CEB-CFB-CGB
25	1	608	CHL	C3A-C2A-CAA-CBA
25	2	607	CHL	C3A-C2A-CAA-CBA
25	5	608	CHL	C3A-C2A-CAA-CBA
25	6	607	CHL	C3A-C2A-CAA-CBA
26	3	603	CLA	C3A-C2A-CAA-CBA
26	A	406	CLA	C3A-C2A-CAA-CBA
26	7	603	CLA	C3A-C2A-CAA-CBA
26	a	406	CLA	C3A-C2A-CAA-CBA
30	3	2630	LHG	O8-C23-C24-C25
30	7	2630	LHG	O8-C23-C24-C25

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Mol	Chain	Res	Type	Atoms
25	1	601	CHL	CAA-CBA-CGA-O2A
25	2	606	CHL	CAA-CBA-CGA-O2A
25	S	601	CHL	CAA-CBA-CGA-O1A
25	5	601	CHL	CAA-CBA-CGA-O2A
25	s	601	CHL	CAA-CBA-CGA-O1A
25	s	606	CHL	CAA-CBA-CGA-O2A
26	2	611	CLA	CAA-CBA-CGA-O2A
26	2	612	CLA	CAA-CBA-CGA-O2A
26	6	611	CLA	CAA-CBA-CGA-O2A
26	6	612	CLA	CAA-CBA-CGA-O2A
25	1	605	CHL	CAD-CBD-CGD-O2D
25	G	606	CHL	CAD-CBD-CGD-O2D
25	5	605	CHL	CAD-CBD-CGD-O2D
25	g	606	CHL	CAD-CBD-CGD-O2D
26	2	604	CLA	CAD-CBD-CGD-O2D
26	2	610	CLA	CAD-CBD-CGD-O2D
26	2	614	CLA	CAD-CBD-CGD-O2D
26	B	607	CLA	CAD-CBD-CGD-O2D
26	B	608	CLA	CAD-CBD-CGD-O2D
26	C	501	CLA	CAD-CBD-CGD-O2D
26	C	502	CLA	CAD-CBD-CGD-O2D
26	C	503	CLA	CAD-CBD-CGD-O2D
26	N	604	CLA	CAD-CBD-CGD-O2D
26	N	614	CLA	CAD-CBD-CGD-O2D
26	R	610	CLA	CAD-CBD-CGD-O2D
26	S	612	CLA	CAD-CBD-CGD-O2D
26	6	604	CLA	CAD-CBD-CGD-O2D
26	6	610	CLA	CAD-CBD-CGD-O2D
26	6	614	CLA	CAD-CBD-CGD-O2D
26	b	607	CLA	CAD-CBD-CGD-O2D
26	b	608	CLA	CAD-CBD-CGD-O2D
26	c	501	CLA	CAD-CBD-CGD-O2D
26	c	502	CLA	CAD-CBD-CGD-O2D
26	c	503	CLA	CAD-CBD-CGD-O2D
26	n	604	CLA	CAD-CBD-CGD-O2D
26	n	614	CLA	CAD-CBD-CGD-O2D
26	r	610	CLA	CAD-CBD-CGD-O2D
26	s	612	CLA	CAD-CBD-CGD-O2D
37	Z	101	LMG	C15-C16-C17-C18
37	z	101	LMG	C15-C16-C17-C18
37	C	521	LMG	C37-C38-C39-C40
35	A	408	PHO	C2-C1-O2A-CGA

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Mol	Chain	Res	Type	Atoms
35	a	408	PHO	C2-C1-O2A-CGA
25	S	606	CHL	CAA-CBA-CGA-O2A
26	4	604	CLA	CAA-CBA-CGA-O2A
26	R	616	CLA	CAA-CBA-CGA-O2A
26	8	604	CLA	CAA-CBA-CGA-O2A
26	r	616	CLA	CAA-CBA-CGA-O2A
36	B	621	SQD	C27-C28-C29-C30
36	b	621	SQD	C27-C28-C29-C30
37	c	521	LMG	C37-C38-C39-C40
26	S	604	CLA	CAA-CBA-CGA-O2A
26	s	604	CLA	CAA-CBA-CGA-O2A
30	D	409	LHG	O8-C23-C24-C25
30	c	2630	LHG	C25-C26-C27-C28
25	G	609	CHL	C4-C3-C5-C6
25	g	609	CHL	C4-C3-C5-C6
26	S	613	CLA	C4-C3-C5-C6
26	G	613	CLA	C16-C17-C18-C20
26	g	613	CLA	C16-C17-C18-C20
30	C	2630	LHG	C25-C26-C27-C28
30	C	523	LHG	C16-C17-C18-C19
25	2	609	CHL	C2-C3-C5-C6
25	G	608	CHL	C2-C3-C5-C6
25	6	609	CHL	C2-C3-C5-C6
25	g	608	CHL	C2-C3-C5-C6
26	C	507	CLA	CAA-CBA-CGA-O2A
27	R	620	LUT	C27-C28-C29-C30
27	r	620	LUT	C27-C28-C29-C30
28	R	622	XAT	C27-C28-C29-C30
28	r	622	XAT	C27-C28-C29-C30
29	3	1623	NEX	C11-C12-C13-C14
29	S	1623	NEX	C11-C12-C13-C14
29	7	1623	NEX	C11-C12-C13-C14
29	s	1623	NEX	C11-C12-C13-C14
31	A	411	BCR	C7-C8-C9-C10
31	a	411	BCR	C7-C8-C9-C10
30	c	523	LHG	C16-C17-C18-C19
29	2	1623	NEX	O24-C26-C27-C28
29	G	1623	NEX	O24-C26-C27-C28
29	N	1623	NEX	O24-C26-C27-C28
29	R	623	NEX	O24-C26-C27-C28
29	Y	1623	NEX	O24-C26-C27-C28
29	6	1623	NEX	O24-C26-C27-C28

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Mol	Chain	Res	Type	Atoms
29	g	1623	NEX	O24-C26-C27-C28
29	n	1623	NEX	O24-C26-C27-C28
29	r	623	NEX	O24-C26-C27-C28
29	y	1623	NEX	O24-C26-C27-C28
25	5	606	CHL	CAA-CBA-CGA-O1A
25	6	608	CHL	CAA-CBA-CGA-O1A
26	n	602	CLA	CBD-CGD-O2D-CED
37	d	411	LMG	O10-C28-O8-C9
36	A	418	SQD	C28-C29-C30-C31
26	c	507	CLA	CAA-CBA-CGA-O2A
30	L	101	LHG	O7-C7-C8-C9
30	l	101	LHG	O7-C7-C8-C9
26	R	611	CLA	O2A-C1-C2-C3
26	r	611	CLA	O2A-C1-C2-C3
25	1	606	CHL	CAA-CBA-CGA-O1A
25	2	608	CHL	CAA-CBA-CGA-O1A
26	S	609	CLA	CAA-CBA-CGA-O1A
26	6	612	CLA	CAA-CBA-CGA-O1A
26	s	609	CLA	CAA-CBA-CGA-O1A
36	a	418	SQD	C28-C29-C30-C31
25	3	601	CHL	O2A-C1-C2-C3
25	3	607	CHL	O2A-C1-C2-C3
25	N	607	CHL	O2A-C1-C2-C3
25	7	601	CHL	O2A-C1-C2-C3
25	7	607	CHL	O2A-C1-C2-C3
25	n	607	CHL	O2A-C1-C2-C3
26	A	405	CLA	O2A-C1-C2-C3
26	a	405	CLA	O2A-C1-C2-C3
37	D	411	LMG	O10-C28-O8-C9
25	R	606	CHL	C2A-CAA-CBA-CGA
25	r	606	CHL	C2A-CAA-CBA-CGA
26	3	610	CLA	C2A-CAA-CBA-CGA
26	S	609	CLA	C2A-CAA-CBA-CGA
26	7	610	CLA	C2A-CAA-CBA-CGA
26	s	609	CLA	C2A-CAA-CBA-CGA
25	1	607	CHL	CAA-CBA-CGA-O2A
25	N	606	CHL	CAA-CBA-CGA-O2A
25	5	607	CHL	CAA-CBA-CGA-O2A
30	D	410	LHG	O8-C23-C24-C25
30	d	410	LHG	O8-C23-C24-C25
26	7	610	CLA	C3-C5-C6-C7
25	1	601	CHL	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	1	606	CHL	CAA-CBA-CGA-O2A
25	5	606	CHL	CAA-CBA-CGA-O2A
26	2	611	CLA	CAA-CBA-CGA-O1A
26	2	612	CLA	CAA-CBA-CGA-O1A
26	4	611	CLA	CAA-CBA-CGA-O1A
26	6	611	CLA	CAA-CBA-CGA-O1A
26	8	611	CLA	CAA-CBA-CGA-O1A
26	C	504	CLA	C16-C17-C18-C19
26	c	504	CLA	C16-C17-C18-C19
26	N	602	CLA	CBD-CGD-O2D-CED
25	2	606	CHL	CHA-CBD-CGD-O1D
25	2	606	CHL	CHA-CBD-CGD-O2D
25	G	605	CHL	CHA-CBD-CGD-O2D
25	N	605	CHL	CHA-CBD-CGD-O1D
25	N	605	CHL	CHA-CBD-CGD-O2D
25	S	607	CHL	CHA-CBD-CGD-O1D
25	S	607	CHL	CHA-CBD-CGD-O2D
25	6	606	CHL	CHA-CBD-CGD-O1D
25	6	606	CHL	CHA-CBD-CGD-O2D
25	g	605	CHL	CHA-CBD-CGD-O2D
25	n	605	CHL	CHA-CBD-CGD-O1D
25	n	605	CHL	CHA-CBD-CGD-O2D
25	s	607	CHL	CHA-CBD-CGD-O1D
25	s	607	CHL	CHA-CBD-CGD-O2D
26	1	613	CLA	CHA-CBD-CGD-O1D
26	1	613	CLA	CHA-CBD-CGD-O2D
26	2	602	CLA	CHA-CBD-CGD-O2D
26	2	612	CLA	CHA-CBD-CGD-O2D
26	3	602	CLA	CHA-CBD-CGD-O1D
26	3	602	CLA	CHA-CBD-CGD-O2D
26	4	602	CLA	CHA-CBD-CGD-O1D
26	4	602	CLA	CHA-CBD-CGD-O2D
26	B	603	CLA	CHA-CBD-CGD-O2D
26	B	610	CLA	CHA-CBD-CGD-O1D
26	B	611	CLA	CHA-CBD-CGD-O2D
26	B	615	CLA	CHA-CBD-CGD-O1D
26	B	615	CLA	CHA-CBD-CGD-O2D
26	C	507	CLA	CHA-CBD-CGD-O1D
26	C	507	CLA	CHA-CBD-CGD-O2D
26	N	603	CLA	CHA-CBD-CGD-O2D
26	R	601	CLA	CHA-CBD-CGD-O2D
26	S	603	CLA	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
26	S	603	CLA	CHA-CBD-CGD-O2D
26	S	611	CLA	CHA-CBD-CGD-O1D
26	S	611	CLA	CHA-CBD-CGD-O2D
26	S	613	CLA	CHA-CBD-CGD-O1D
26	S	613	CLA	CHA-CBD-CGD-O2D
26	Y	602	CLA	CHA-CBD-CGD-O2D
26	5	613	CLA	CHA-CBD-CGD-O1D
26	5	613	CLA	CHA-CBD-CGD-O2D
26	6	602	CLA	CHA-CBD-CGD-O2D
26	6	612	CLA	CHA-CBD-CGD-O2D
26	7	602	CLA	CHA-CBD-CGD-O1D
26	7	602	CLA	CHA-CBD-CGD-O2D
26	8	602	CLA	CHA-CBD-CGD-O1D
26	8	602	CLA	CHA-CBD-CGD-O2D
26	b	603	CLA	CHA-CBD-CGD-O2D
26	b	610	CLA	CHA-CBD-CGD-O1D
26	b	611	CLA	CHA-CBD-CGD-O2D
26	b	615	CLA	CHA-CBD-CGD-O1D
26	b	615	CLA	CHA-CBD-CGD-O2D
26	c	507	CLA	CHA-CBD-CGD-O1D
26	c	507	CLA	CHA-CBD-CGD-O2D
26	n	603	CLA	CHA-CBD-CGD-O2D
26	r	601	CLA	CHA-CBD-CGD-O2D
26	s	603	CLA	CHA-CBD-CGD-O1D
26	s	603	CLA	CHA-CBD-CGD-O2D
26	s	611	CLA	CHA-CBD-CGD-O1D
26	s	611	CLA	CHA-CBD-CGD-O2D
26	s	613	CLA	CHA-CBD-CGD-O1D
26	s	613	CLA	CHA-CBD-CGD-O2D
26	y	602	CLA	CHA-CBD-CGD-O2D
29	R	623	NEX	C13-C14-C15-C35
25	1	605	CHL	CAA-CBA-CGA-O2A
25	2	606	CHL	CAA-CBA-CGA-O1A
25	5	601	CHL	CAA-CBA-CGA-O1A
25	5	605	CHL	CAA-CBA-CGA-O2A
25	6	606	CHL	CAA-CBA-CGA-O1A
26	2	604	CLA	CAA-CBA-CGA-O2A
26	4	604	CLA	CAA-CBA-CGA-O1A
26	6	604	CLA	CAA-CBA-CGA-O2A
26	8	604	CLA	CAA-CBA-CGA-O1A
25	Y	607	CHL	C4-C3-C5-C6
25	y	607	CHL	C4-C3-C5-C6

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Mol	Chain	Res	Type	Atoms
25	n	606	CHL	CAA-CBA-CGA-O2A
26	C	501	CLA	CAA-CBA-CGA-O2A
26	c	501	CLA	CAA-CBA-CGA-O2A
30	C	2630	LHG	O8-C23-C24-C25
30	c	2630	LHG	O8-C23-C24-C25
30	D	408	LHG	C33-C34-C35-C36
30	d	408	LHG	C33-C34-C35-C36
25	N	608	CHL	C2-C3-C5-C6
25	n	608	CHL	C2-C3-C5-C6
26	3	610	CLA	C3-C5-C6-C7
30	D	410	LHG	C8-C7-O7-C5
36	b	621	SQD	C31-C32-C33-C34
30	D	410	LHG	O6-C4-C5-C6
30	d	410	LHG	O6-C4-C5-C6
26	N	614	CLA	O2A-C1-C2-C3
26	n	614	CLA	O2A-C1-C2-C3
25	7	601	CHL	CAA-CBA-CGA-O2A
26	1	602	CLA	CAA-CBA-CGA-O2A
26	1	613	CLA	CAA-CBA-CGA-O2A
26	2	603	CLA	CAA-CBA-CGA-O2A
26	B	617	CLA	CAA-CBA-CGA-O2A
26	G	611	CLA	CAA-CBA-CGA-O2A
26	R	603	CLA	CAA-CBA-CGA-O2A
26	6	603	CLA	CAA-CBA-CGA-O2A
26	b	617	CLA	CAA-CBA-CGA-O2A
26	g	611	CLA	CAA-CBA-CGA-O2A
26	r	603	CLA	CAA-CBA-CGA-O2A
30	C	523	LHG	C13-C14-C15-C16
36	B	621	SQD	C31-C32-C33-C34
37	A	413	LMG	C31-C32-C33-C34
30	c	523	LHG	C13-C14-C15-C16
37	a	413	LMG	C31-C32-C33-C34
25	8	607	CHL	CBD-CGD-O2D-CED
25	3	601	CHL	CAA-CBA-CGA-O2A
26	5	602	CLA	CAA-CBA-CGA-O2A
37	A	415	LMG	O8-C28-C29-C30
25	3	606	CHL	CAA-CBA-CGA-O2A
25	7	606	CHL	CAA-CBA-CGA-O2A
26	3	612	CLA	CAA-CBA-CGA-O2A
26	7	612	CLA	CAA-CBA-CGA-O2A
35	A	409	PHO	CHA-CBD-CGD-O1D
35	a	409	PHO	CHA-CBD-CGD-O1D

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Mol	Chain	Res	Type	Atoms
25	Y	607	CHL	C8-C10-C11-C12
25	y	607	CHL	C8-C10-C11-C12
26	A	410	CLA	C8-C10-C11-C12
30	s	2630	LHG	C12-C13-C14-C15
26	5	613	CLA	CAA-CBA-CGA-O2A
37	a	415	LMG	O8-C28-C29-C30
30	S	2630	LHG	C12-C13-C14-C15
25	4	607	CHL	CBD-CGD-O2D-CED
26	B	609	CLA	C4-C3-C5-C6
26	b	609	CLA	C4-C3-C5-C6
37	a	413	LMG	C35-C36-C37-C38
25	3	607	CHL	C2-C3-C5-C6
25	7	607	CHL	C2-C3-C5-C6
26	B	602	CLA	C12-C13-C15-C16
26	C	501	CLA	C2-C3-C5-C6
26	C	508	CLA	C11-C12-C13-C15
26	b	602	CLA	C12-C13-C15-C16
26	c	501	CLA	C2-C3-C5-C6
26	c	508	CLA	C11-C12-C13-C15
30	2	2630	LHG	C16-C17-C18-C19
30	6	2630	LHG	C16-C17-C18-C19
37	A	413	LMG	C35-C36-C37-C38
30	C	522	LHG	C14-C15-C16-C17
30	c	522	LHG	C14-C15-C16-C17
25	G	608	CHL	C11-C12-C13-C14
25	S	607	CHL	C6-C7-C8-C9
25	g	608	CHL	C11-C12-C13-C14
25	s	607	CHL	C6-C7-C8-C9
26	B	614	CLA	C11-C12-C13-C14
26	C	503	CLA	C6-C7-C8-C9
26	C	503	CLA	C14-C13-C15-C16
26	C	504	CLA	C14-C13-C15-C16
26	C	511	CLA	C14-C13-C15-C16
26	N	613	CLA	C11-C10-C8-C9
26	b	614	CLA	C11-C12-C13-C14
26	c	503	CLA	C6-C7-C8-C9
26	c	504	CLA	C14-C13-C15-C16
26	c	511	CLA	C14-C13-C15-C16
26	n	613	CLA	C11-C10-C8-C9
29	2	1623	NEX	C9-C10-C11-C12
29	6	1623	NEX	C9-C10-C11-C12
29	r	623	NEX	C13-C14-C15-C35

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Mol	Chain	Res	Type	Atoms
26	a	410	CLA	C8-C10-C11-C12
35	A	409	PHO	C8-C10-C11-C12
35	a	409	PHO	C8-C10-C11-C12
30	G	2630	LHG	C31-C32-C33-C34
30	g	2630	LHG	C31-C32-C33-C34
30	D	408	LHG	C24-C23-O8-C6
30	d	408	LHG	C24-C23-O8-C6
37	B	2633	LMG	C29-C28-O8-C9
37	b	2633	LMG	C29-C28-O8-C9
26	C	501	CLA	CAA-CBA-CGA-O1A
36	B	621	SQD	C5-C6-S-O8
36	b	621	SQD	C5-C6-S-O8
30	Y	2630	LHG	O10-C23-O8-C6
30	y	2630	LHG	O10-C23-O8-C6
25	2	601	CHL	CAA-CBA-CGA-O2A
25	4	609	CHL	CAA-CBA-CGA-O2A
25	S	606	CHL	CAA-CBA-CGA-O1A
25	6	601	CHL	CAA-CBA-CGA-O2A
25	8	609	CHL	CAA-CBA-CGA-O2A
25	s	606	CHL	CAA-CBA-CGA-O1A
26	1	611	CLA	CAA-CBA-CGA-O1A
26	5	611	CLA	CAA-CBA-CGA-O1A
26	1	612	CLA	C2A-CAA-CBA-CGA
26	5	612	CLA	C2A-CAA-CBA-CGA
38	D	405	PL9	C46-C47-C48-C49
38	d	405	PL9	C46-C47-C48-C49
25	1	607	CHL	CAA-CBA-CGA-O1A
25	5	607	CHL	CAA-CBA-CGA-O1A
26	C	507	CLA	CAA-CBA-CGA-O1A
26	c	501	CLA	CAA-CBA-CGA-O1A
26	G	612	CLA	CAA-CBA-CGA-O2A
26	g	612	CLA	CAA-CBA-CGA-O2A
36	B	623	SQD	O47-C7-C8-C9
36	b	623	SQD	O47-C7-C8-C9
27	R	620	LUT	C27-C28-C29-C39
30	B	2631	LHG	C23-C24-C25-C26
30	b	2631	LHG	C23-C24-C25-C26
26	c	507	CLA	CAA-CBA-CGA-O1A
30	S	2630	LHG	O10-C23-C24-C25
36	B	623	SQD	O49-C7-C8-C9
36	b	623	SQD	O49-C7-C8-C9
26	3	603	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
26	B	616	CLA	C4-C3-C5-C6
26	b	616	CLA	C4-C3-C5-C6
26	R	616	CLA	CAA-CBA-CGA-O1A
26	r	616	CLA	CAA-CBA-CGA-O1A
30	s	2630	LHG	O10-C23-C24-C25
31	C	515	BCR	C17-C18-C19-C20
31	c	515	BCR	C17-C18-C19-C20
39	b	626	DGD	C3B-C4B-C5B-C6B
25	3	607	CHL	C1A-C2A-CAA-CBA
25	G	609	CHL	C1A-C2A-CAA-CBA
25	7	607	CHL	C1A-C2A-CAA-CBA
25	g	609	CHL	C1A-C2A-CAA-CBA
26	3	603	CLA	C1A-C2A-CAA-CBA
26	C	512	CLA	C1A-C2A-CAA-CBA
26	7	603	CLA	C1A-C2A-CAA-CBA
26	c	512	CLA	C1A-C2A-CAA-CBA
36	a	418	SQD	C11-C12-C13-C14
39	B	626	DGD	C3B-C4B-C5B-C6B
26	B	614	CLA	CAA-CBA-CGA-O1A
26	b	614	CLA	CAA-CBA-CGA-O1A
26	y	612	CLA	CAA-CBA-CGA-O1A
26	7	603	CLA	C5-C6-C7-C8
26	B	605	CLA	C2-C1-O2A-CGA
26	C	506	CLA	C2-C1-O2A-CGA
26	C	511	CLA	C2-C1-O2A-CGA
26	b	605	CLA	C2-C1-O2A-CGA
26	c	506	CLA	C2-C1-O2A-CGA
26	c	511	CLA	C2-C1-O2A-CGA
26	Y	612	CLA	CAA-CBA-CGA-O1A
30	D	410	LHG	O10-C23-C24-C25
30	d	410	LHG	O10-C23-C24-C25
37	A	415	LMG	O10-C28-C29-C30
37	a	415	LMG	O10-C28-C29-C30
30	4	2630	LHG	C4-C5-C6-O8
30	8	2630	LHG	C4-C5-C6-O8
39	C	519	DGD	O1G-C1A-C2A-C3A
36	A	418	SQD	C11-C12-C13-C14
26	8	610	CLA	C2A-CAA-CBA-CGA
26	5	611	CLA	CBD-CGD-O2D-CED
26	B	617	CLA	C16-C17-C18-C20
26	b	617	CLA	C16-C17-C18-C20
35	A	408	PHO	C16-C17-C18-C19

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Mol	Chain	Res	Type	Atoms
35	a	408	PHO	C16-C17-C18-C19
25	N	606	CHL	CAA-CBA-CGA-O1A
25	n	606	CHL	CAA-CBA-CGA-O1A
39	c	519	DGD	O1G-C1A-C2A-C3A
26	1	602	CLA	CAA-CBA-CGA-O1A
26	S	604	CLA	CAA-CBA-CGA-O1A
26	5	602	CLA	CAA-CBA-CGA-O1A
26	s	604	CLA	CAA-CBA-CGA-O1A
37	Z	101	LMG	O10-C28-C29-C30
36	B	621	SQD	C2-C1-O6-C44
36	b	621	SQD	C2-C1-O6-C44
30	2	2630	LHG	C3-O3-P-O5
30	B	2631	LHG	C4-O6-P-O5
30	D	409	LHG	C3-O3-P-O5
30	D	410	LHG	C3-O3-P-O5
30	L	101	LHG	C4-O6-P-O5
30	R	2630	LHG	C3-O3-P-O5
30	6	2630	LHG	C3-O3-P-O5
30	b	2631	LHG	C4-O6-P-O5
30	d	409	LHG	C3-O3-P-O5
30	d	410	LHG	C3-O3-P-O5
30	l	101	LHG	C4-O6-P-O5
30	r	2630	LHG	C3-O3-P-O5
26	C	507	CLA	C16-C17-C18-C20
26	c	507	CLA	C16-C17-C18-C20
26	R	603	CLA	CAA-CBA-CGA-O1A
26	r	603	CLA	CAA-CBA-CGA-O1A
30	N	2630	LHG	O10-C23-C24-C25
30	n	2630	LHG	O10-C23-C24-C25
37	z	101	LMG	O10-C28-C29-C30
37	b	622	LMG	C31-C32-C33-C34
26	C	503	CLA	C13-C15-C16-C17
26	c	503	CLA	C13-C15-C16-C17
26	B	617	CLA	CAA-CBA-CGA-O1A
26	b	617	CLA	CAA-CBA-CGA-O1A
30	G	2630	LHG	O10-C23-C24-C25
30	g	2630	LHG	O10-C23-C24-C25
30	Y	2630	LHG	C11-C12-C13-C14
37	B	622	LMG	C31-C32-C33-C34
36	B	621	SQD	O47-C7-C8-C9
36	b	621	SQD	O47-C7-C8-C9
30	y	2630	LHG	C11-C12-C13-C14

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Mol	Chain	Res	Type	Atoms
26	S	610	CLA	C5-C6-C7-C8
26	s	610	CLA	C5-C6-C7-C8
25	1	605	CHL	CAA-CBA-CGA-O1A
25	5	605	CHL	CAA-CBA-CGA-O1A
26	3	612	CLA	CAA-CBA-CGA-O1A
26	7	612	CLA	CAA-CBA-CGA-O1A
30	N	2630	LHG	C16-C17-C18-C19
30	Y	2630	LHG	C11-C10-C9-C8
26	4	610	CLA	C2A-CAA-CBA-CGA
39	c	519	DGD	O1B-C1B-C2B-C3B
26	C	502	CLA	C3-C5-C6-C7
26	B	607	CLA	C10-C11-C12-C13
30	n	2630	LHG	C16-C17-C18-C19
30	y	2630	LHG	C11-C10-C9-C8
26	B	606	CLA	C13-C15-C16-C17
26	G	603	CLA	C5-C6-C7-C8
26	b	606	CLA	C13-C15-C16-C17
26	b	607	CLA	C10-C11-C12-C13
36	b	621	SQD	O49-C7-C8-C9
39	C	519	DGD	O1B-C1B-C2B-C3B
39	C	520	DGD	C3A-C4A-C5A-C6A
39	c	520	DGD	C3A-C4A-C5A-C6A
25	3	606	CHL	CAA-CBA-CGA-O1A
25	7	606	CHL	CAA-CBA-CGA-O1A
26	2	611	CLA	CAD-CBD-CGD-O1D
26	B	610	CLA	CAD-CBD-CGD-O1D
26	B	613	CLA	CAD-CBD-CGD-O1D
26	B	615	CLA	CAD-CBD-CGD-O1D
26	C	505	CLA	CAD-CBD-CGD-O1D
26	R	601	CLA	CAD-CBD-CGD-O1D
26	6	611	CLA	CAD-CBD-CGD-O1D
26	b	610	CLA	CAD-CBD-CGD-O1D
26	b	613	CLA	CAD-CBD-CGD-O1D
26	c	505	CLA	CAD-CBD-CGD-O1D
26	r	601	CLA	CAD-CBD-CGD-O1D
37	B	2633	LMG	C9-C8-O7-C10
37	b	2633	LMG	C9-C8-O7-C10
26	1	611	CLA	CBD-CGD-O2D-CED
26	g	612	CLA	CAA-CBA-CGA-O1A
36	B	621	SQD	O49-C7-C8-C9
37	a	413	LMG	C34-C35-C36-C37
26	g	603	CLA	C5-C6-C7-C8

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Mol	Chain	Res	Type	Atoms
30	C	522	LHG	O2-C2-C3-O3
30	c	522	LHG	O2-C2-C3-O3
26	B	609	CLA	C11-C12-C13-C14
26	D	403	CLA	C11-C10-C8-C9
26	N	602	CLA	C11-C12-C13-C14
26	N	603	CLA	C6-C7-C8-C9
26	b	609	CLA	C11-C12-C13-C14
26	d	403	CLA	C11-C10-C8-C9
26	n	602	CLA	C11-C12-C13-C14
26	n	603	CLA	C6-C7-C8-C9
37	A	413	LMG	C34-C35-C36-C37
26	G	610	CLA	C13-C15-C16-C17
26	g	610	CLA	C13-C15-C16-C17
26	G	612	CLA	CAA-CBA-CGA-O1A
26	3	603	CLA	C3-C5-C6-C7
26	7	603	CLA	C3-C5-C6-C7
26	c	502	CLA	C3-C5-C6-C7
25	N	601	CHL	CAA-CBA-CGA-O2A
26	3	602	CLA	CAA-CBA-CGA-O2A
26	C	510	CLA	CAA-CBA-CGA-O2A
26	7	602	CLA	CAA-CBA-CGA-O2A
26	c	510	CLA	CAA-CBA-CGA-O2A
36	A	412	SQD	O47-C7-C8-C9
36	a	412	SQD	O47-C7-C8-C9
37	Z	101	LMG	O8-C28-C29-C30
37	z	101	LMG	O8-C28-C29-C30
25	2	609	CHL	C5-C6-C7-C8
25	6	609	CHL	C5-C6-C7-C8
26	G	611	CLA	CAA-CBA-CGA-O1A
36	A	418	SQD	C17-C18-C19-C20
25	2	607	CHL	CAA-CBA-CGA-O2A
25	G	601	CHL	CAA-CBA-CGA-O2A
25	6	607	CHL	CAA-CBA-CGA-O2A
25	g	601	CHL	CAA-CBA-CGA-O2A
30	B	2630	LHG	C9-C10-C11-C12
30	b	2630	LHG	C9-C10-C11-C12
36	a	418	SQD	C17-C18-C19-C20
25	3	601	CHL	CAA-CBA-CGA-O1A
25	7	601	CHL	CAA-CBA-CGA-O1A
26	1	613	CLA	CAA-CBA-CGA-O1A
26	5	613	CLA	CAA-CBA-CGA-O1A
30	N	2630	LHG	C2-C3-O3-P

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Mol	Chain	Res	Type	Atoms
30	d	410	LHG	C2-C3-O3-P
30	n	2630	LHG	C2-C3-O3-P
25	g	607	CHL	C4C-C3C-CAC-CBC
25	n	609	CHL	C12-C13-C15-C16
26	3	602	CLA	C2-C3-C5-C6
26	B	602	CLA	C11-C10-C8-C7
26	B	603	CLA	C6-C7-C8-C10
26	B	605	CLA	C3A-C2A-CAA-CBA
26	B	609	CLA	C11-C12-C13-C15
26	C	503	CLA	C6-C7-C8-C10
26	C	512	CLA	C3A-C2A-CAA-CBA
26	D	403	CLA	C12-C13-C15-C16
26	N	602	CLA	C11-C12-C13-C15
26	Y	613	CLA	C11-C10-C8-C7
26	7	602	CLA	C2-C3-C5-C6
26	b	602	CLA	C11-C10-C8-C7
26	b	603	CLA	C6-C7-C8-C10
26	b	605	CLA	C3A-C2A-CAA-CBA
26	b	609	CLA	C11-C12-C13-C15
26	c	503	CLA	C6-C7-C8-C10
26	c	512	CLA	C3A-C2A-CAA-CBA
26	d	403	CLA	C12-C13-C15-C16
26	n	602	CLA	C11-C12-C13-C15
26	y	613	CLA	C11-C10-C8-C7
26	g	611	CLA	CAA-CBA-CGA-O1A
25	S	607	CHL	CAA-CBA-CGA-O2A
25	Y	601	CHL	CAA-CBA-CGA-O2A
25	n	601	CHL	CAA-CBA-CGA-O2A
25	s	607	CHL	CAA-CBA-CGA-O2A
25	y	601	CHL	CAA-CBA-CGA-O2A
30	B	2631	LHG	O7-C7-C8-C9
30	b	2631	LHG	O7-C7-C8-C9
37	A	413	LMG	O7-C10-C11-C12
37	D	411	LMG	O7-C10-C11-C12
37	a	413	LMG	O7-C10-C11-C12
37	d	411	LMG	O7-C10-C11-C12
31	4	623	BCR	C17-C18-C19-C20
31	8	623	BCR	C17-C18-C19-C20
25	G	601	CHL	CAA-CBA-CGA-O1A
25	N	601	CHL	CAA-CBA-CGA-O1A
25	n	601	CHL	CAA-CBA-CGA-O1A
26	6	603	CLA	CAA-CBA-CGA-O1A

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Mol	Chain	Res	Type	Atoms
25	R	608	CHL	C11-C12-C13-C14
25	r	608	CHL	C11-C12-C13-C14
26	R	611	CLA	CAA-CBA-CGA-O2A
26	r	611	CLA	CAA-CBA-CGA-O2A
26	S	611	CLA	C5-C6-C7-C8
26	s	611	CLA	C5-C6-C7-C8
25	g	601	CHL	CAA-CBA-CGA-O1A
26	2	603	CLA	CAA-CBA-CGA-O1A
26	7	602	CLA	CAA-CBA-CGA-O1A
30	C	522	LHG	O9-C7-C8-C9
30	c	522	LHG	O9-C7-C8-C9
39	C	519	DGD	O1A-C1A-C2A-C3A
39	c	519	DGD	O1A-C1A-C2A-C3A
26	B	605	CLA	C5-C6-C7-C8
26	C	509	CLA	C13-C15-C16-C17
26	b	605	CLA	C5-C6-C7-C8
26	c	509	CLA	C13-C15-C16-C17
26	2	602	CLA	CAA-CBA-CGA-O2A
26	R	601	CLA	CAA-CBA-CGA-O2A
26	Y	602	CLA	CAA-CBA-CGA-O2A
26	6	602	CLA	CAA-CBA-CGA-O2A
26	y	602	CLA	CAA-CBA-CGA-O2A
30	C	523	LHG	O7-C7-C8-C9
30	c	523	LHG	O7-C7-C8-C9
37	Z	101	LMG	O7-C10-C11-C12
37	z	101	LMG	O7-C10-C11-C12
25	G	607	CHL	C2C-C3C-CAC-CBC
25	2	607	CHL	CAA-CBA-CGA-O1A
25	6	607	CHL	CAA-CBA-CGA-O1A
26	3	602	CLA	CAA-CBA-CGA-O1A
26	C	510	CLA	CAA-CBA-CGA-O1A
25	3	607	CHL	C4C-C3C-CAC-CBC
25	G	607	CHL	C4C-C3C-CAC-CBC
25	7	607	CHL	C4C-C3C-CAC-CBC
25	r	607	CHL	C4C-C3C-CAC-CBC
26	N	610	CLA	C8-C10-C11-C12
26	n	610	CLA	C8-C10-C11-C12
25	g	607	CHL	C2C-C3C-CAC-CBC
25	S	607	CHL	CAA-CBA-CGA-O1A
25	s	607	CHL	CAA-CBA-CGA-O1A
30	B	2631	LHG	O9-C7-C8-C9
25	R	607	CHL	C4C-C3C-CAC-CBC

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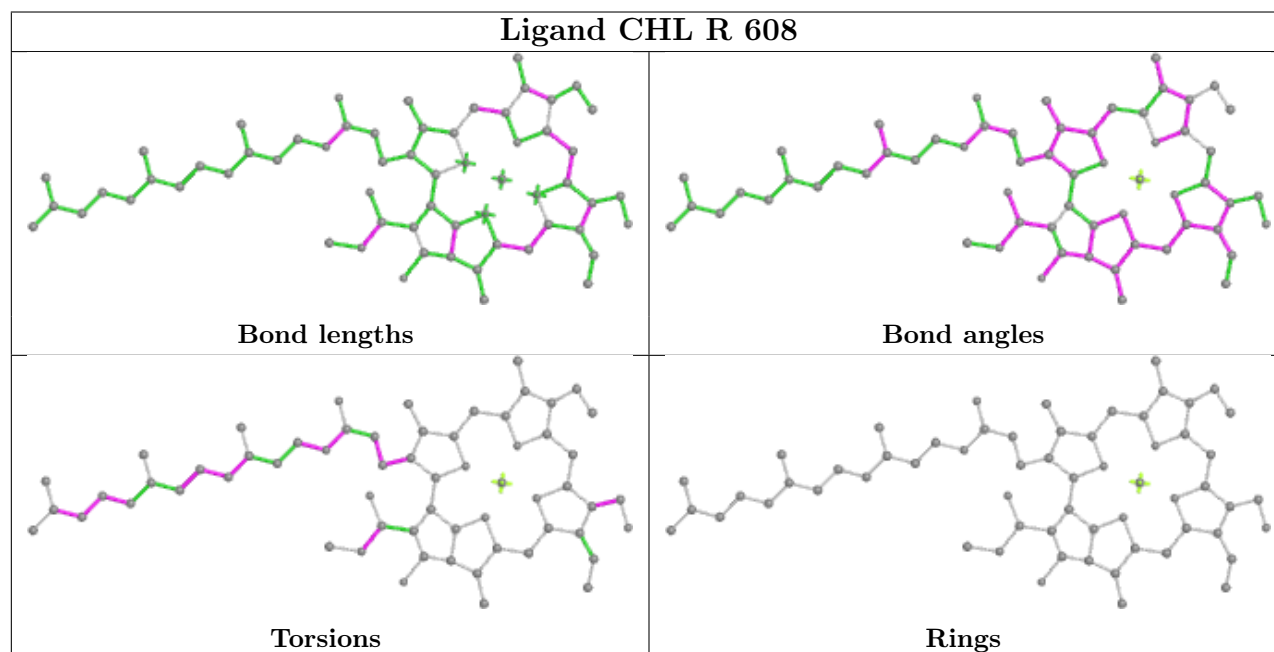
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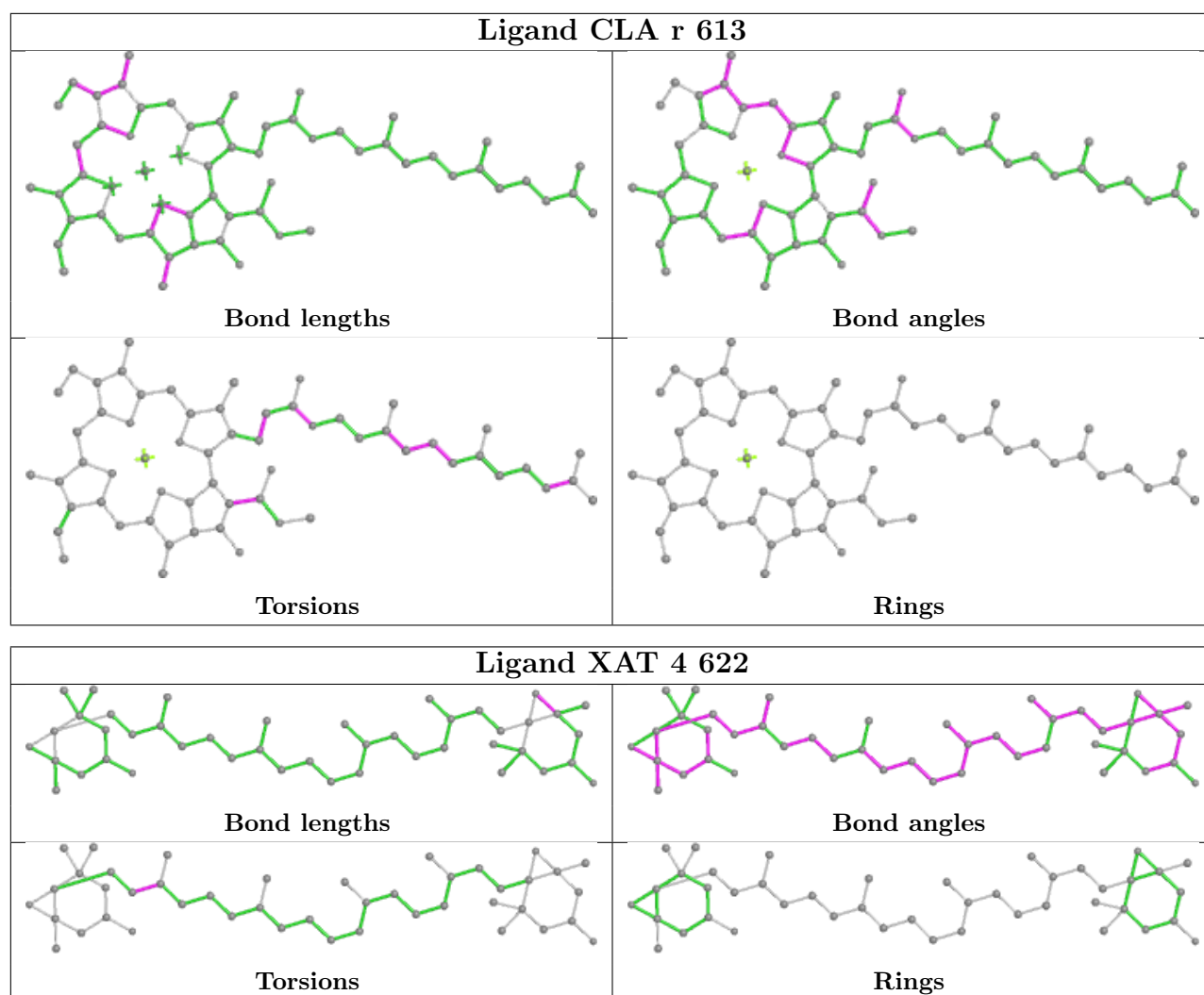
Mol	Chain	Res	Type	Atoms
26	B	613	CLA	CAA-CBA-CGA-O2A
26	N	602	CLA	CAA-CBA-CGA-O2A
26	b	613	CLA	CAA-CBA-CGA-O2A
26	r	601	CLA	CAA-CBA-CGA-O2A

There are no ring outliers.

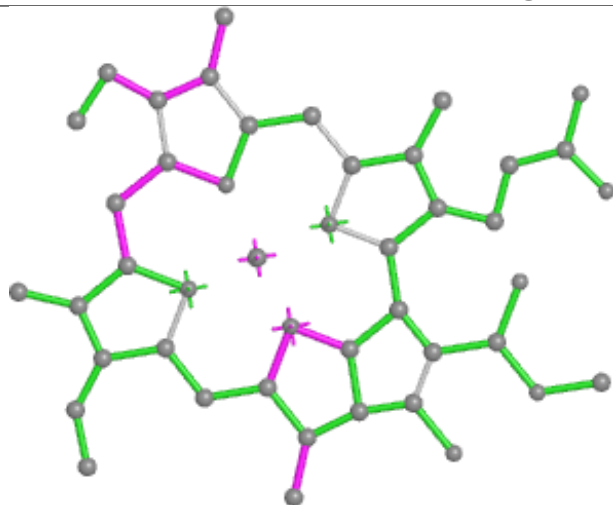
No monomer is involved in short contacts.

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.

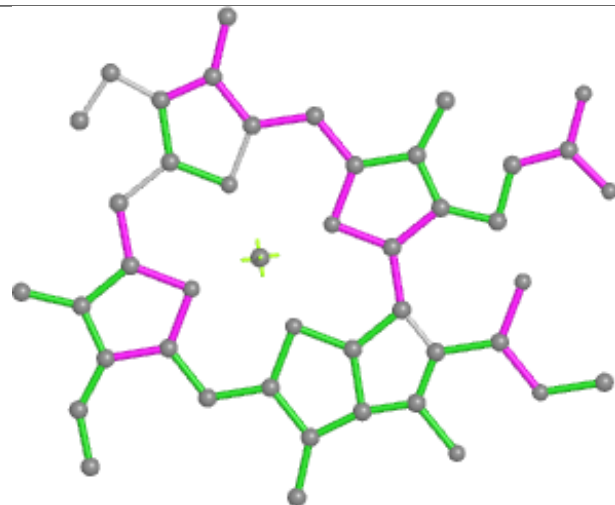




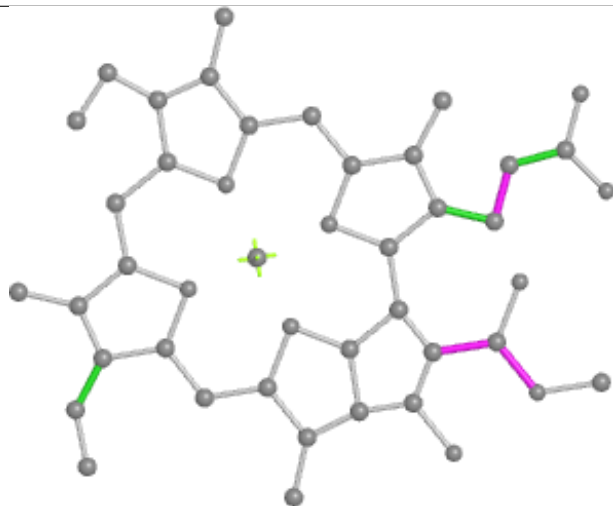
Ligand CLA s 603



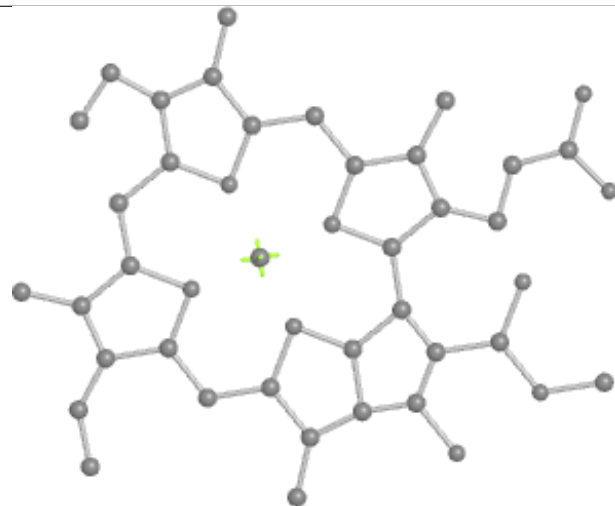
Bond lengths



Bond angles

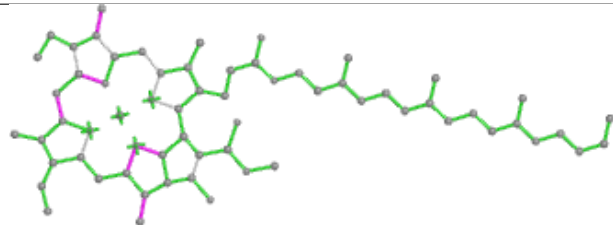


Torsions

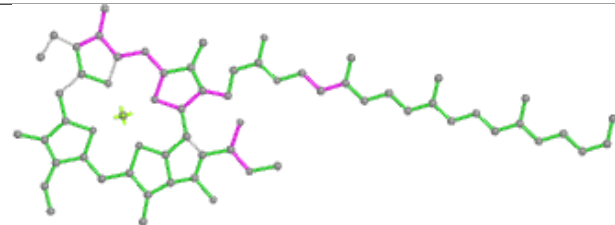


Rings

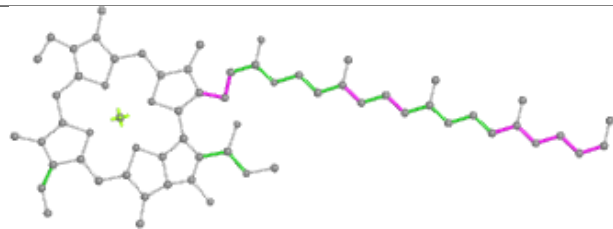
Ligand CLA g 610



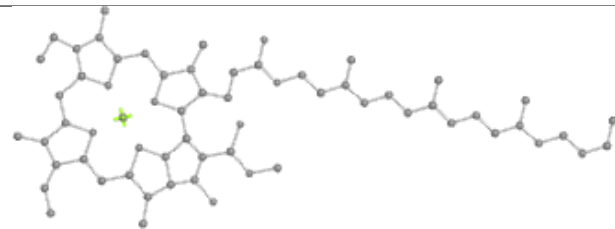
Bond lengths



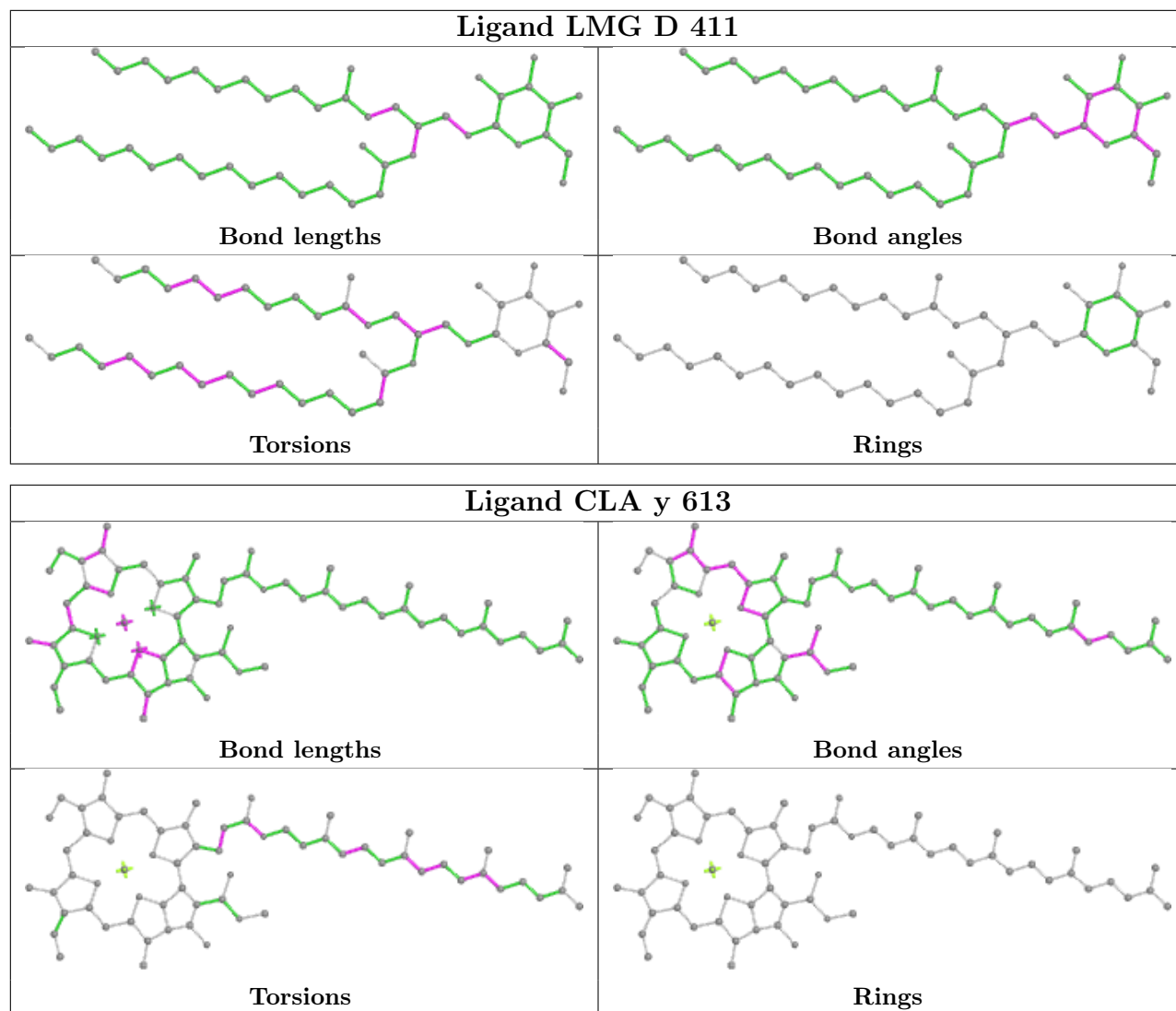
Bond angles



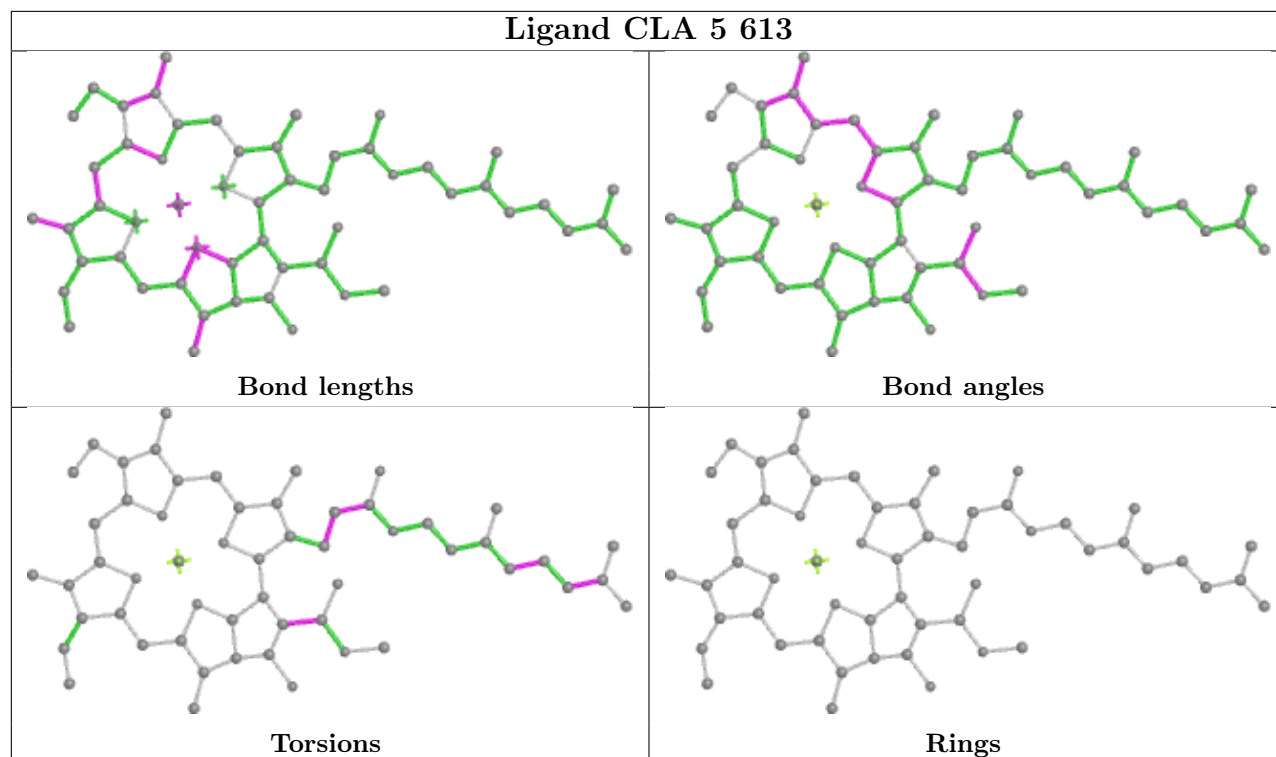
Torsions



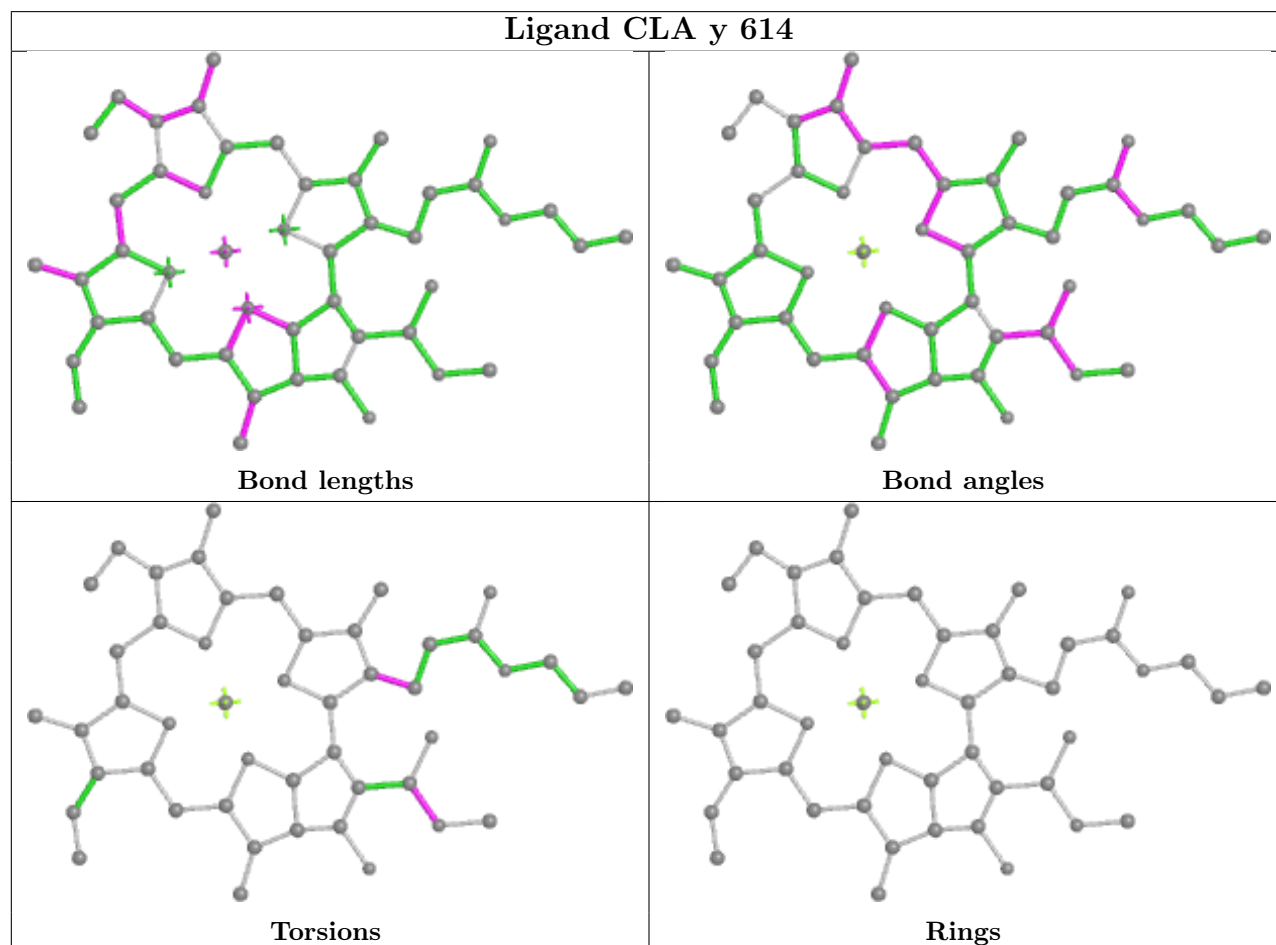
Rings

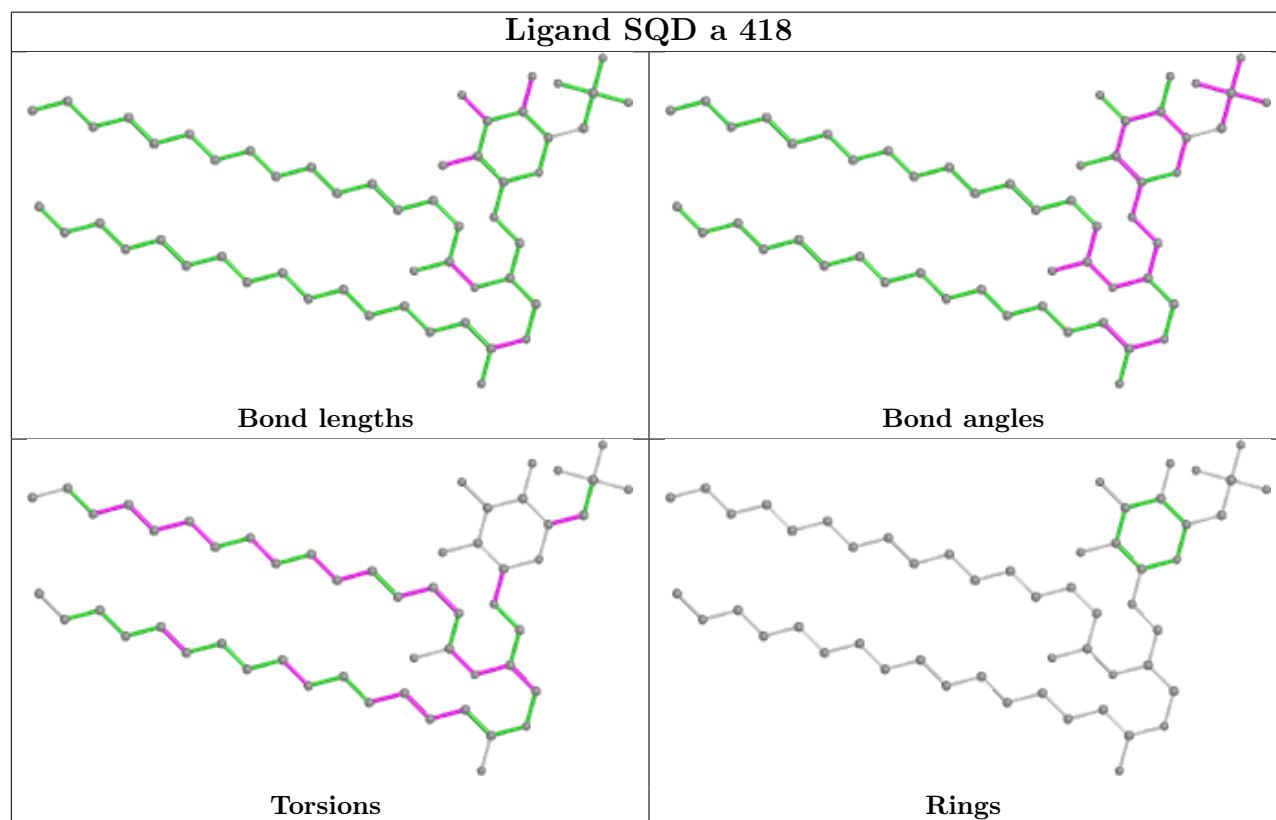
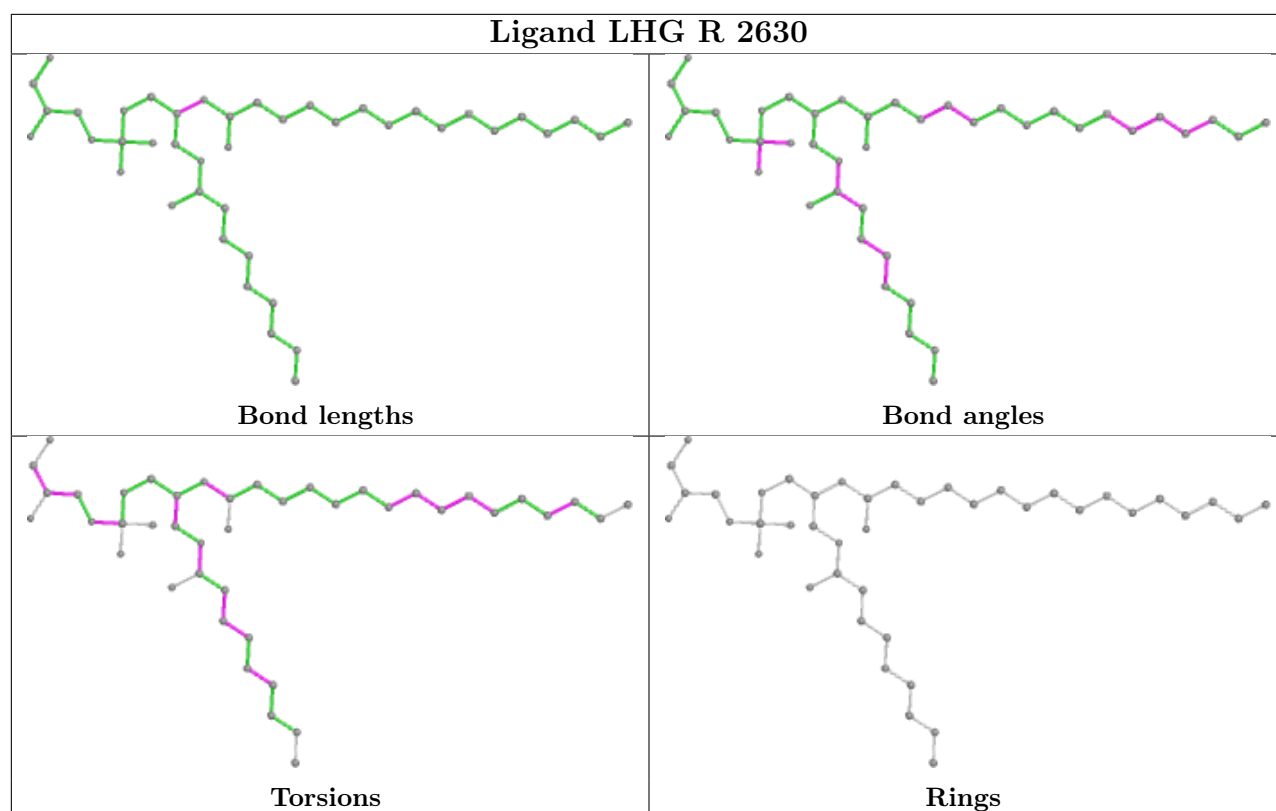


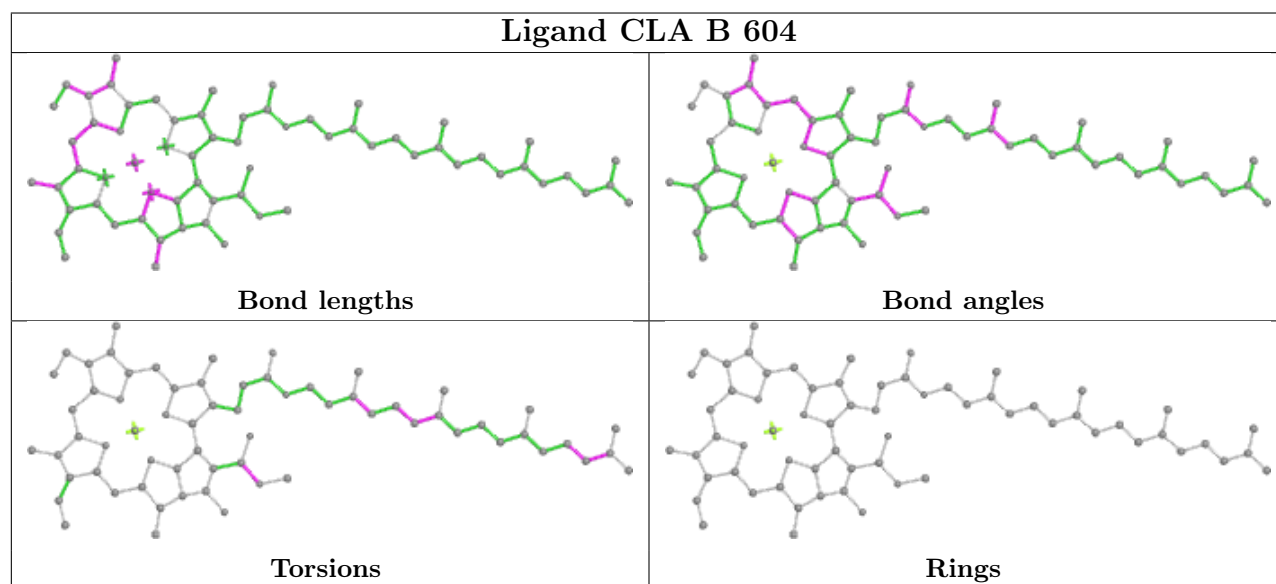
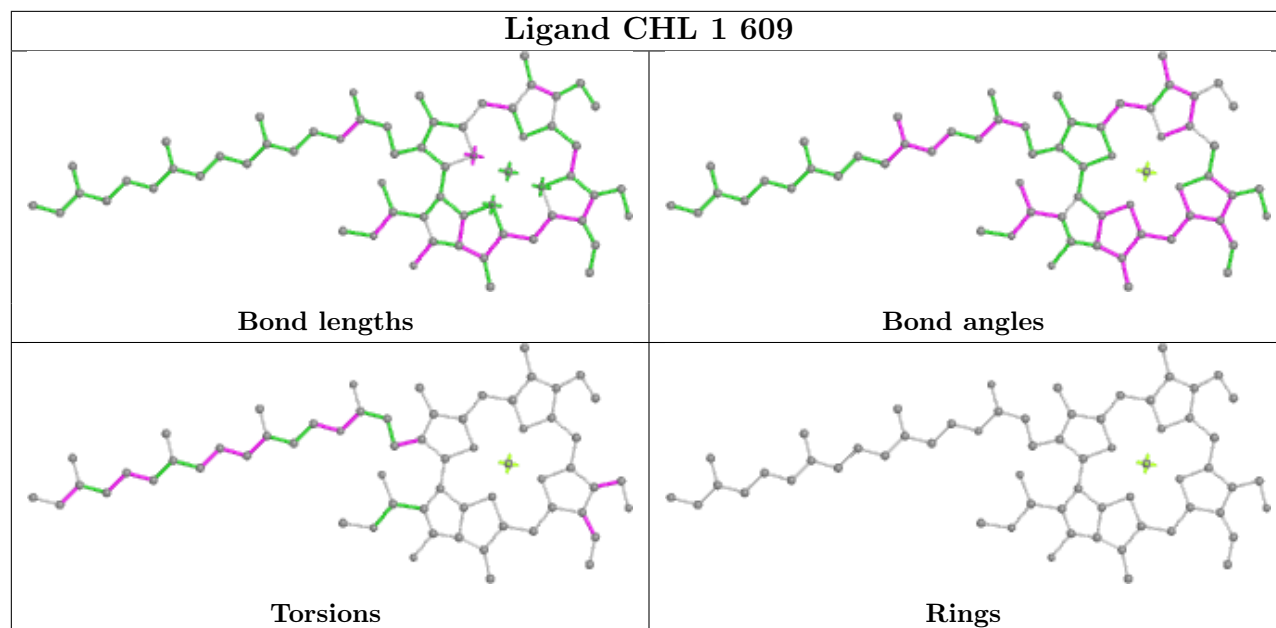
Ligand CLA 5 613

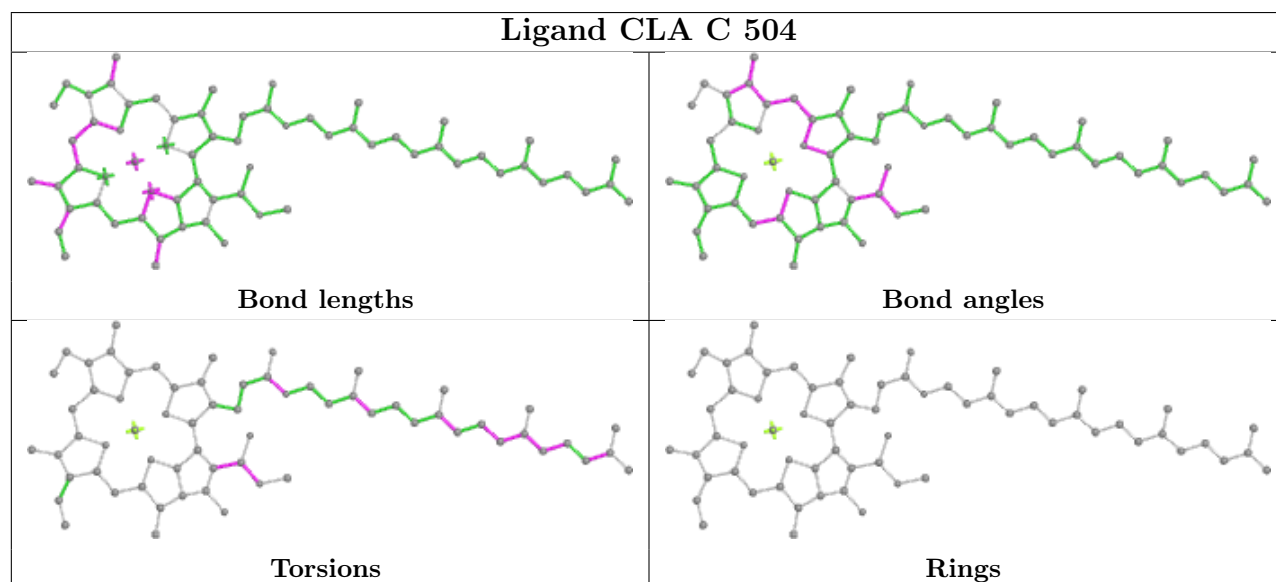
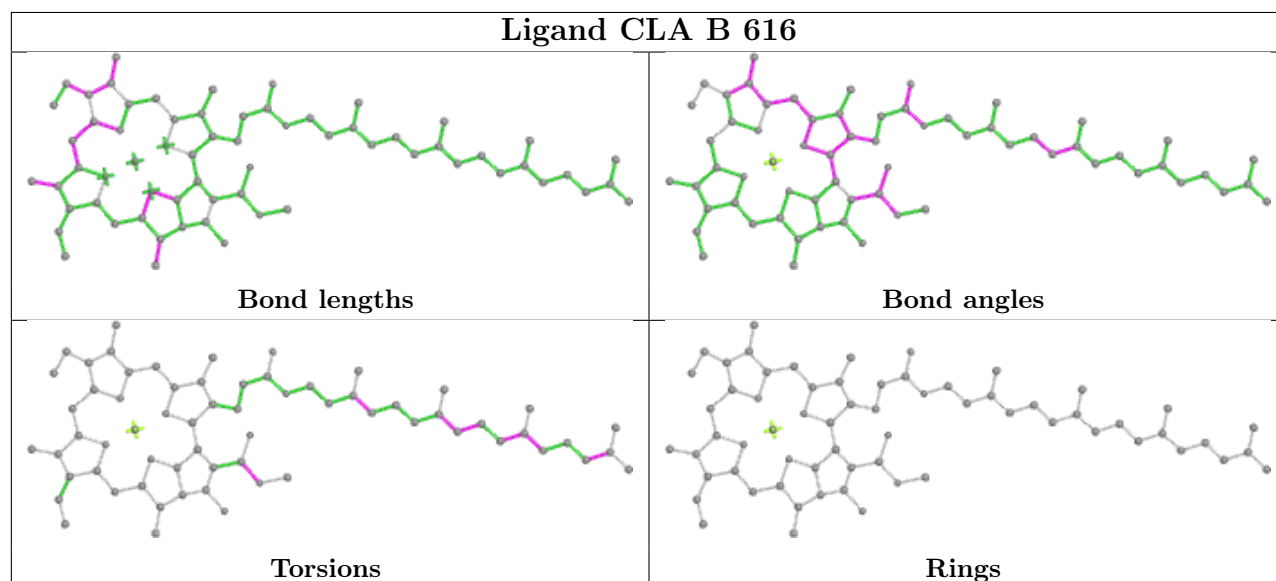
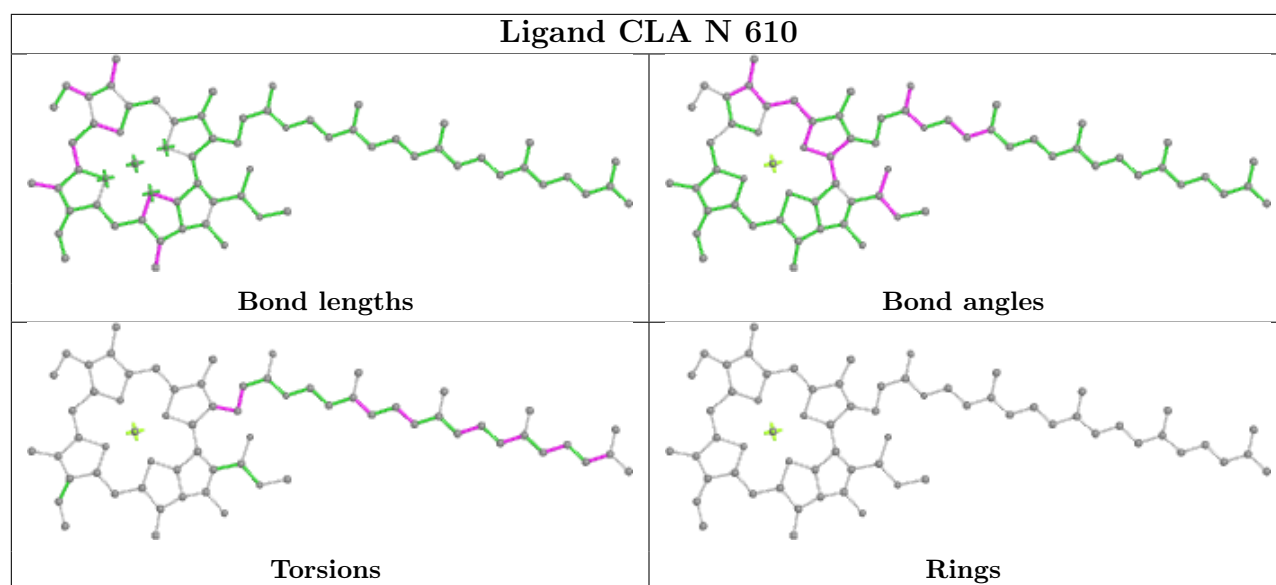


Ligand CLA y 614

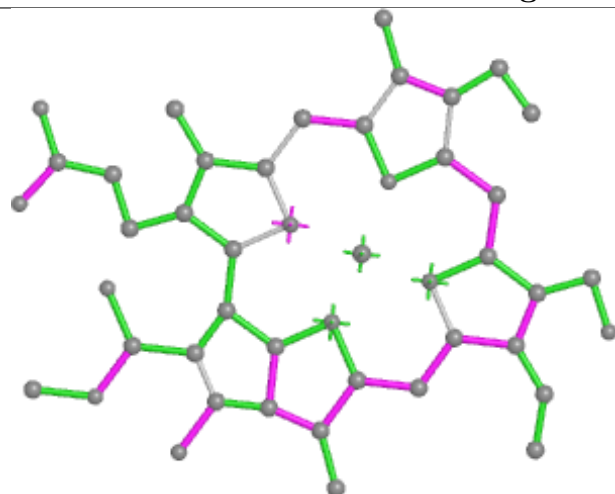




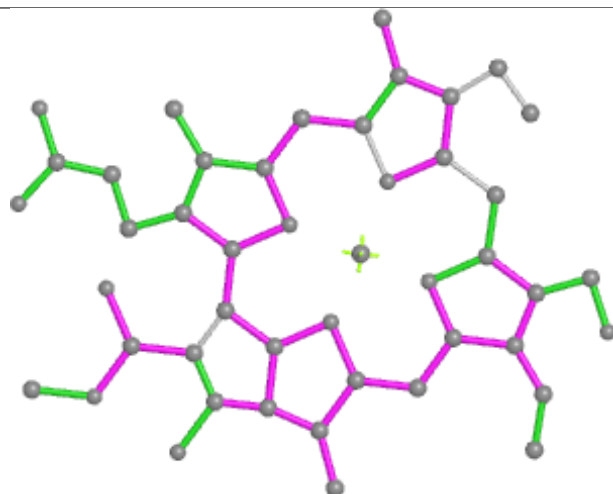




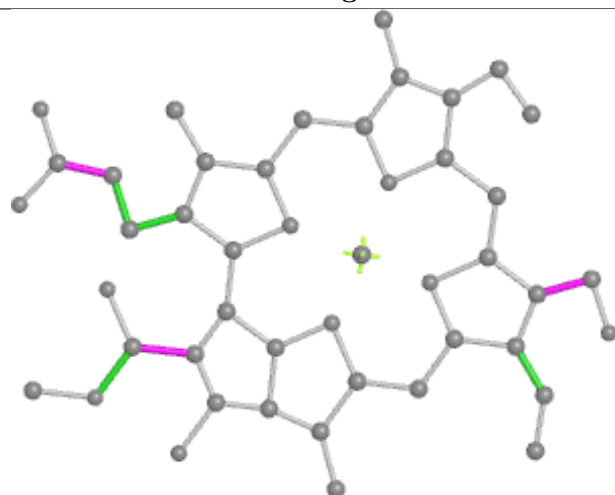
Ligand CHL 1 601



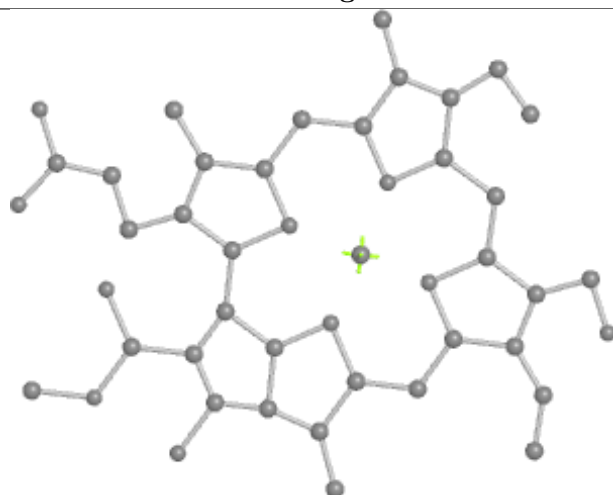
Bond lengths



Bond angles

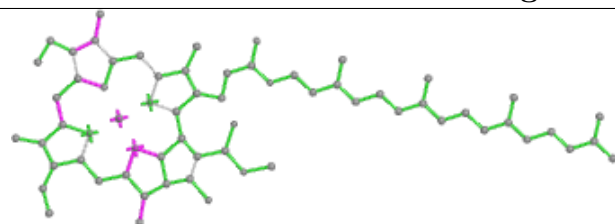


Torsions

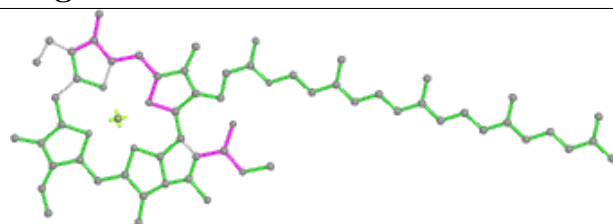


Rings

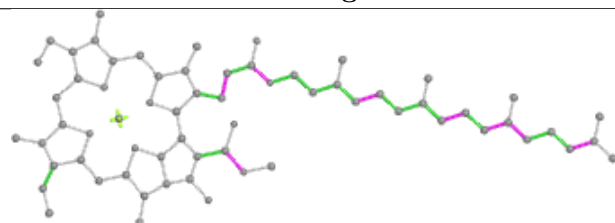
Ligand CLA g 613



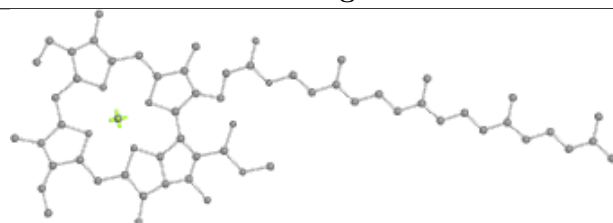
Bond lengths



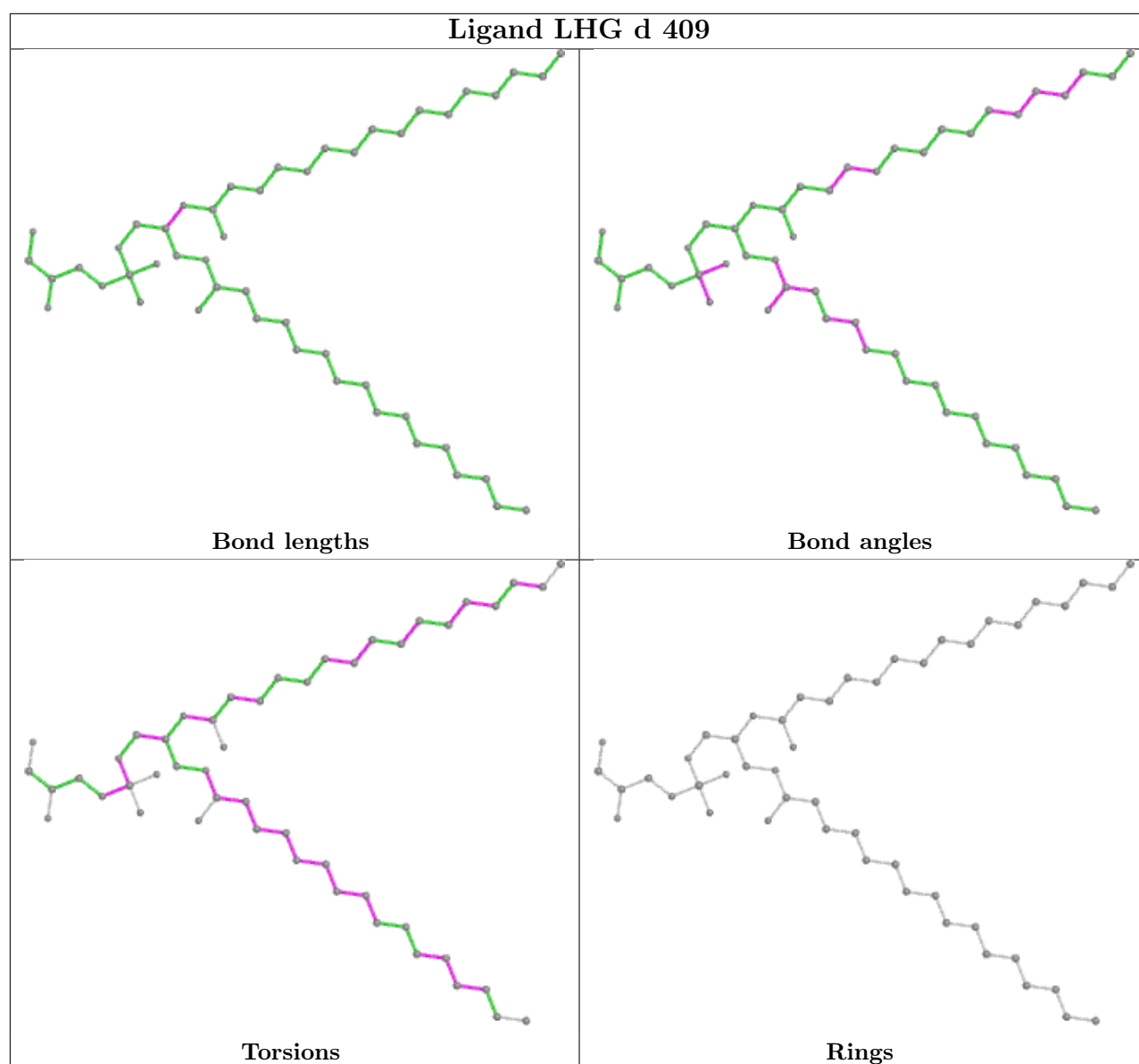
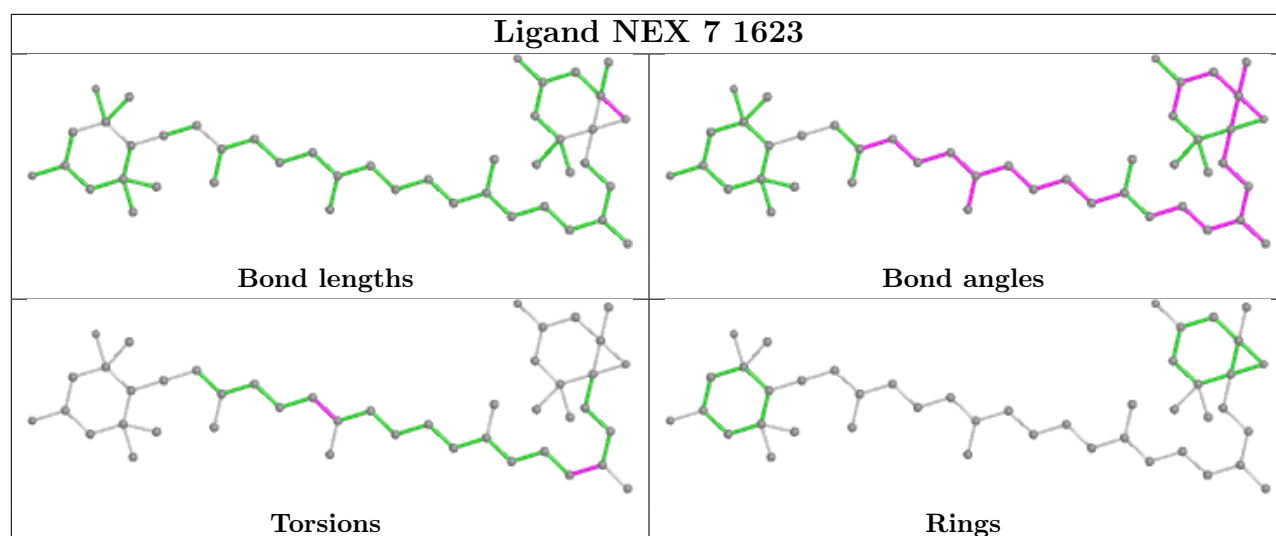
Bond angles

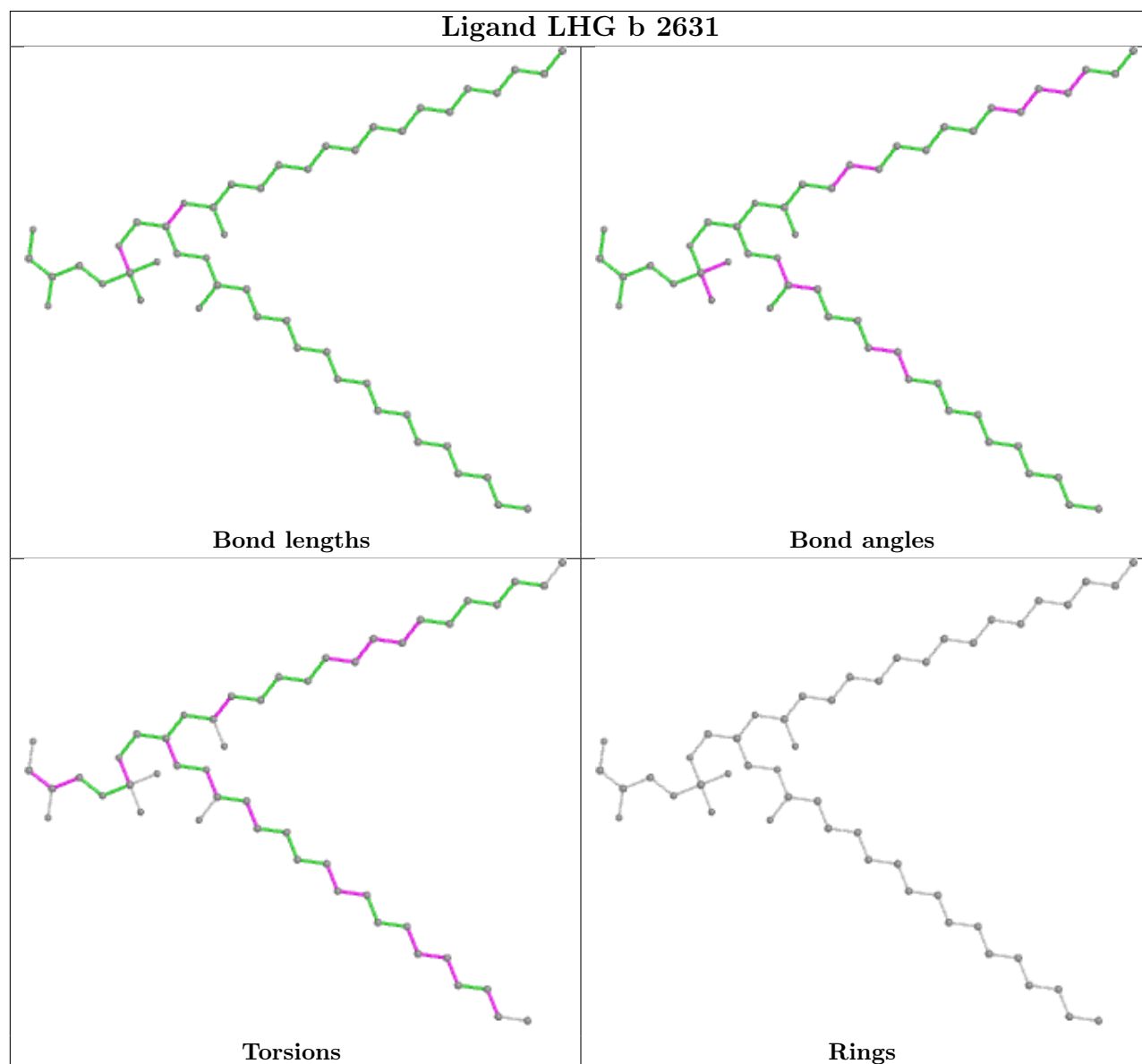
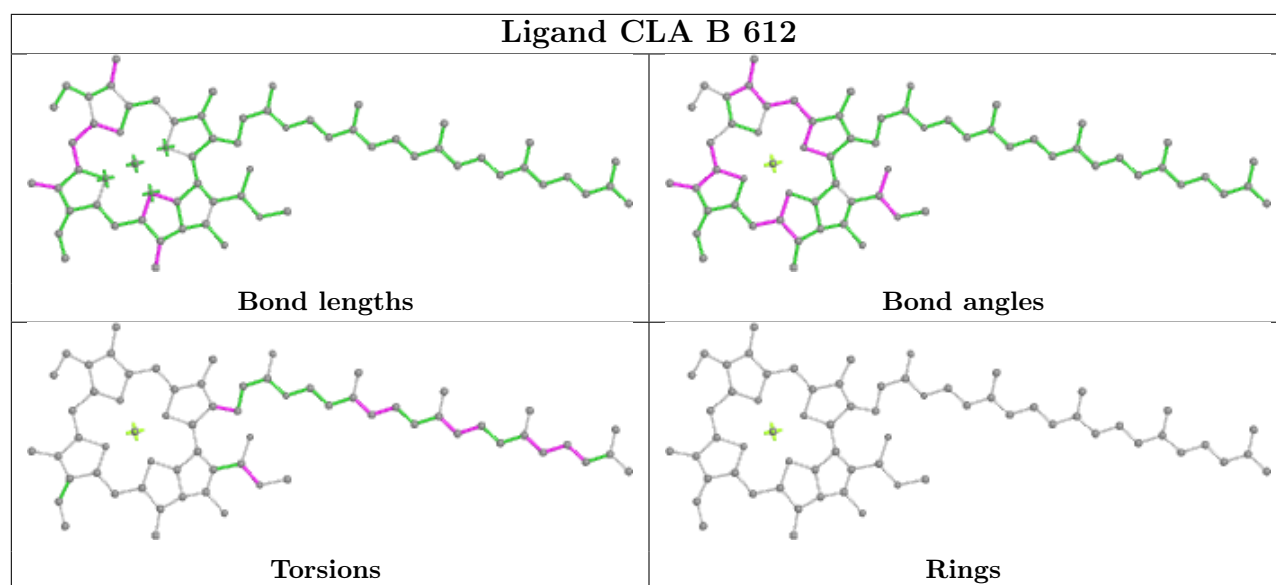


Torsions

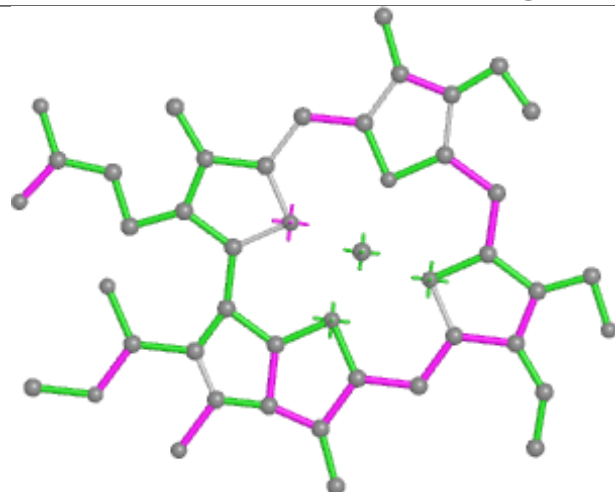


Rings

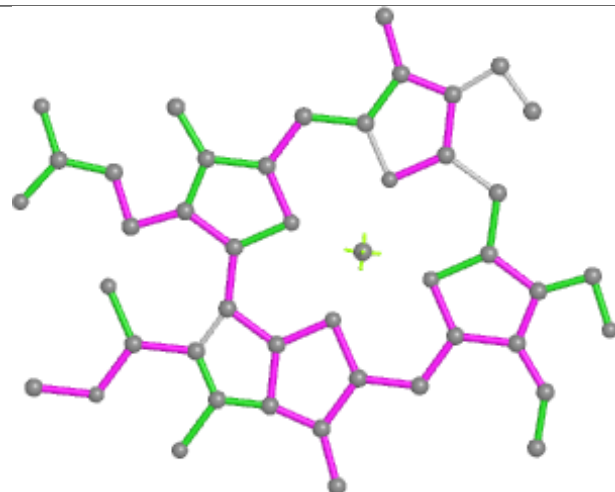




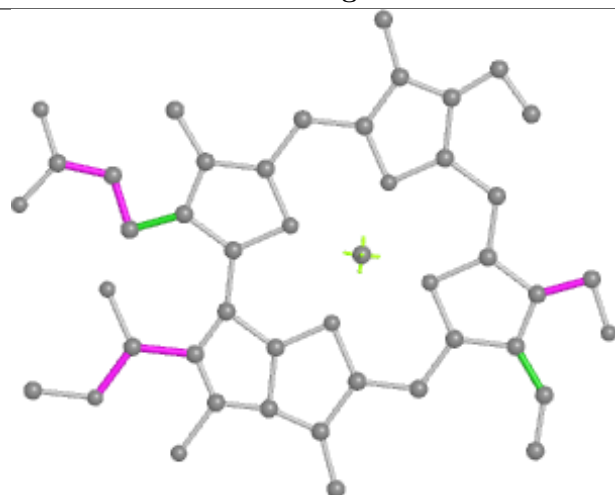
Ligand CHL 1 606



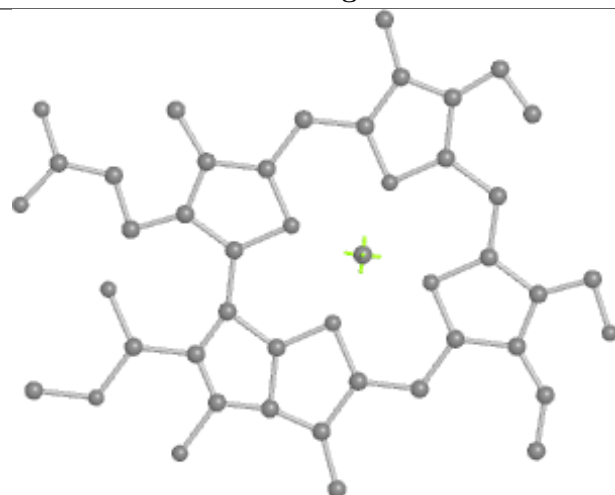
Bond lengths



Bond angles

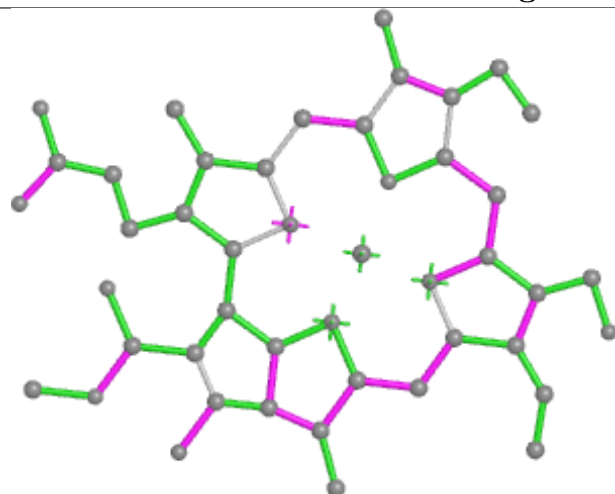


Torsions

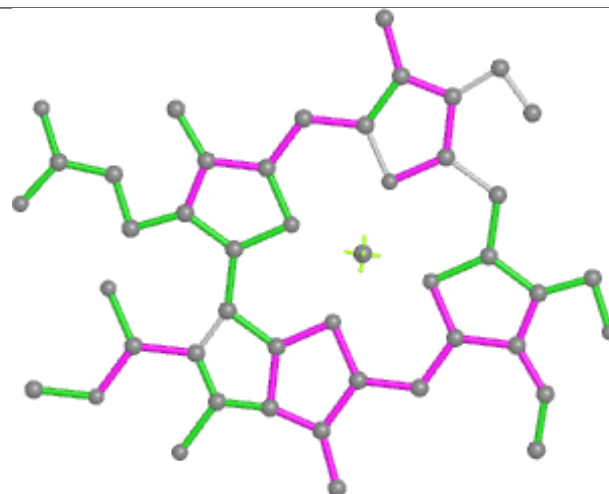


Rings

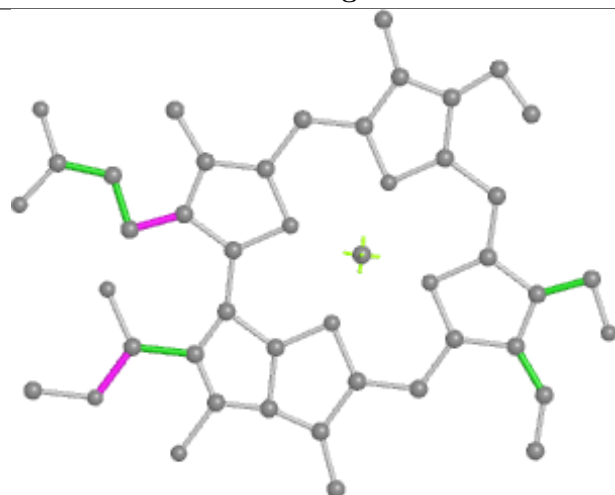
Ligand CHL S 608



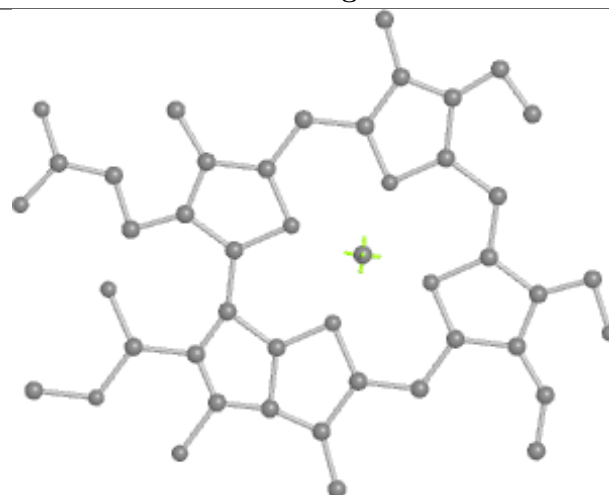
Bond lengths



Bond angles

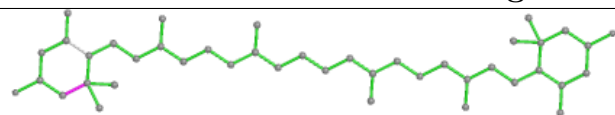


Torsions

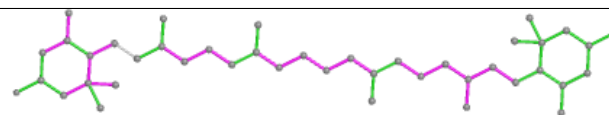


Rings

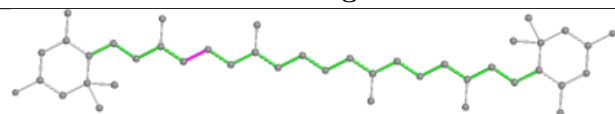
Ligand LUT Y 1621



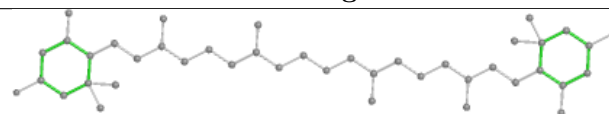
Bond lengths



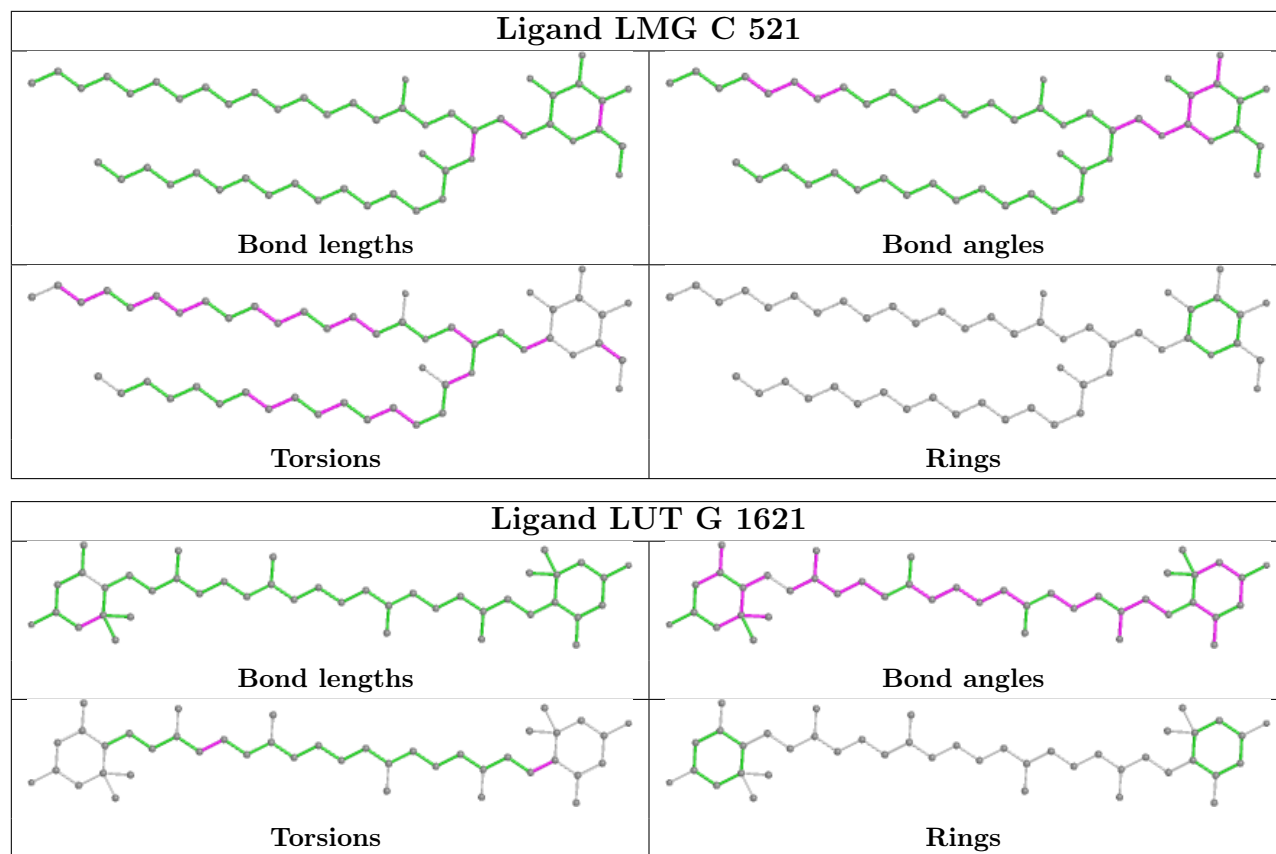
Bond angles

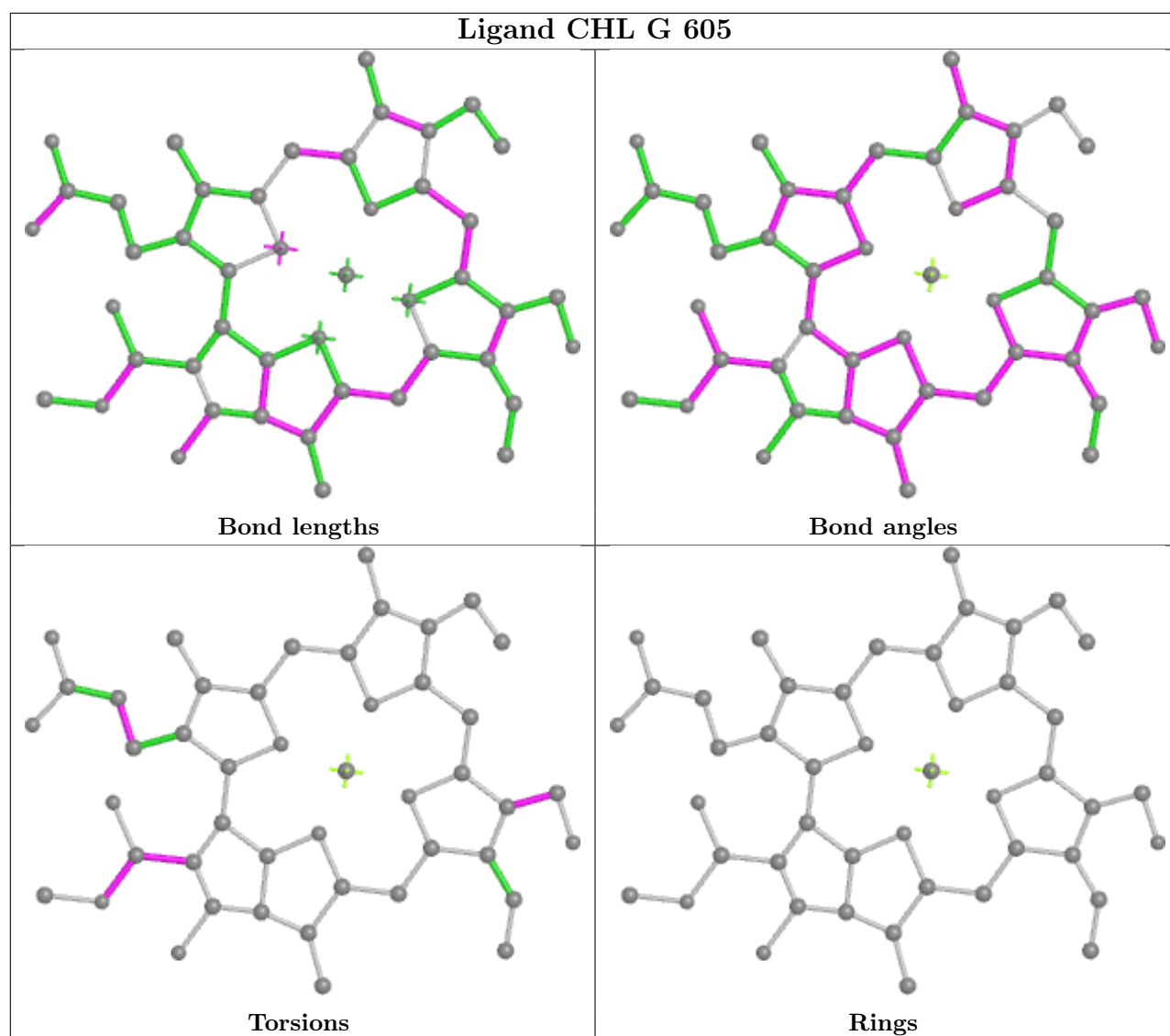


Torsions

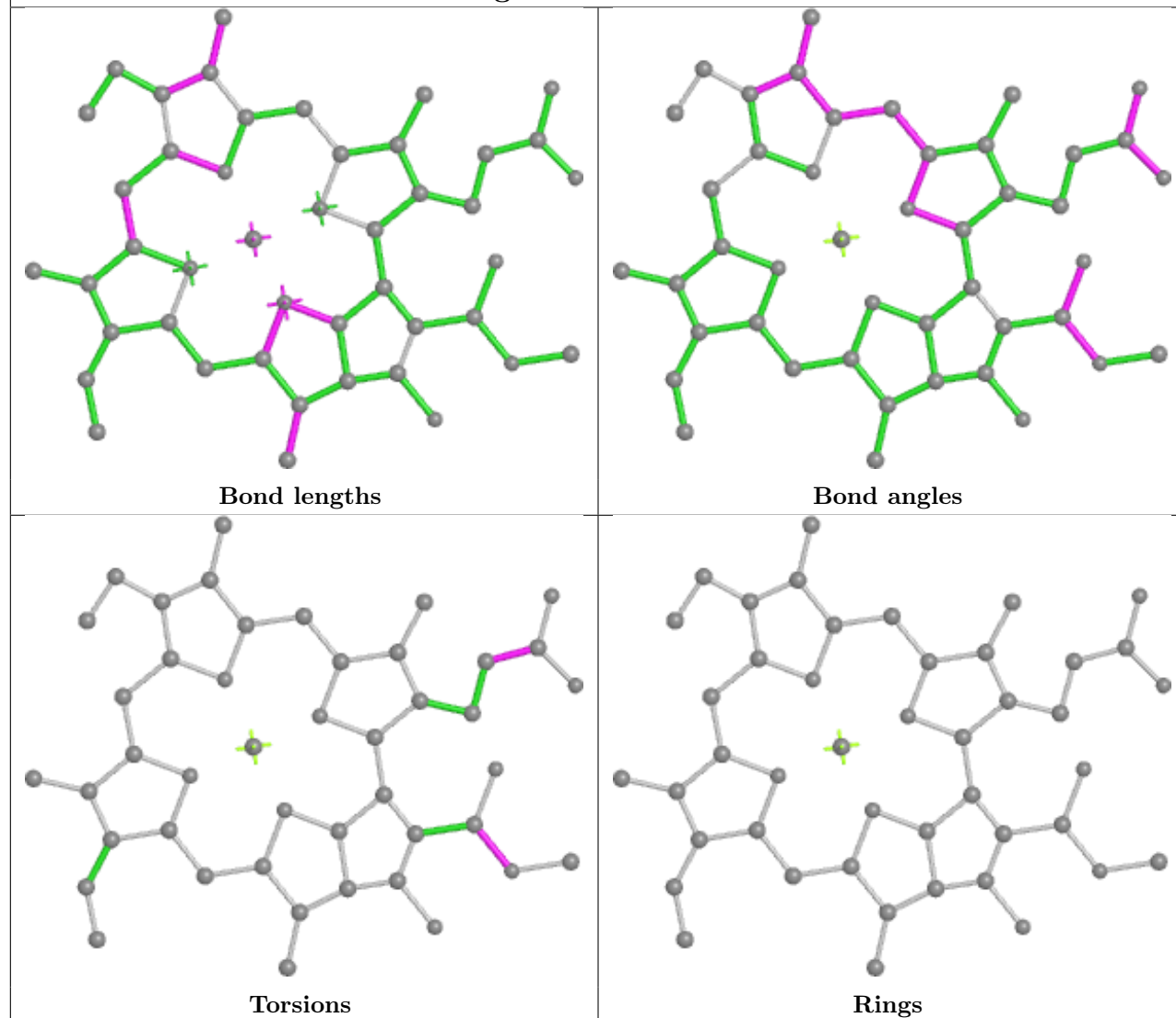


Rings

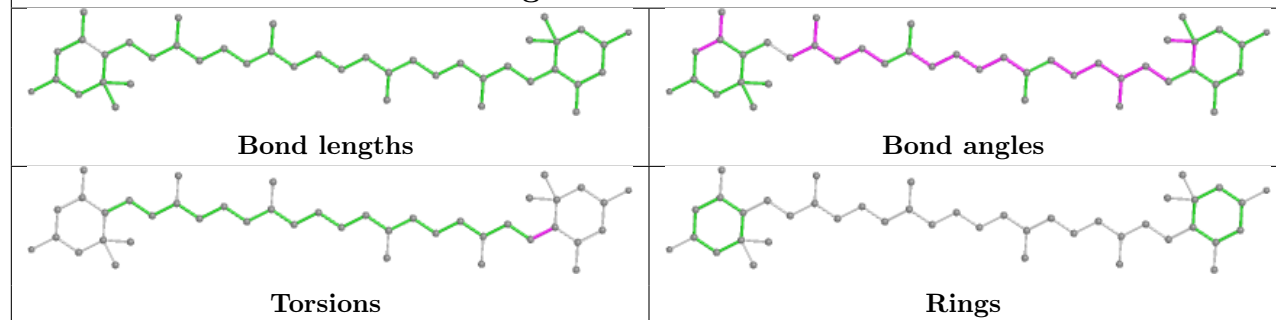


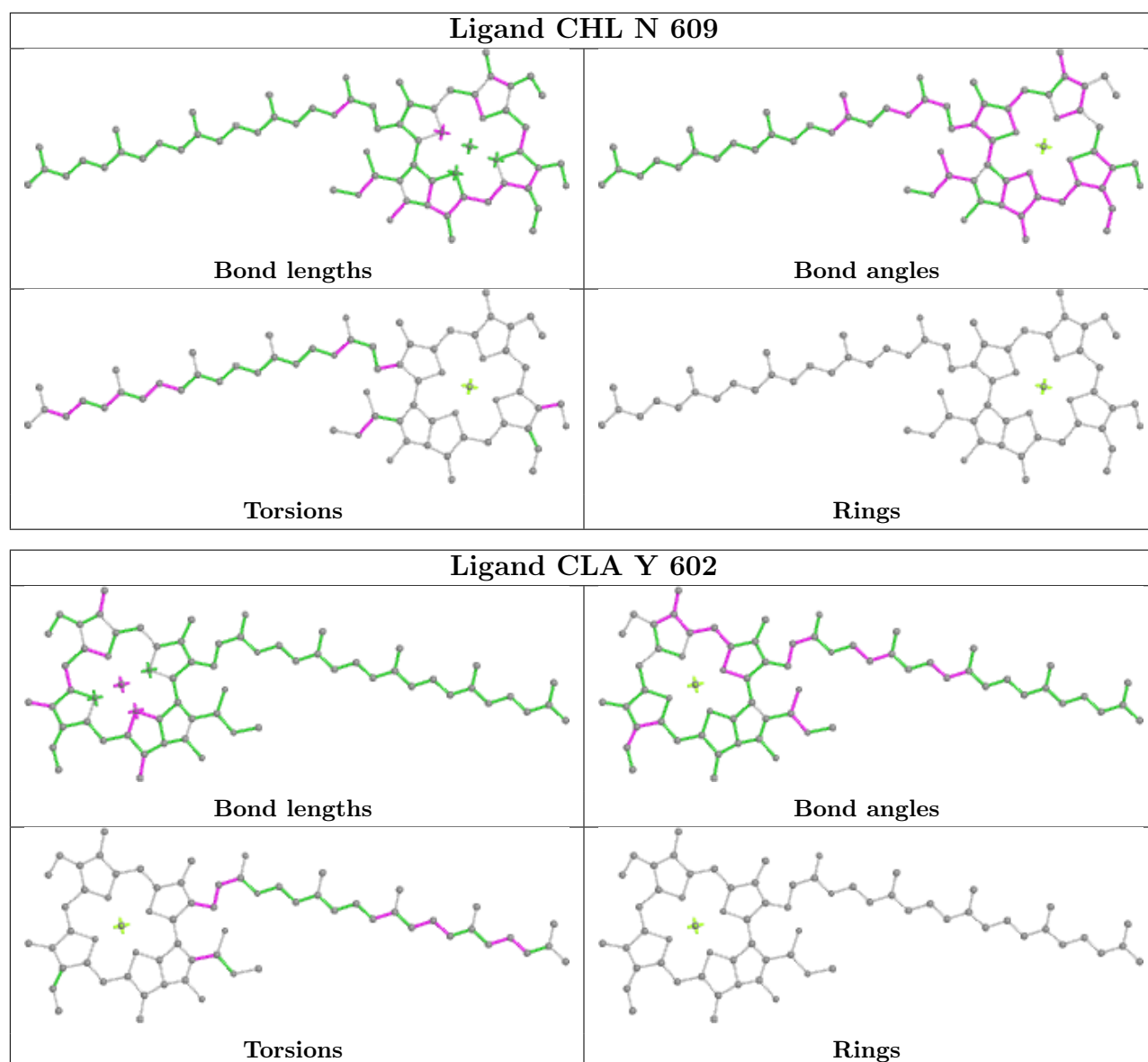


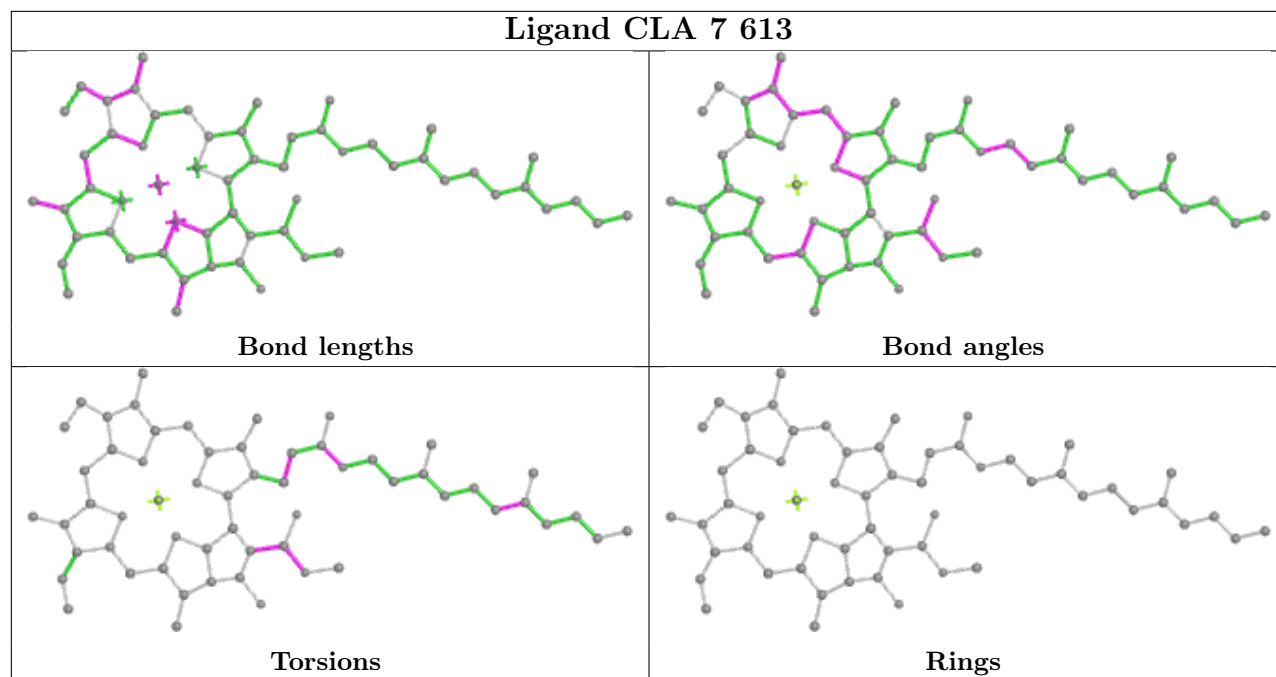
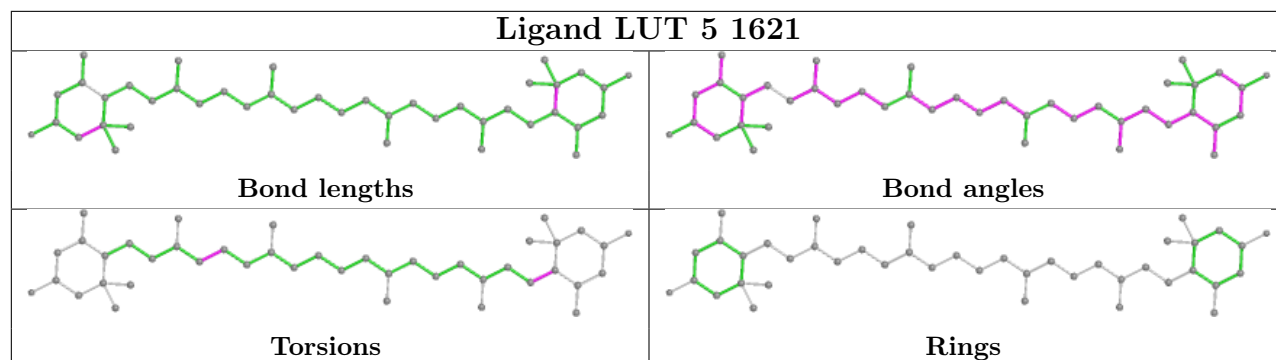
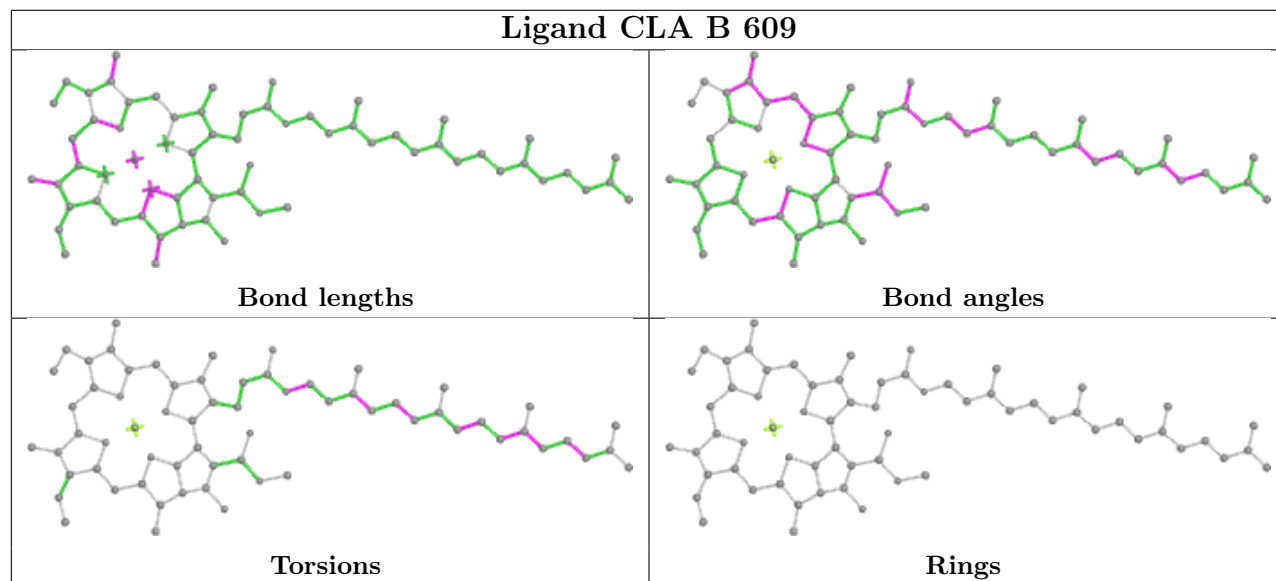
Ligand CLA 4 611

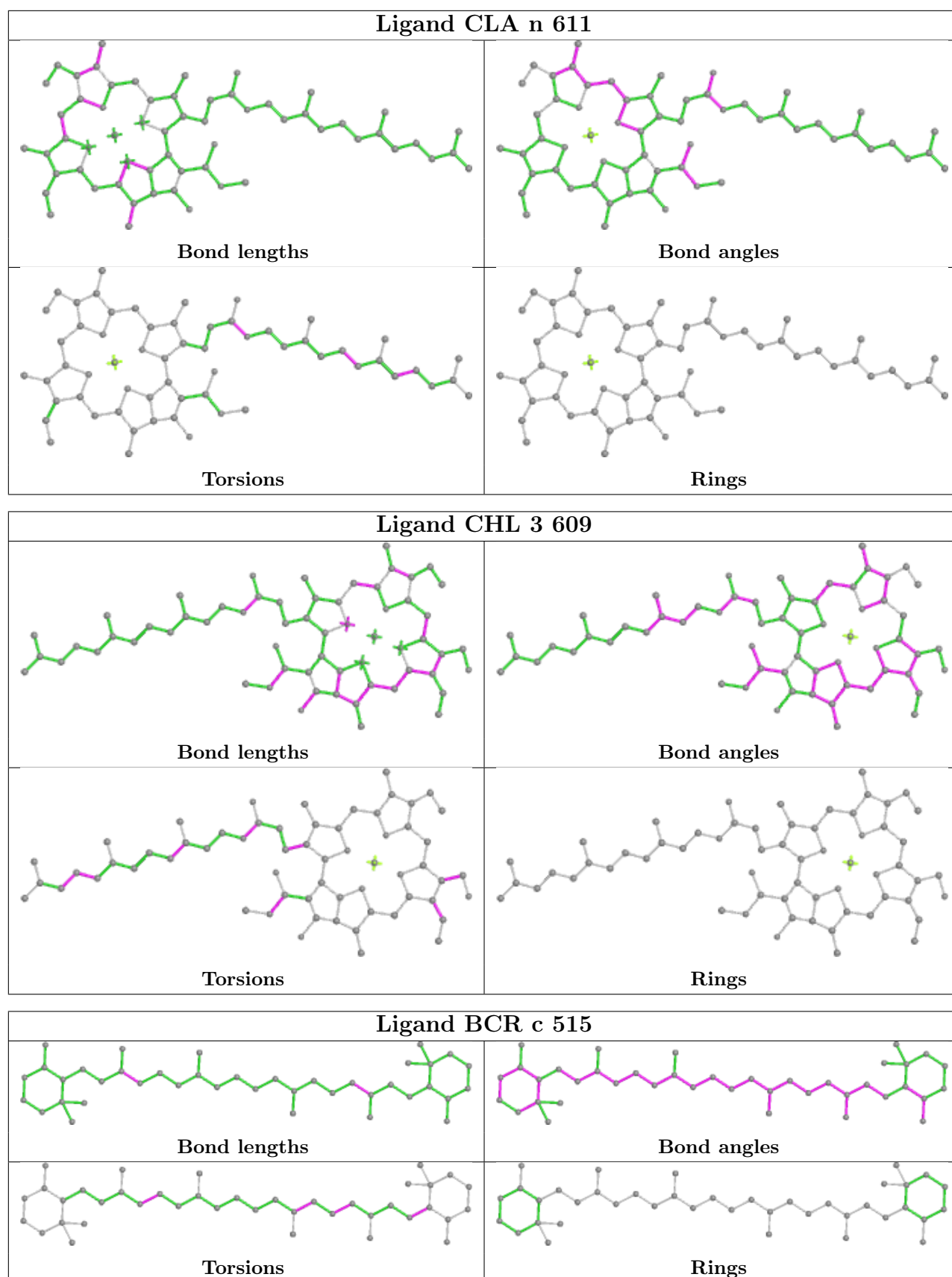


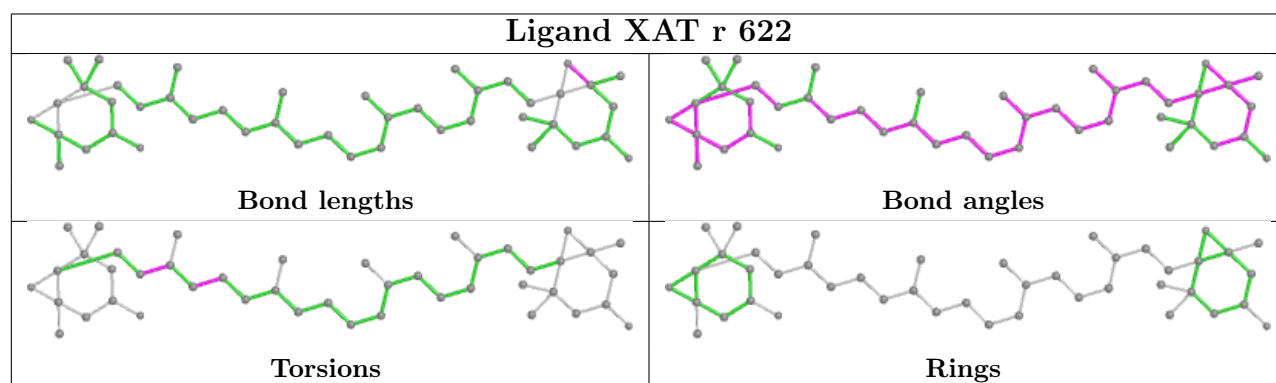
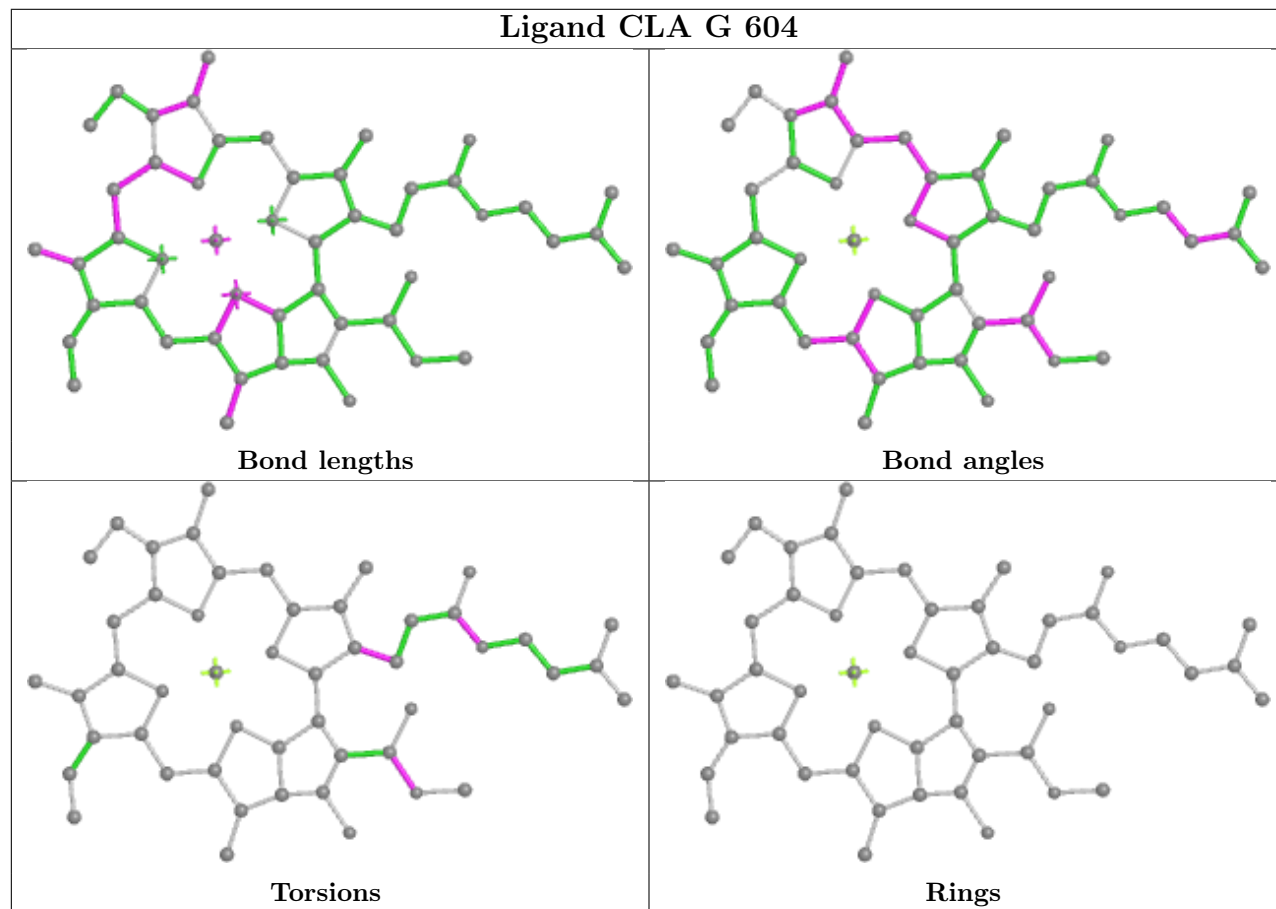
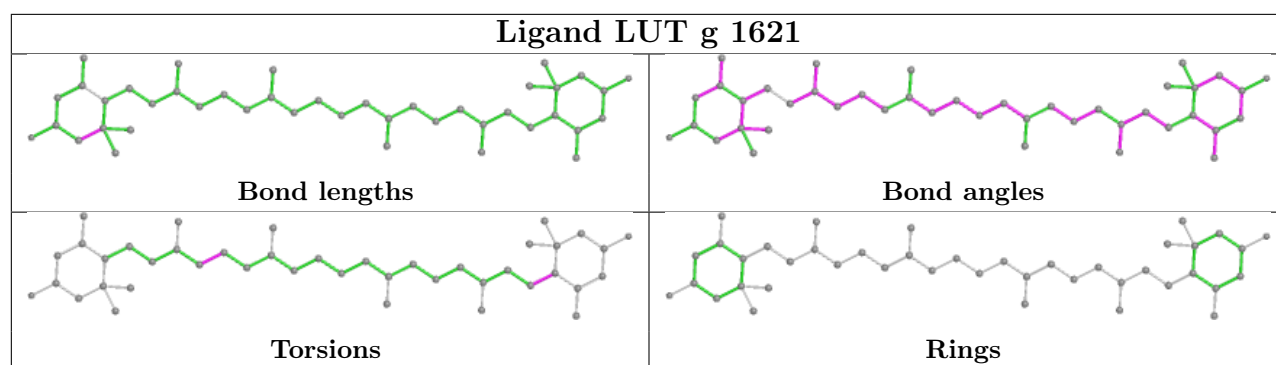
Ligand LUT N 1620

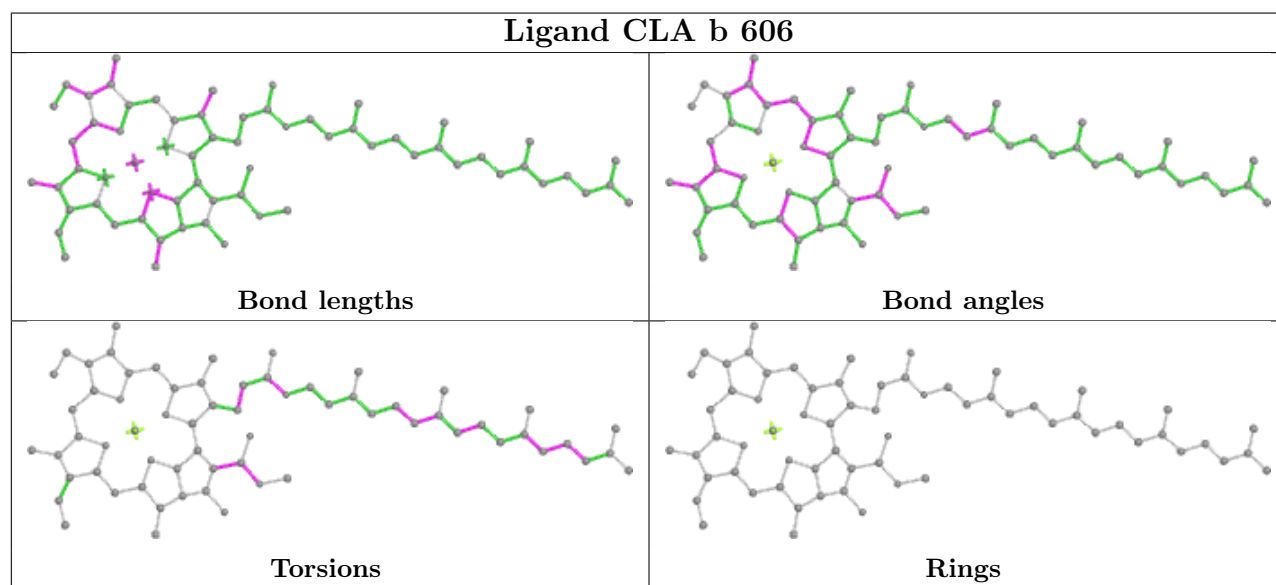
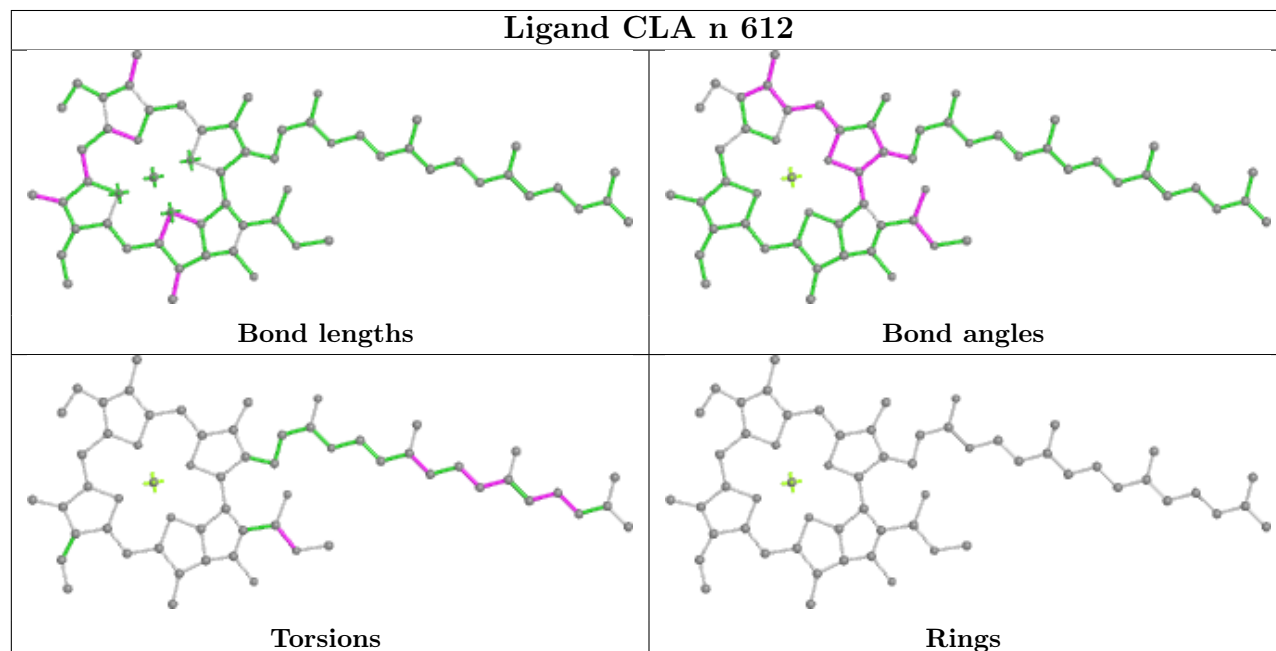
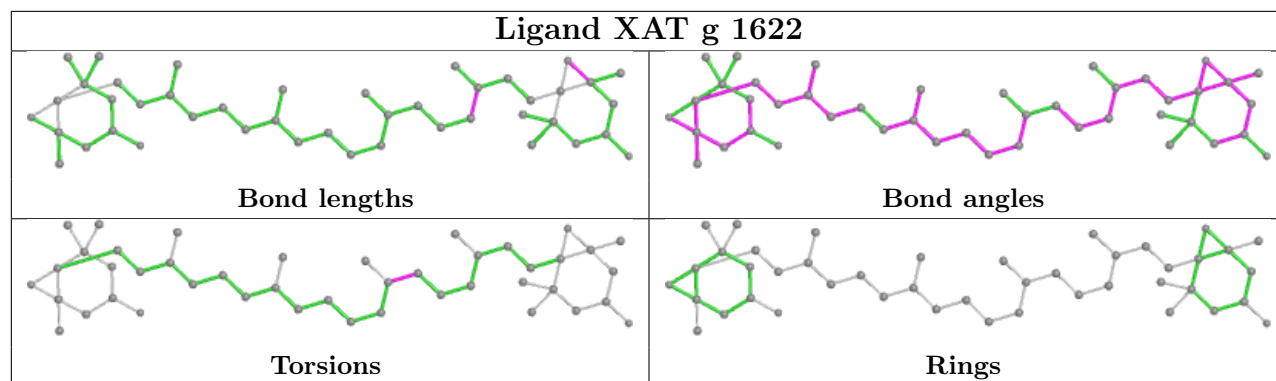




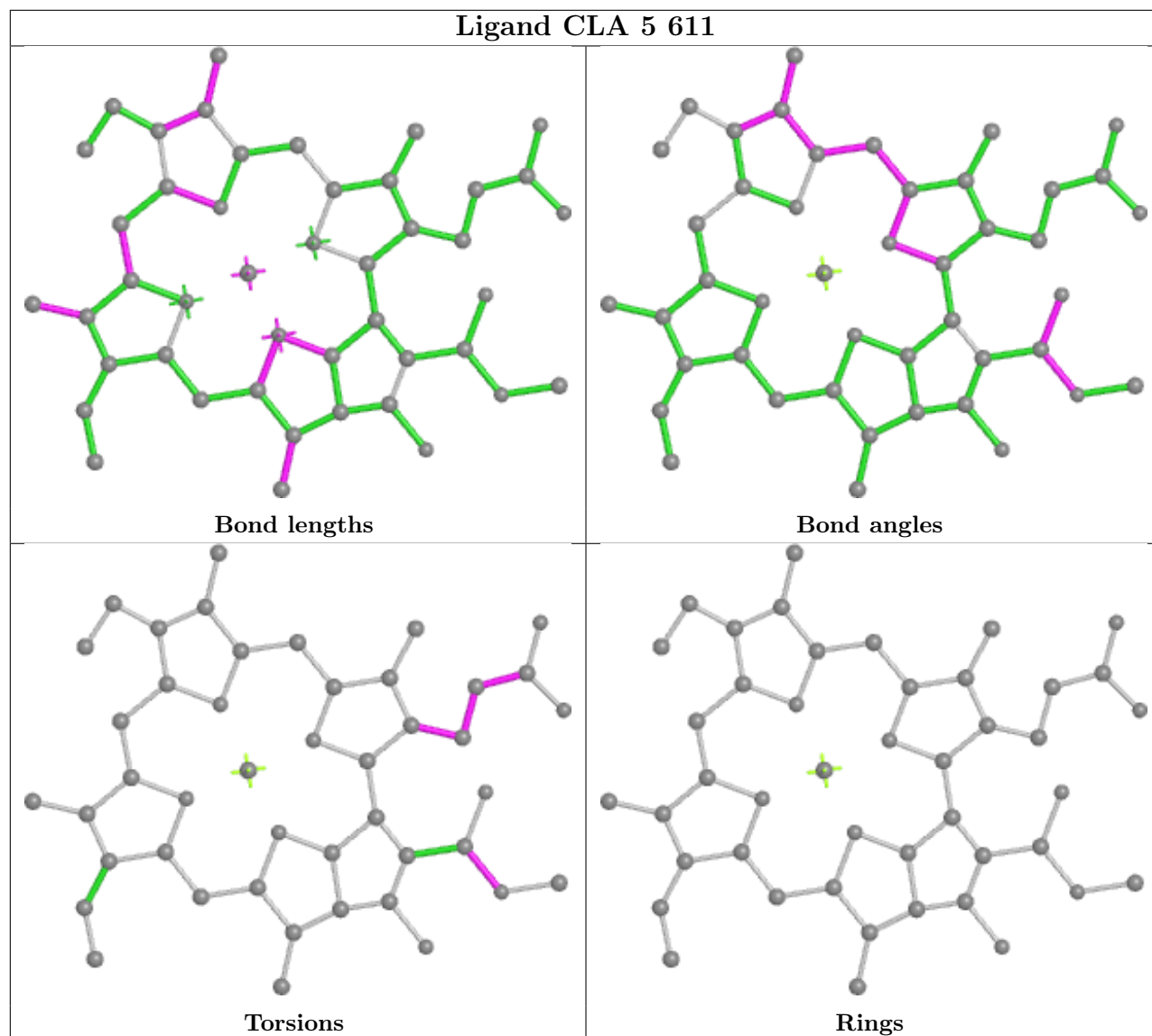
Ligand CLA 7 613**Ligand LUT 5 1621****Ligand CLA B 609**

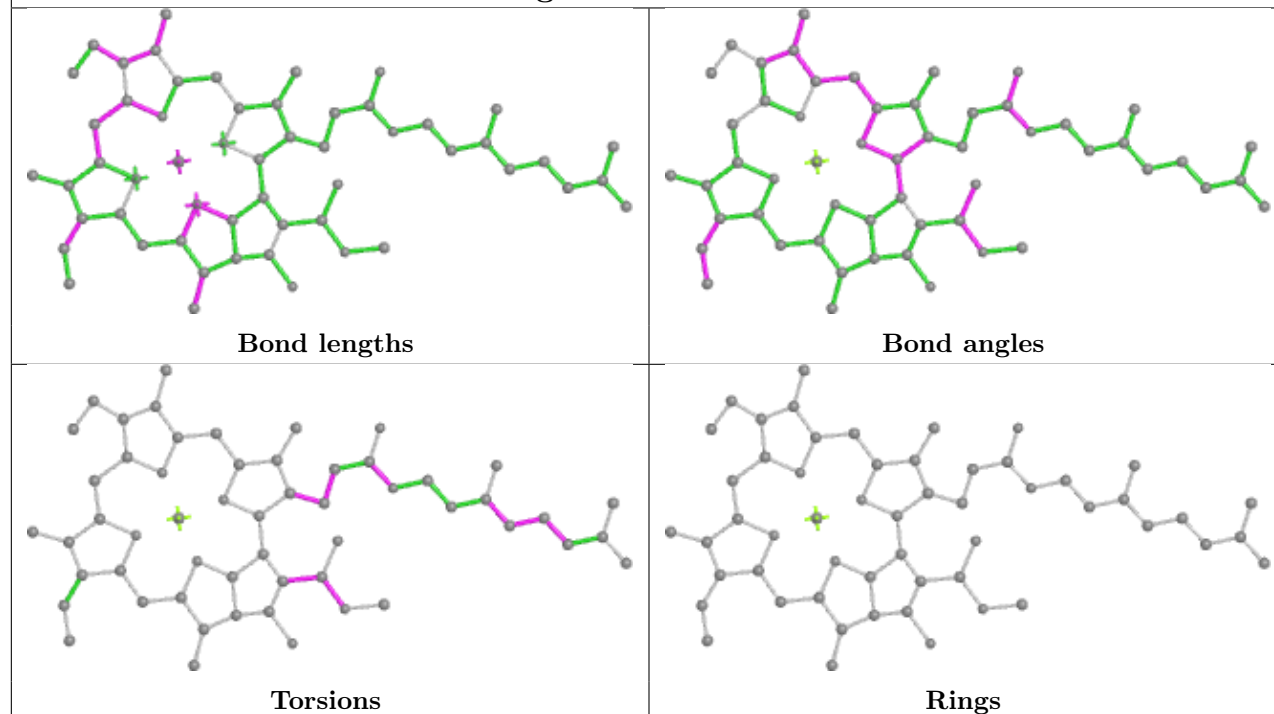
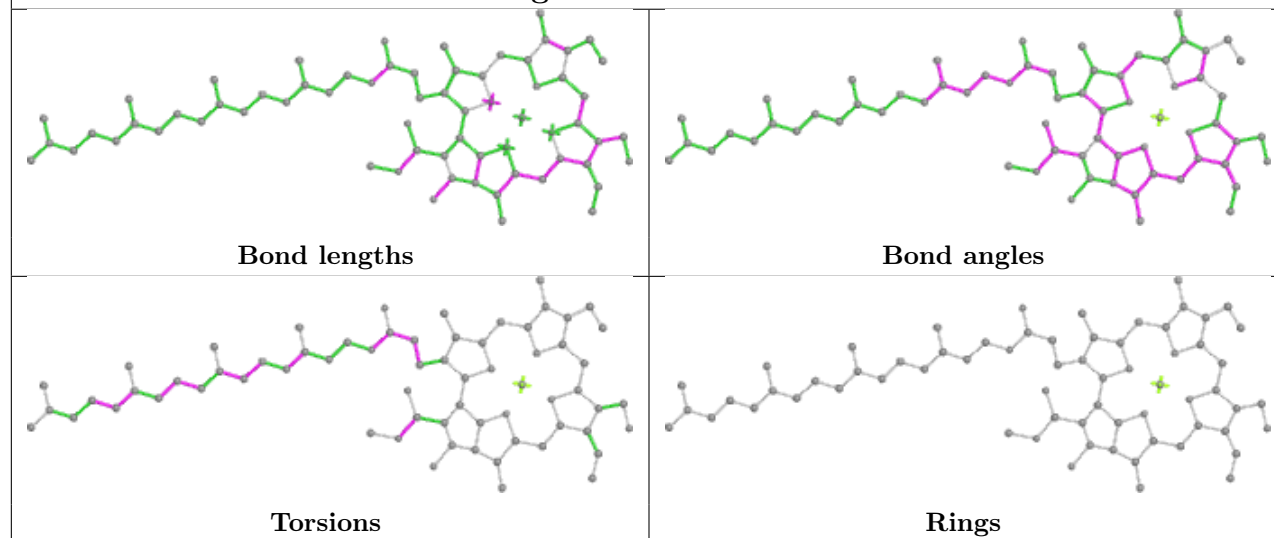




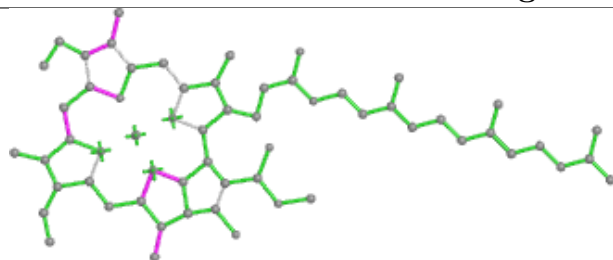


Ligand CLA 5 611

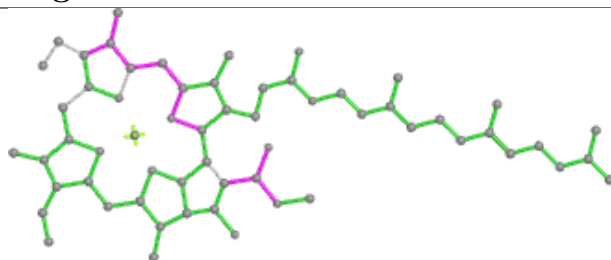


Ligand CLA 3 603**Ligand CHL Y 601**

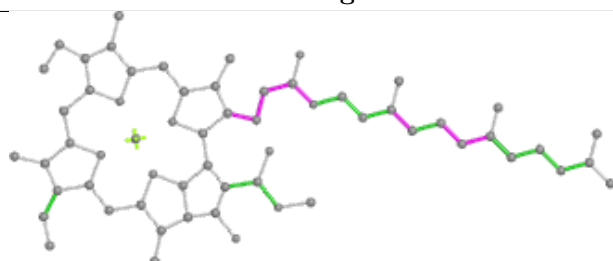
Ligand CLA g 611



Bond lengths



Bond angles

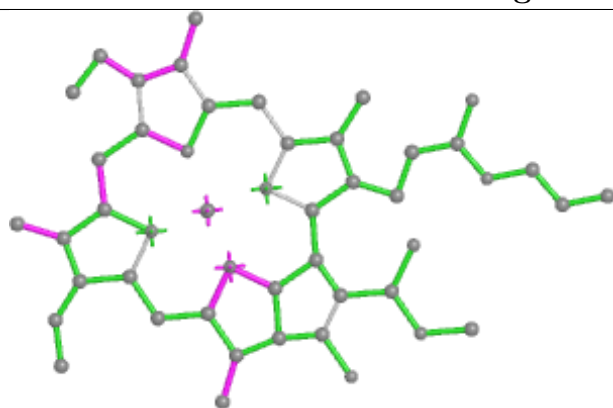


Torsions

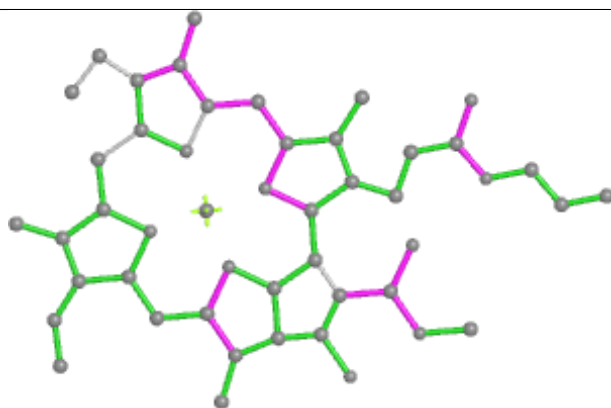


Rings

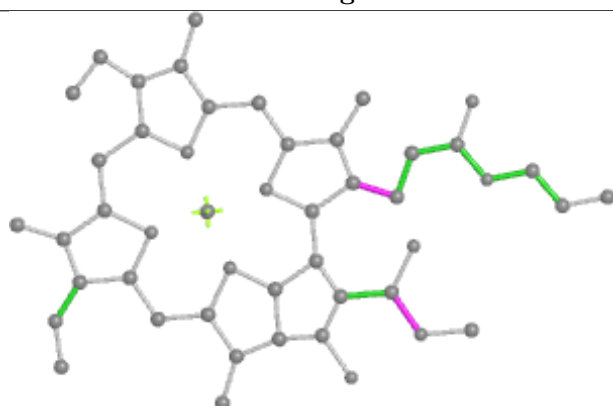
Ligand CLA Y 614



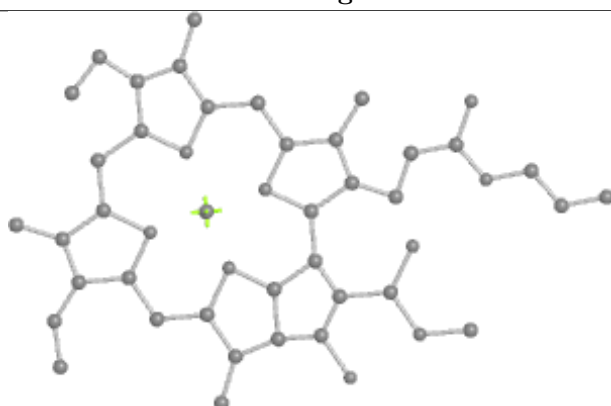
Bond lengths



Bond angles

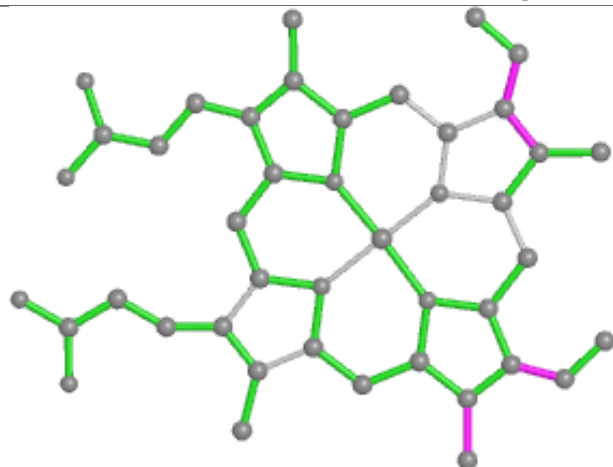


Torsions

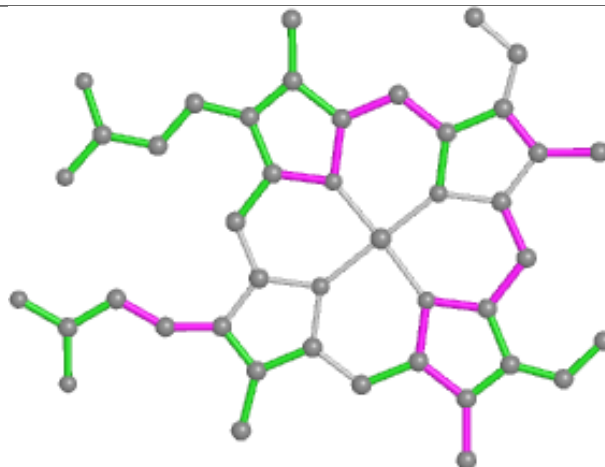


Rings

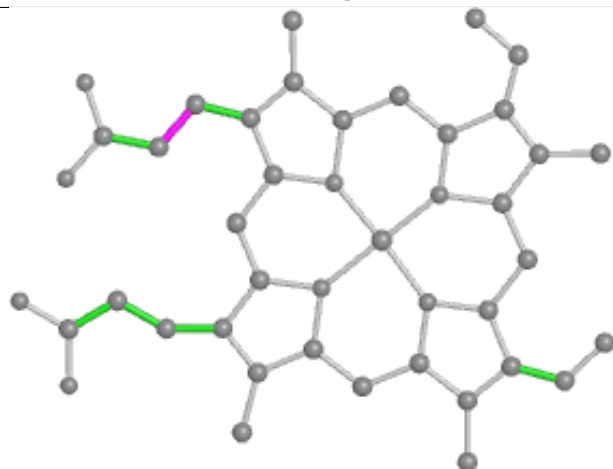
Ligand HEM f 101



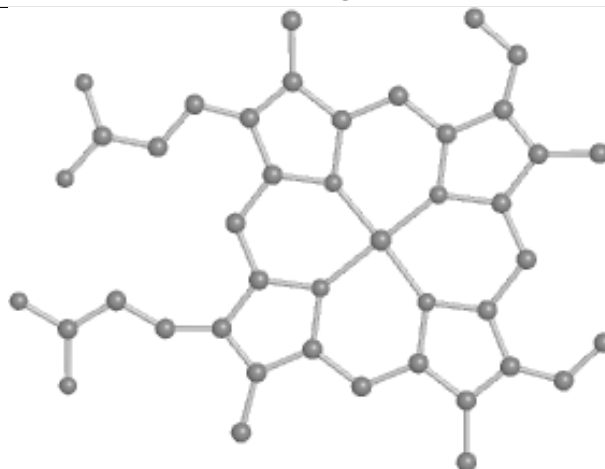
Bond lengths



Bond angles

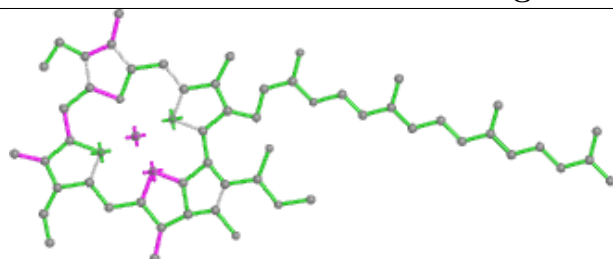


Torsions

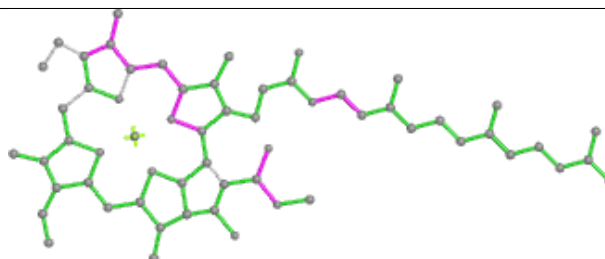


Rings

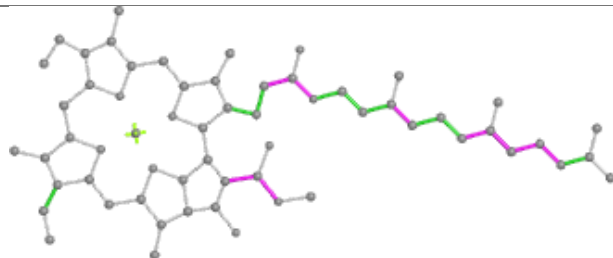
Ligand CLA Y 612



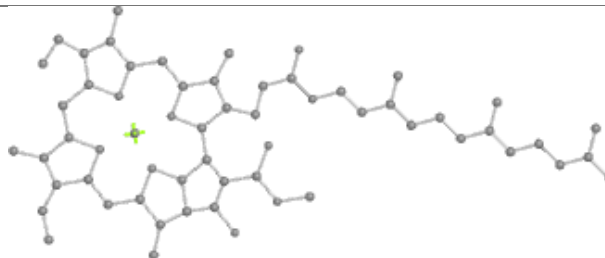
Bond lengths



Bond angles

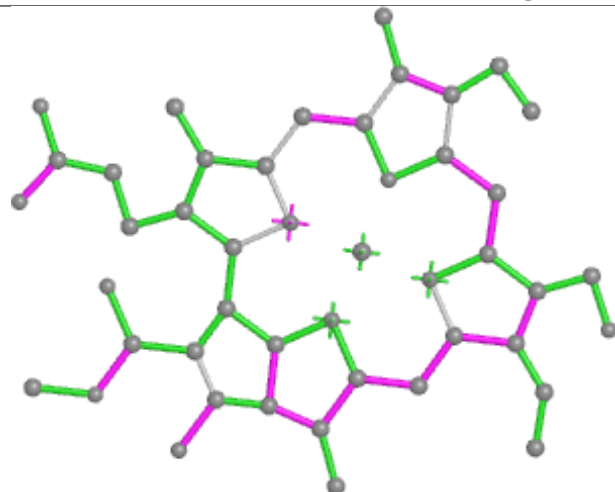


Torsions

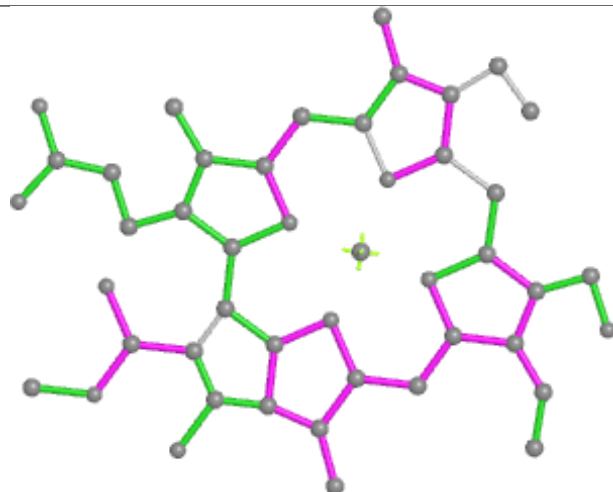


Rings

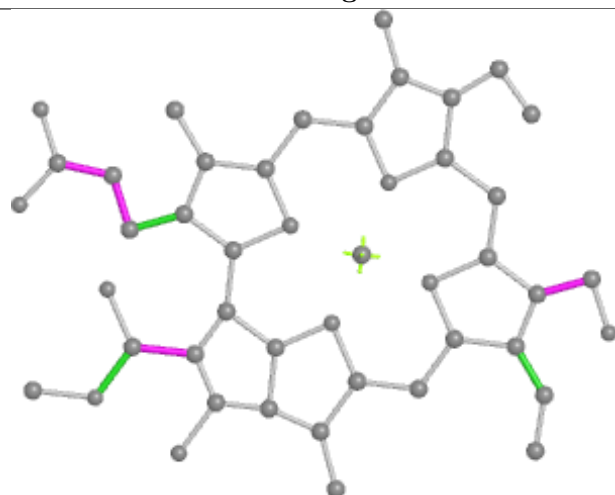
Ligand CHL 6 606



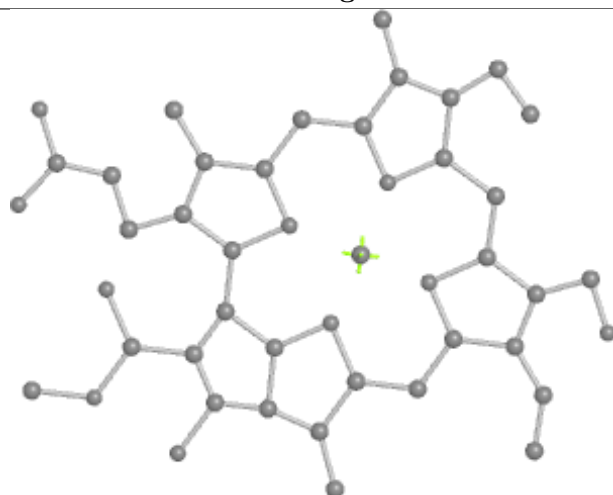
Bond lengths



Bond angles

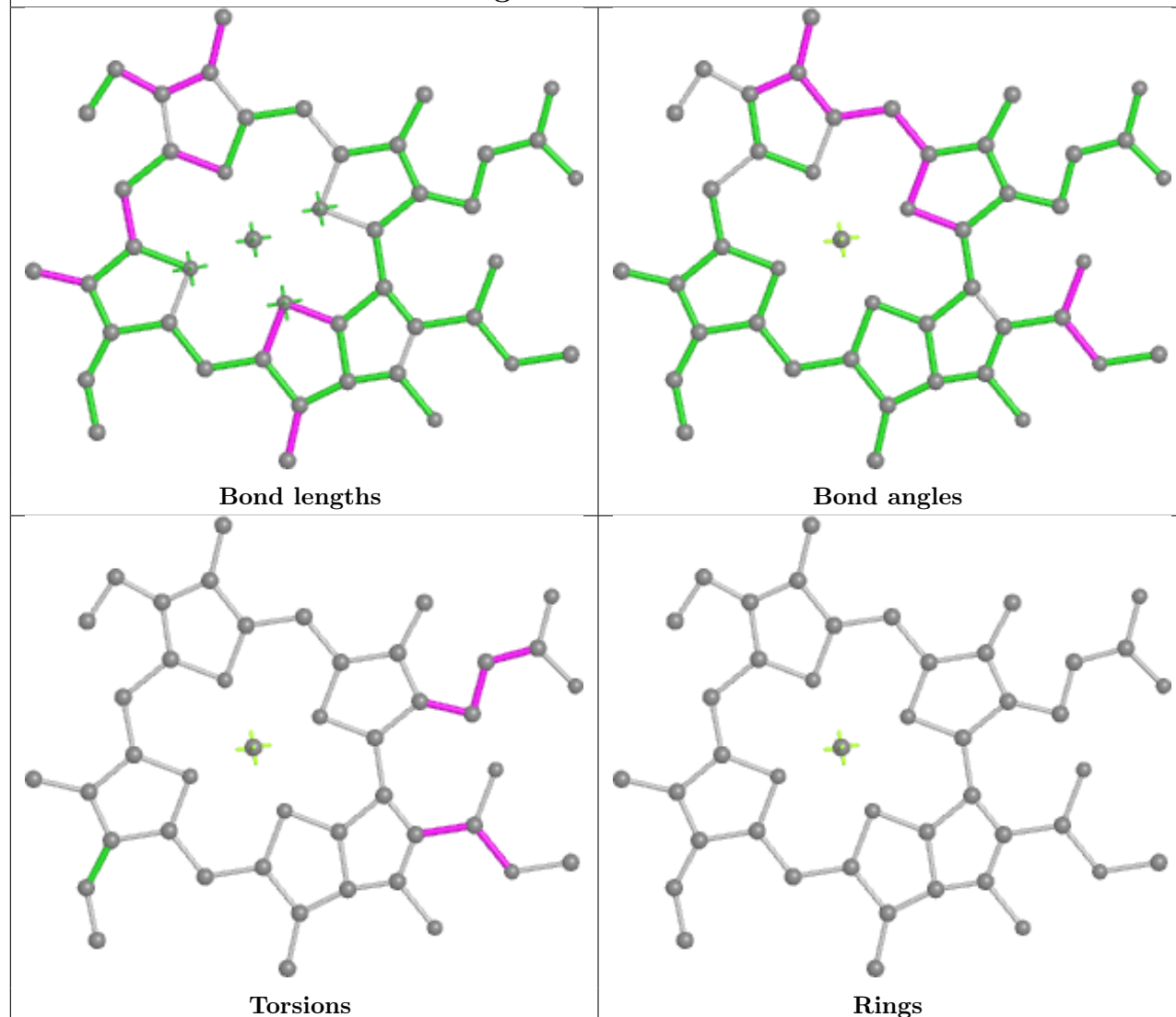


Torsions

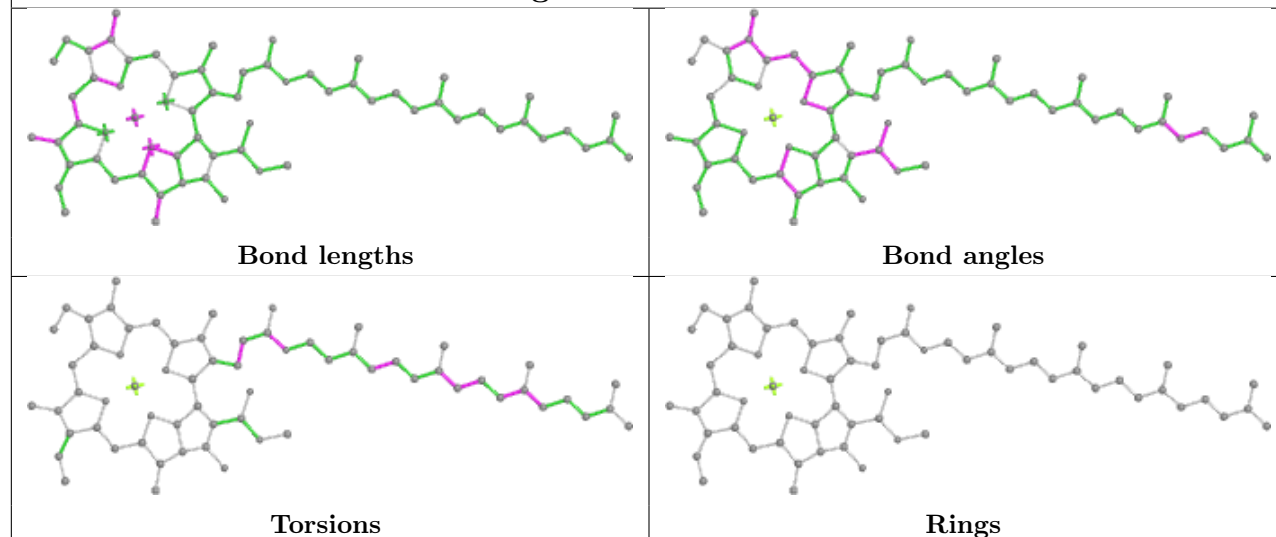


Rings

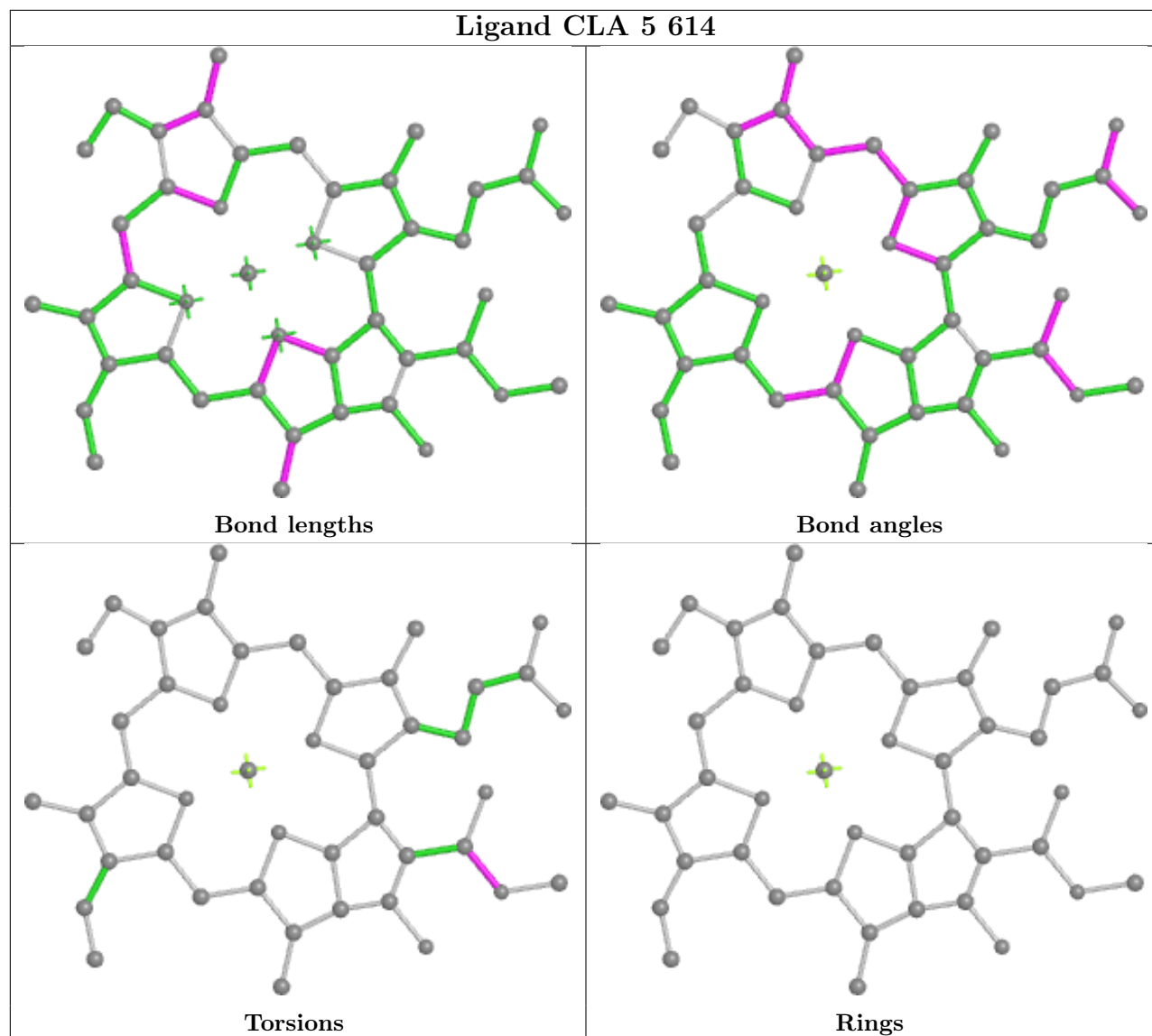
Ligand CLA 3 604

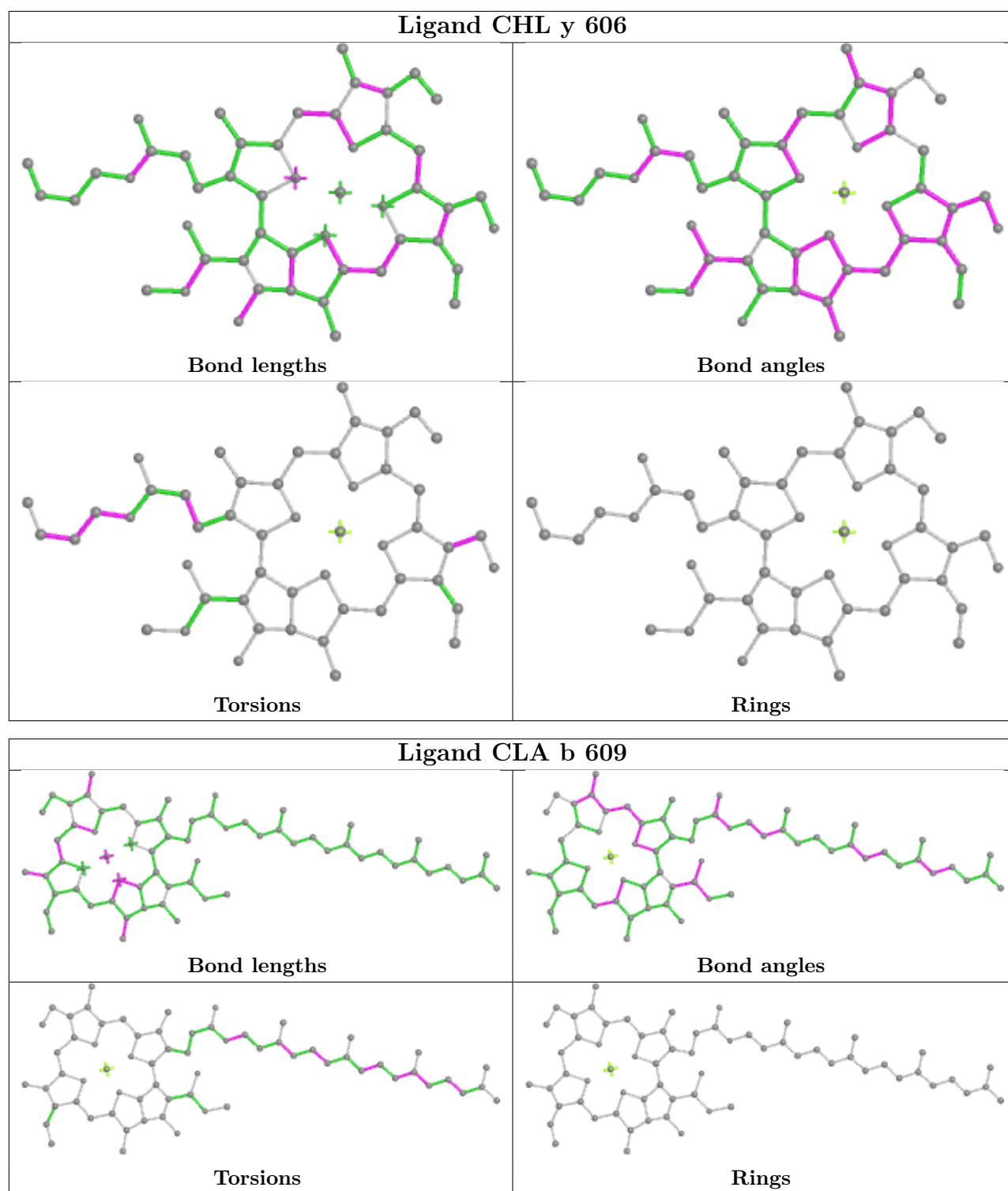


Ligand CLA Y 613

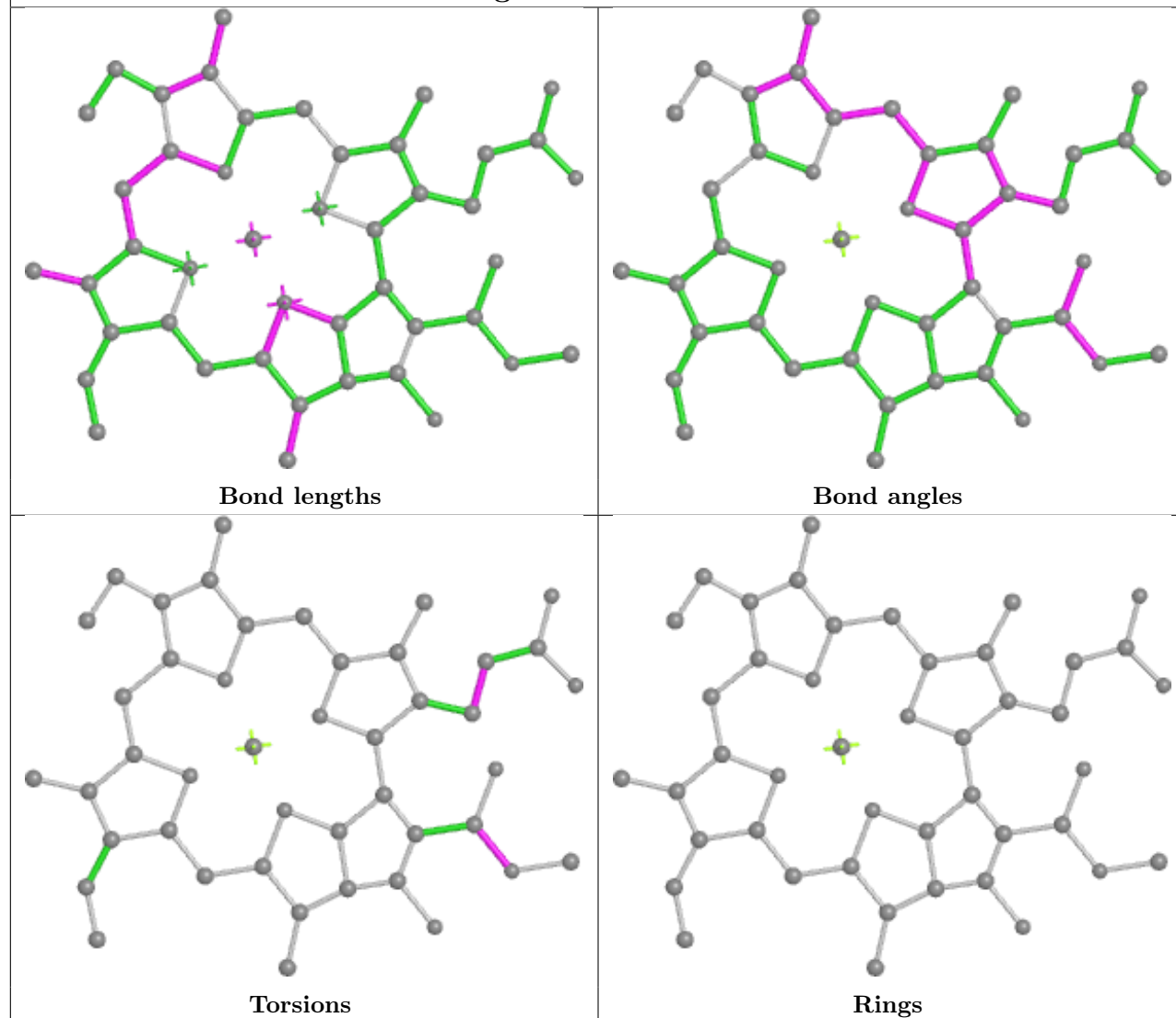


Ligand CLA 5 614

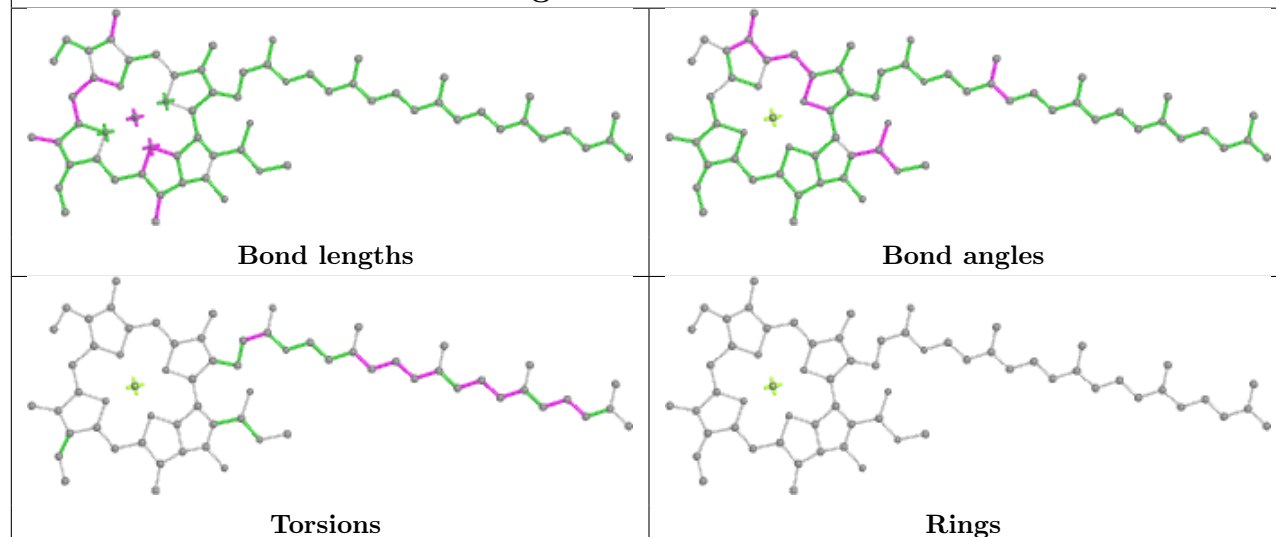




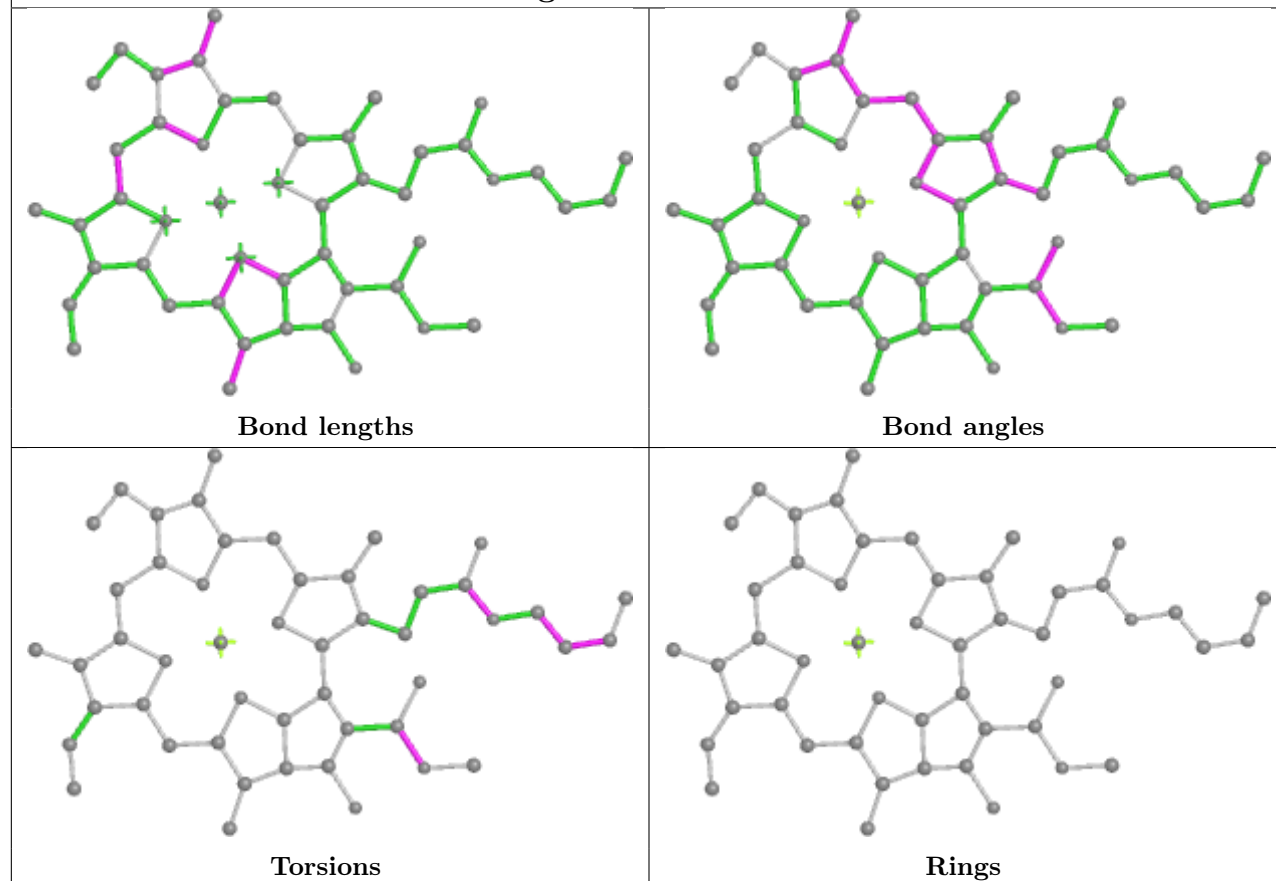
Ligand CLA 5 612



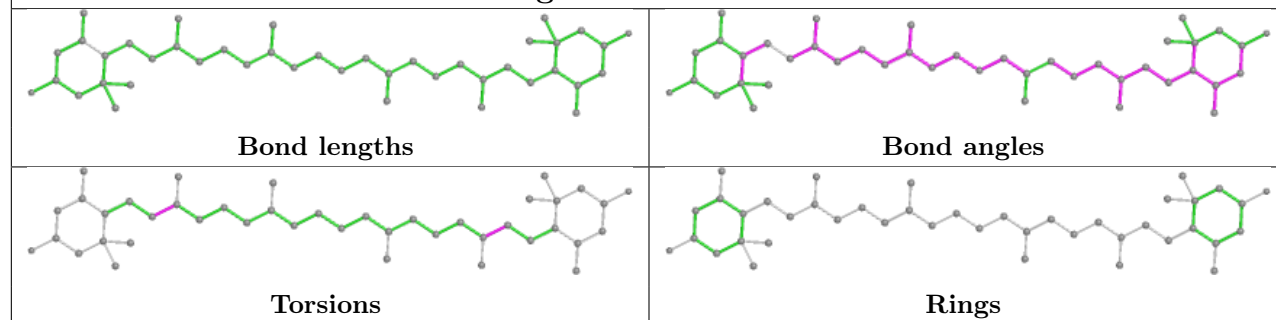
Ligand CLA B 614

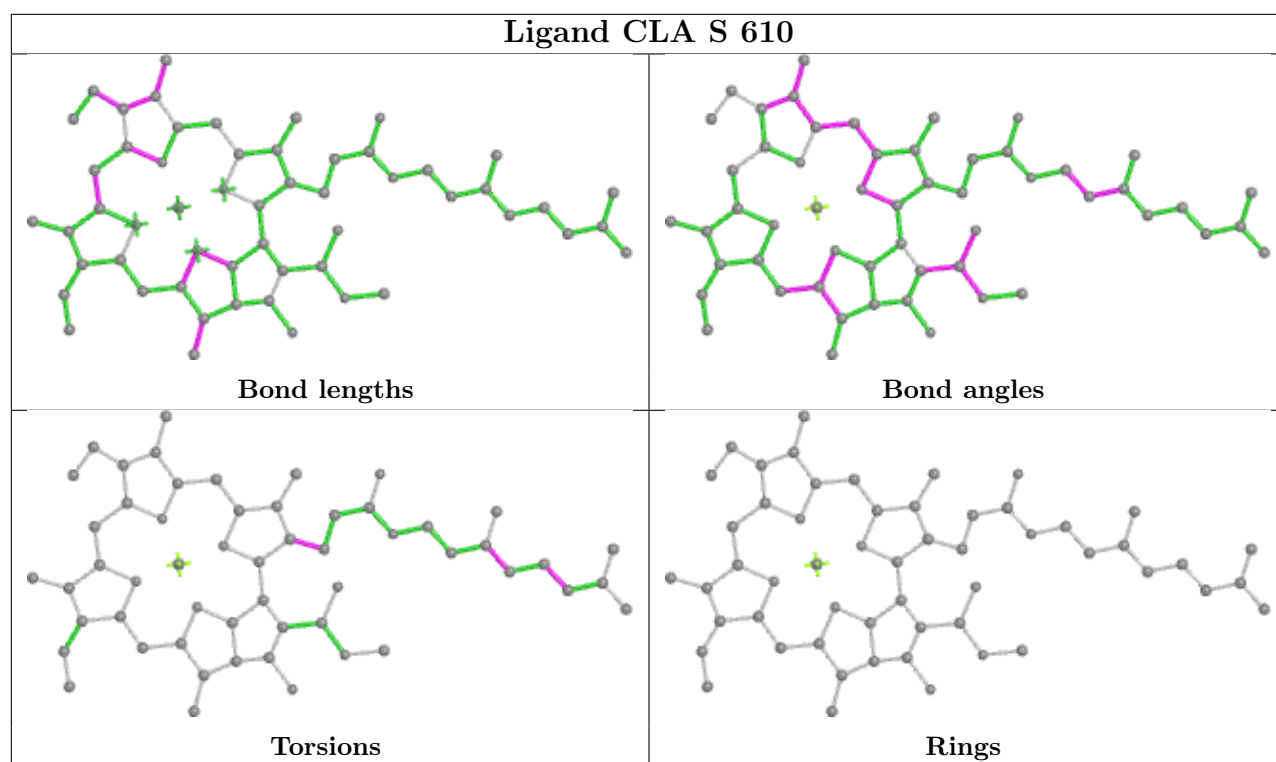


Ligand CLA r 612

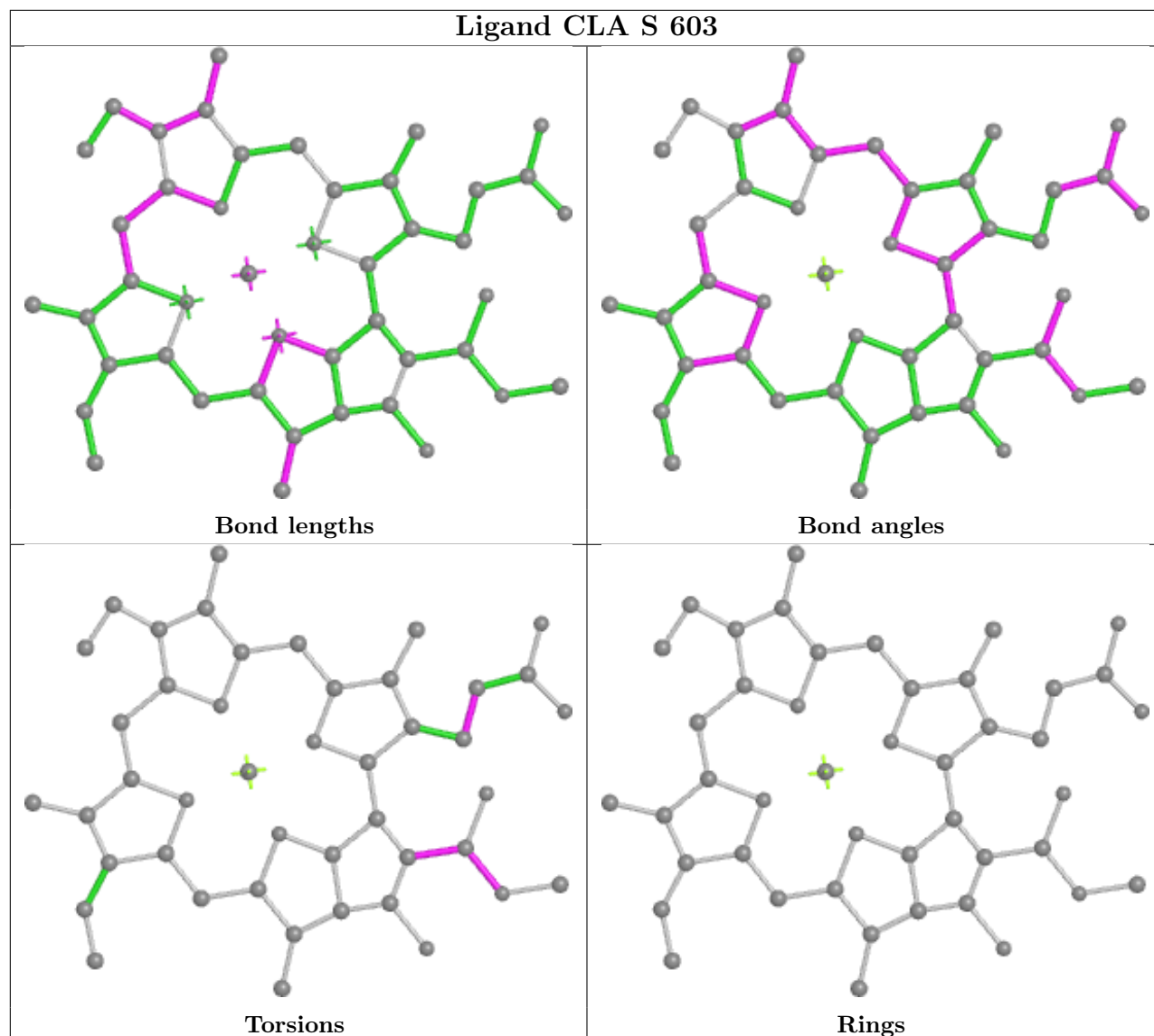


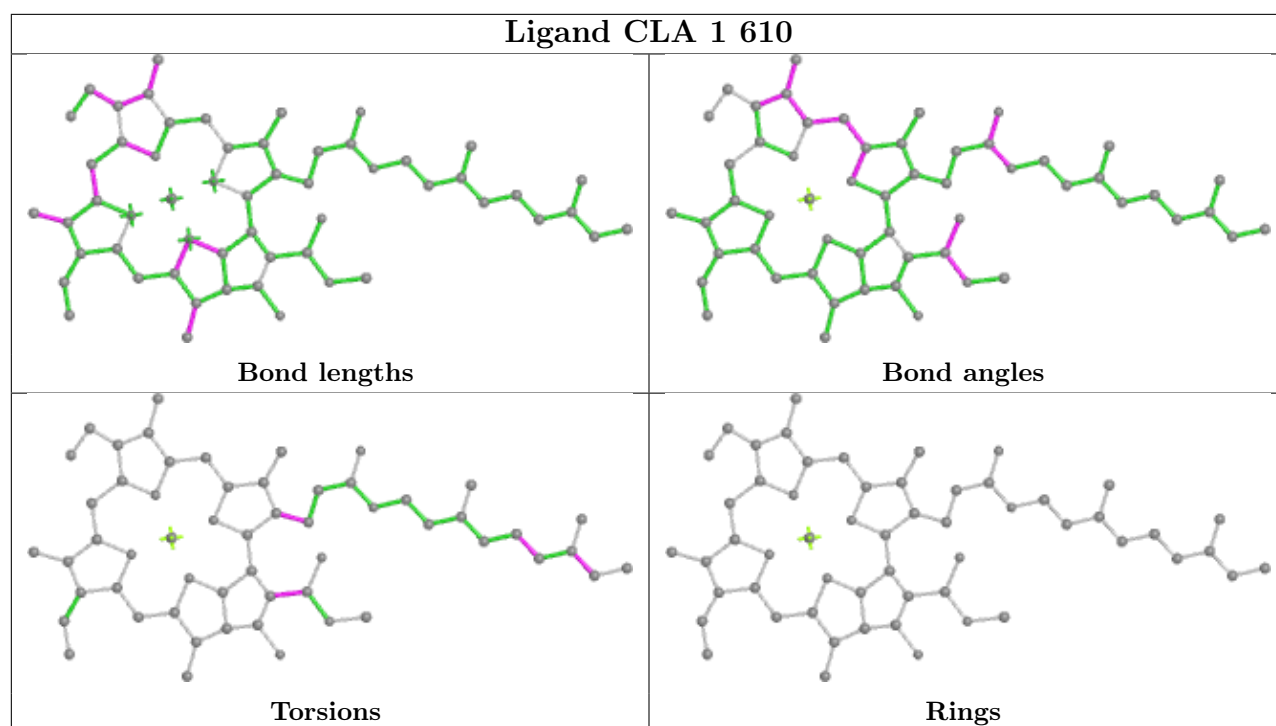
Ligand LUT 8 620



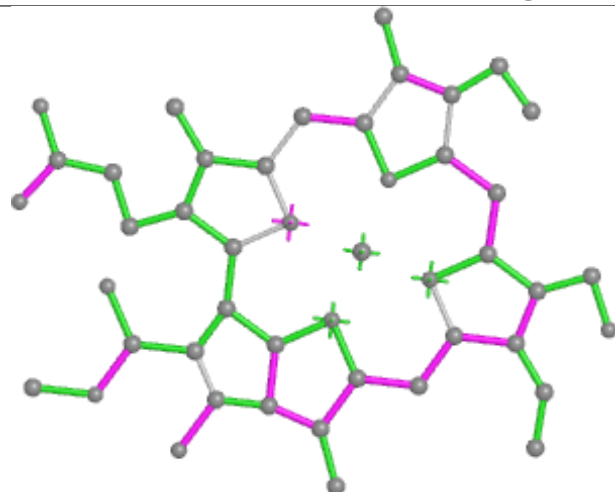


Ligand CLA S 603

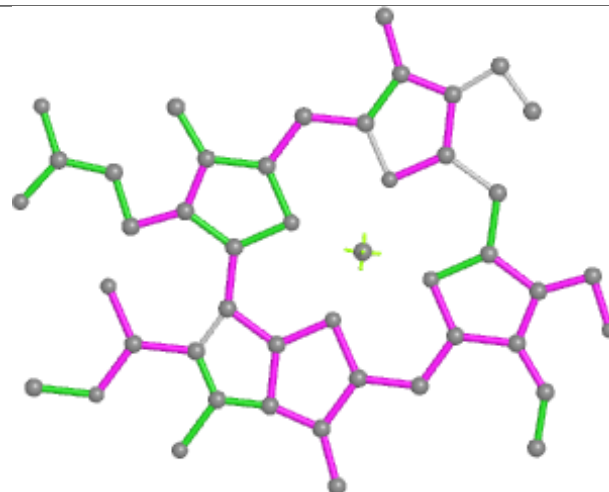




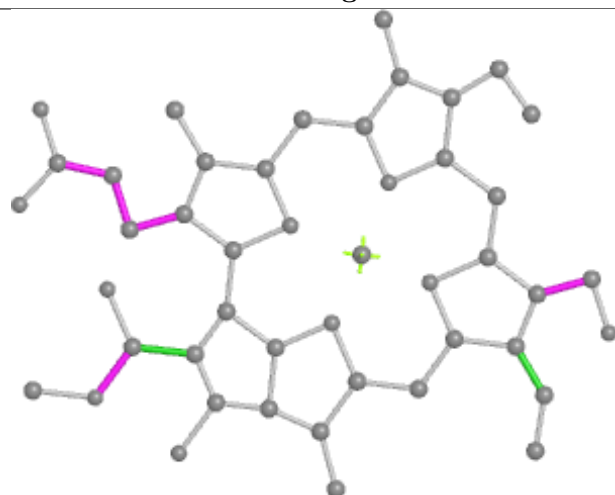
Ligand CHL 3 605



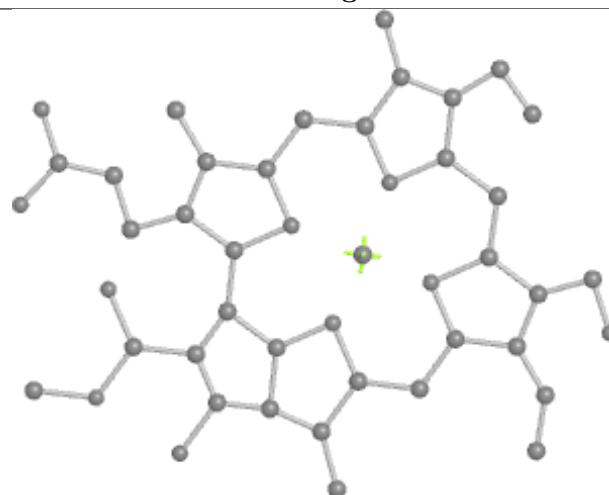
Bond lengths



Bond angles

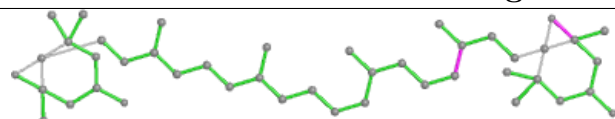


Torsions

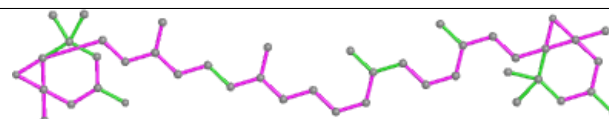


Rings

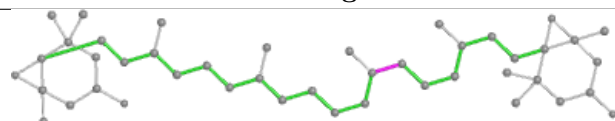
Ligand XAT G 1622



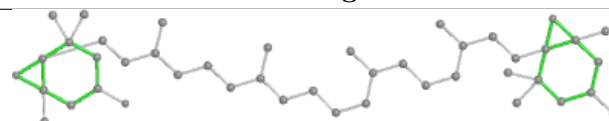
Bond lengths



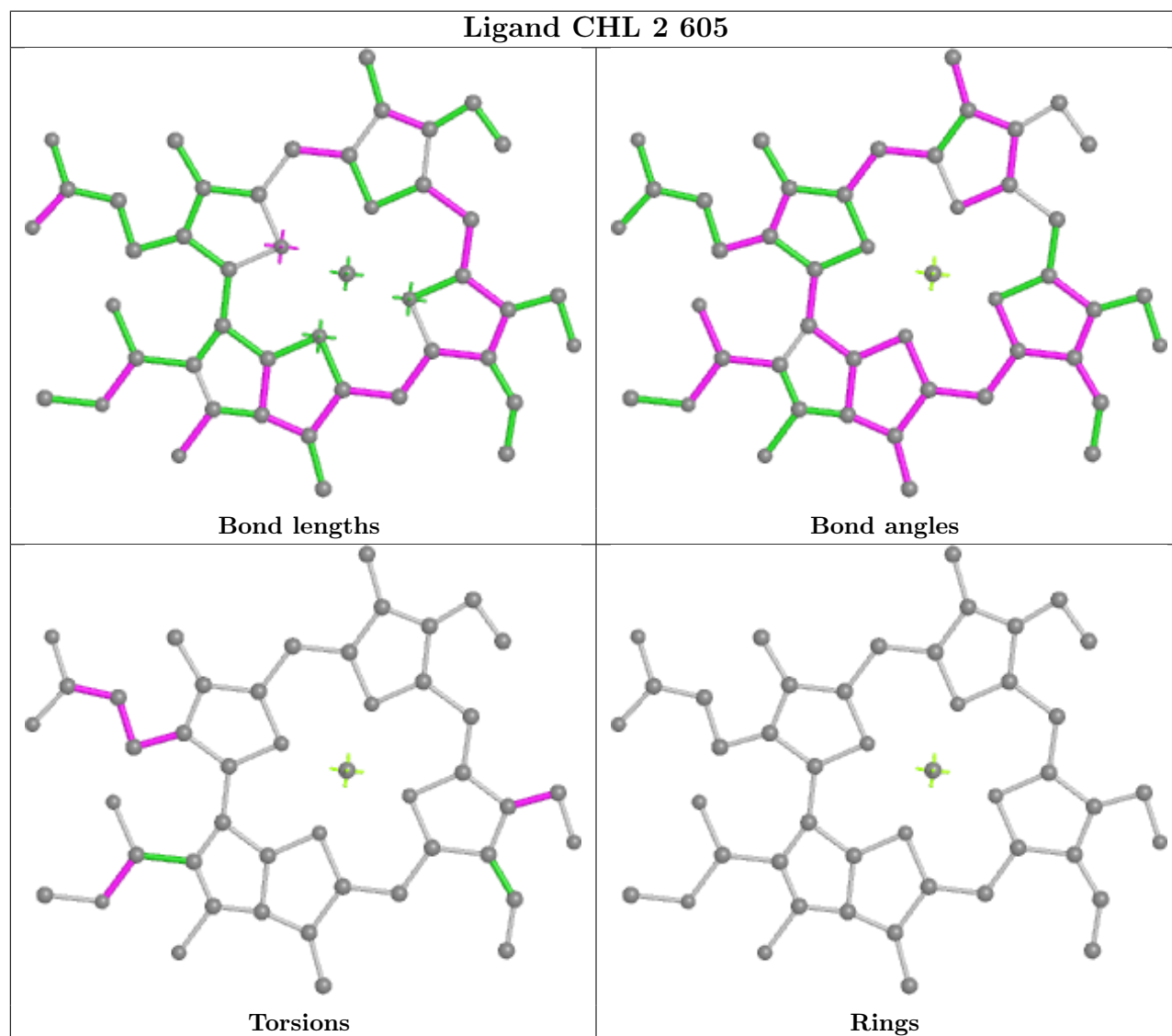
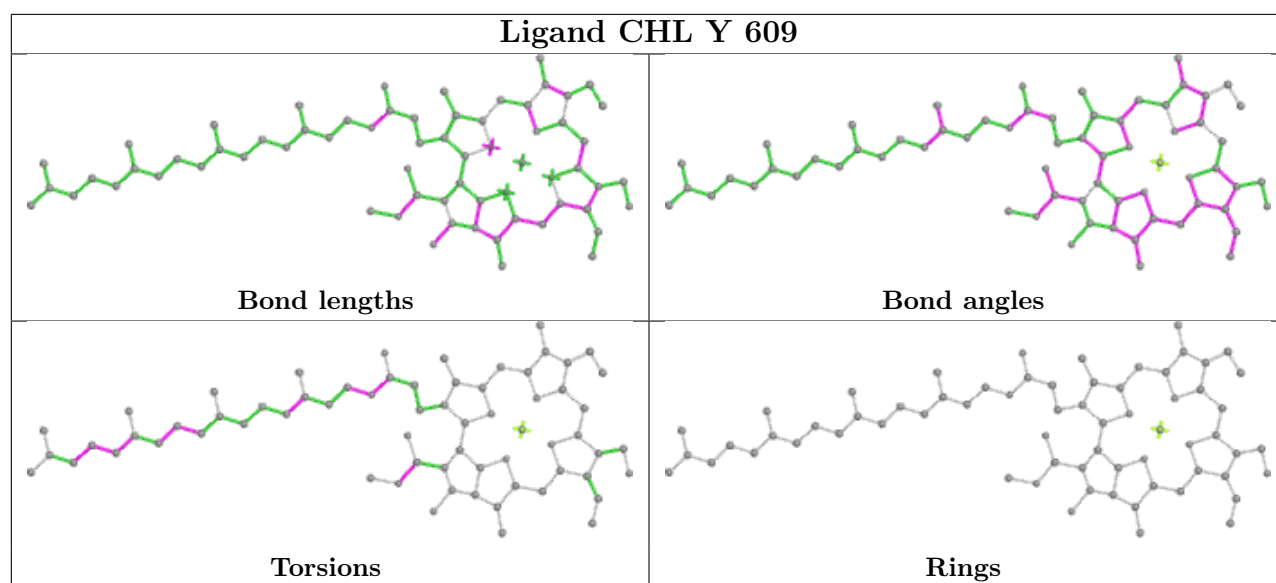
Bond angles



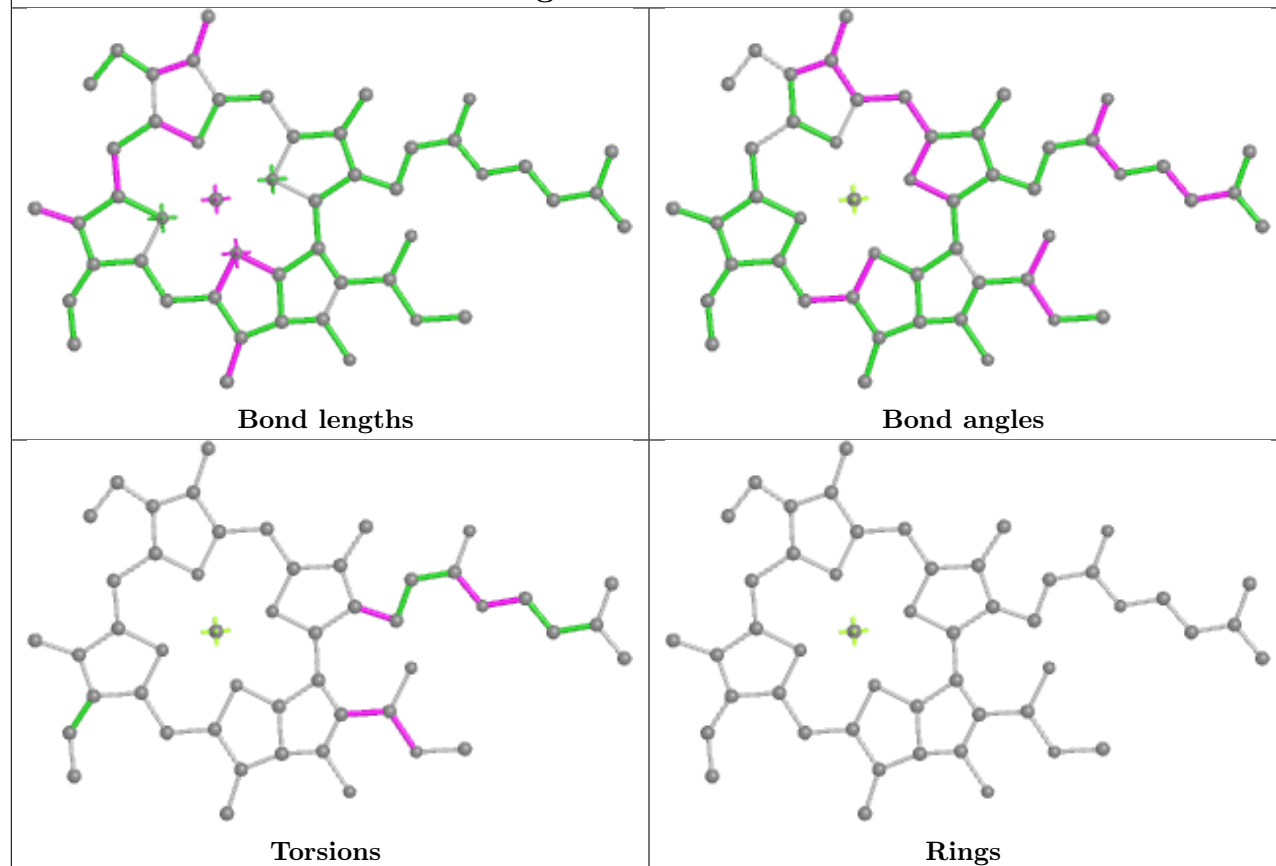
Torsions



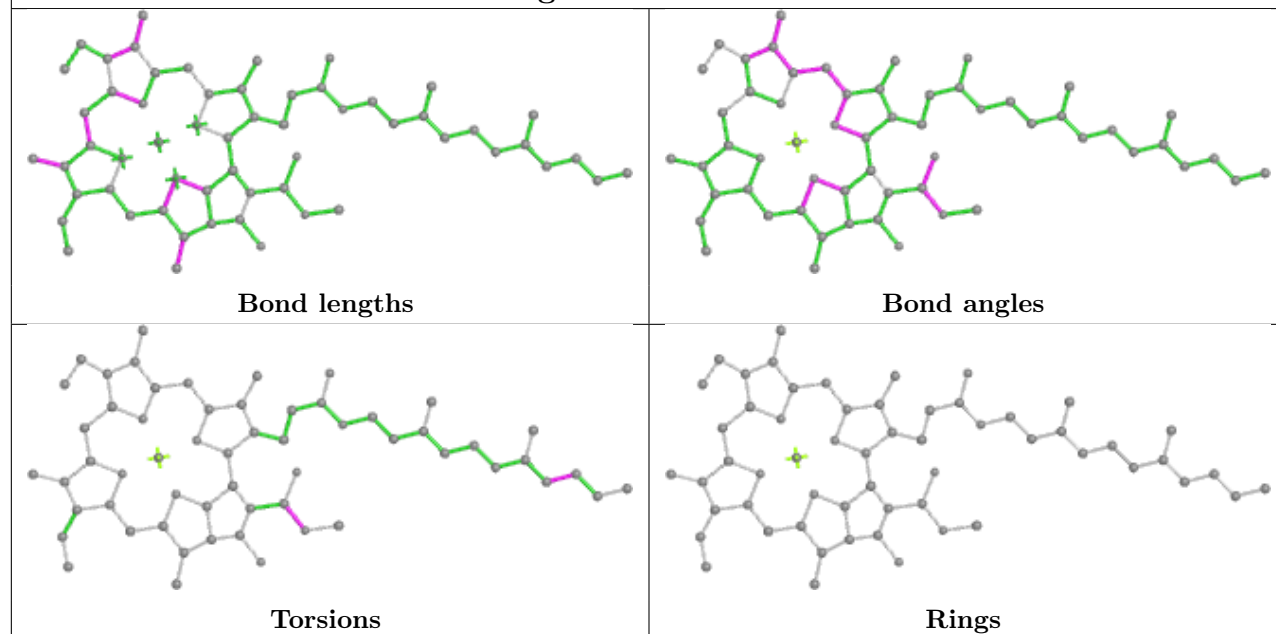
Rings

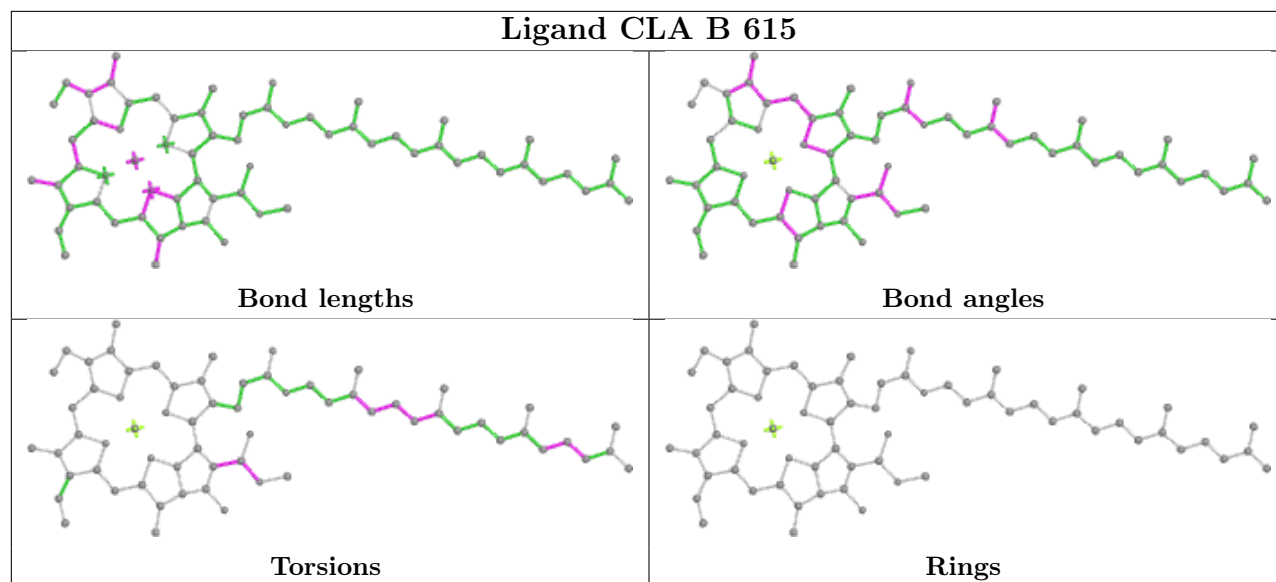
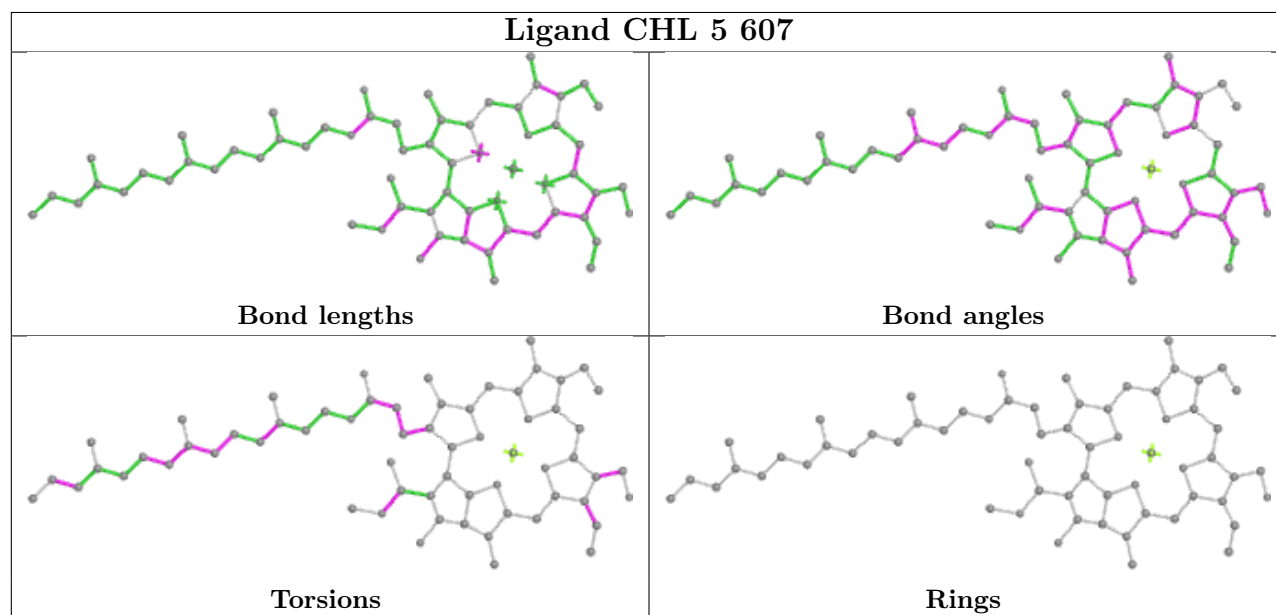


Ligand CLA 1 604

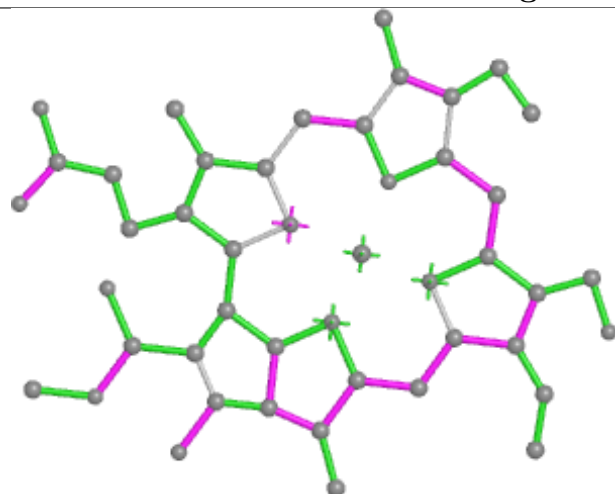


Ligand CLA r 609

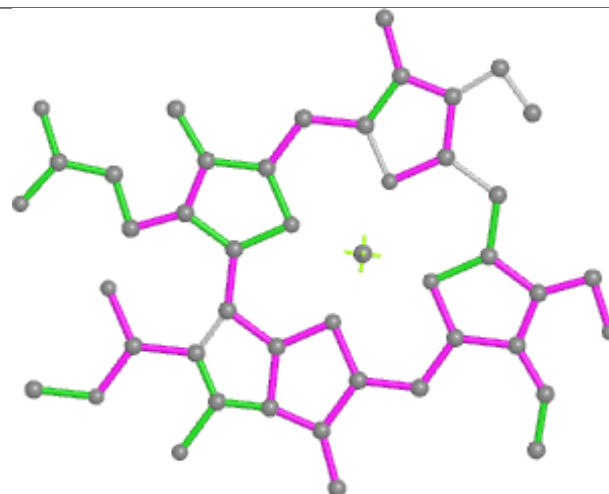


Ligand CLA B 615**Ligand CHL 5 607**

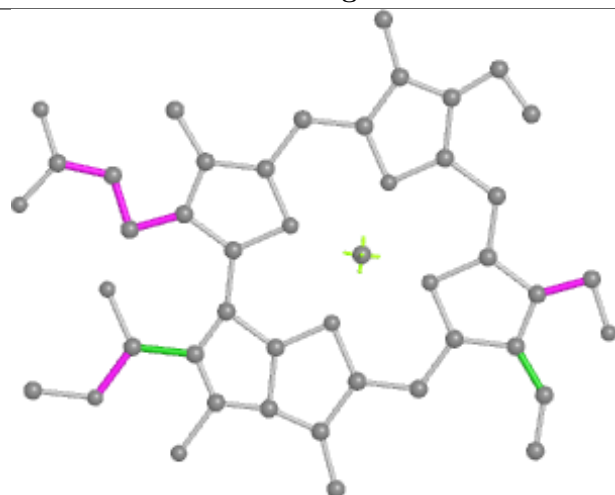
Ligand CHL 7 605



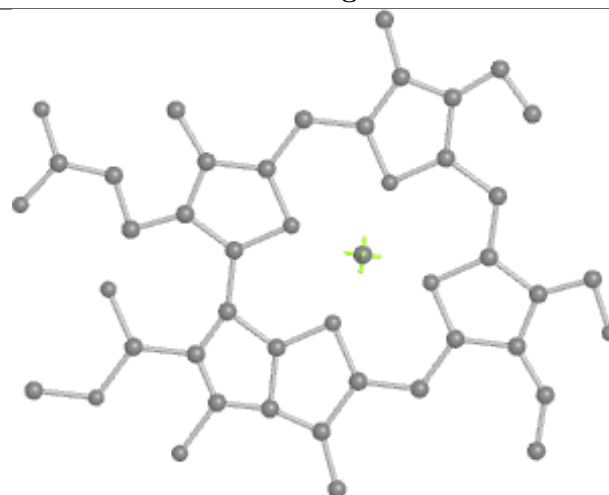
Bond lengths



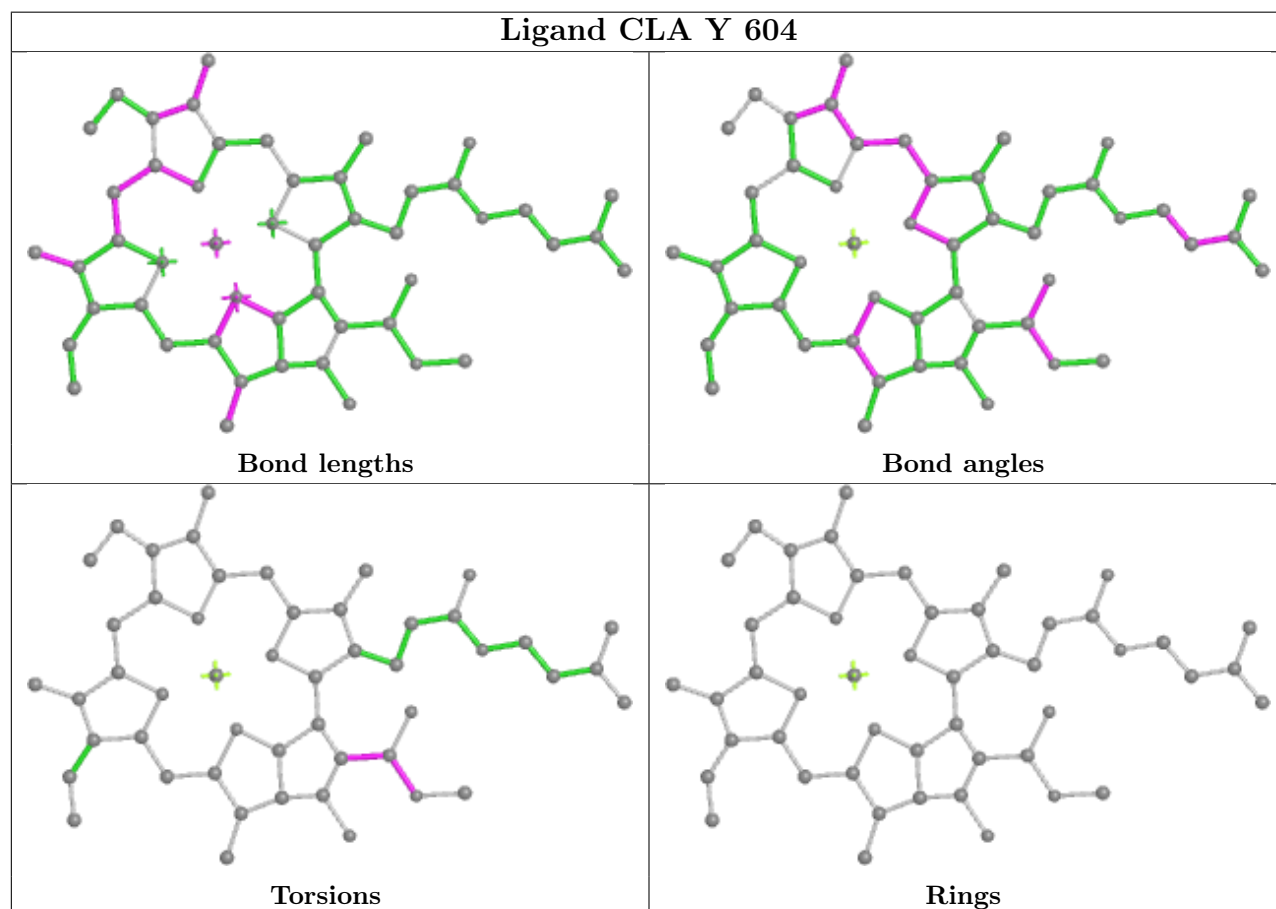
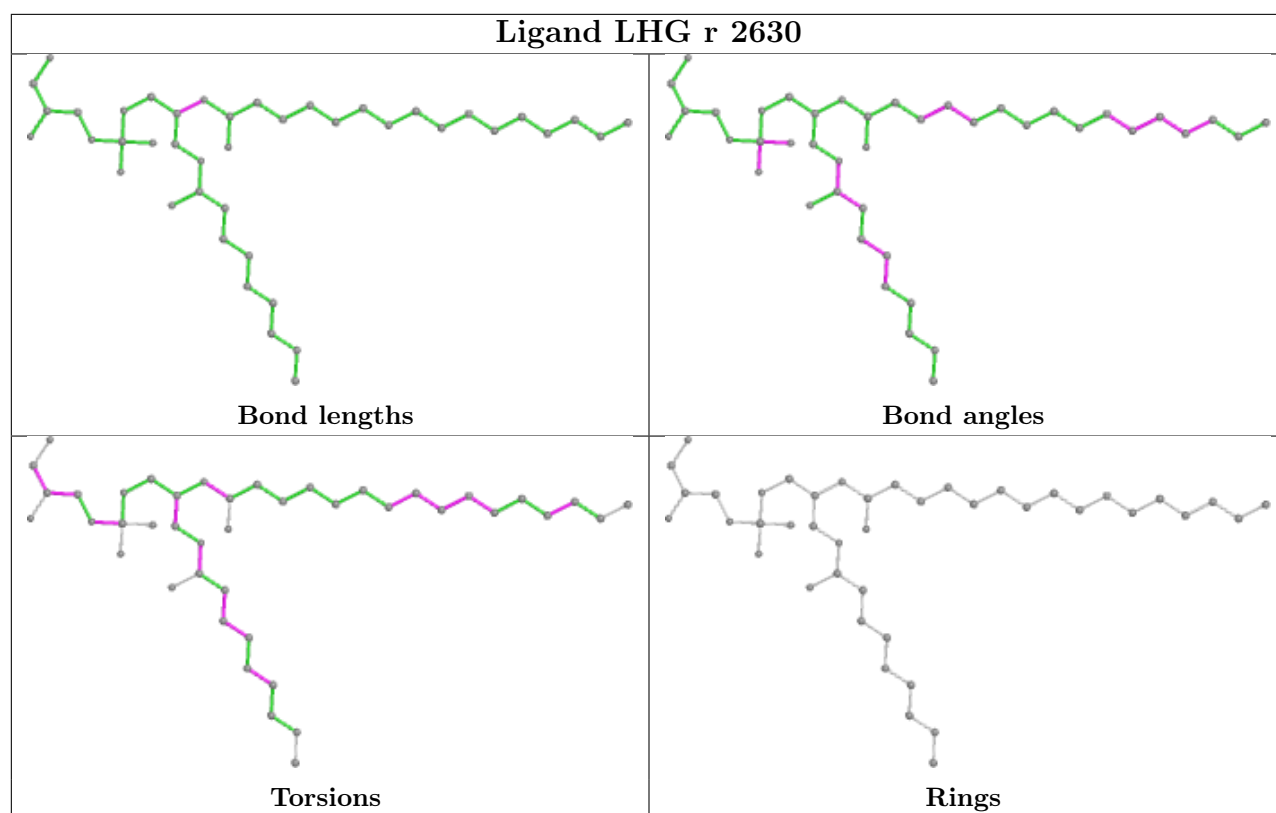
Bond angles

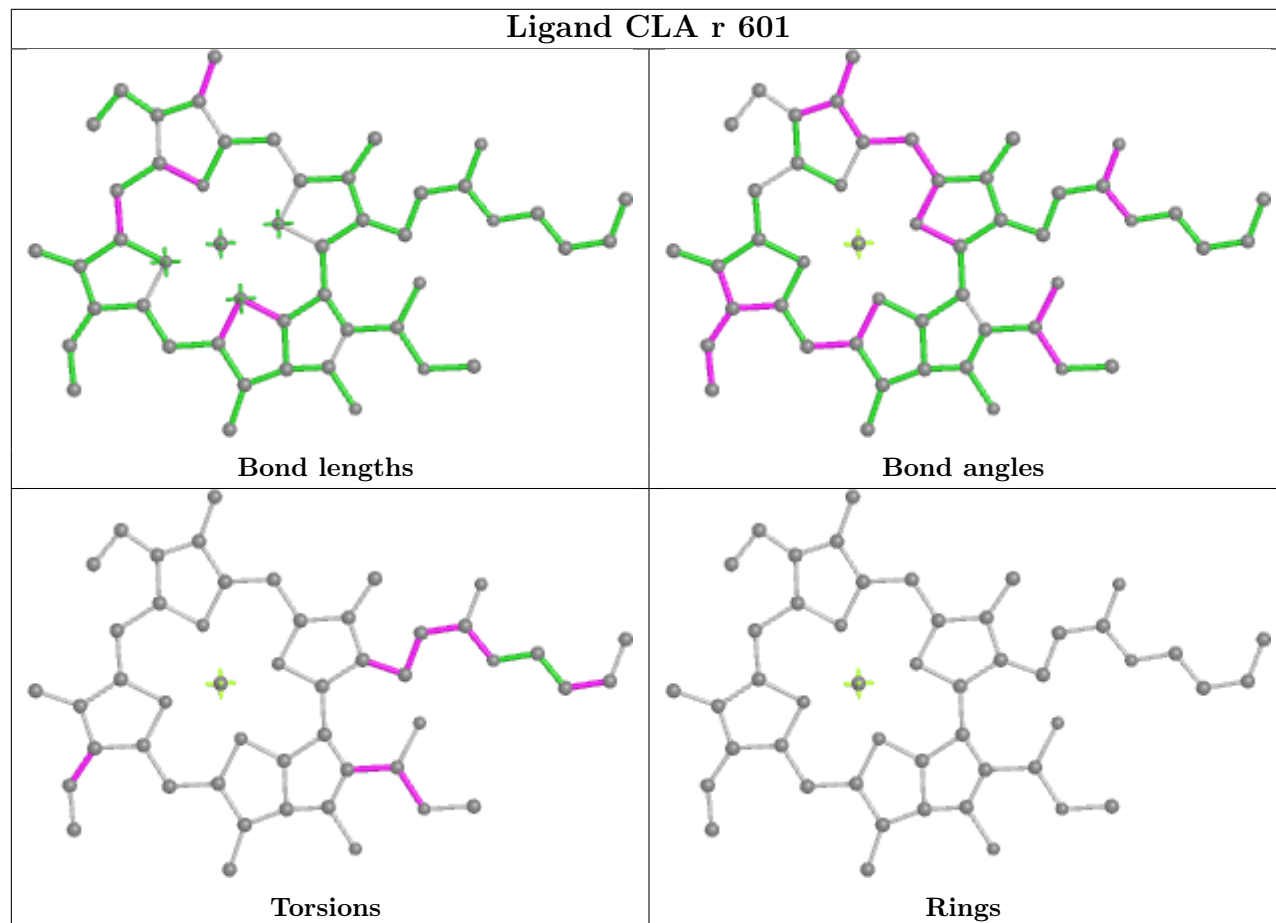
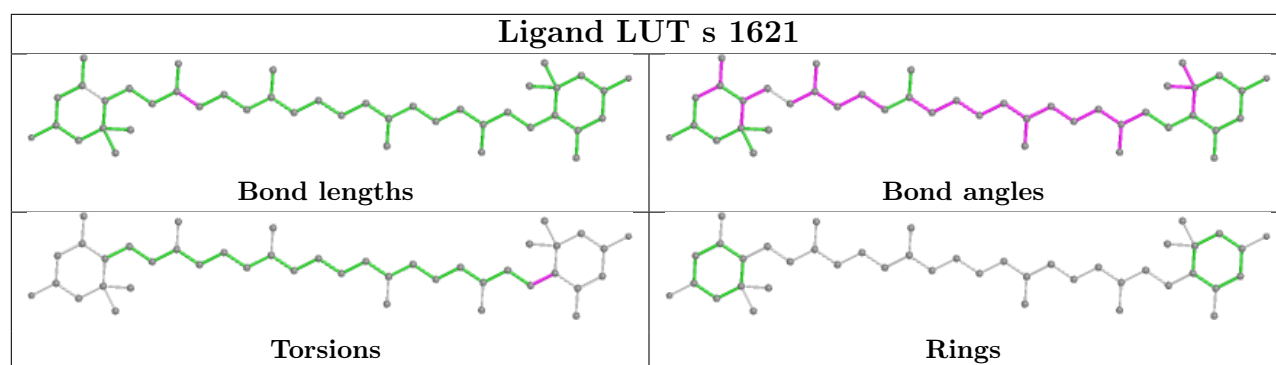


Torsions

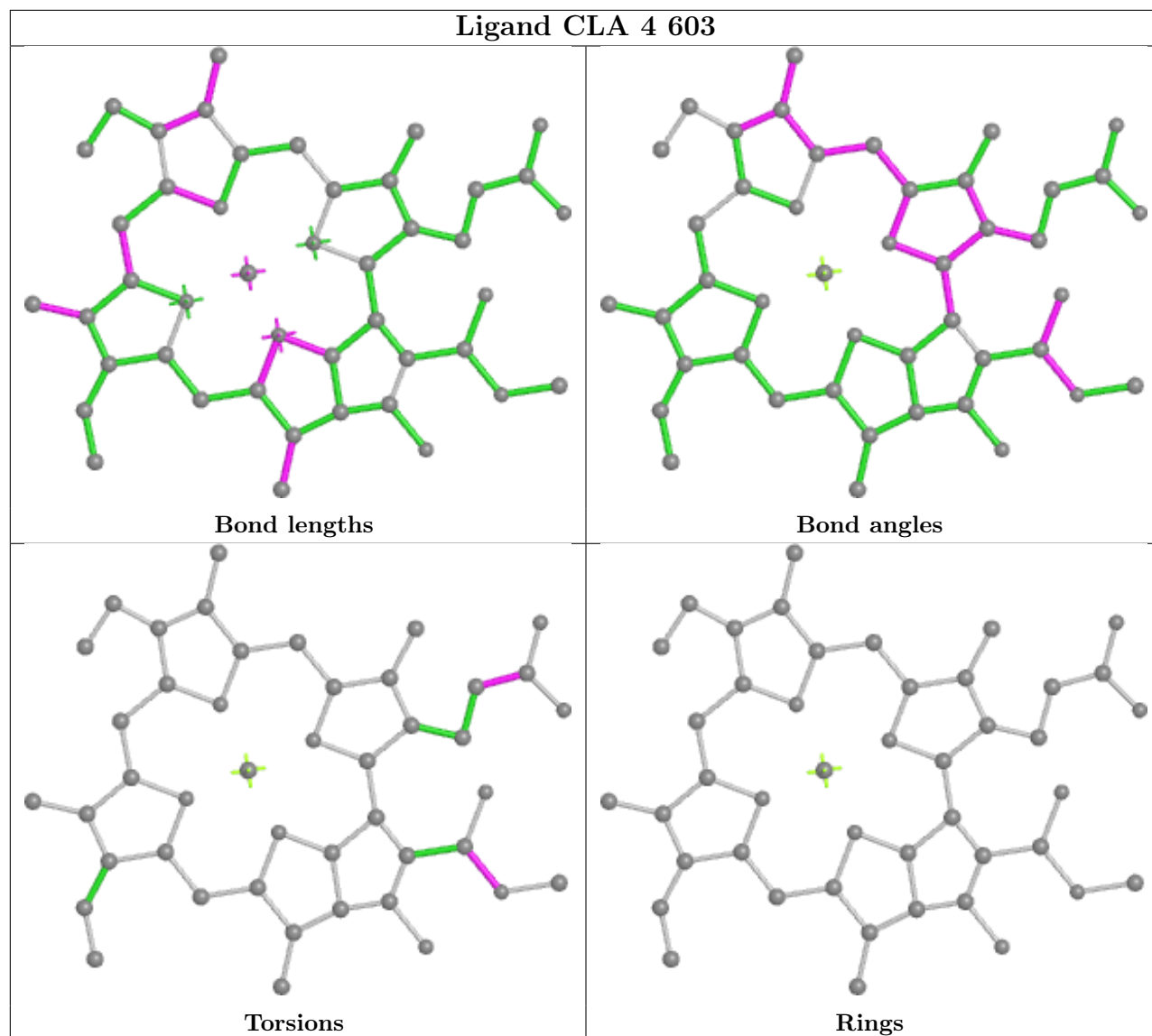


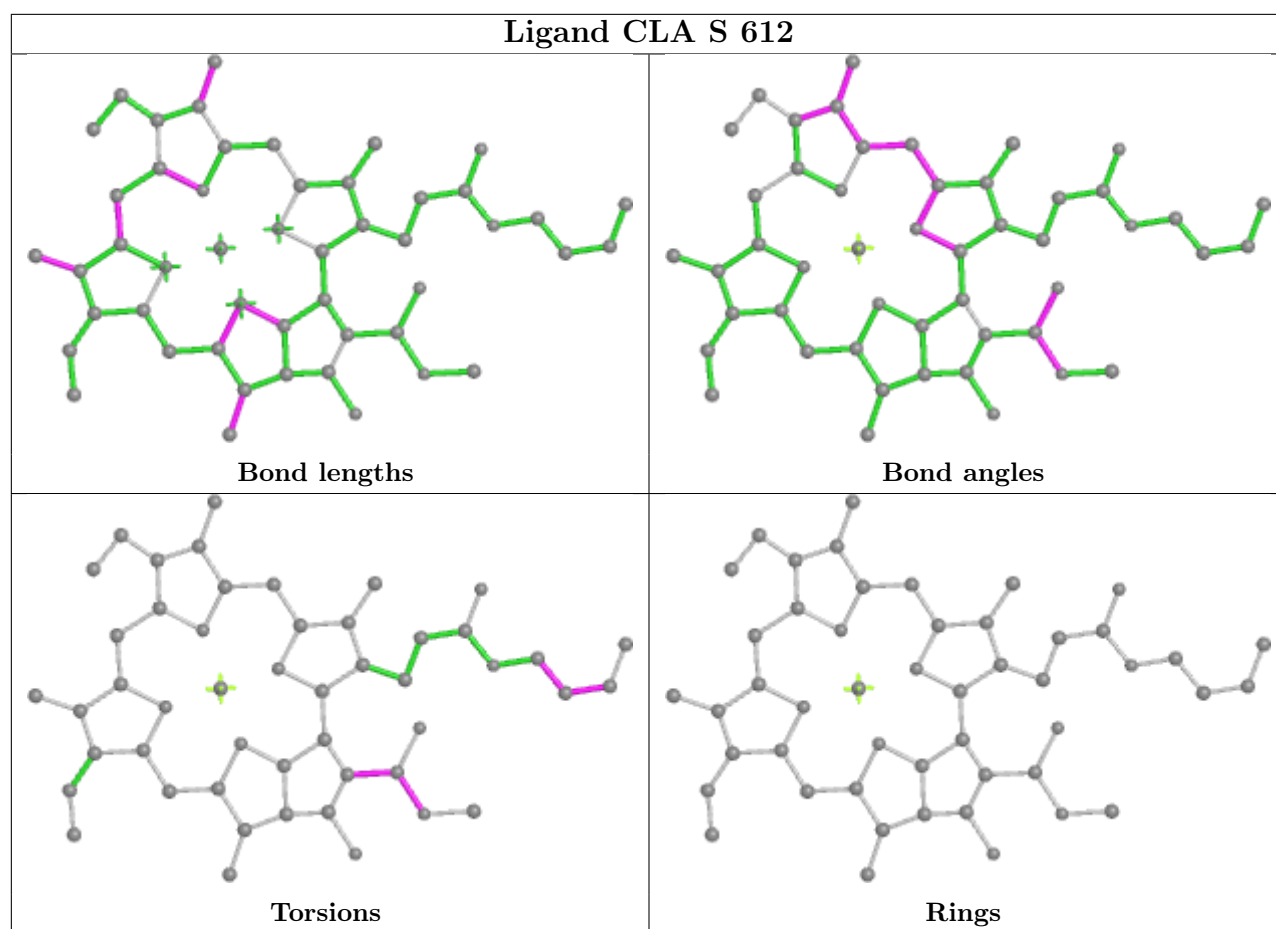
Rings

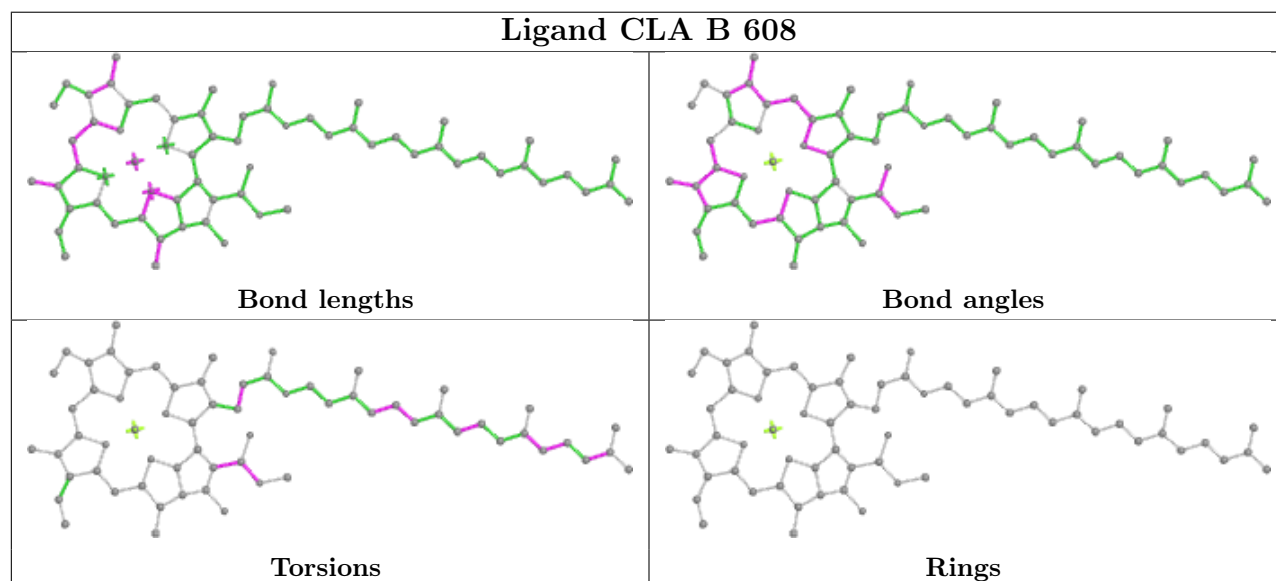
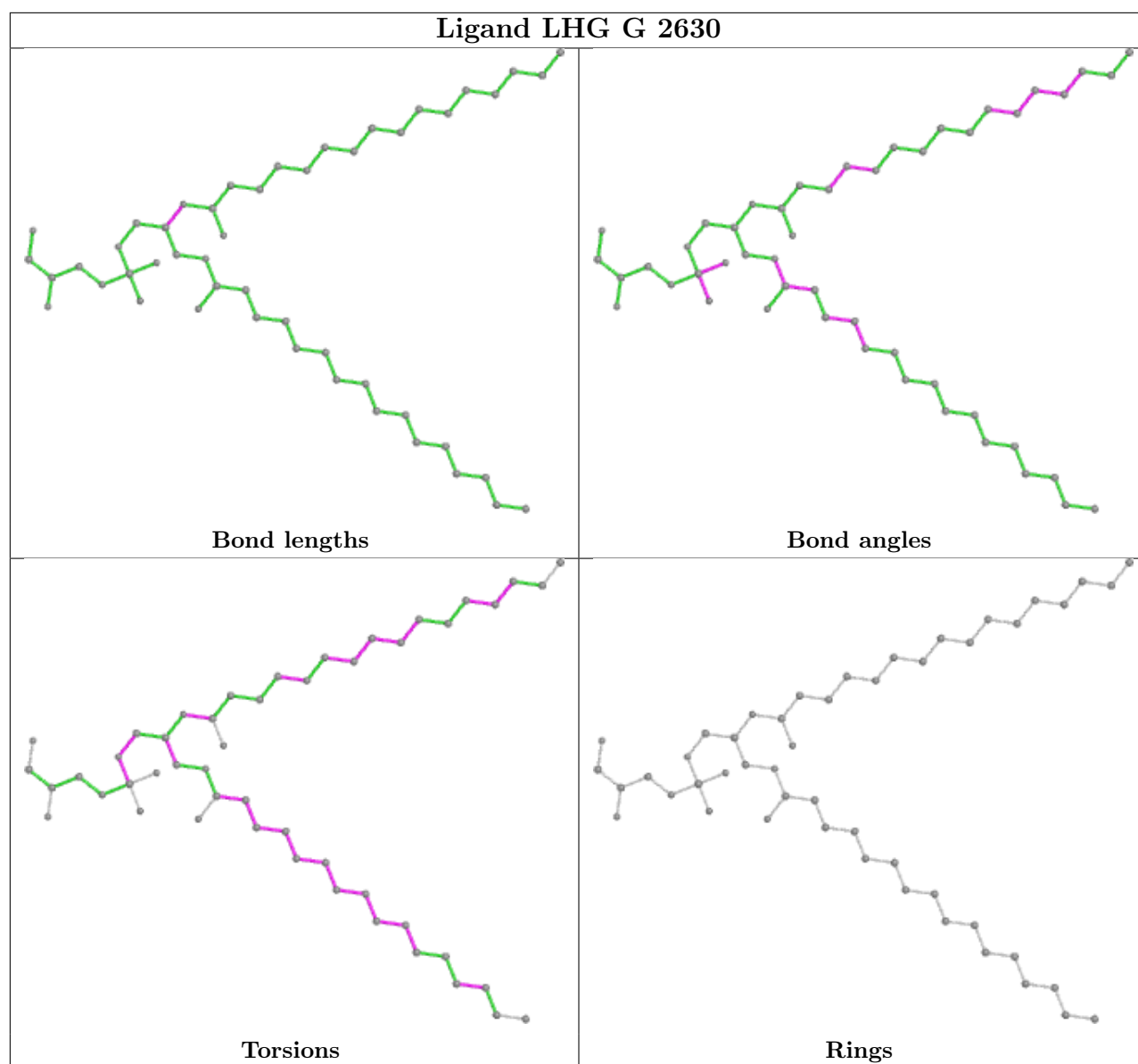


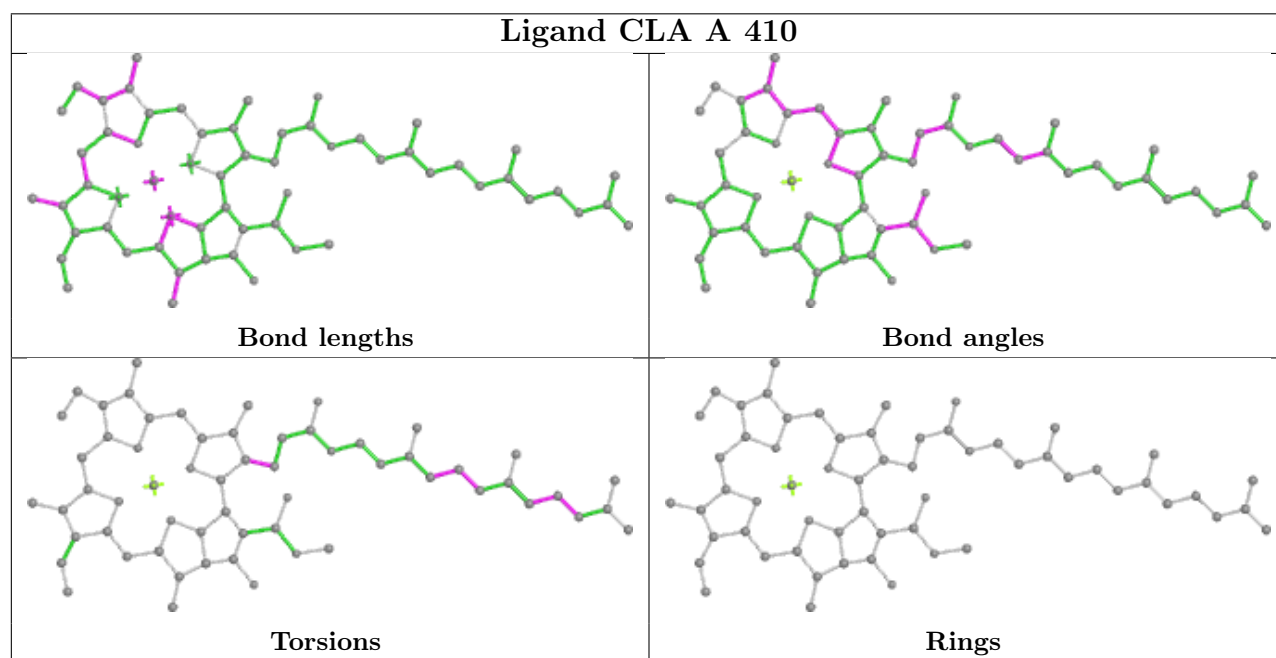
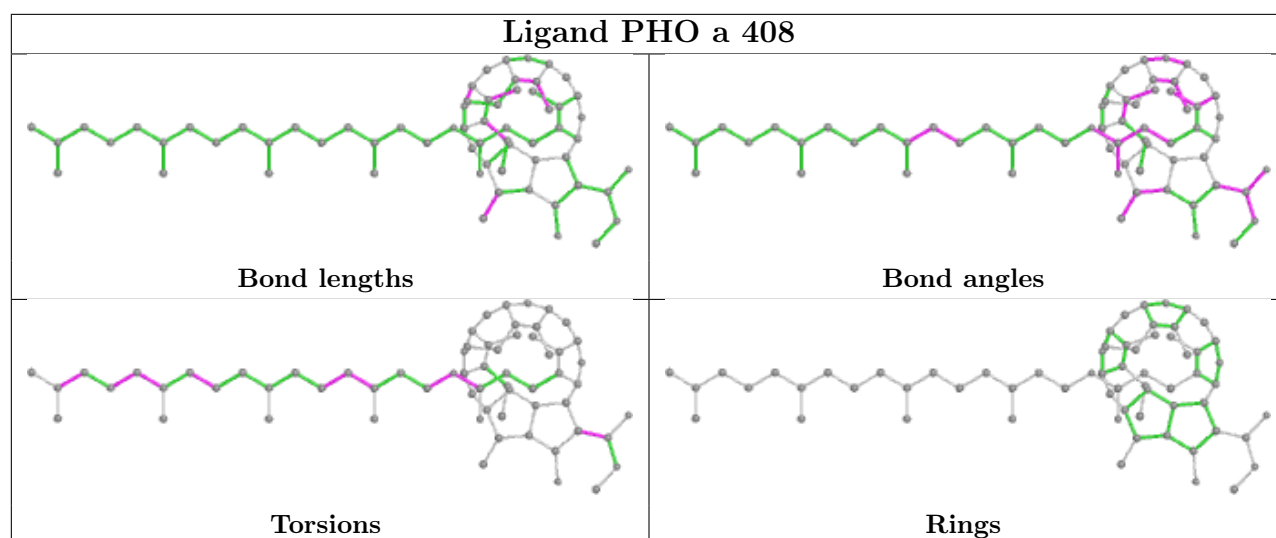


Ligand CLA 4 603

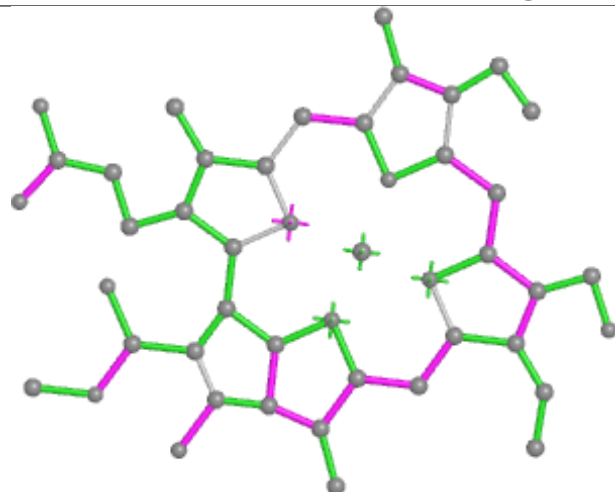




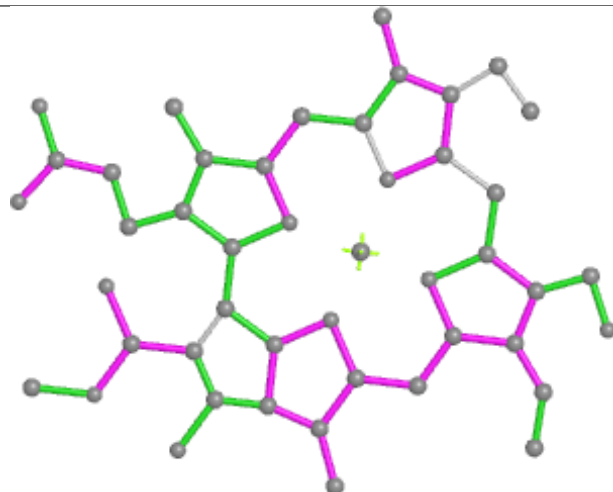




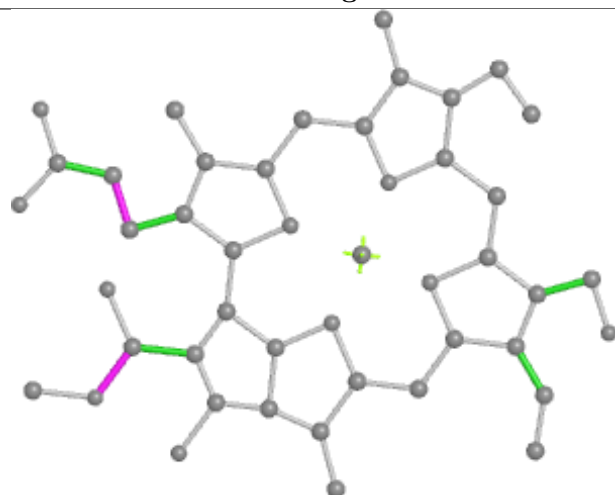
Ligand CHL 3 608



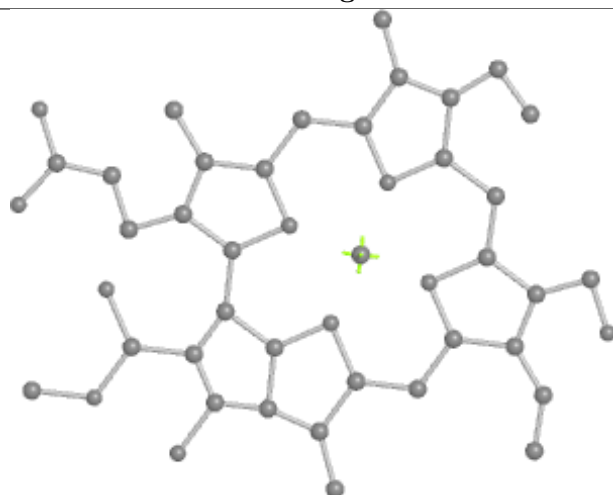
Bond lengths



Bond angles

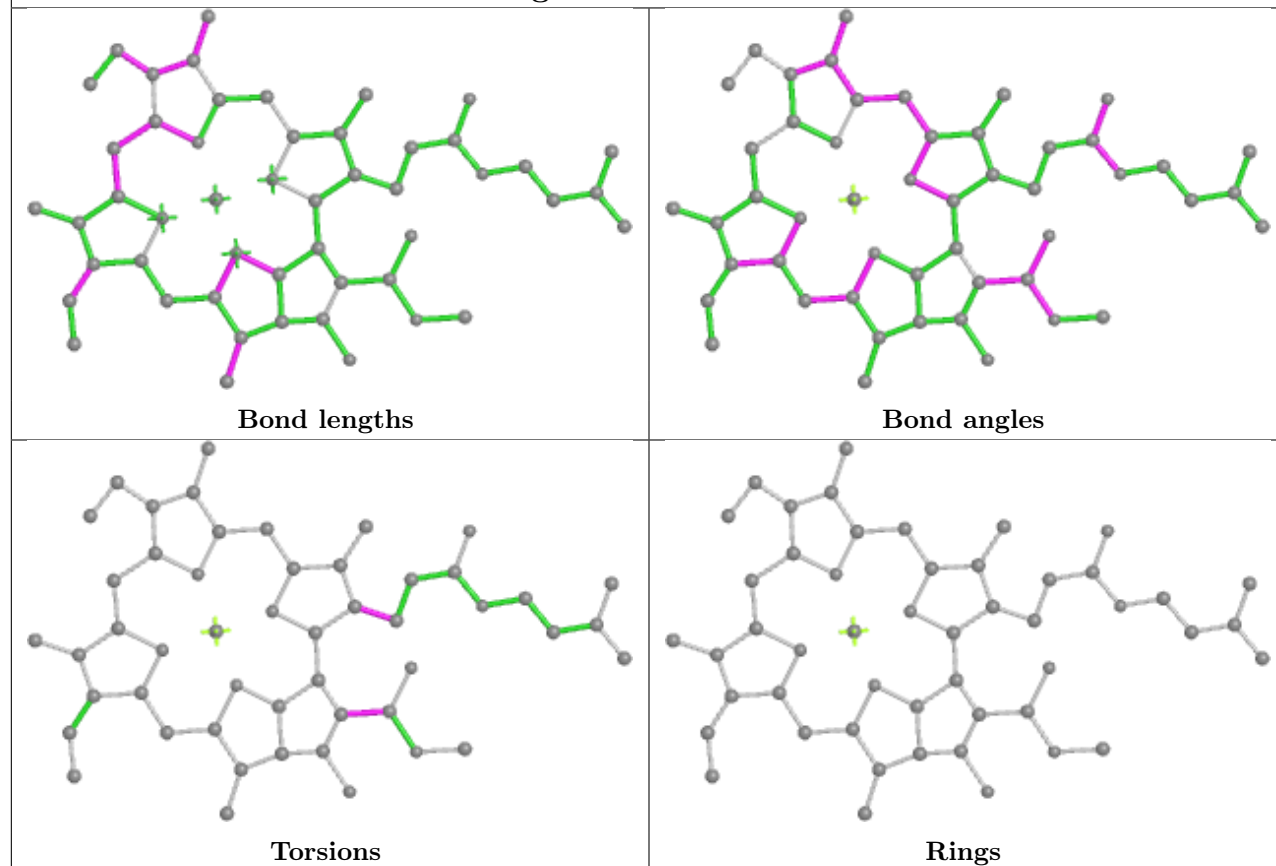


Torsions

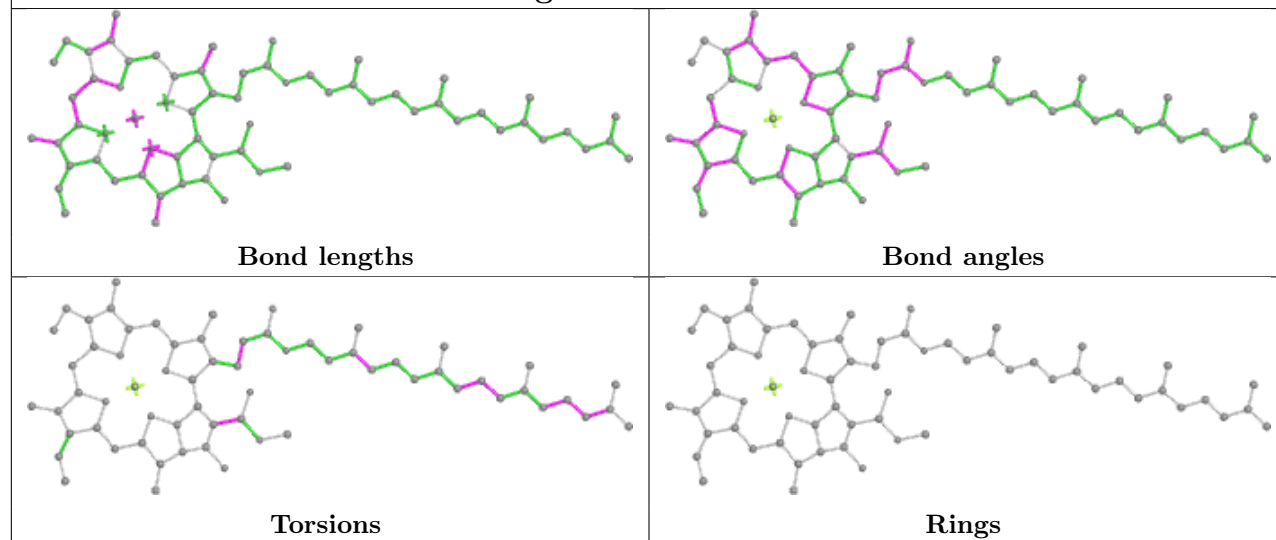


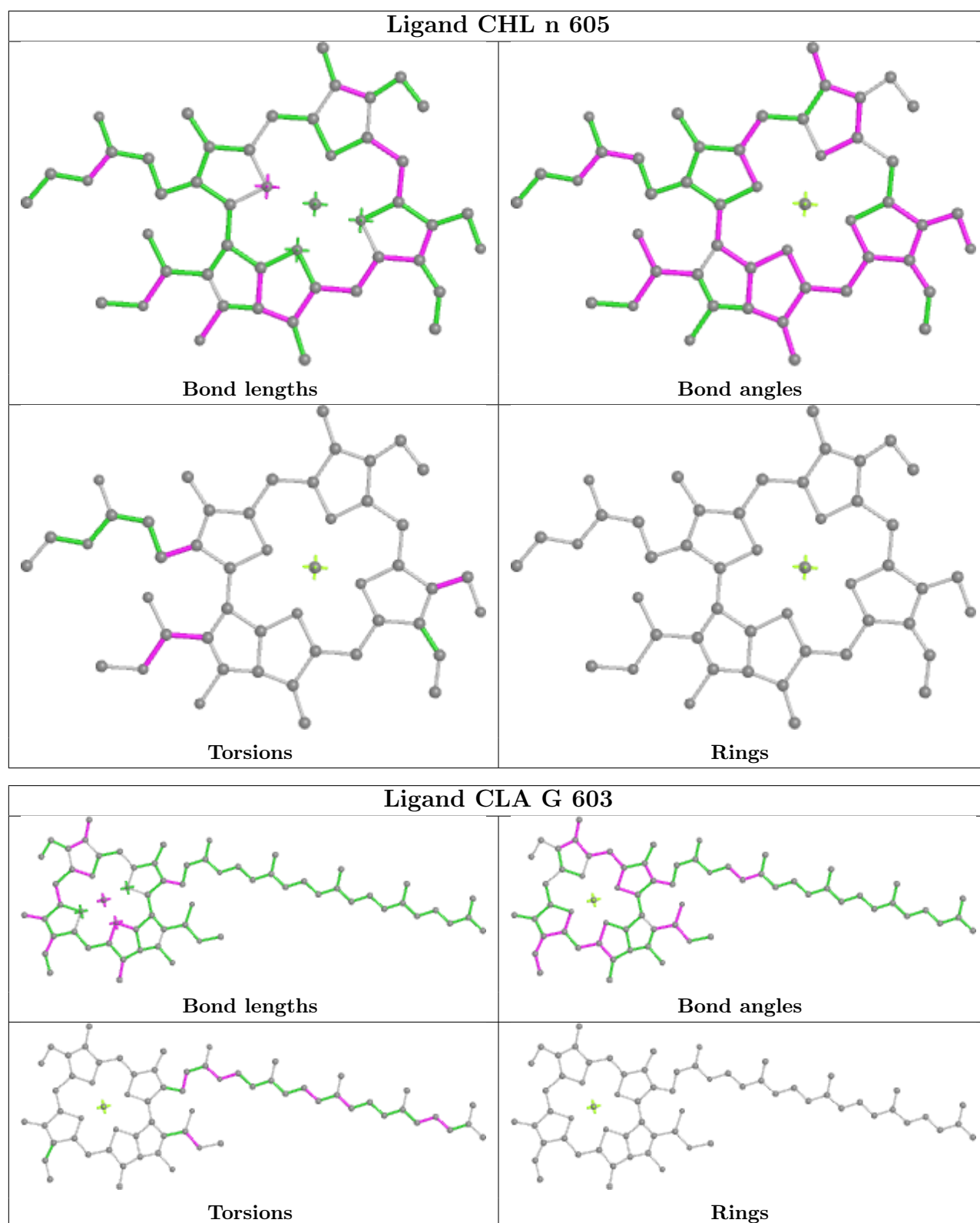
Rings

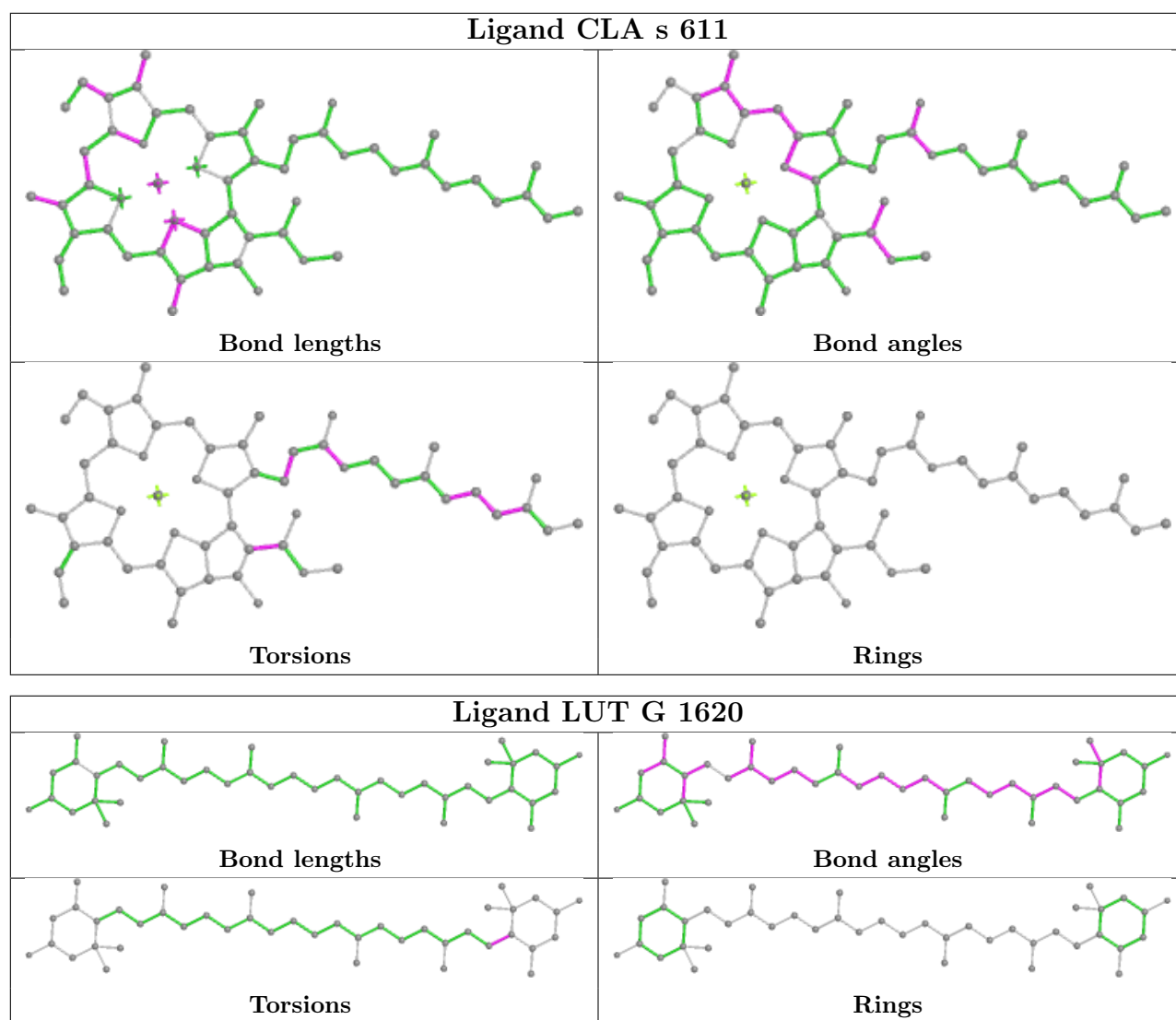
Ligand CLA A 407

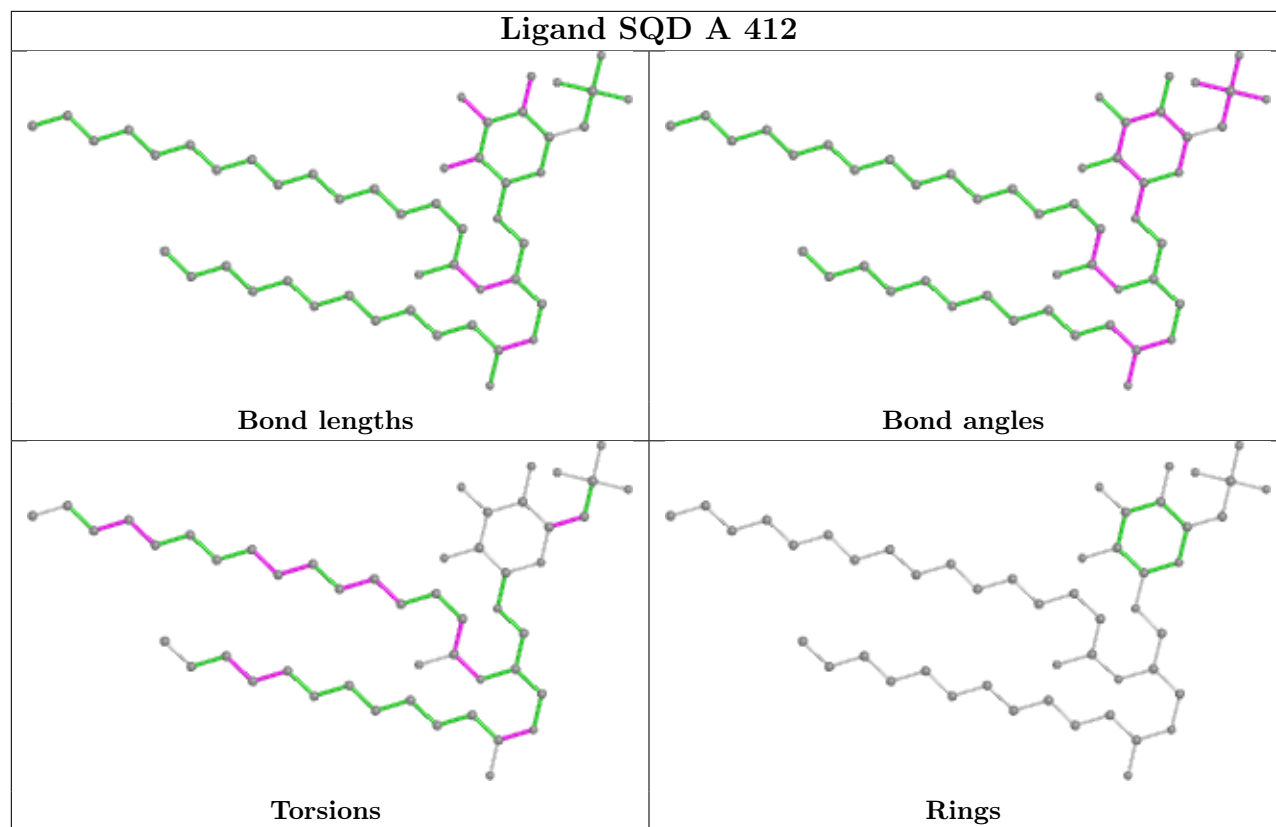


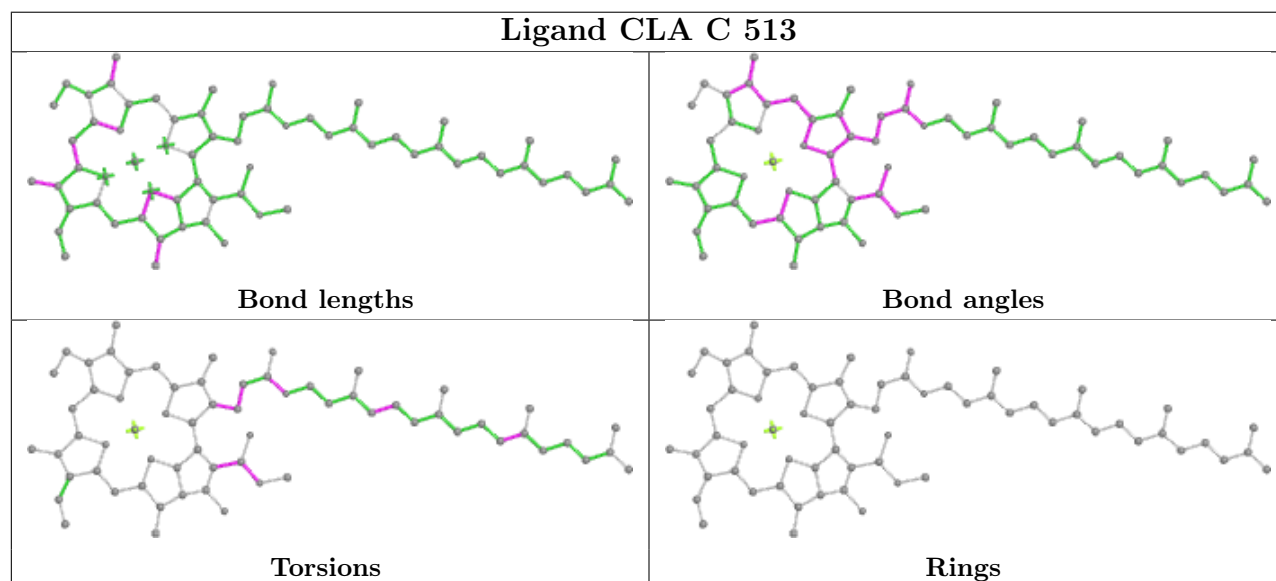
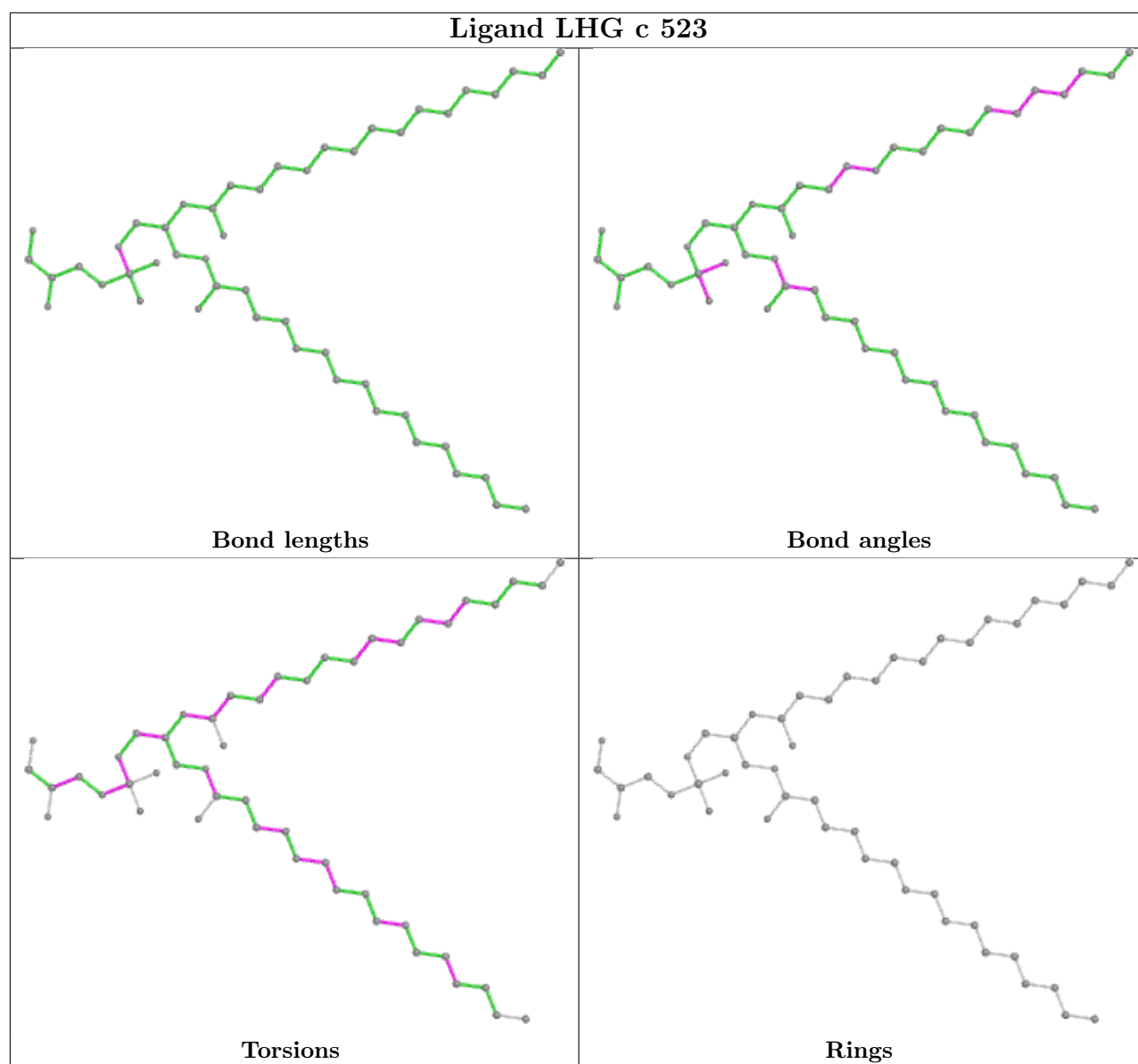
Ligand CLA b 607



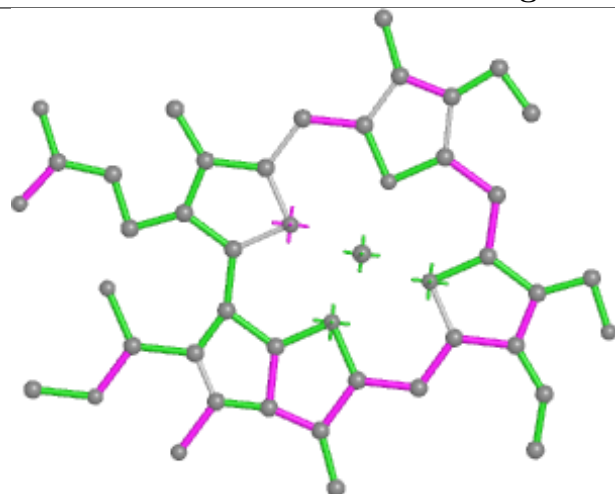




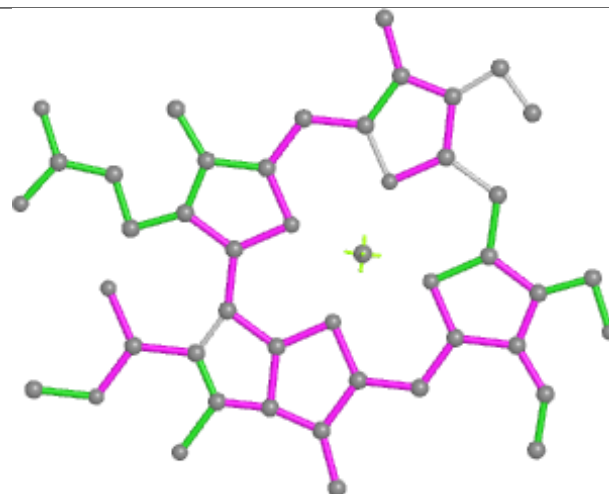




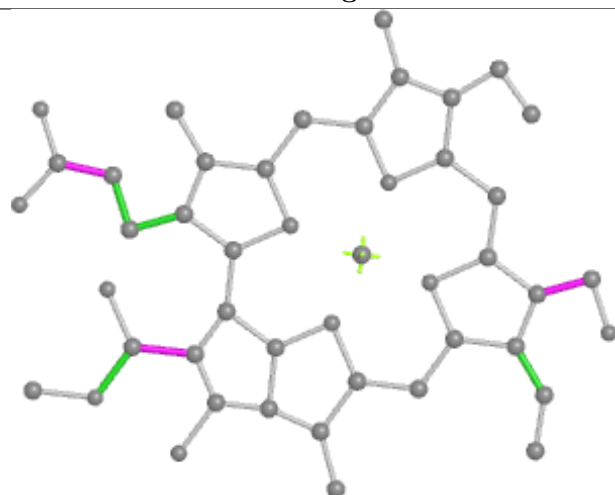
Ligand CHL 5 601



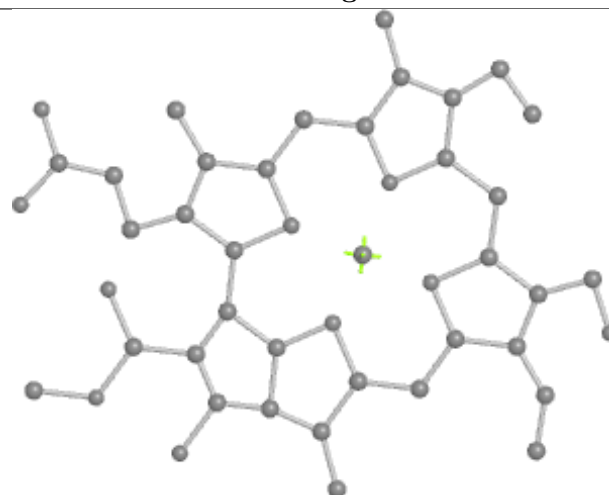
Bond lengths



Bond angles

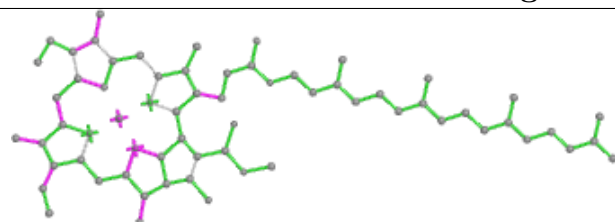


Torsions

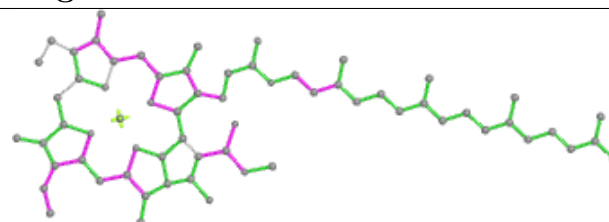


Rings

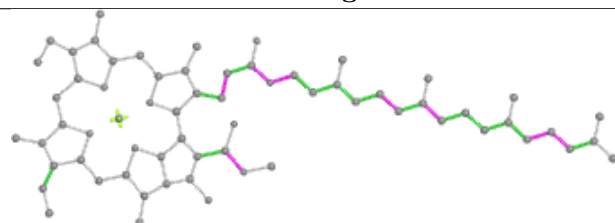
Ligand CLA g 603



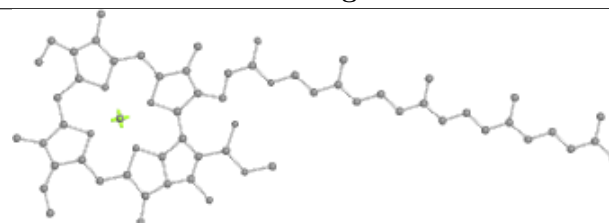
Bond lengths



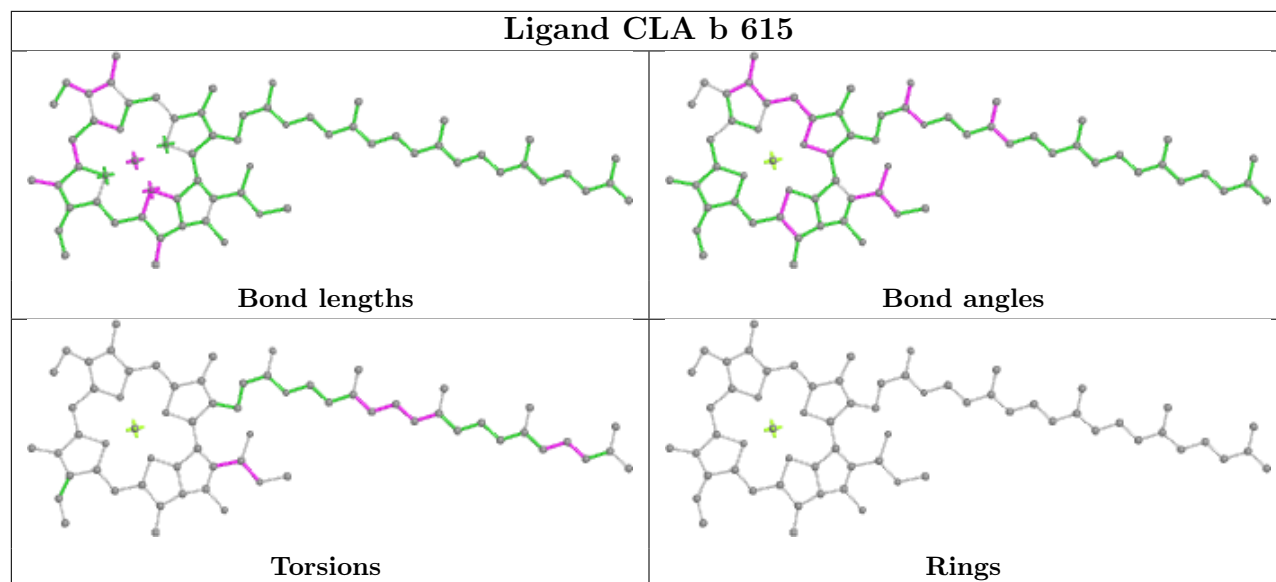
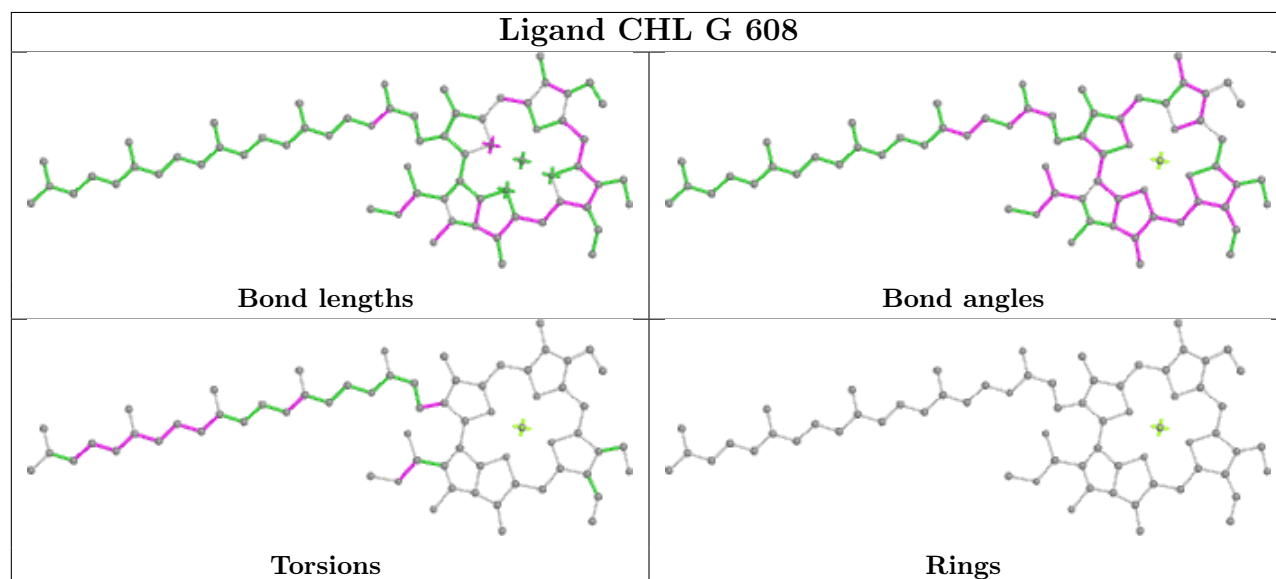
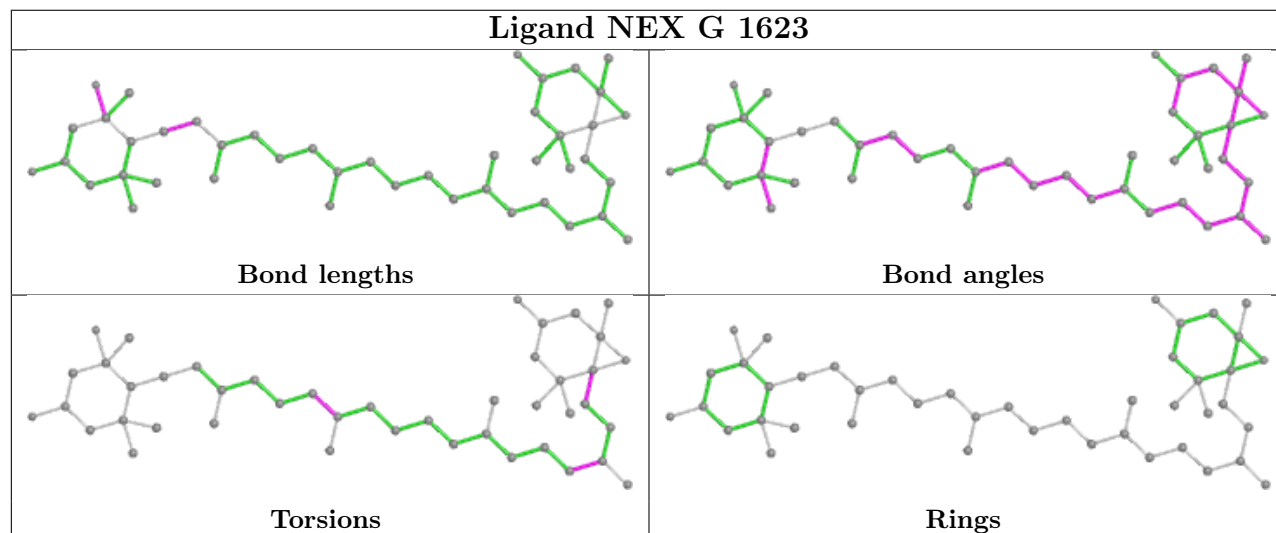
Bond angles



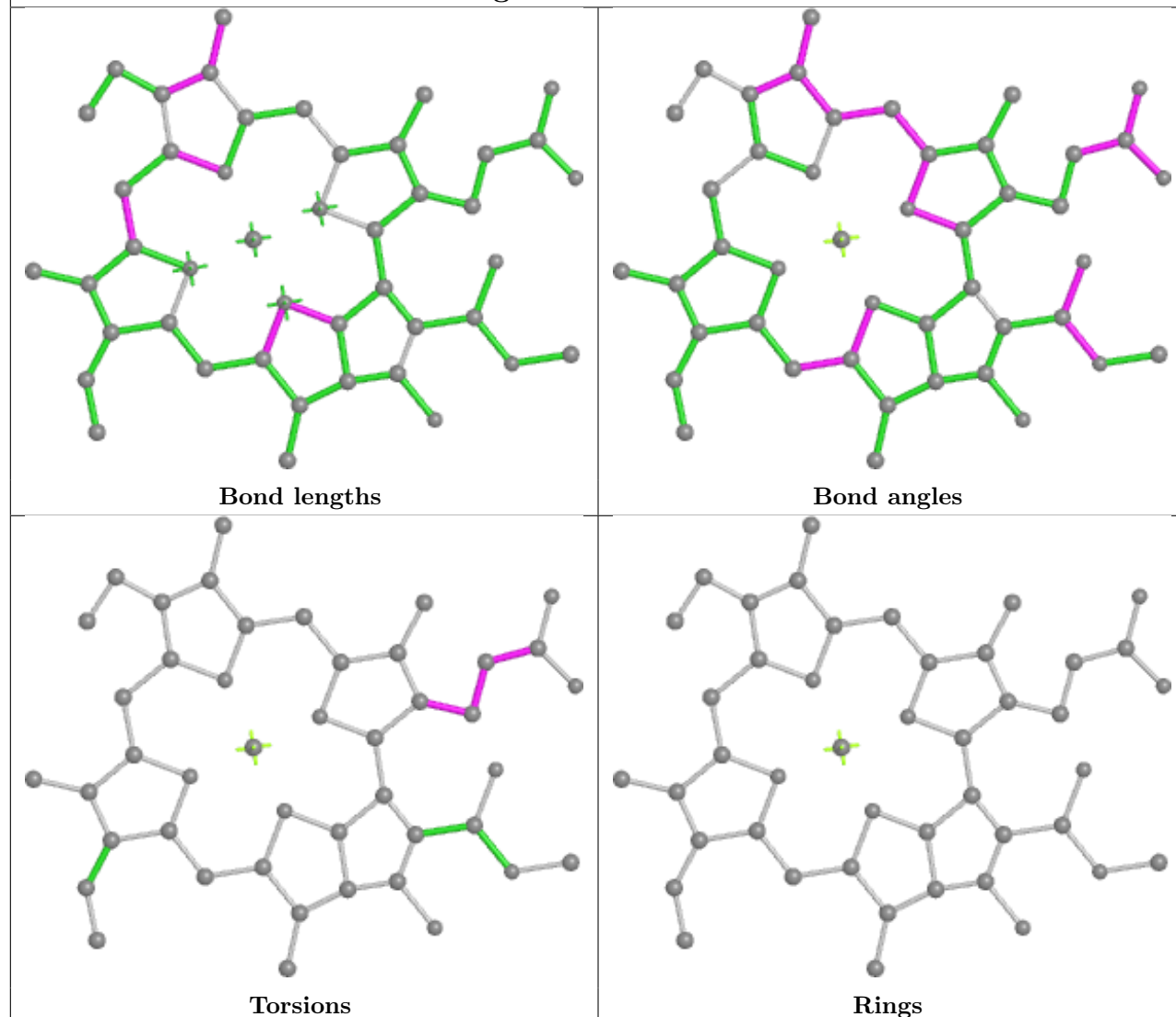
Torsions



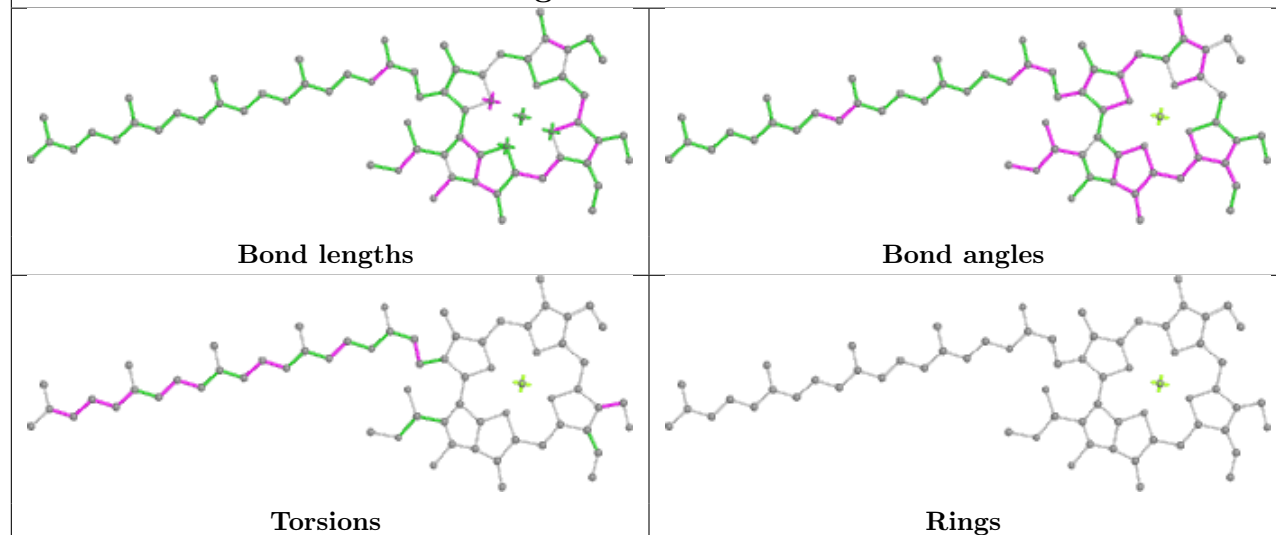
Rings

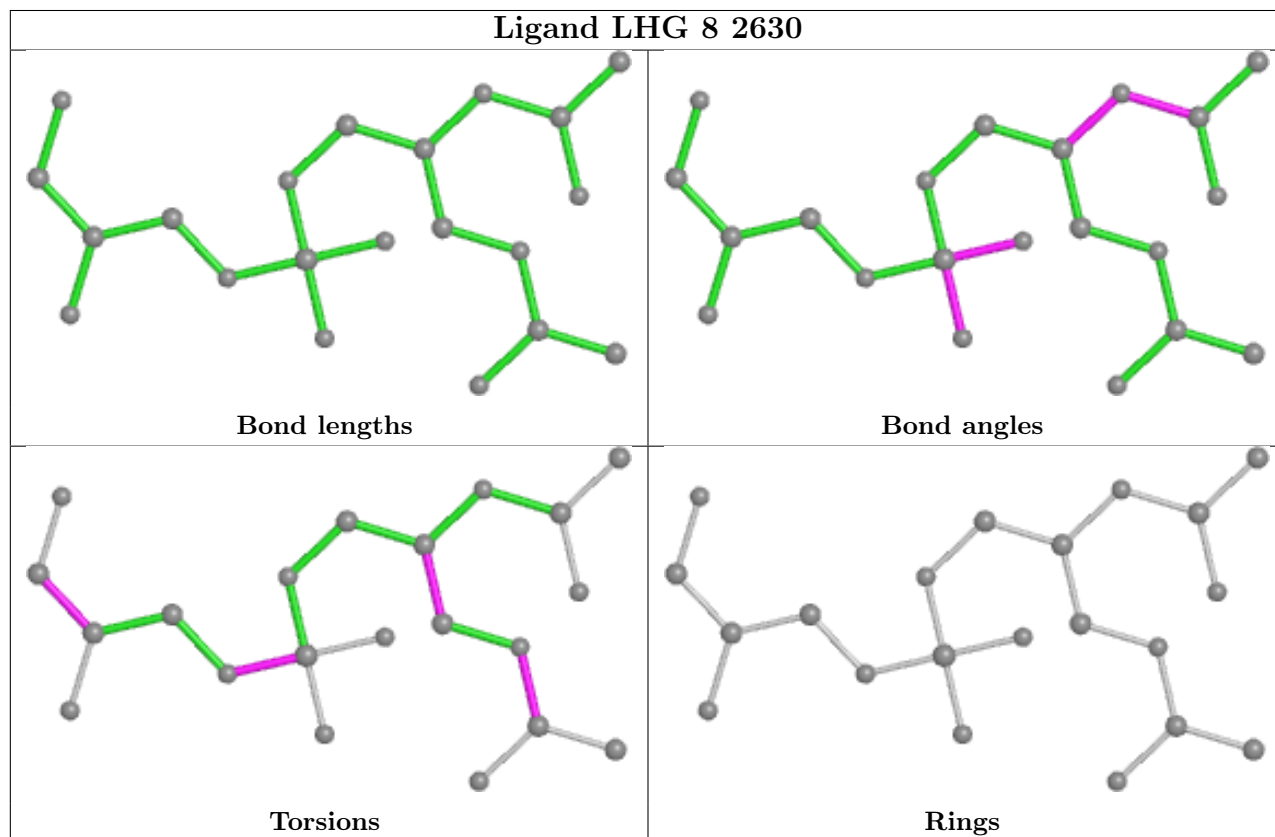
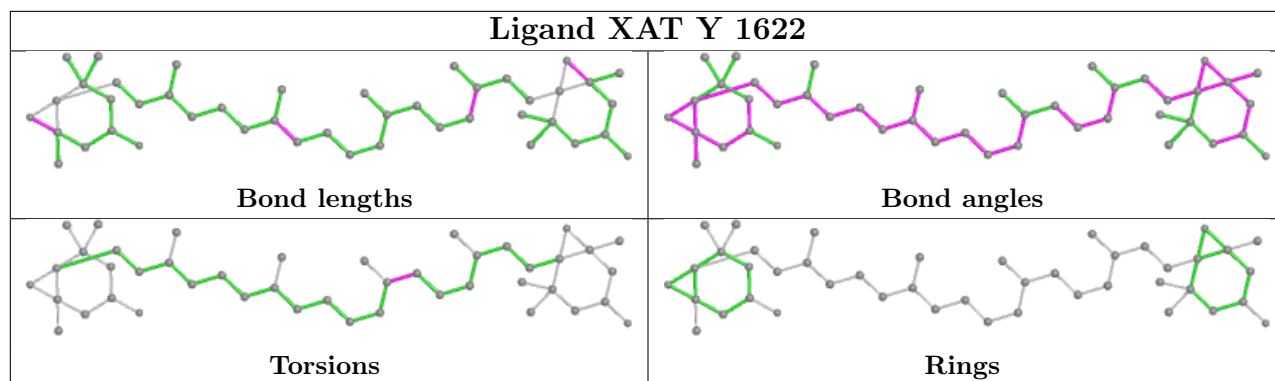
Ligand CLA b 615**Ligand CHL G 608****Ligand NEX G 1623**

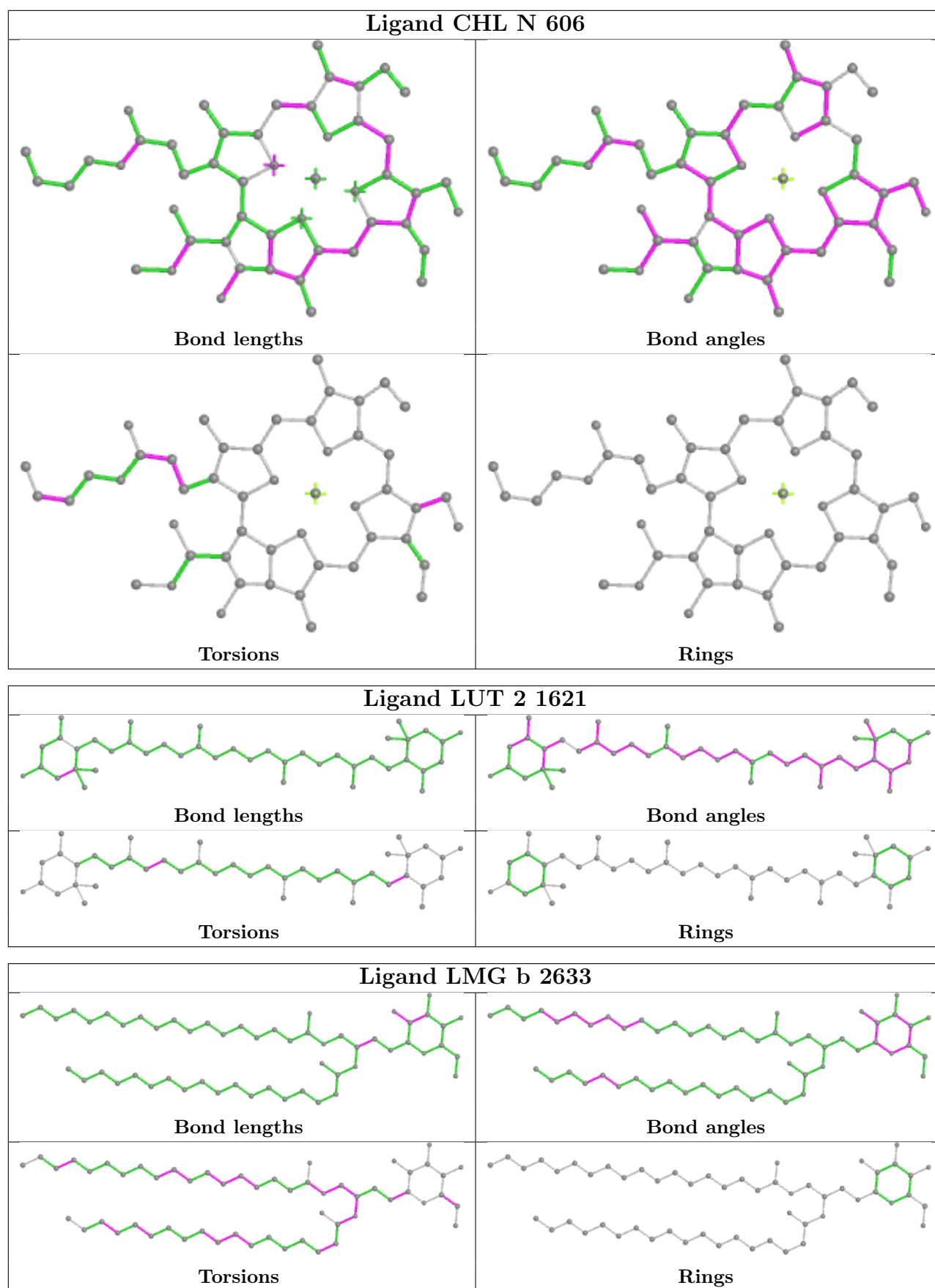
Ligand CLA S 609



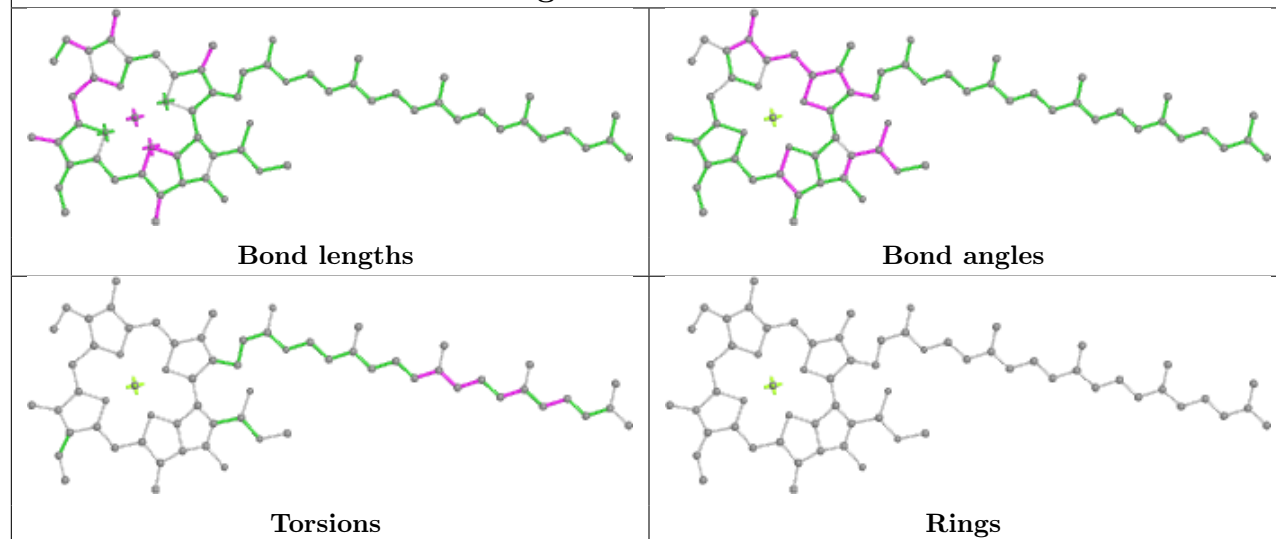
Ligand CHL n 607



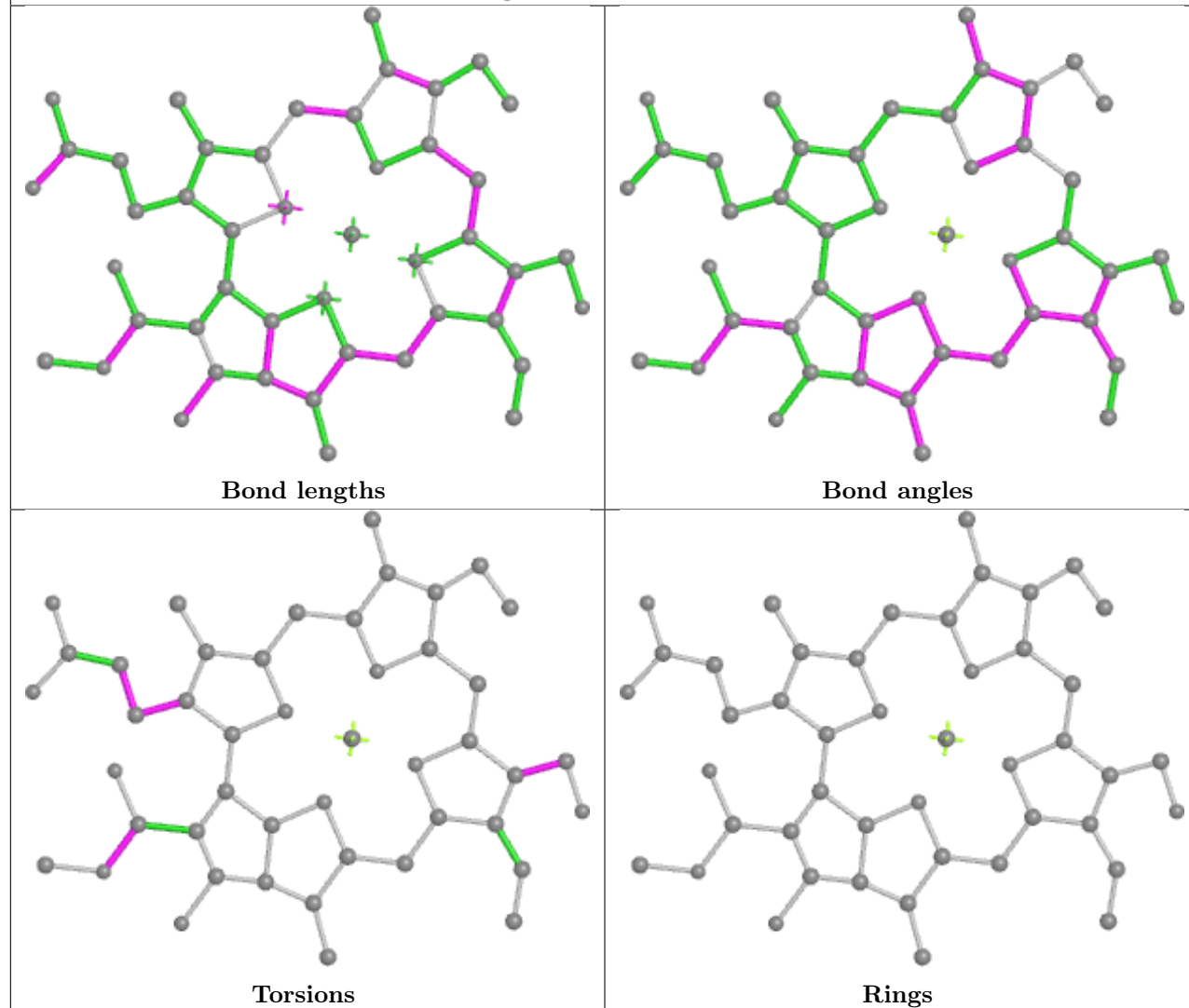


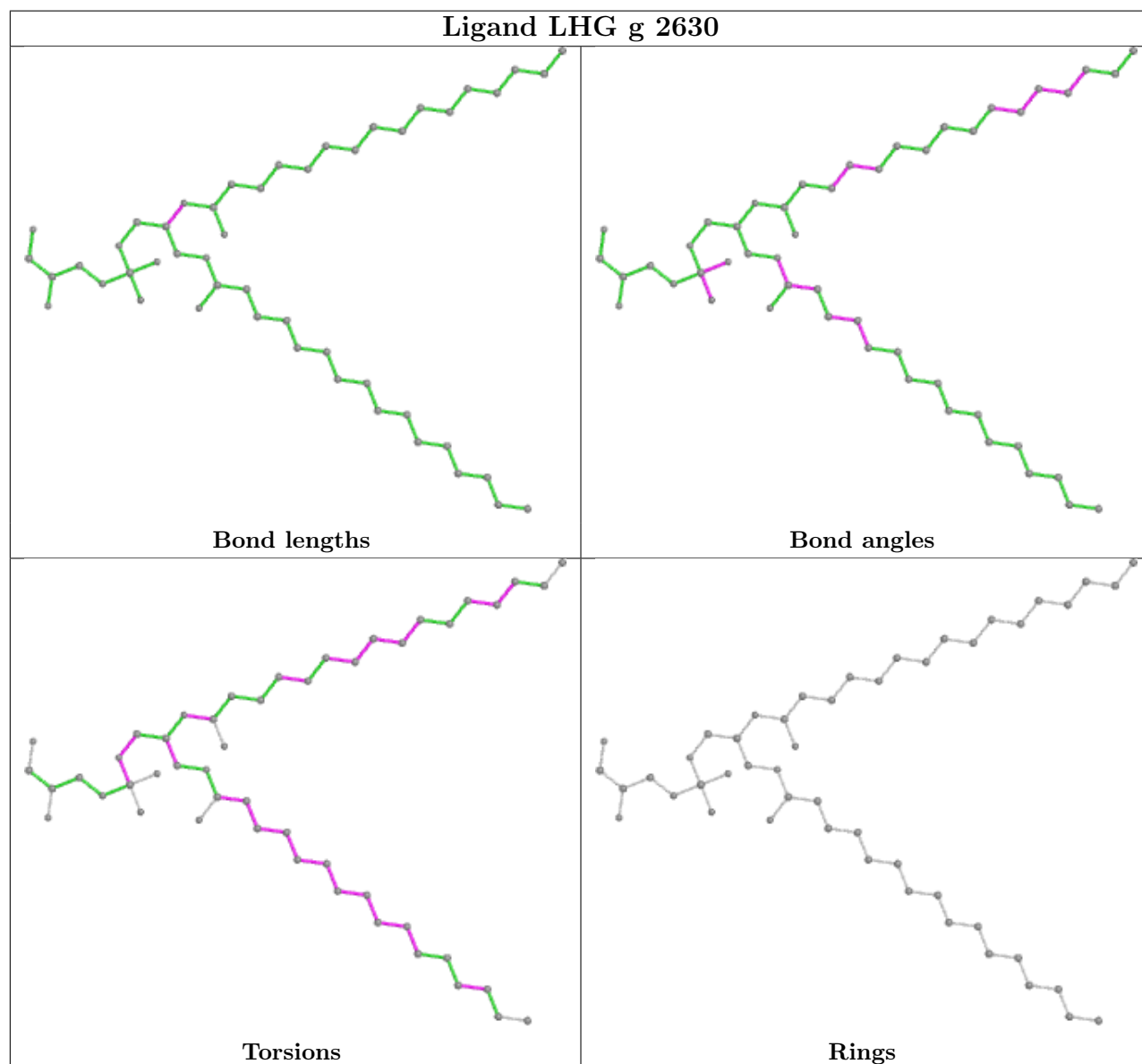
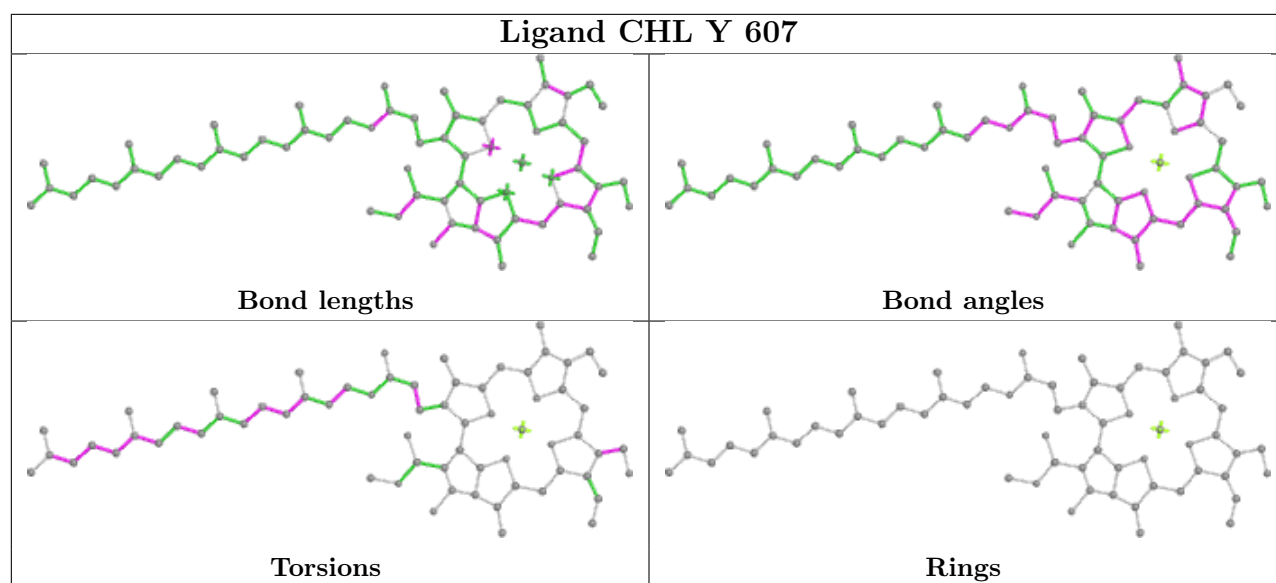


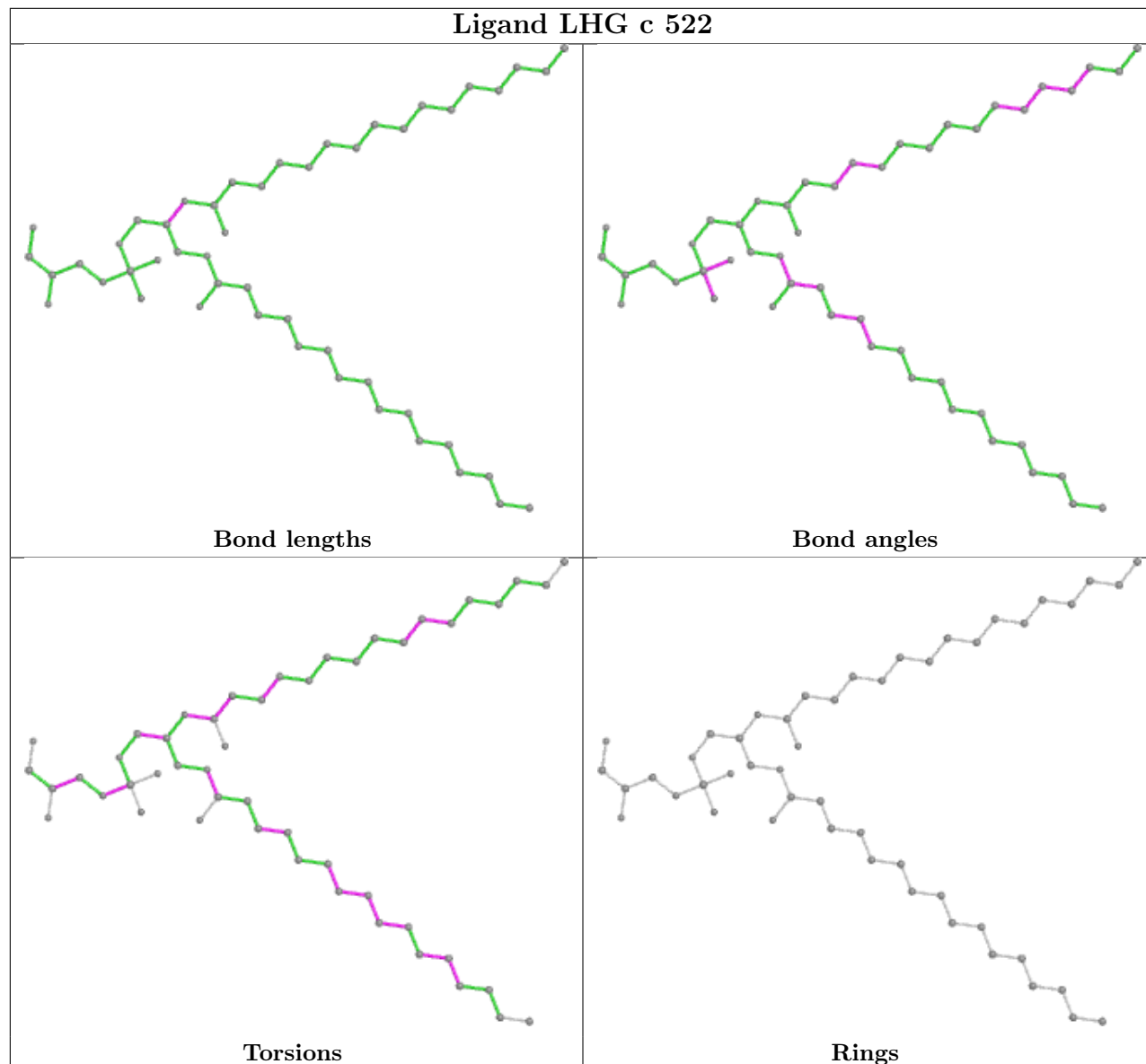
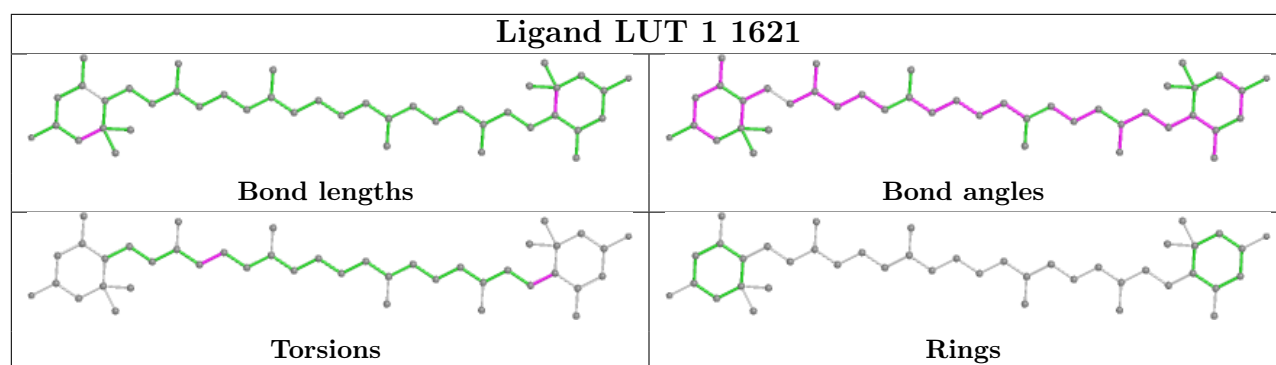
Ligand CLA c 509

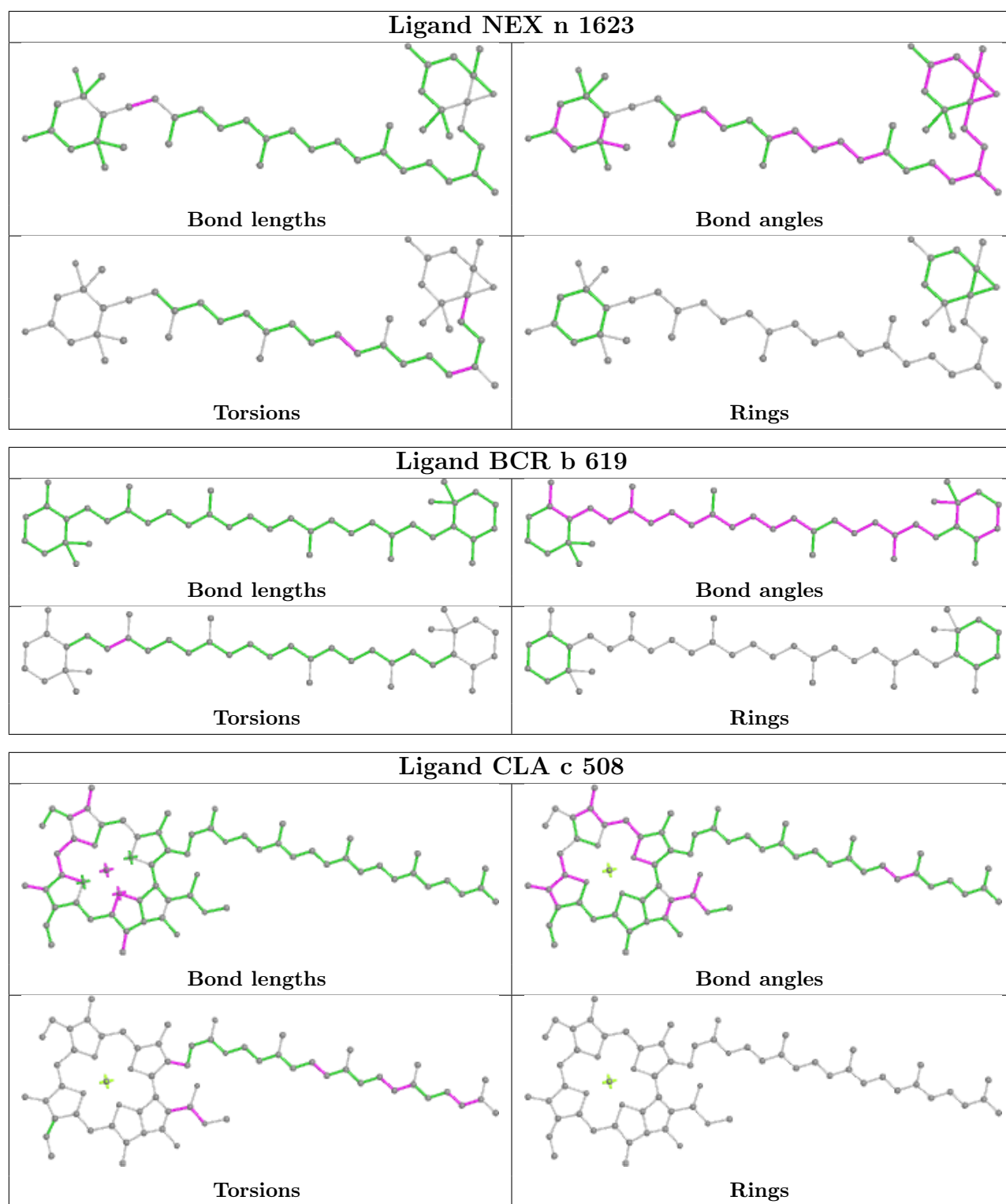


Ligand CHL 5 608

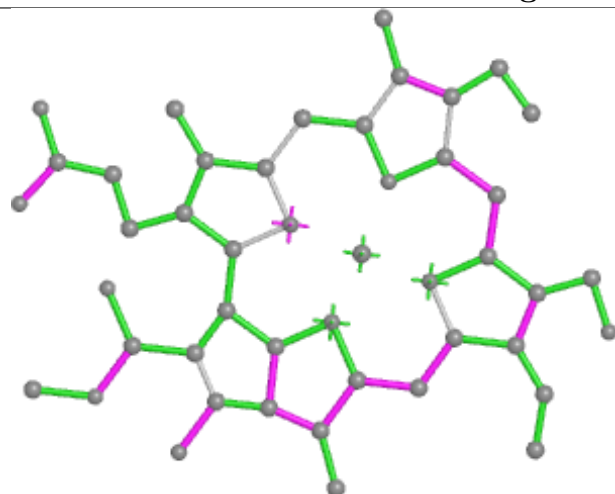




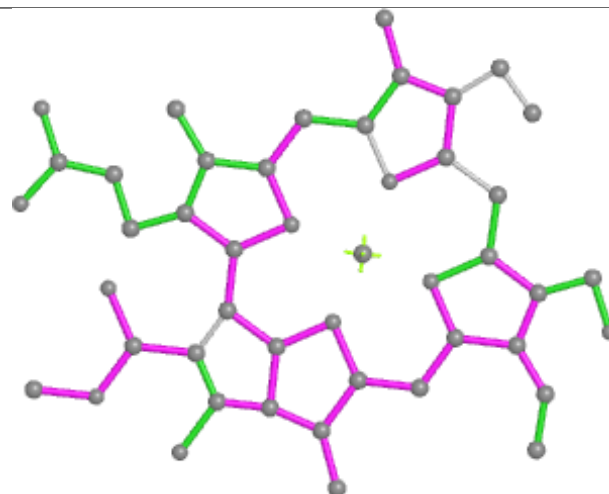




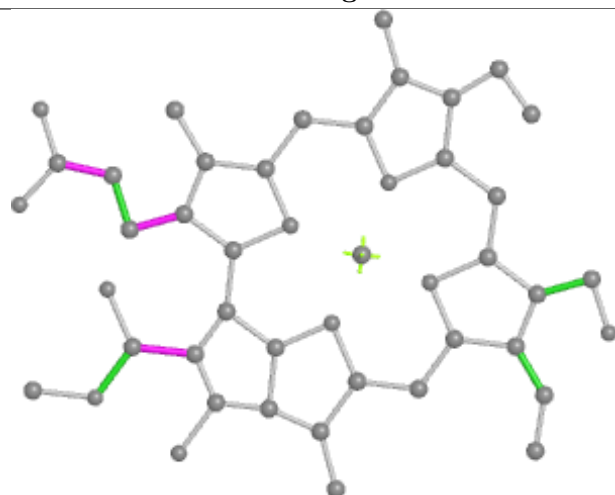
Ligand CHL 6 601



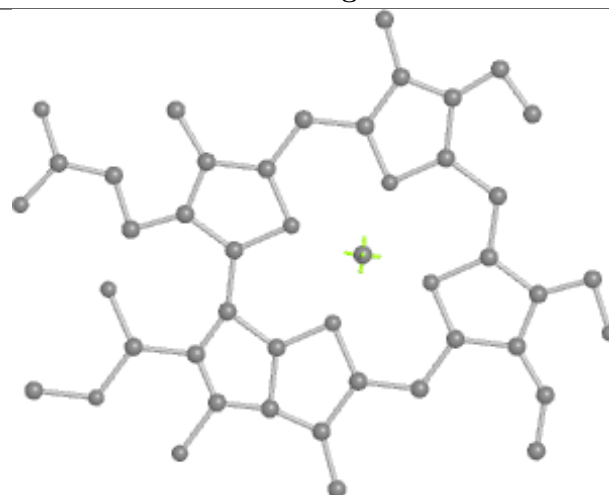
Bond lengths



Bond angles

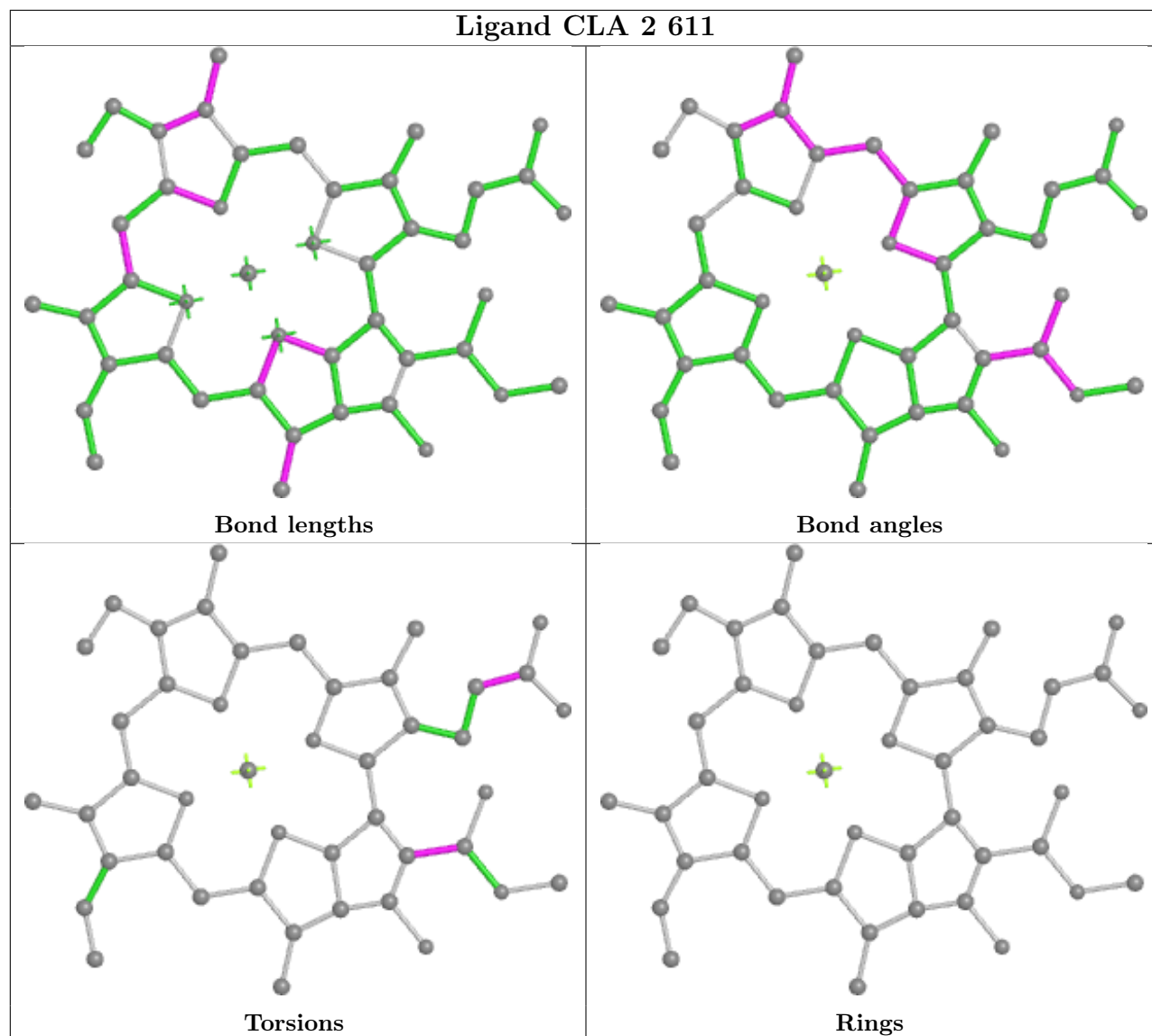


Torsions

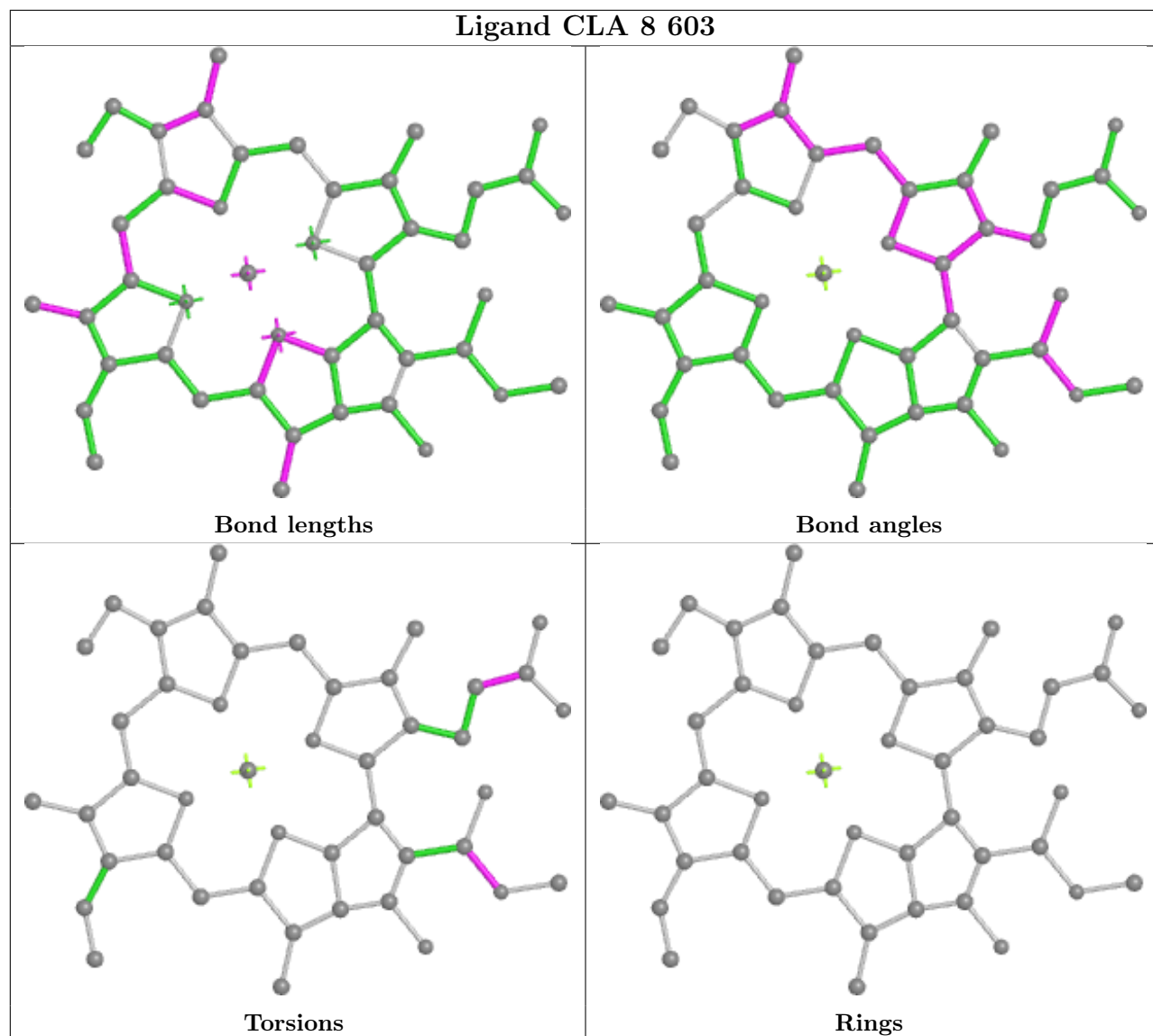


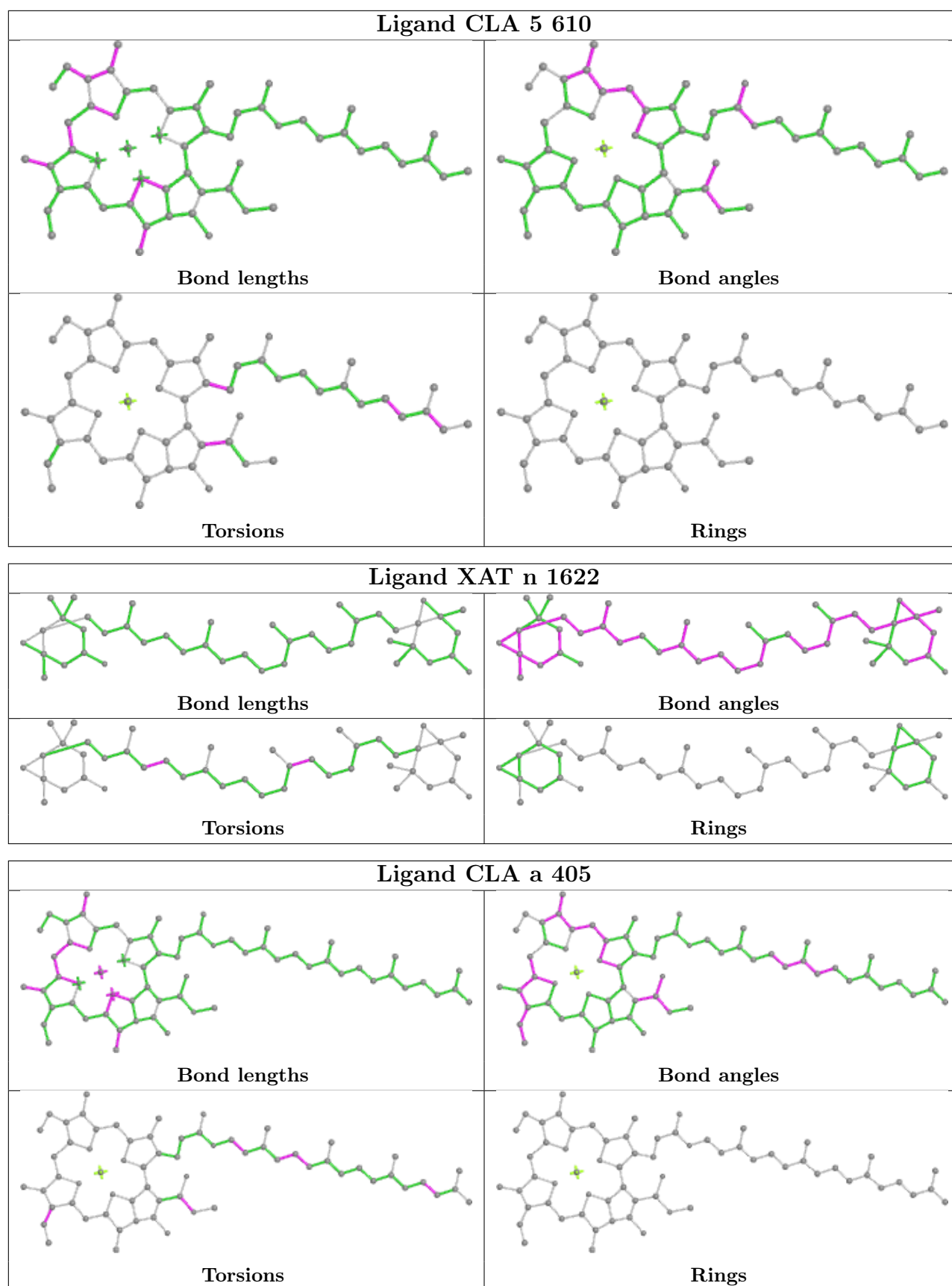
Rings

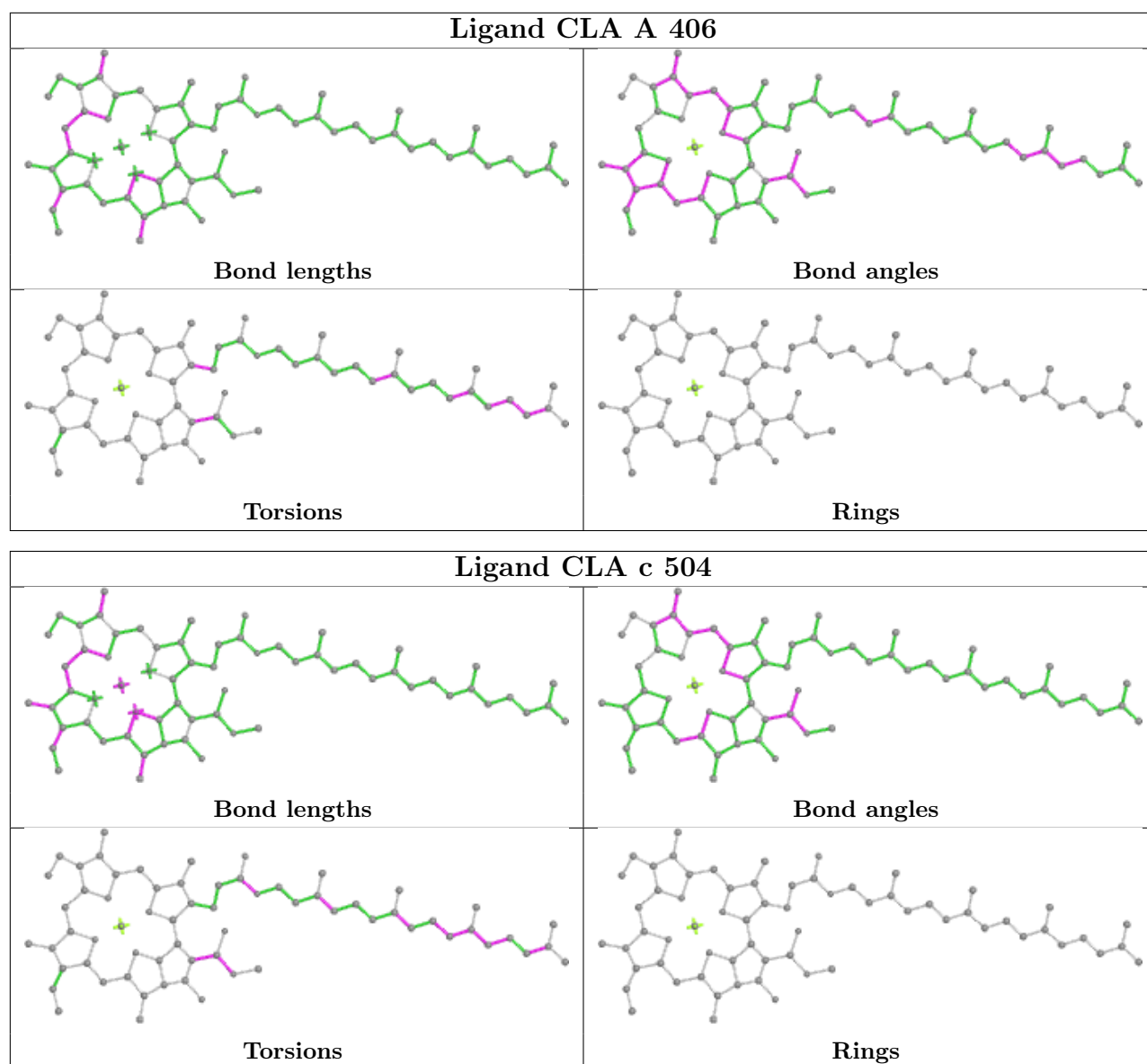
Ligand CLA 2 611

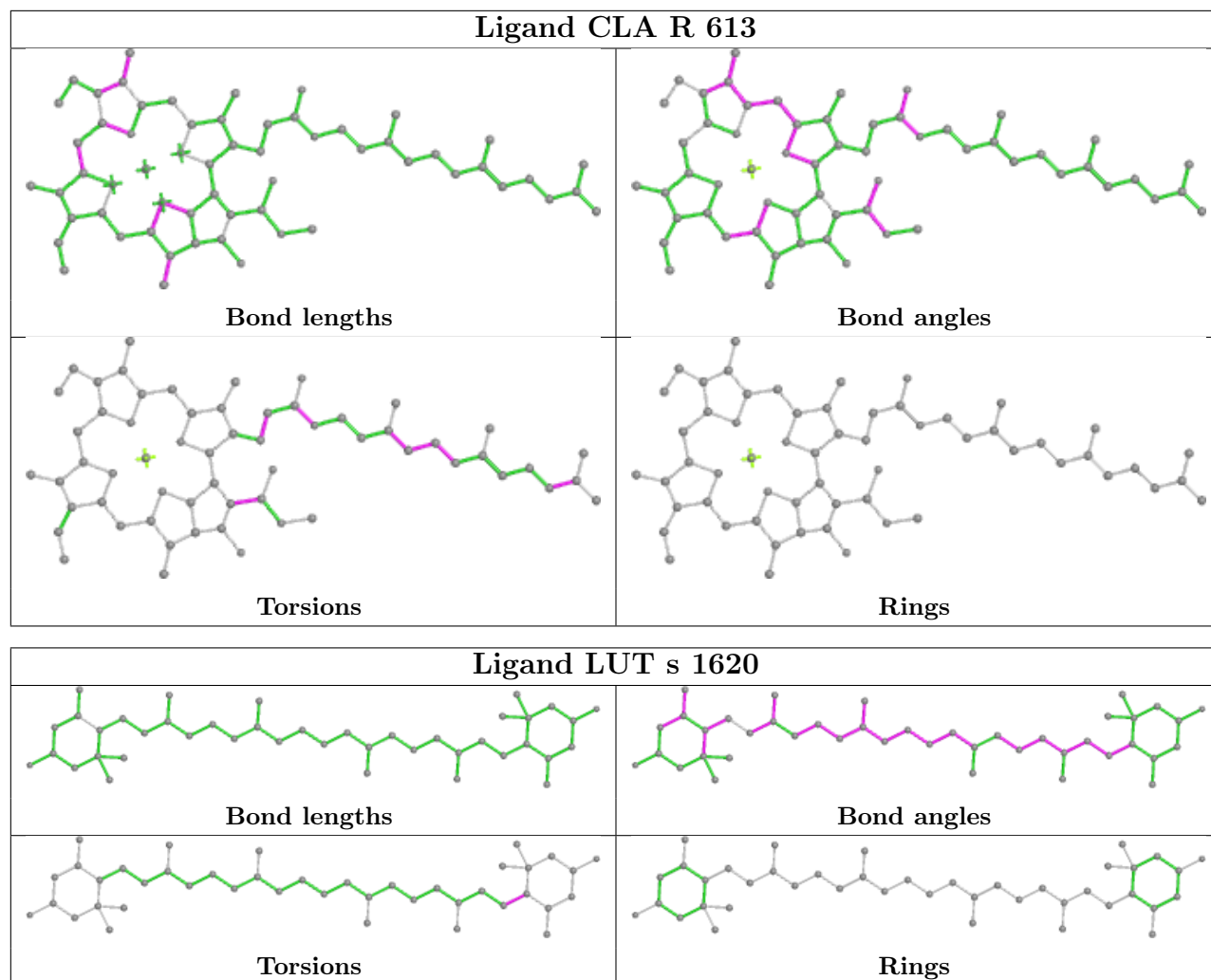


Ligand CLA 8 603

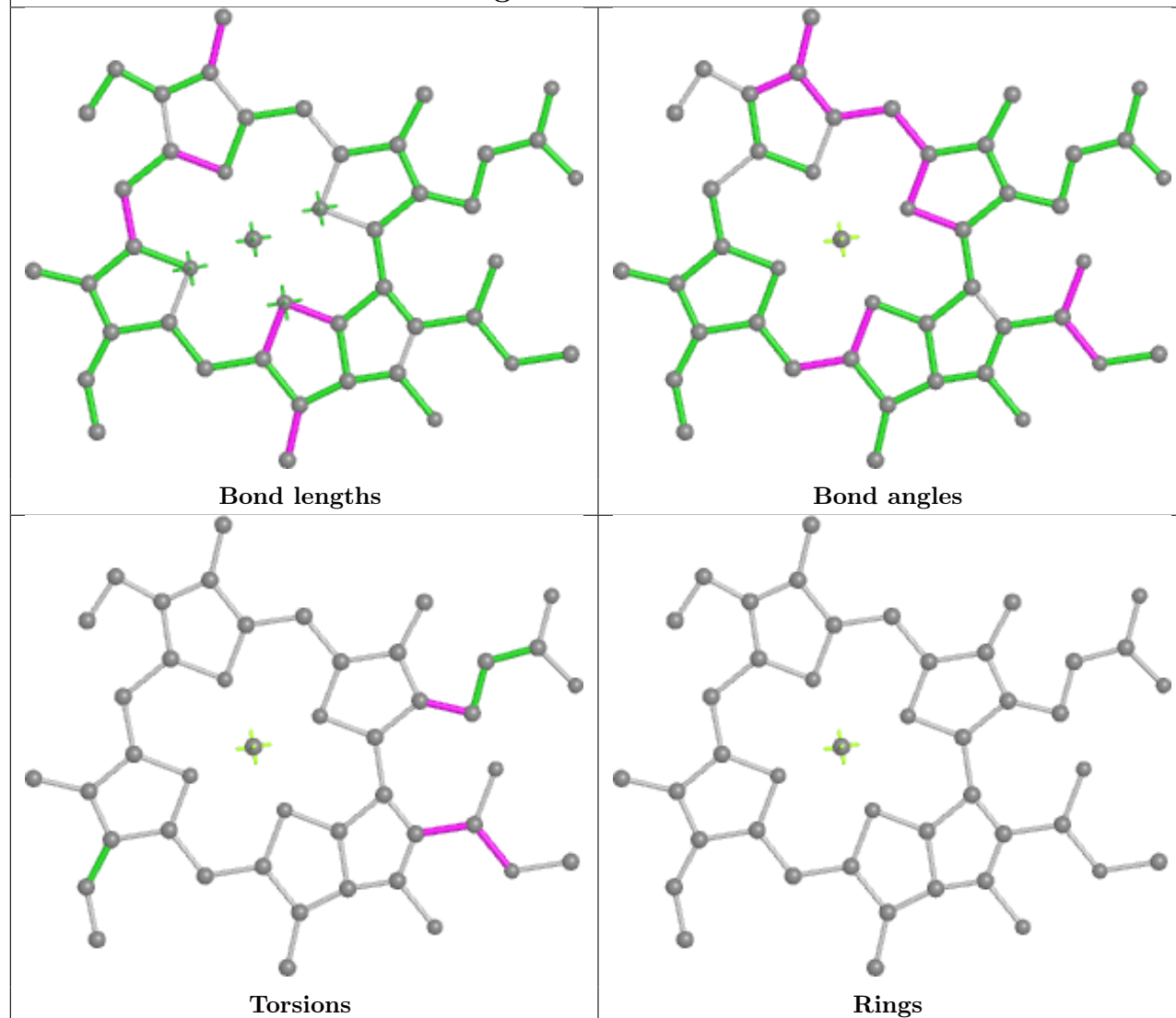




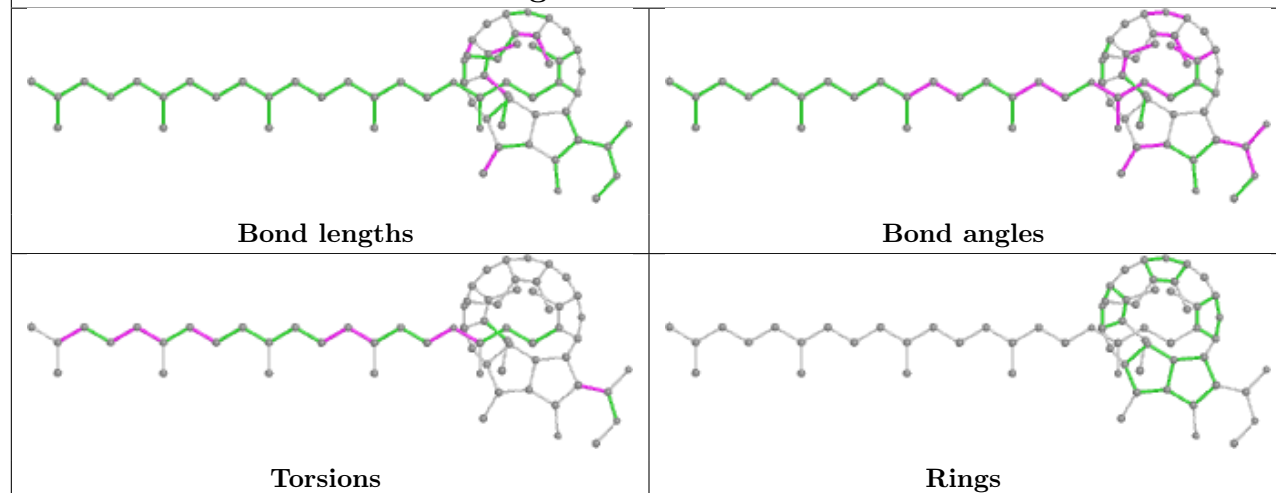




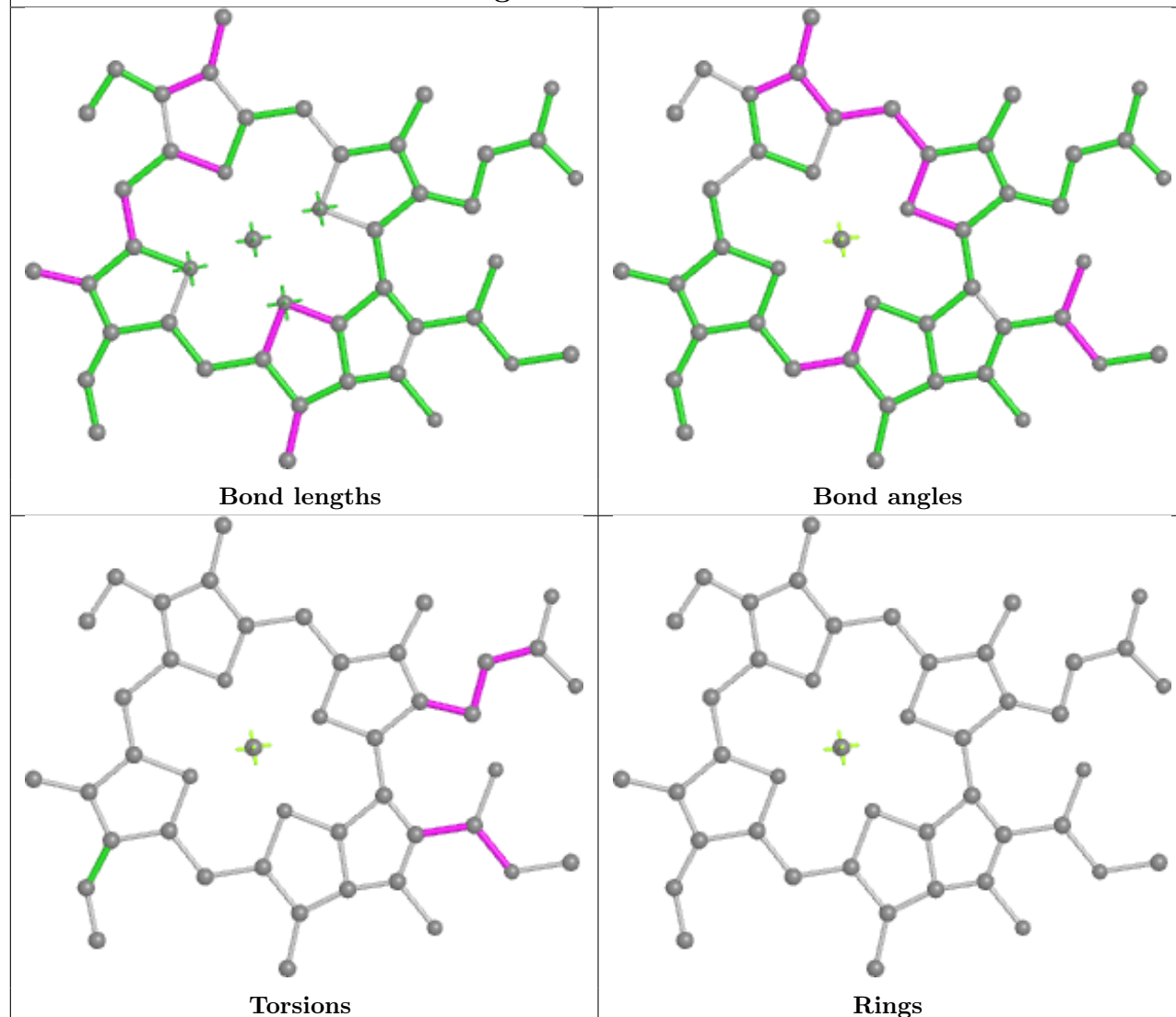
Ligand CLA 2 614



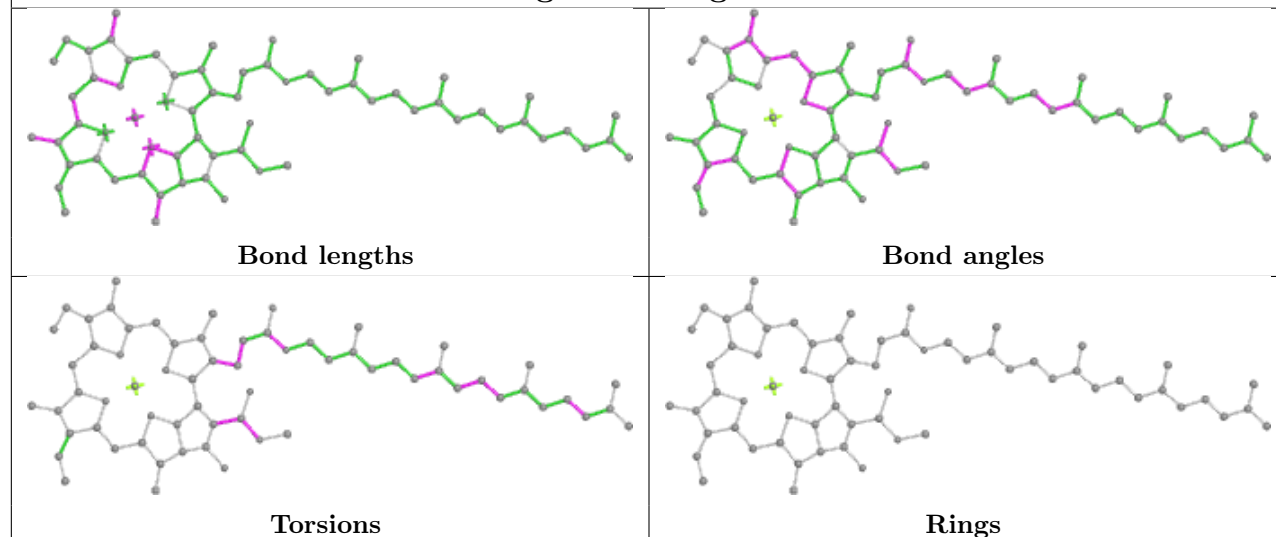
Ligand PHO A 408

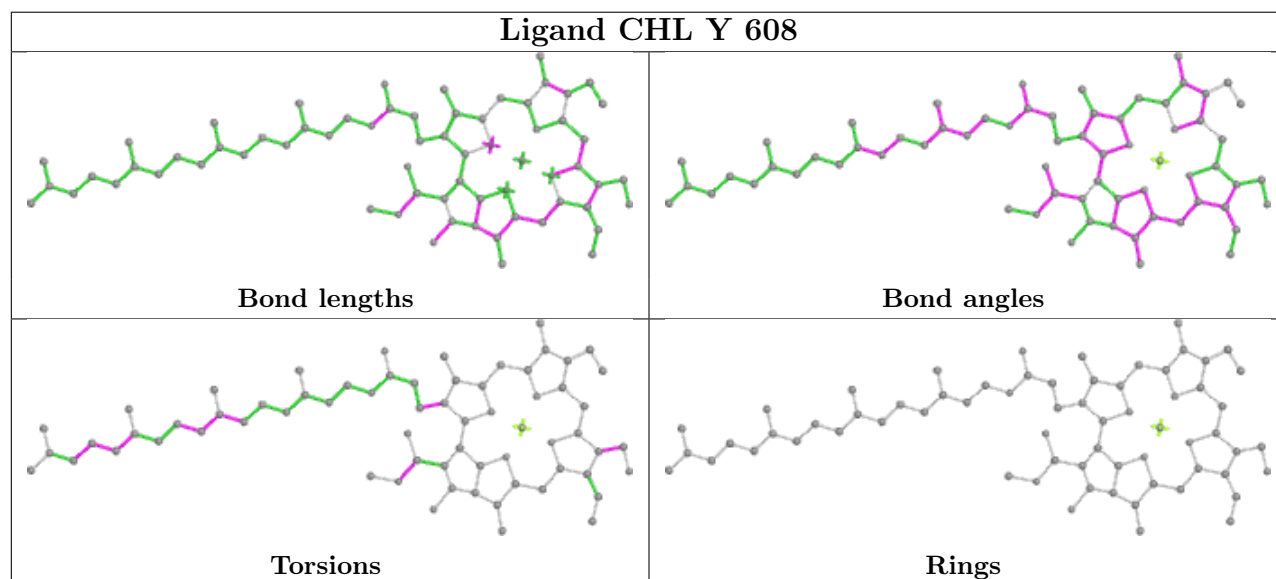
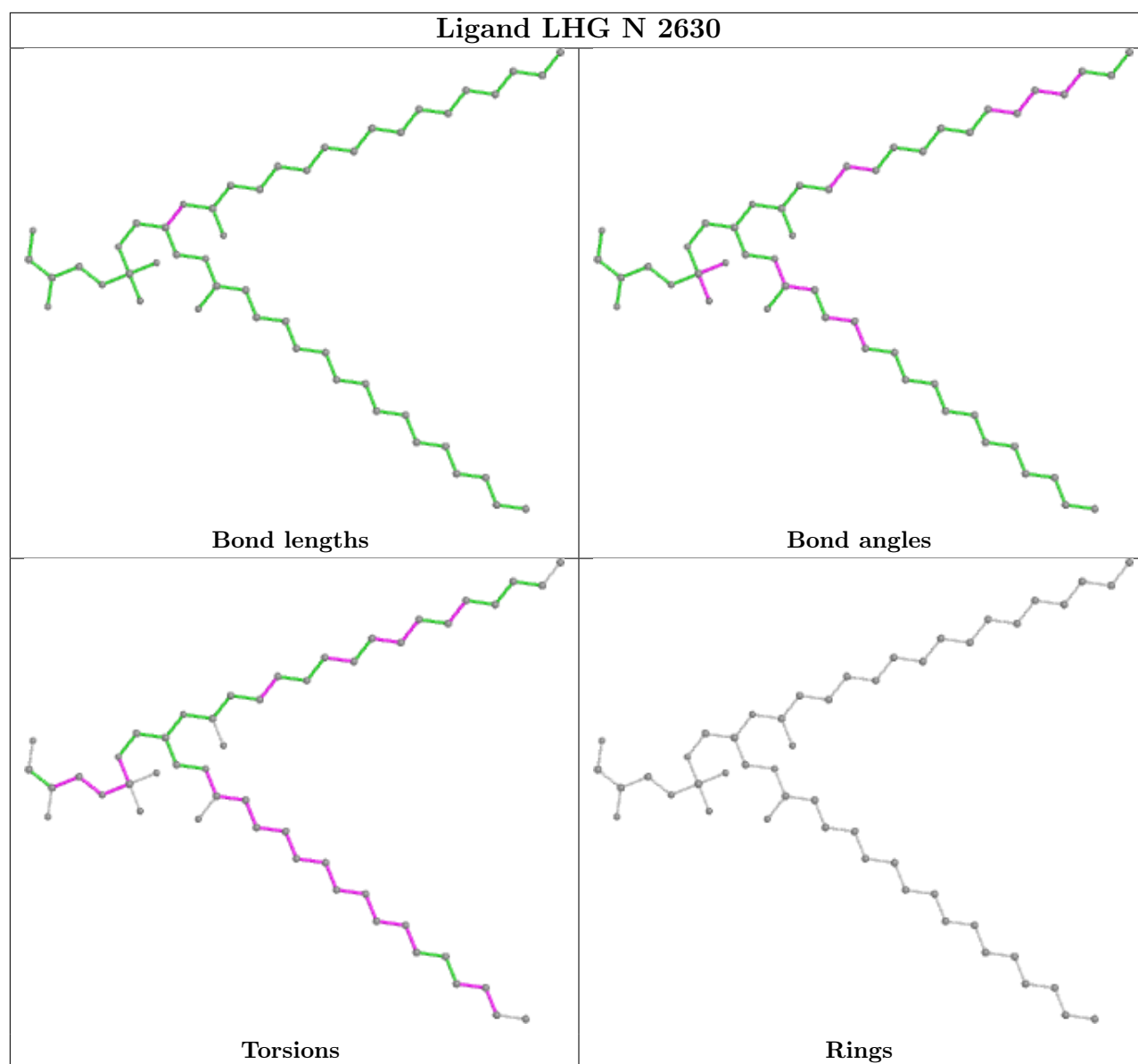


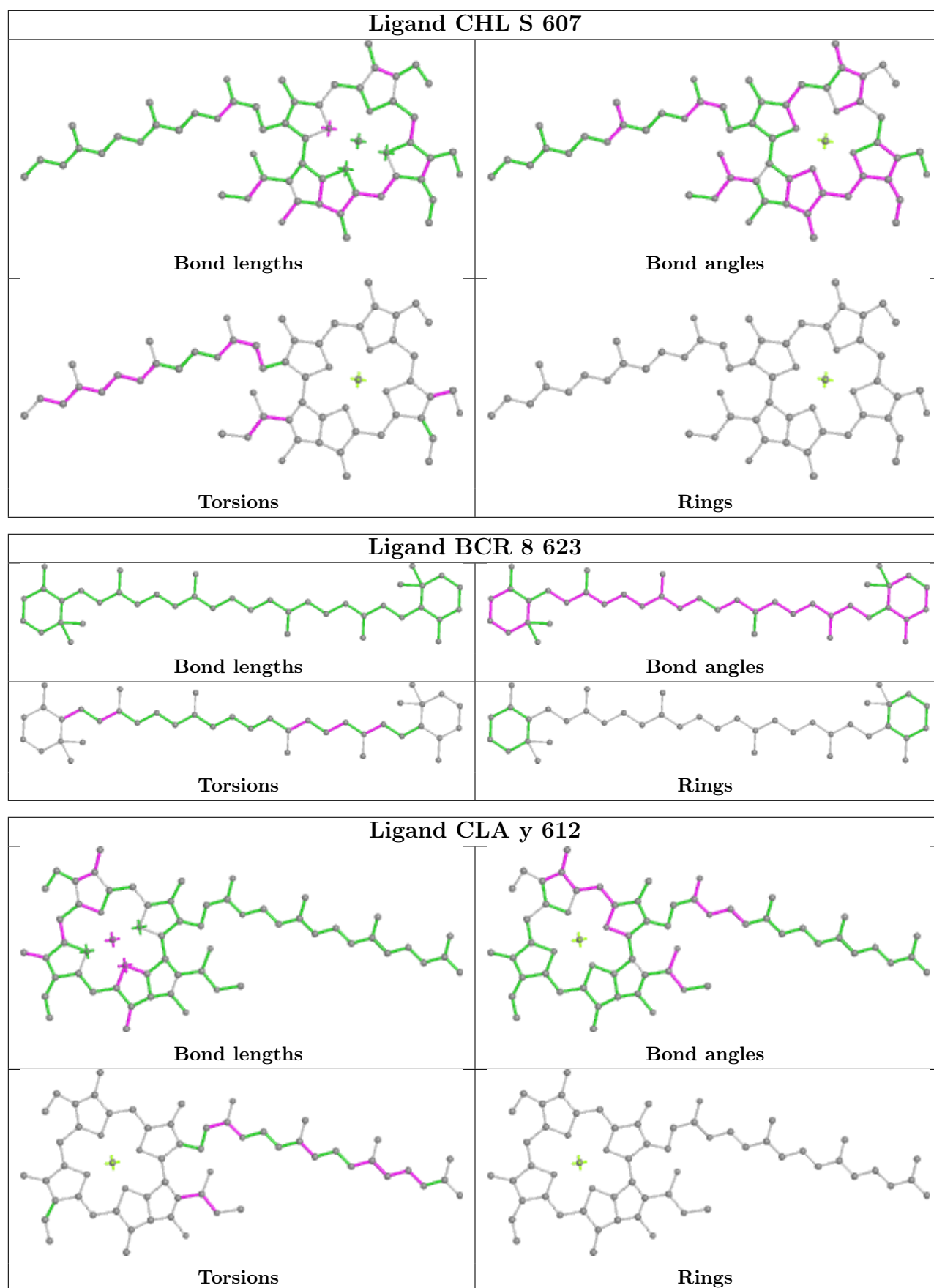
Ligand CLA 4 604



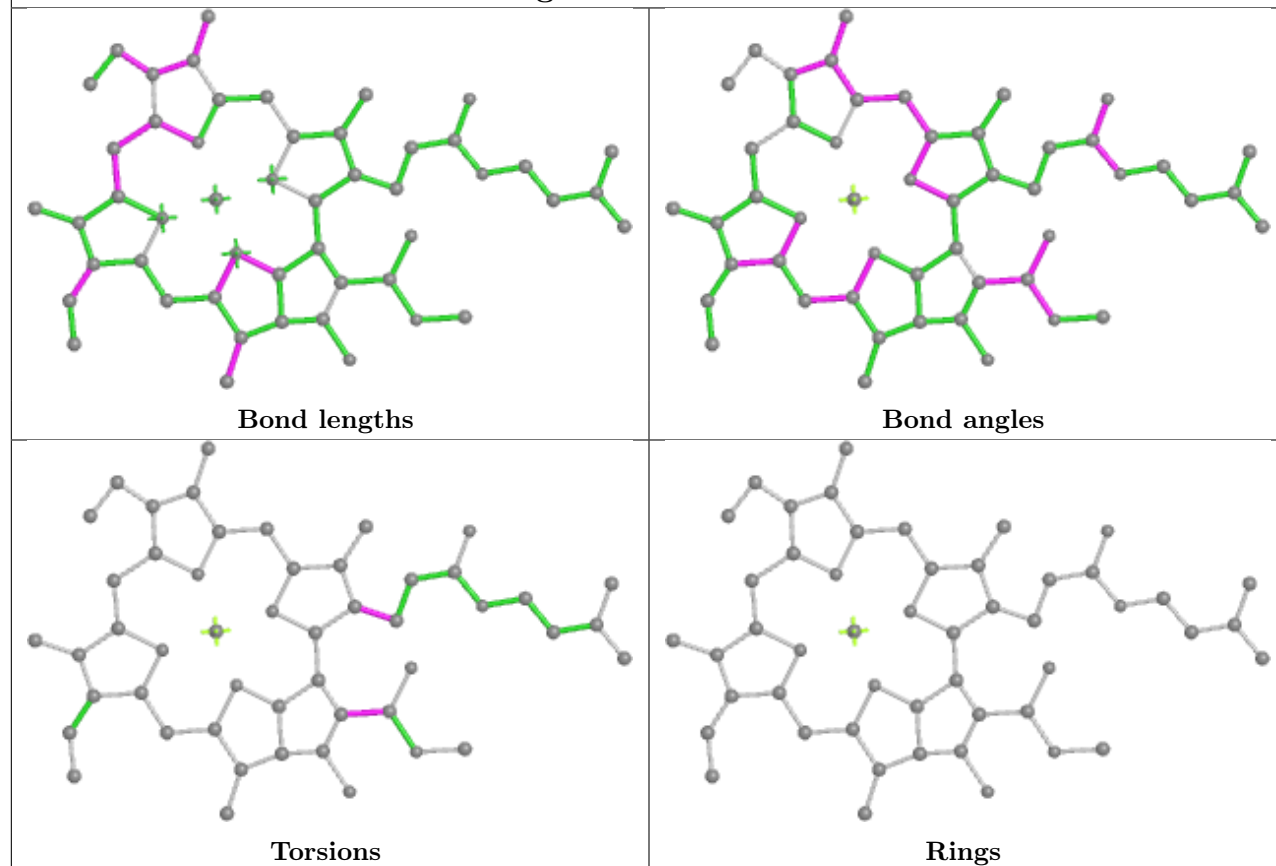
Ligand CLA g 602



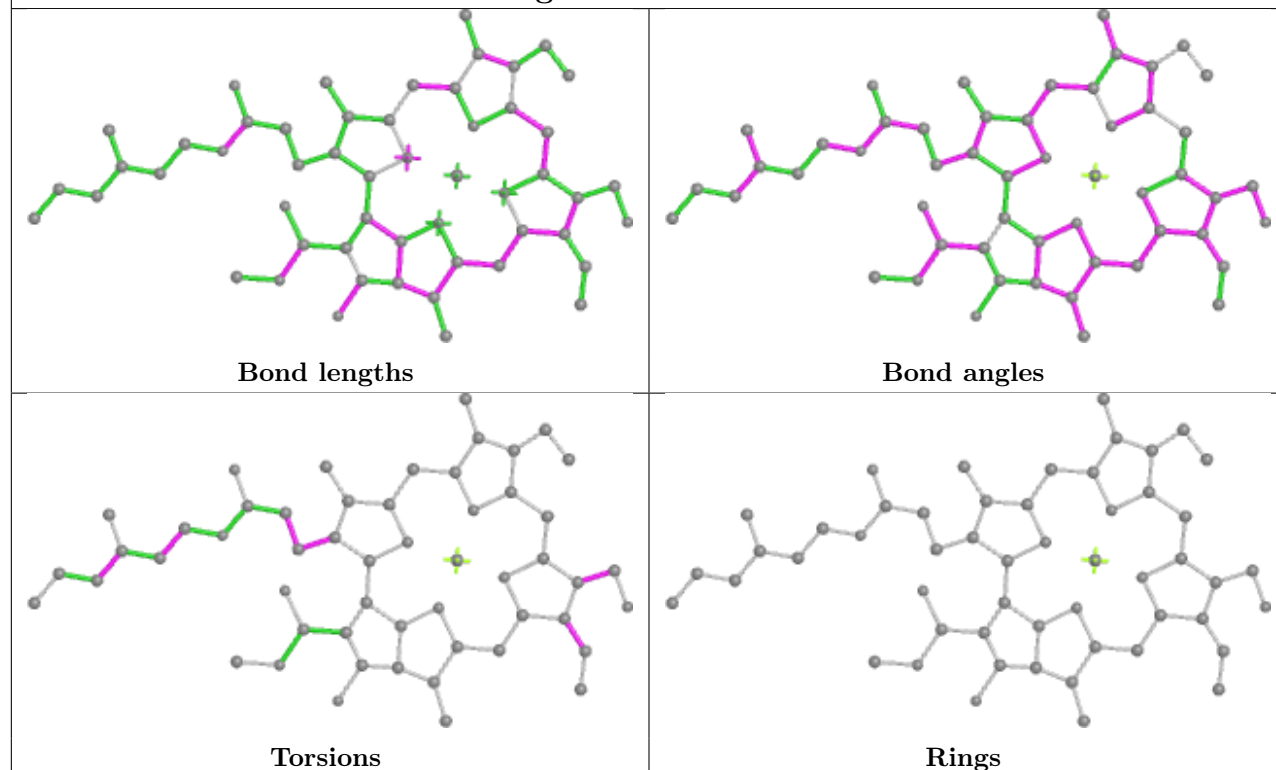




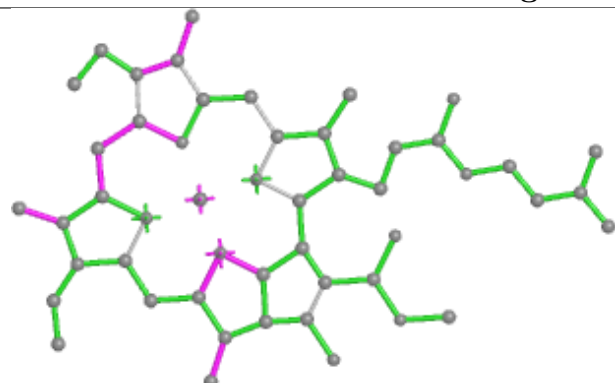
Ligand CLA a 407



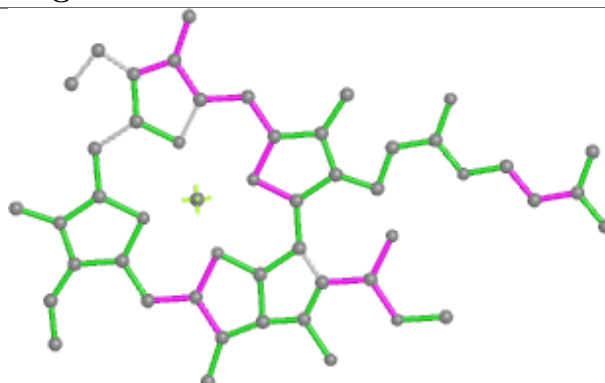
Ligand CHL 3 607



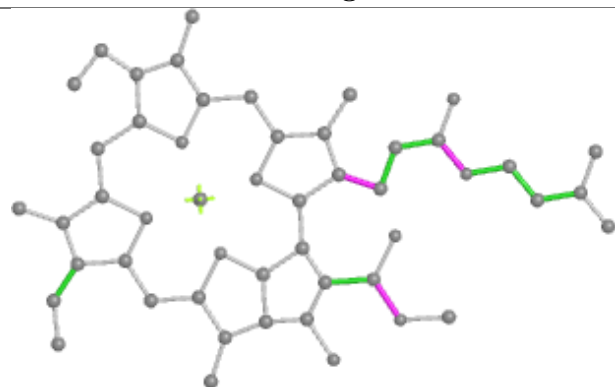
Ligand CLA g 604



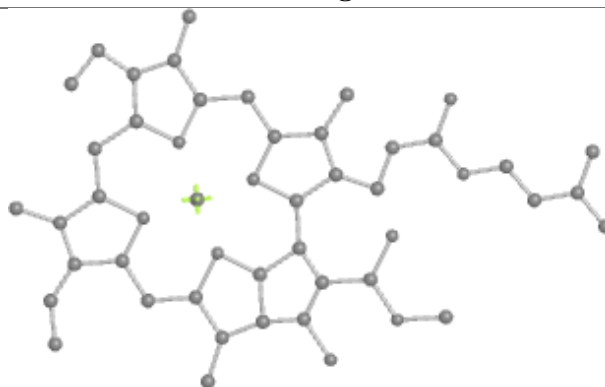
Bond lengths



Bond angles

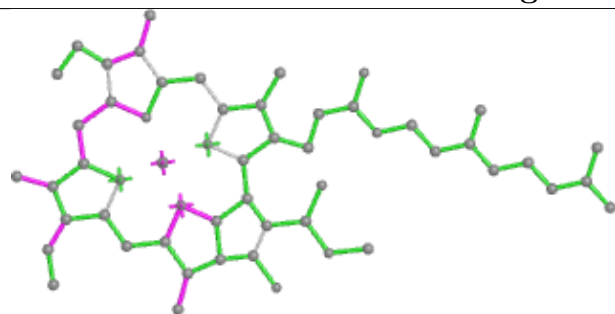


Torsions

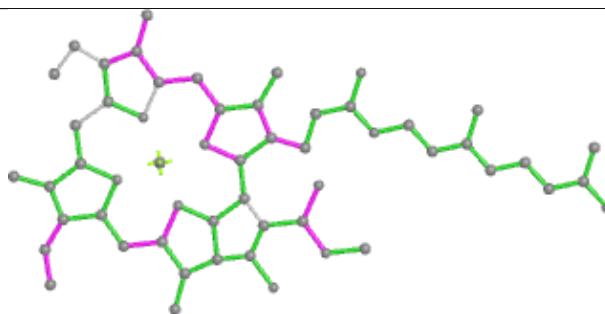


Rings

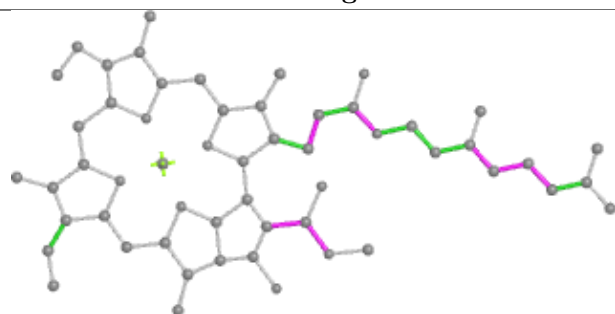
Ligand CLA 5 603



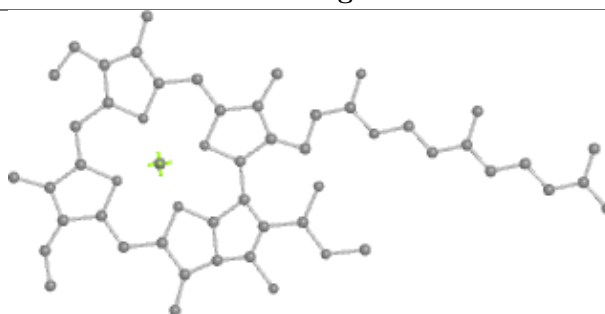
Bond lengths



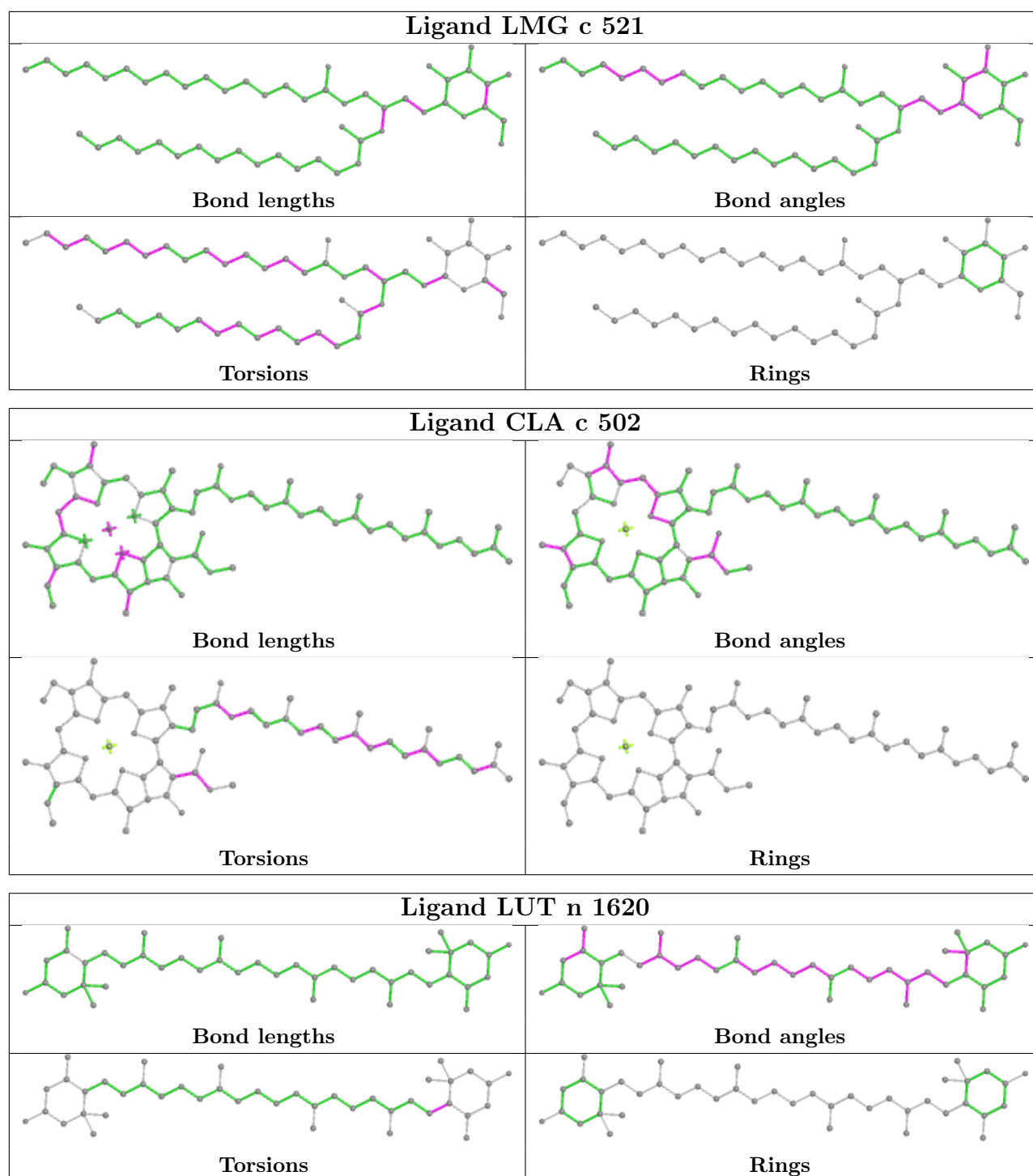
Bond angles



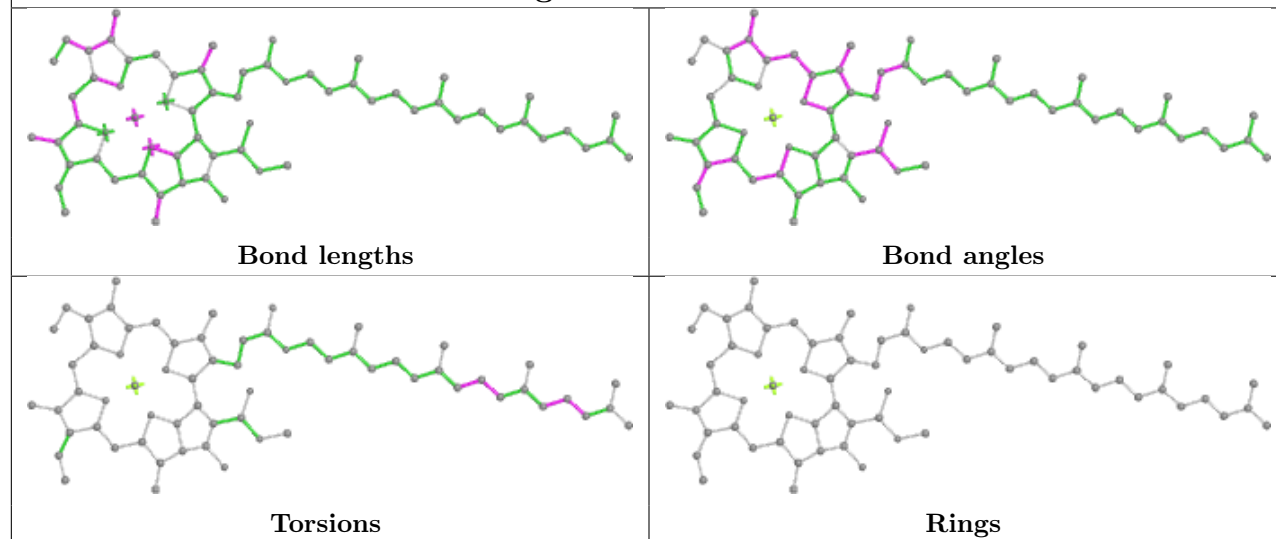
Torsions



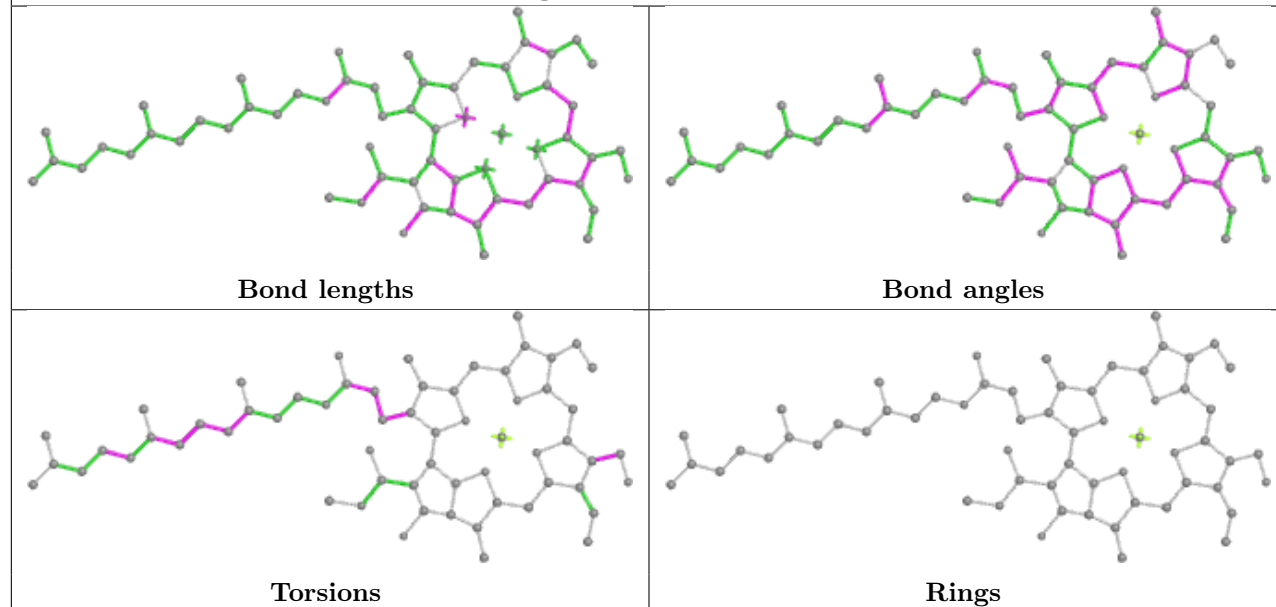
Rings



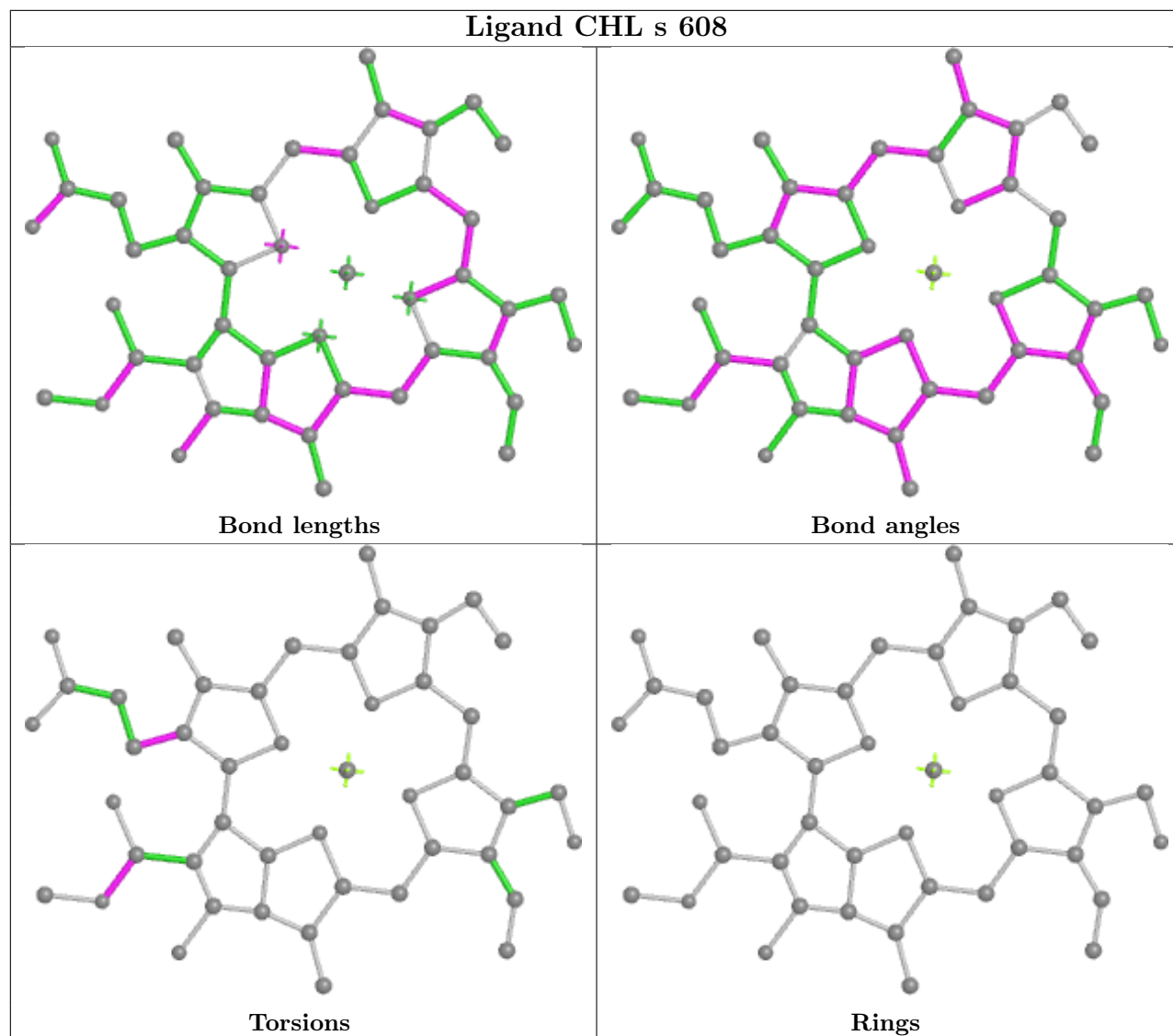
Ligand CLA d 402



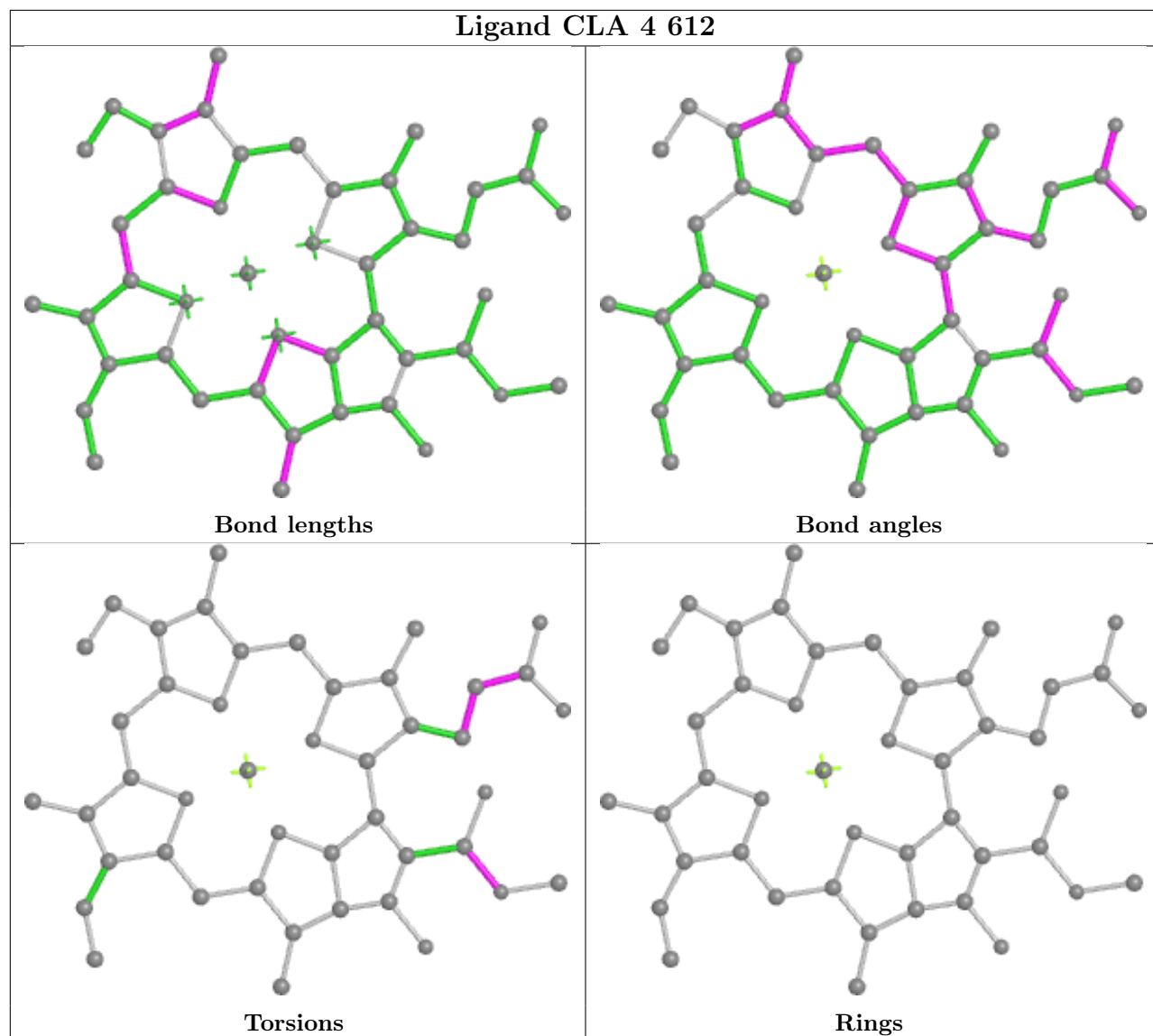
Ligand CHL 2 607

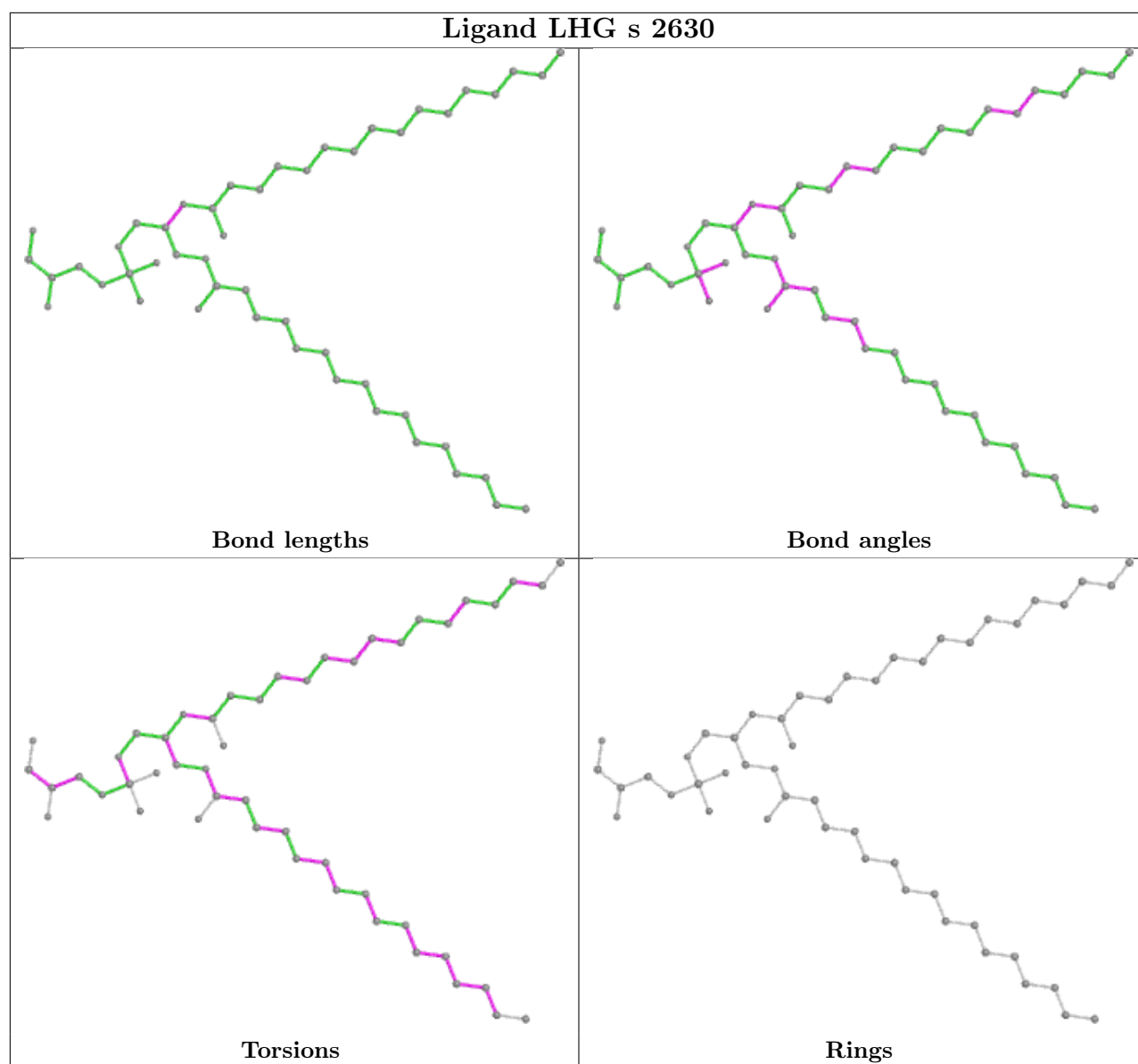


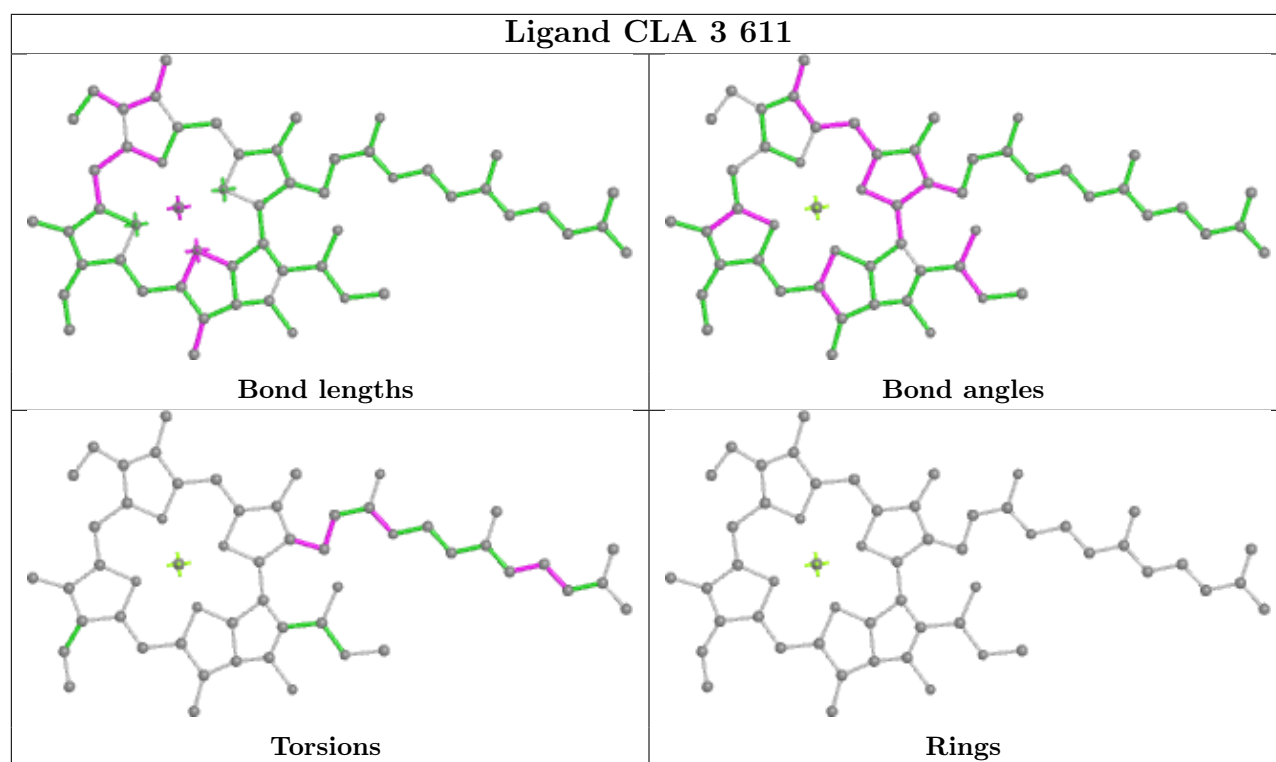
Ligand CHL s 608



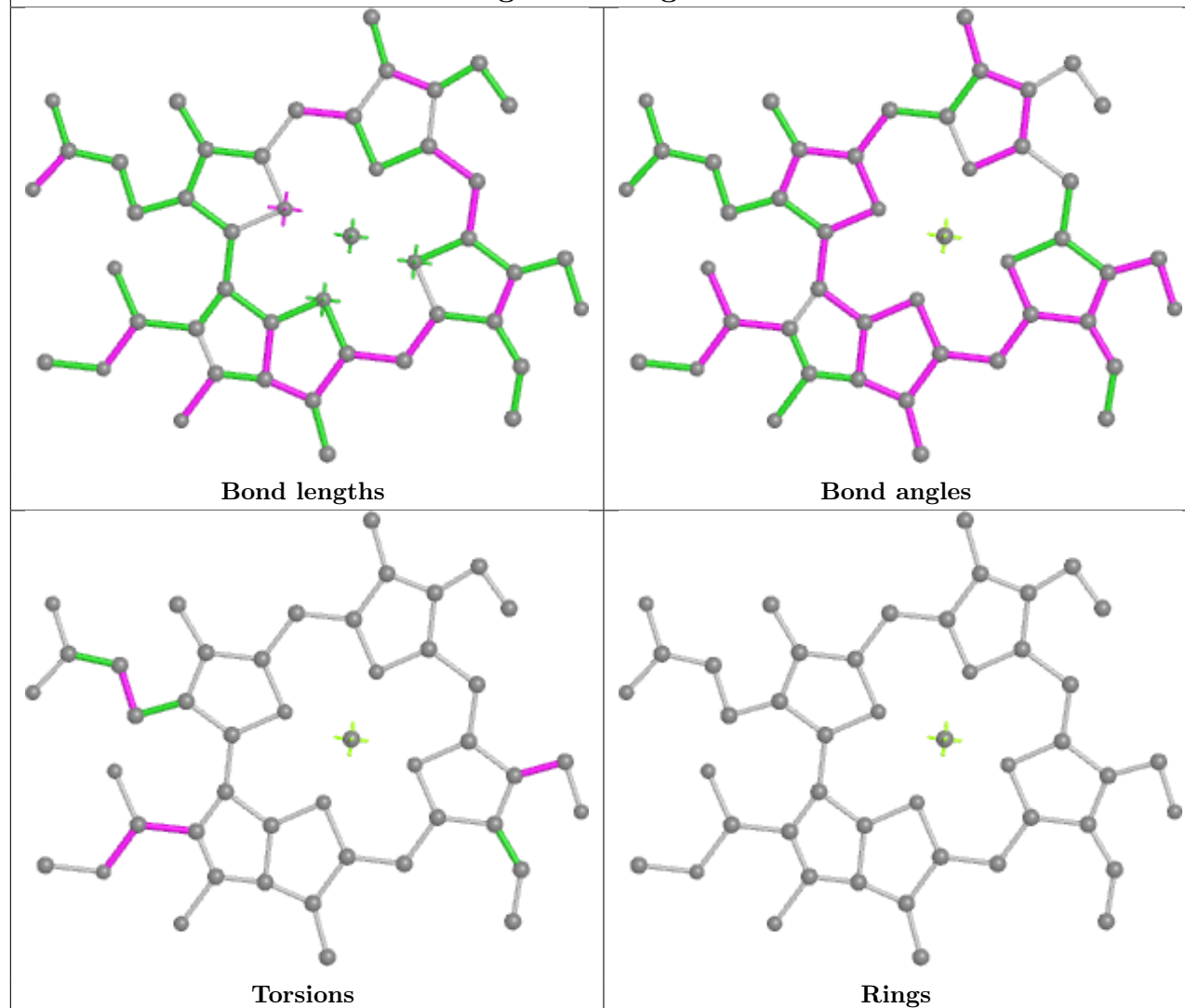
Ligand CLA 4 612



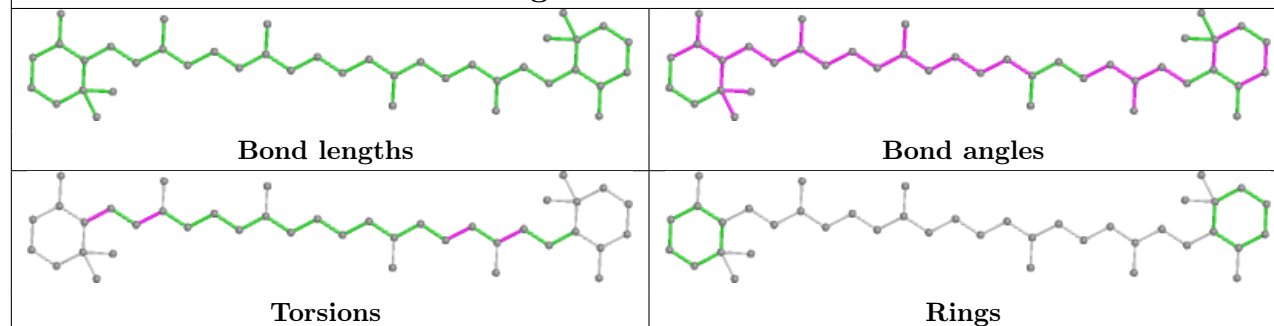


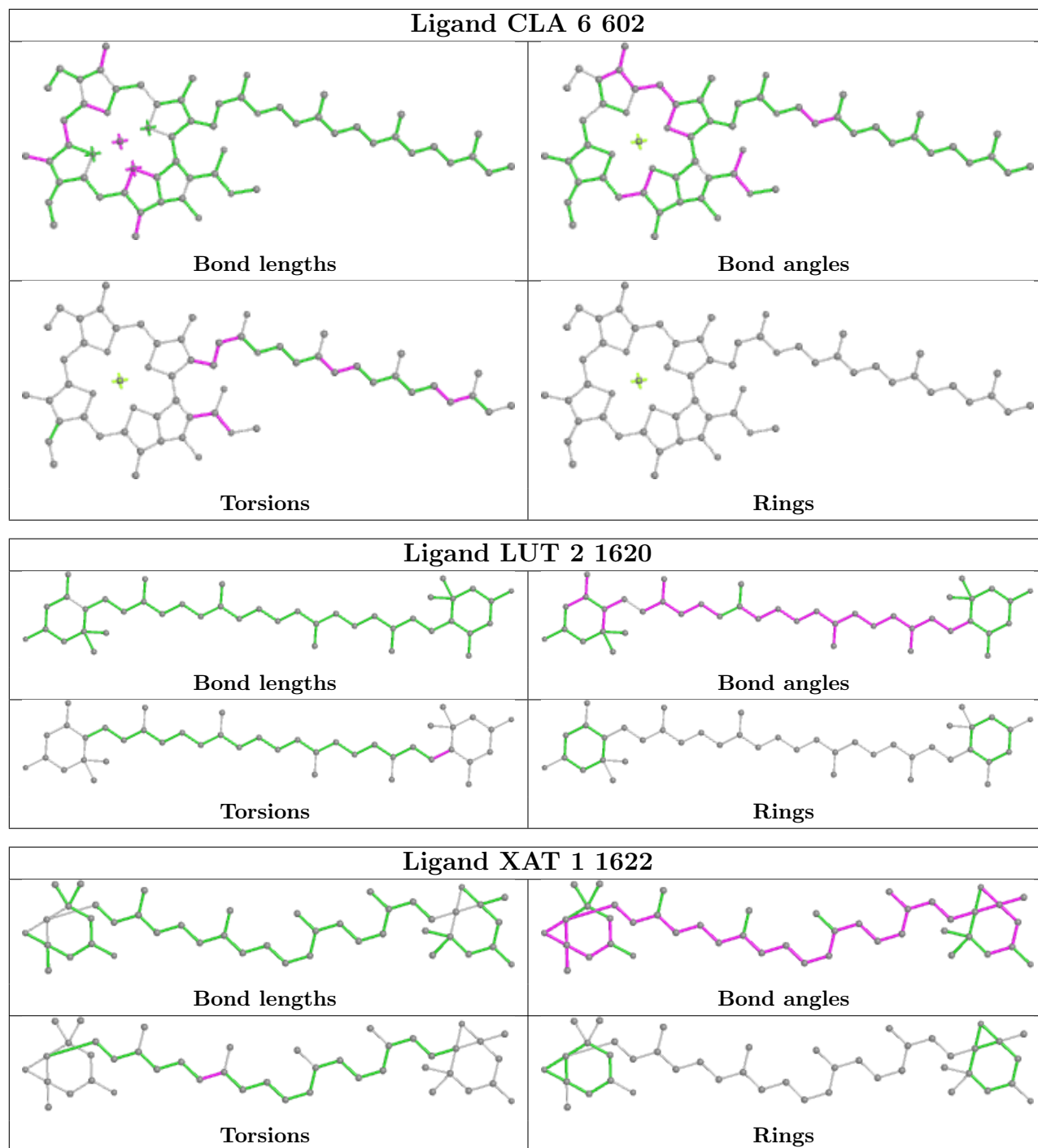


Ligand CHL g 605

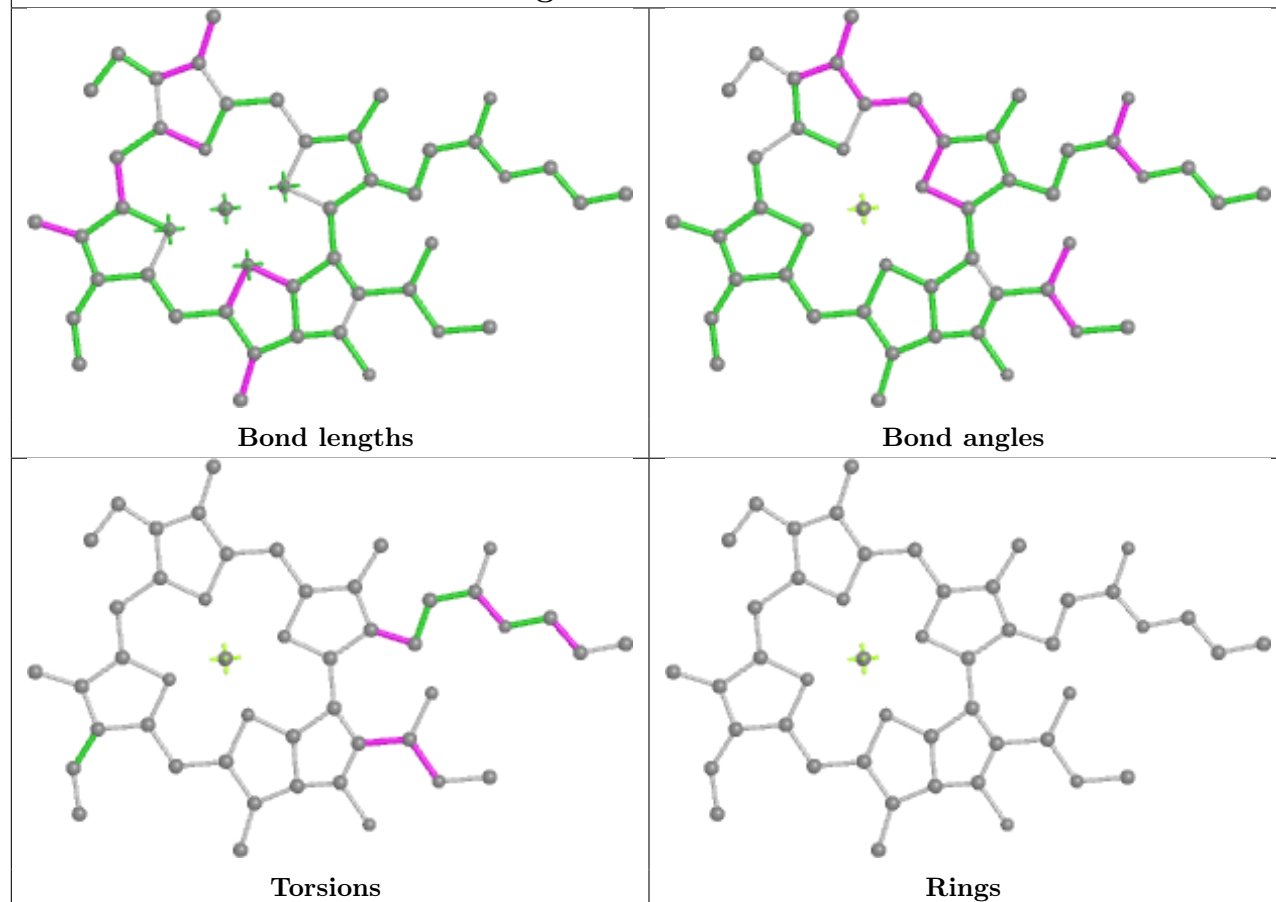


Ligand BCR C 516

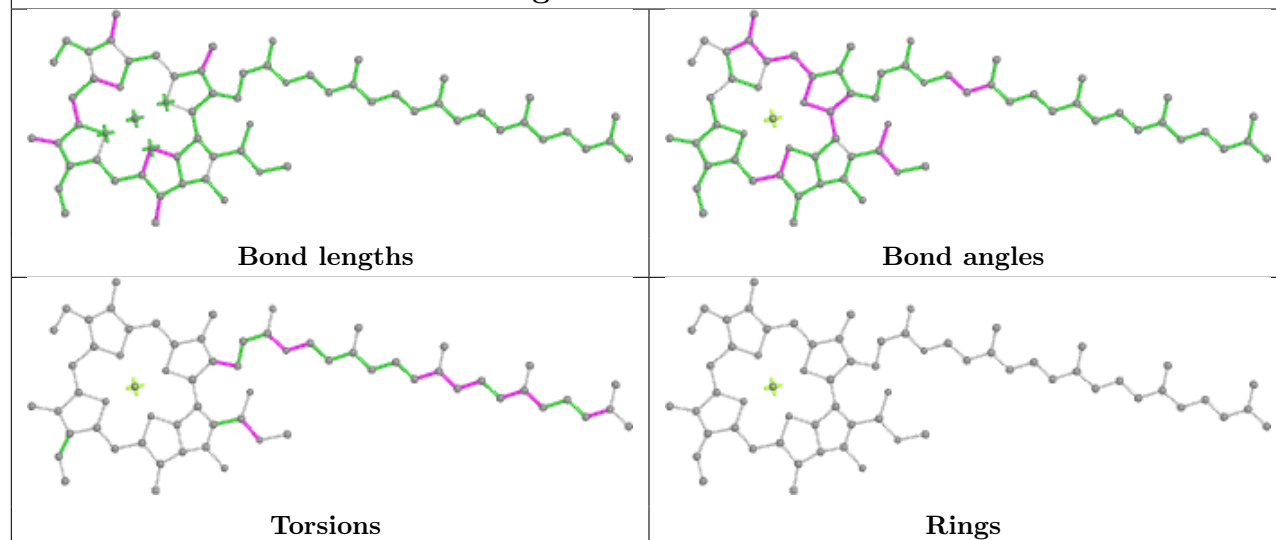


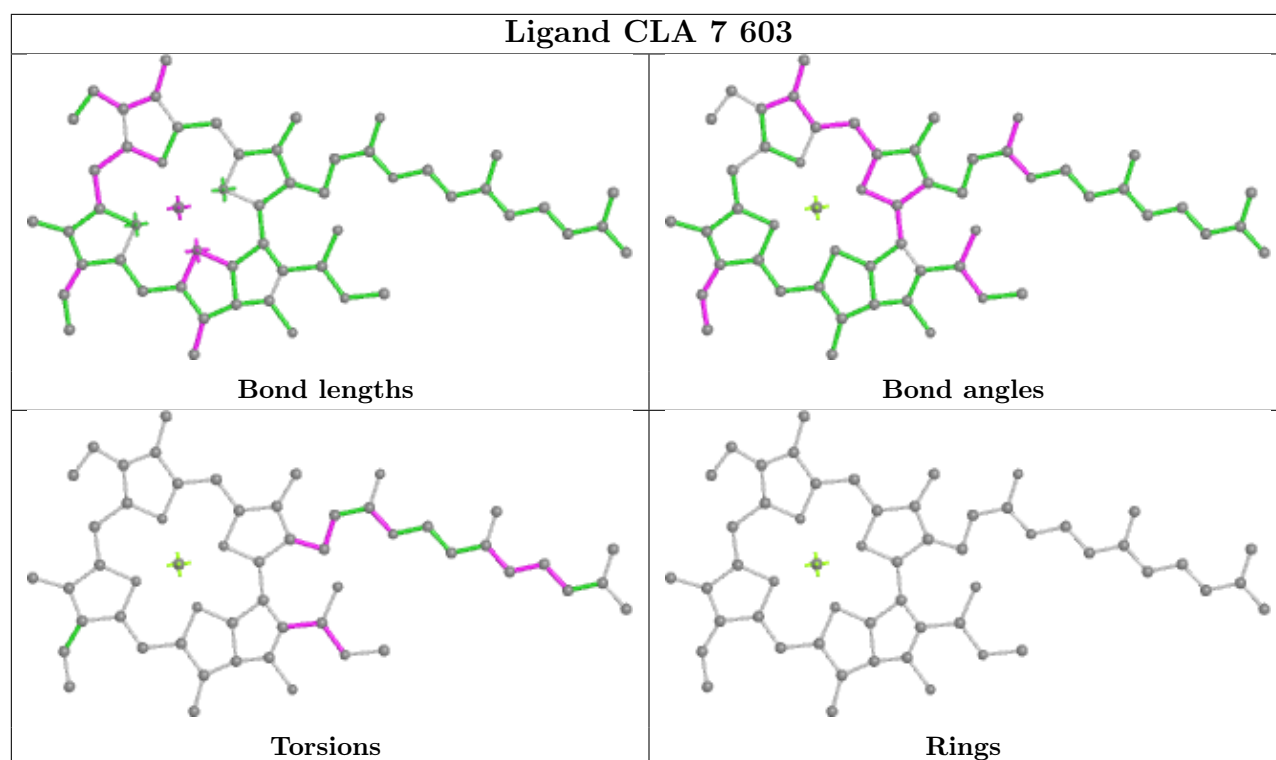


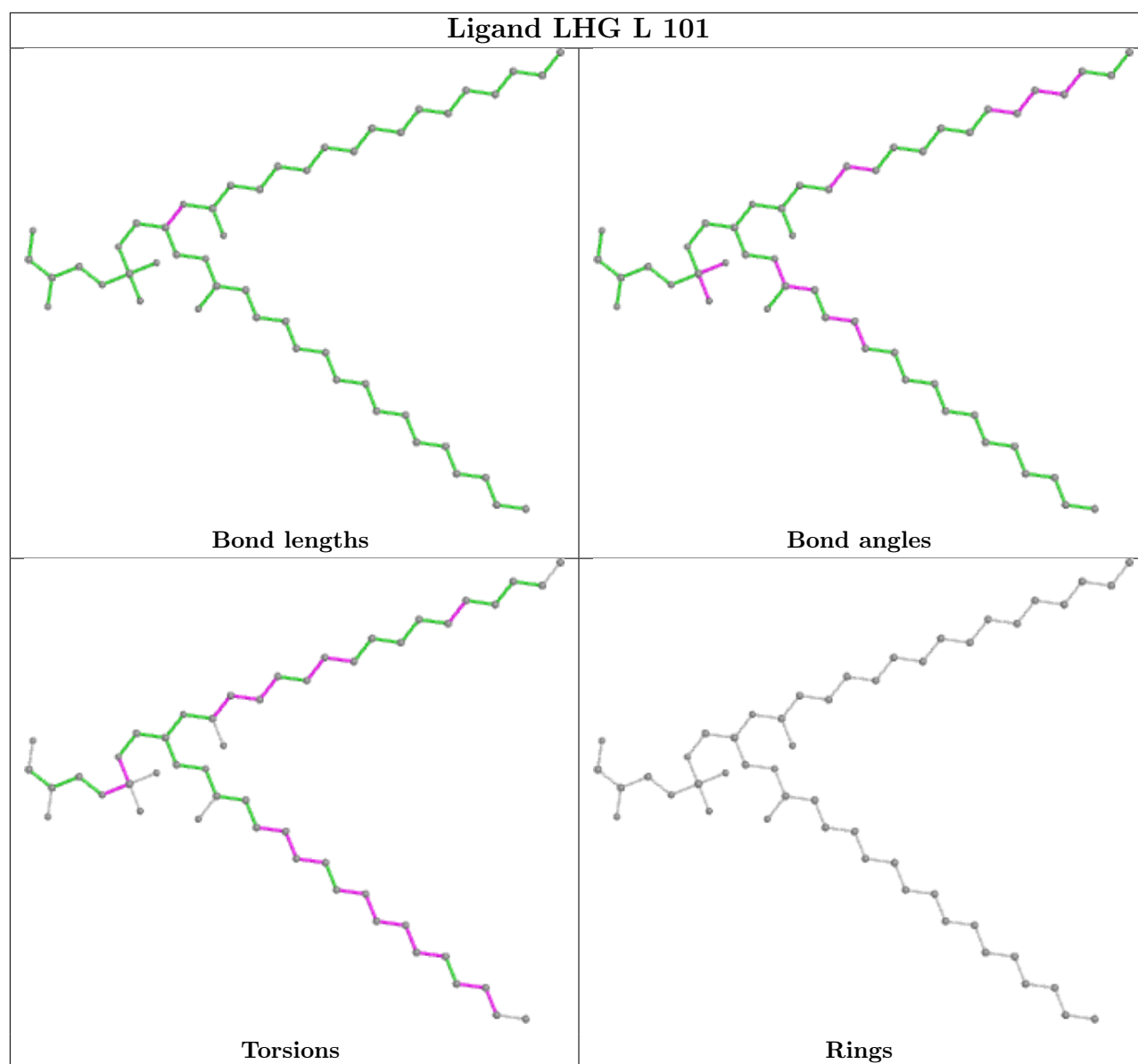
Ligand CLA 3 614

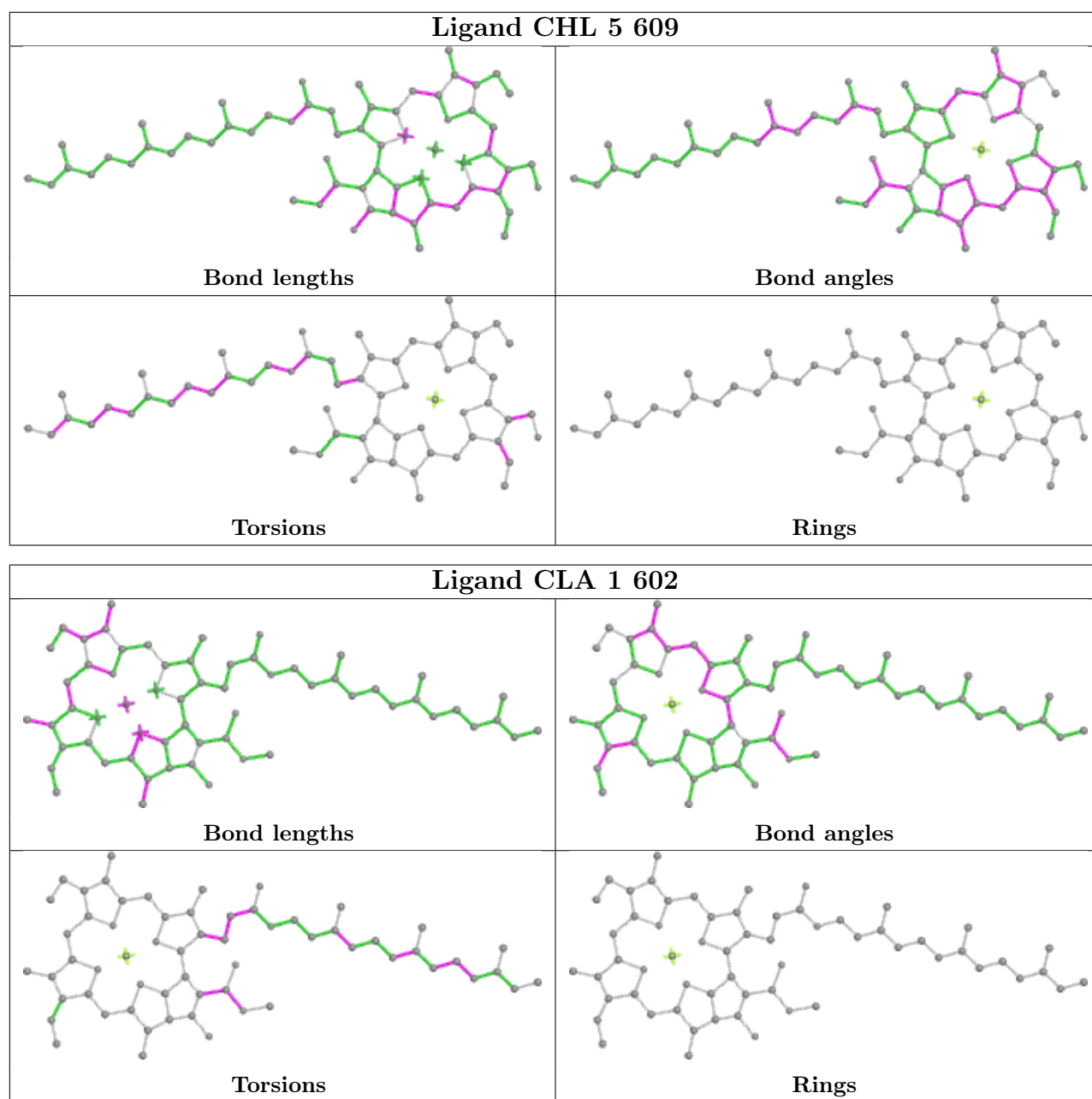


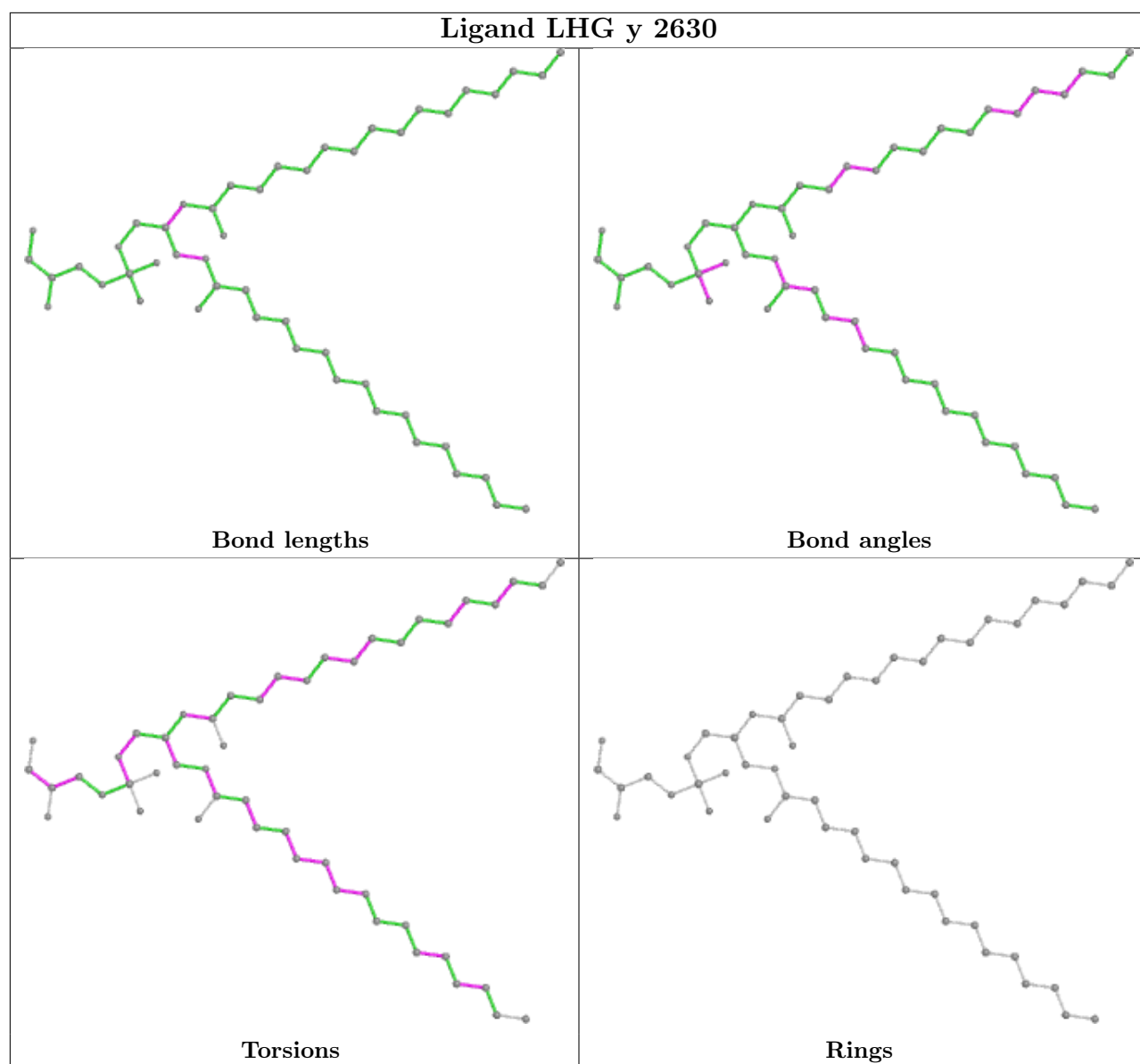
Ligand CLA C 511



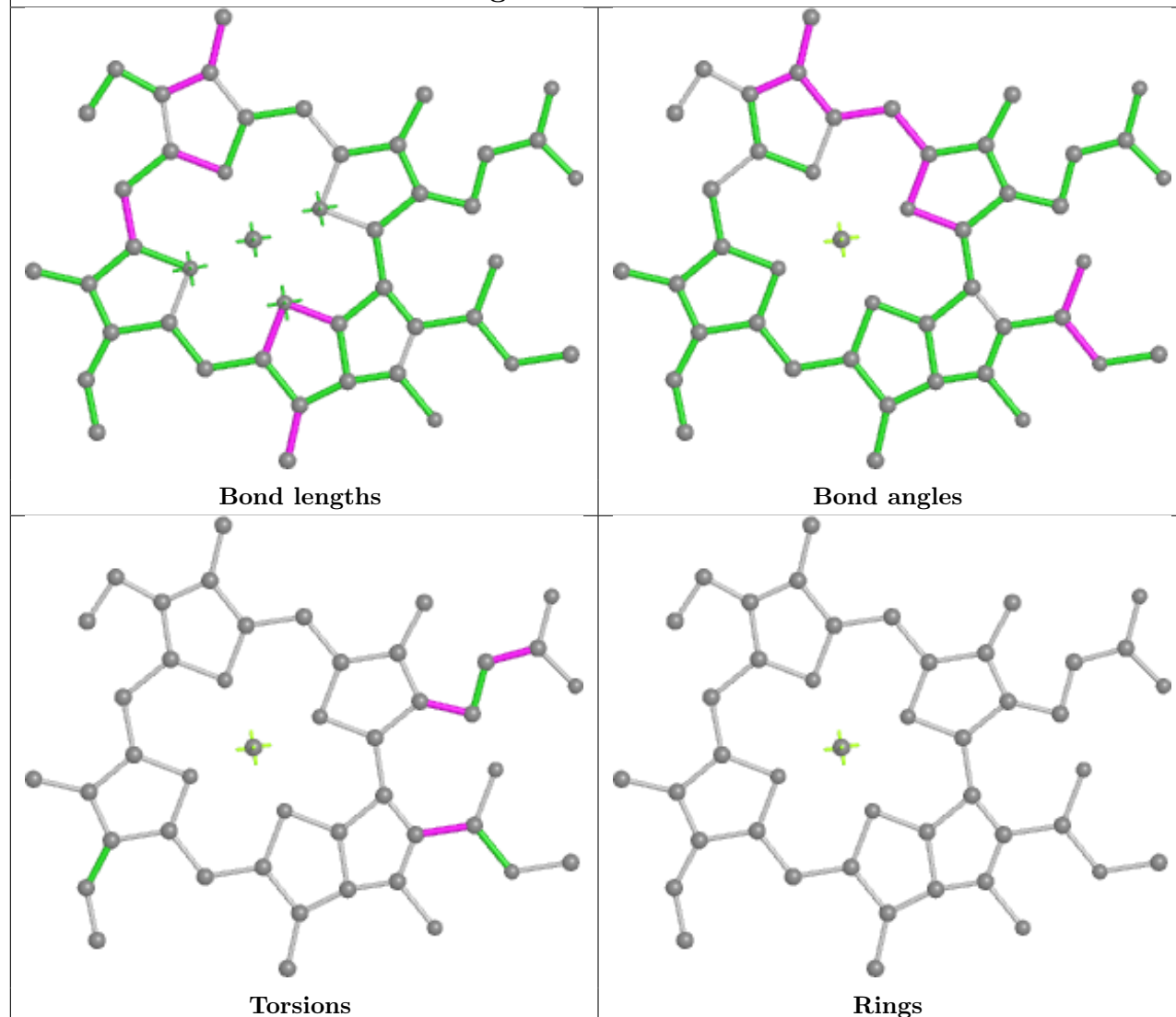




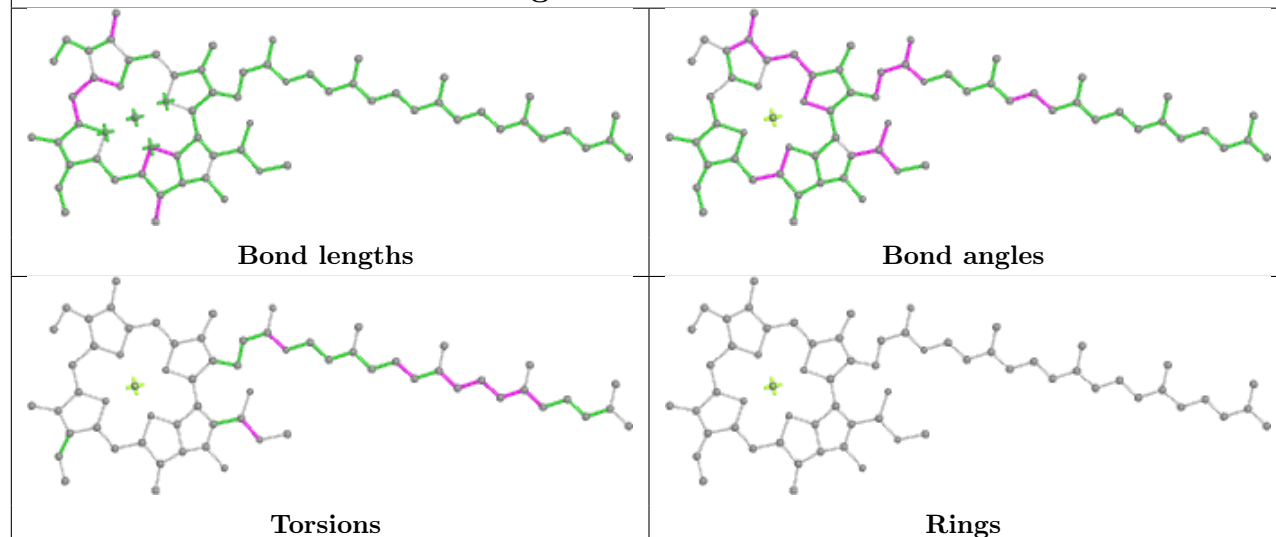




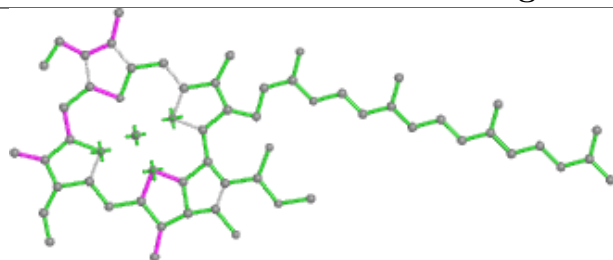
Ligand CLA R 616



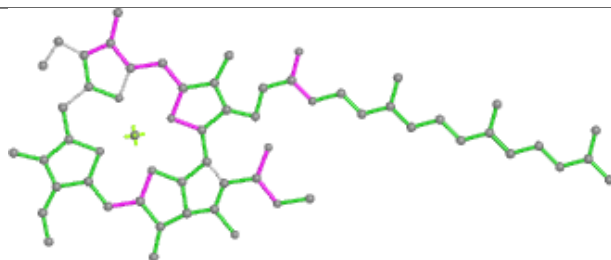
Ligand CLA D 403



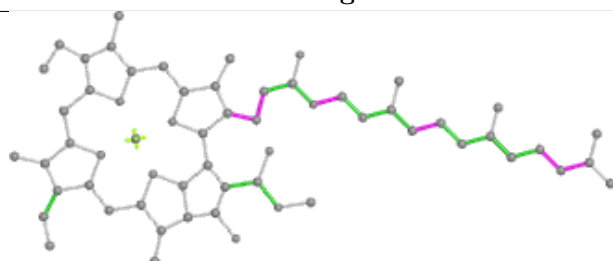
Ligand CLA 7 610



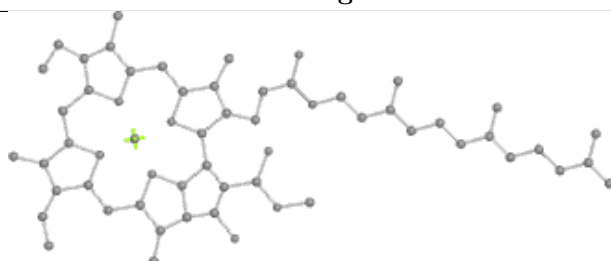
Bond lengths



Bond angles

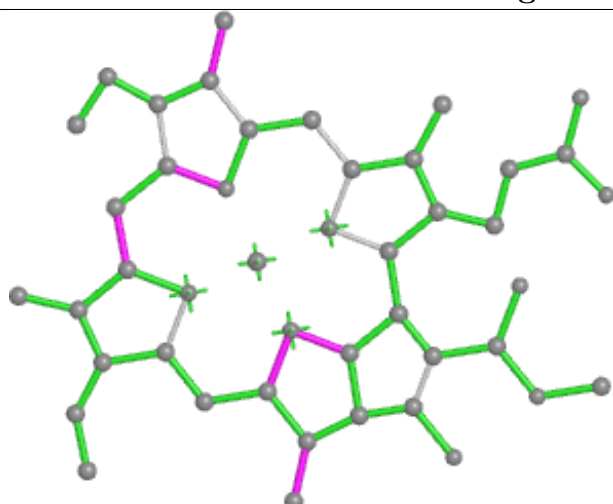


Torsions

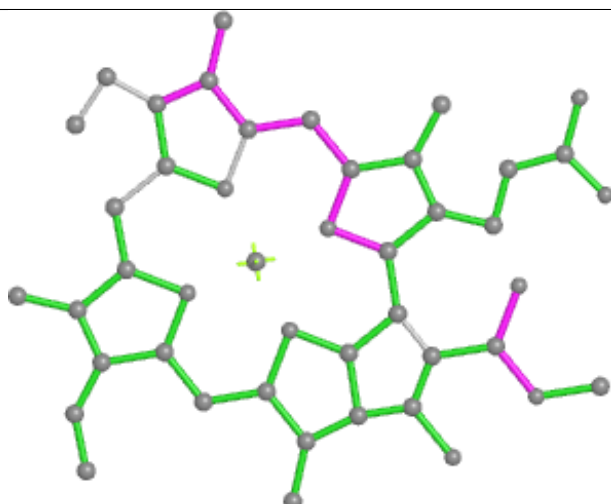


Rings

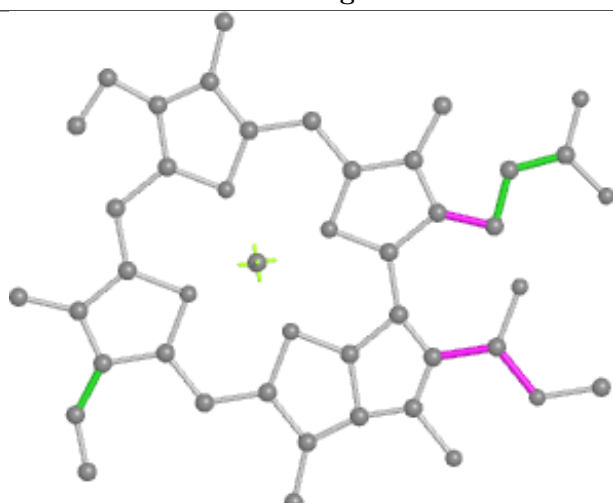
Ligand CLA 6 614



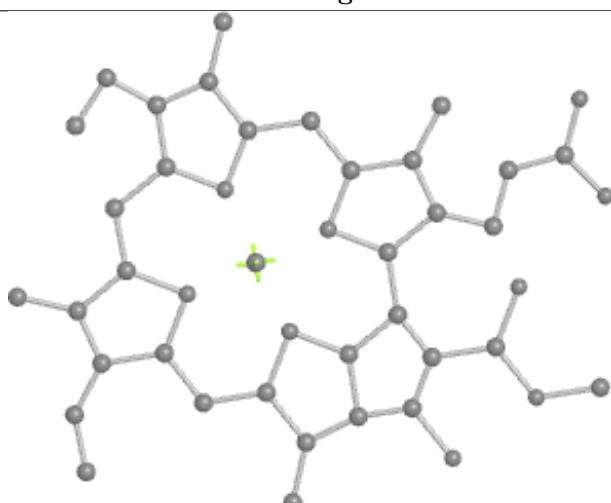
Bond lengths



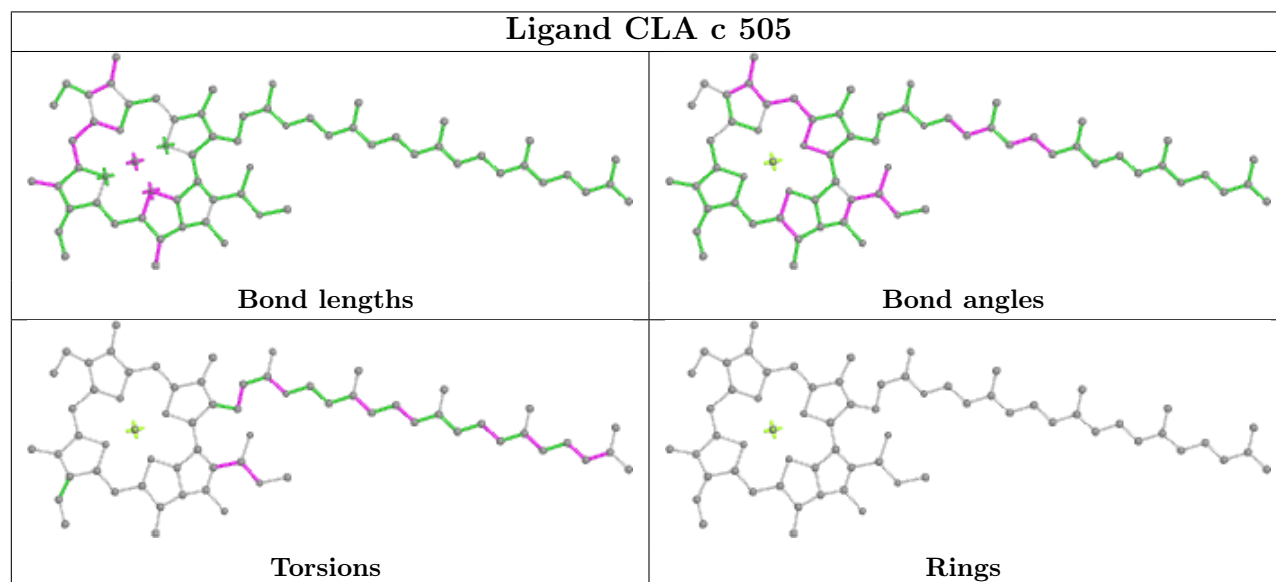
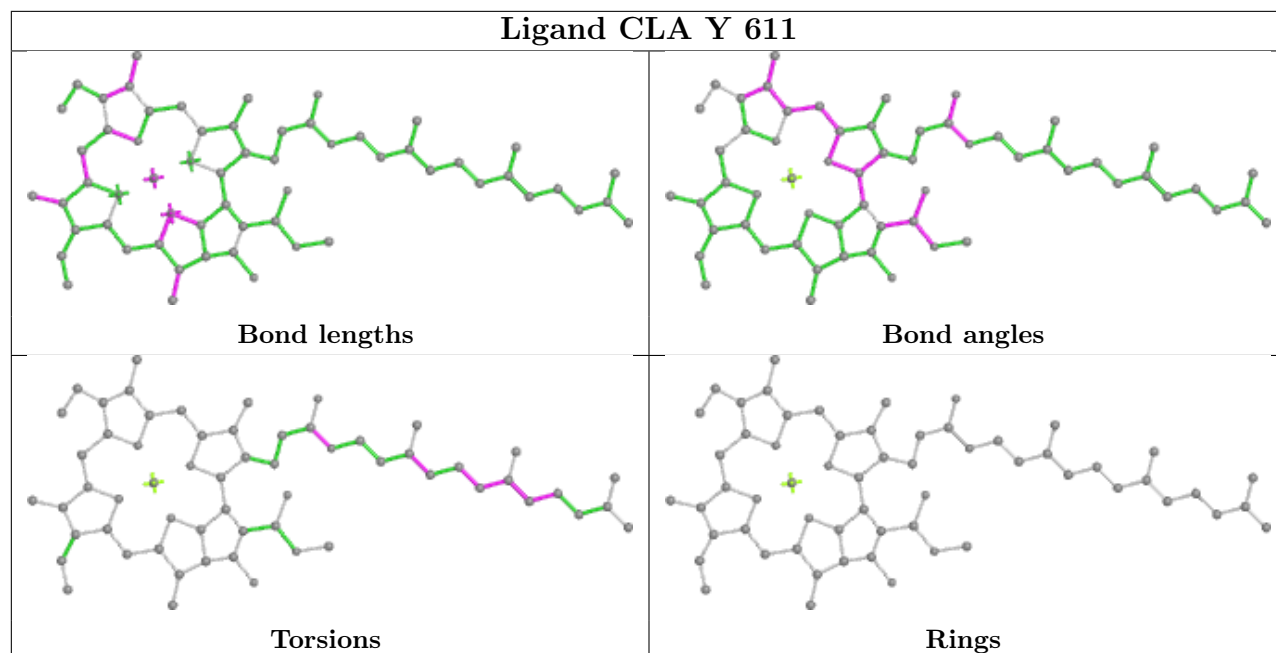
Bond angles

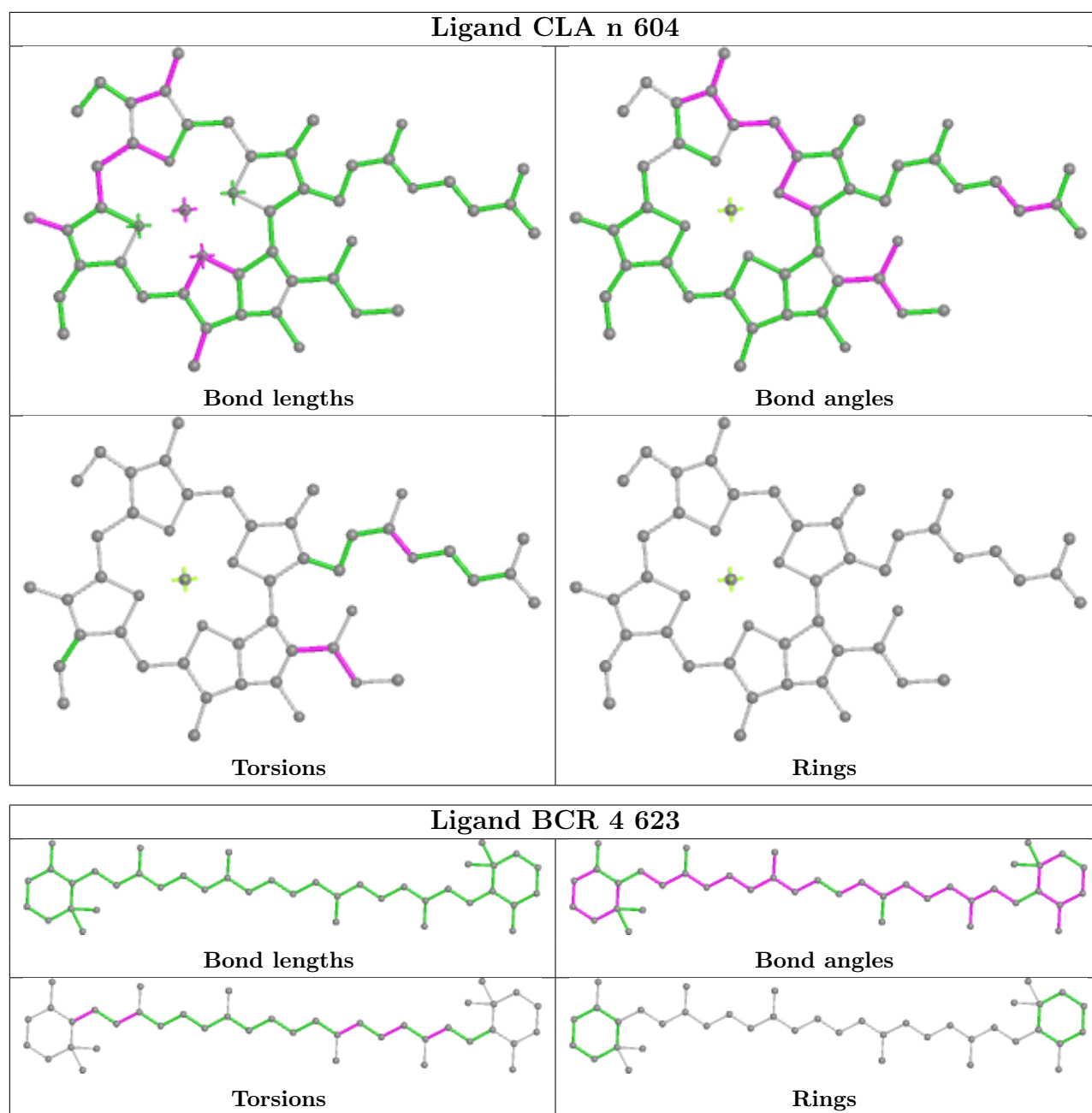


Torsions

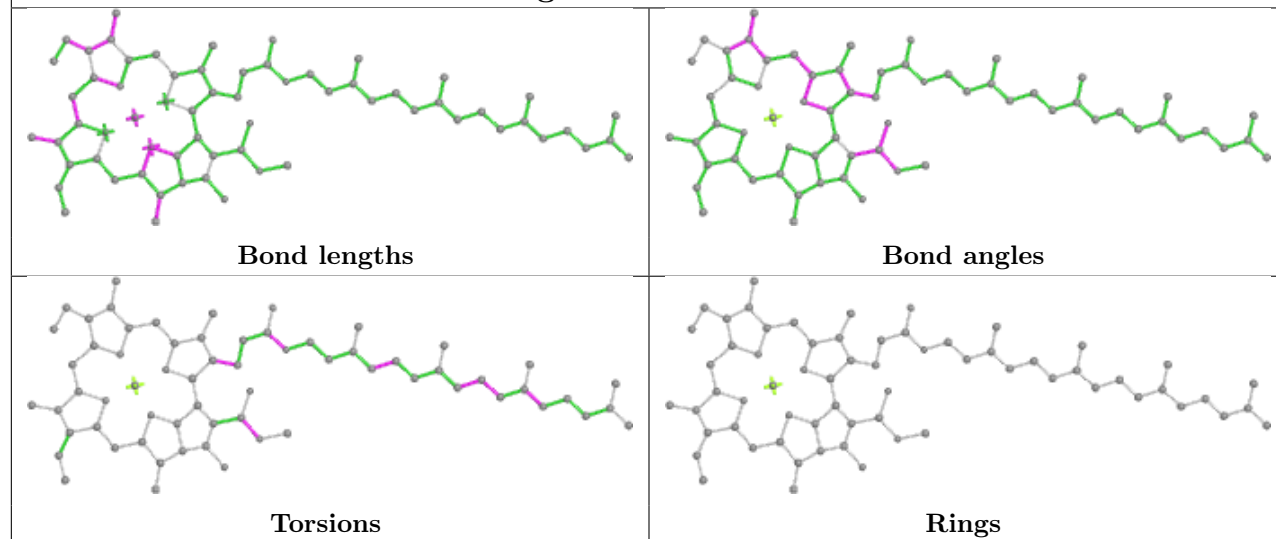


Rings

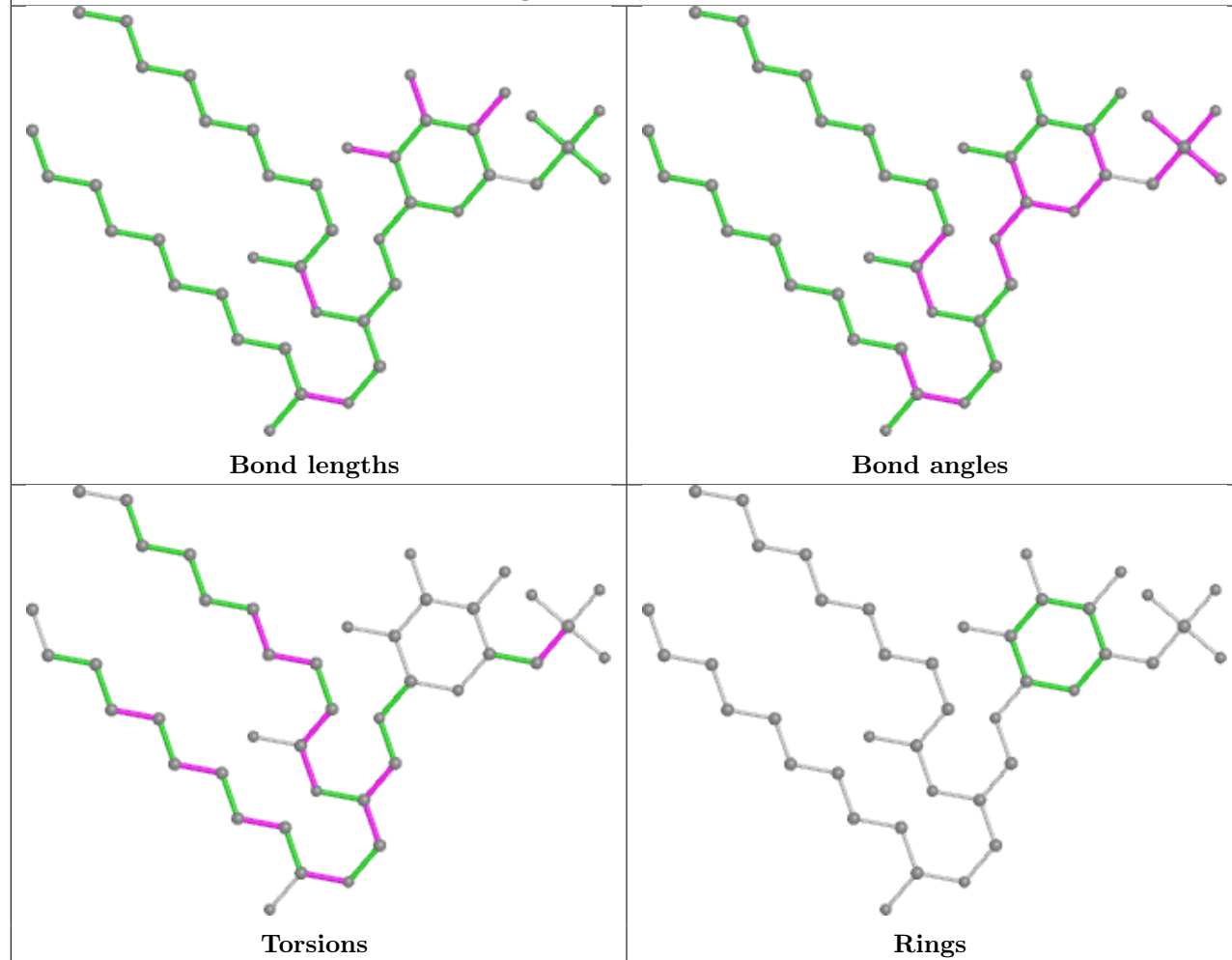


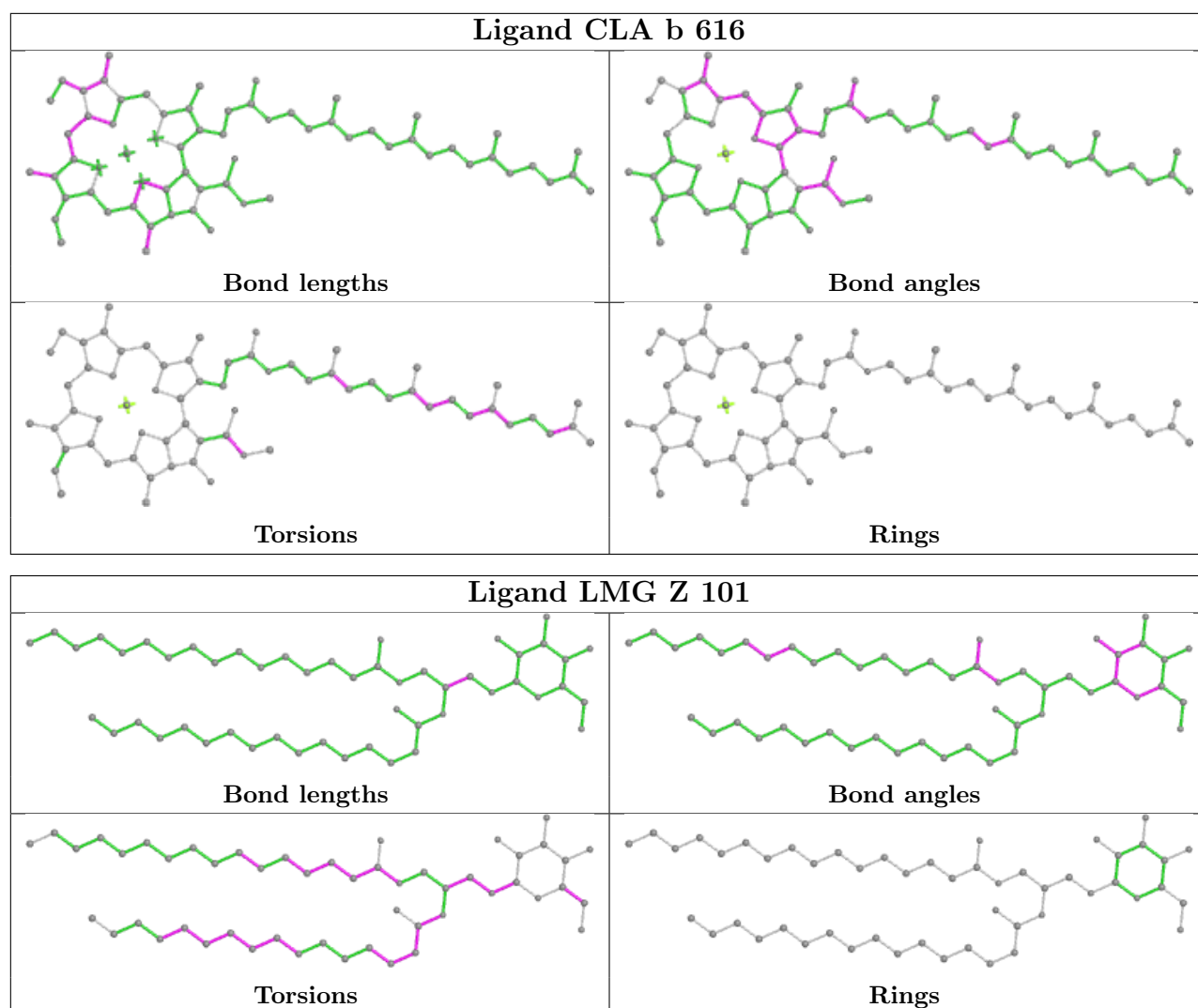


Ligand CLA c 512

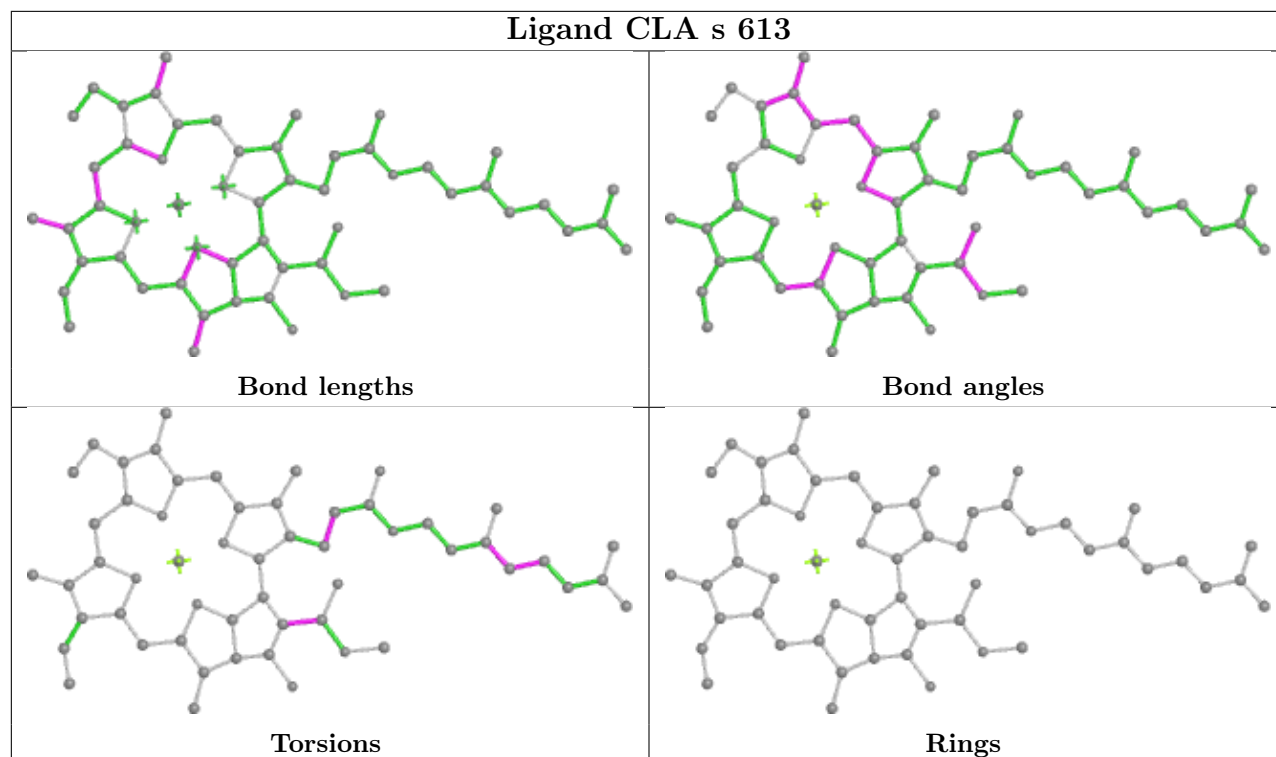


Ligand SQD b 623

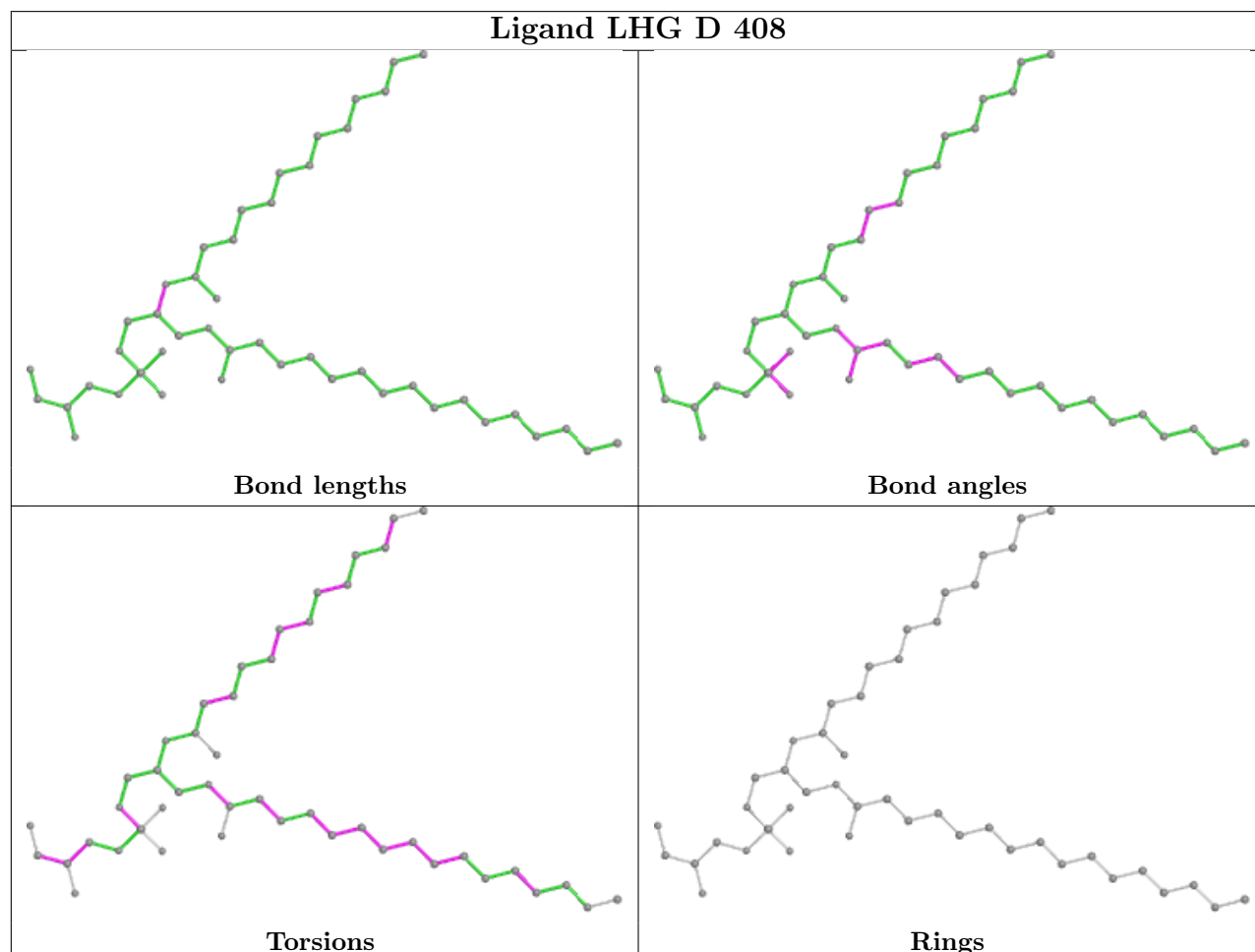


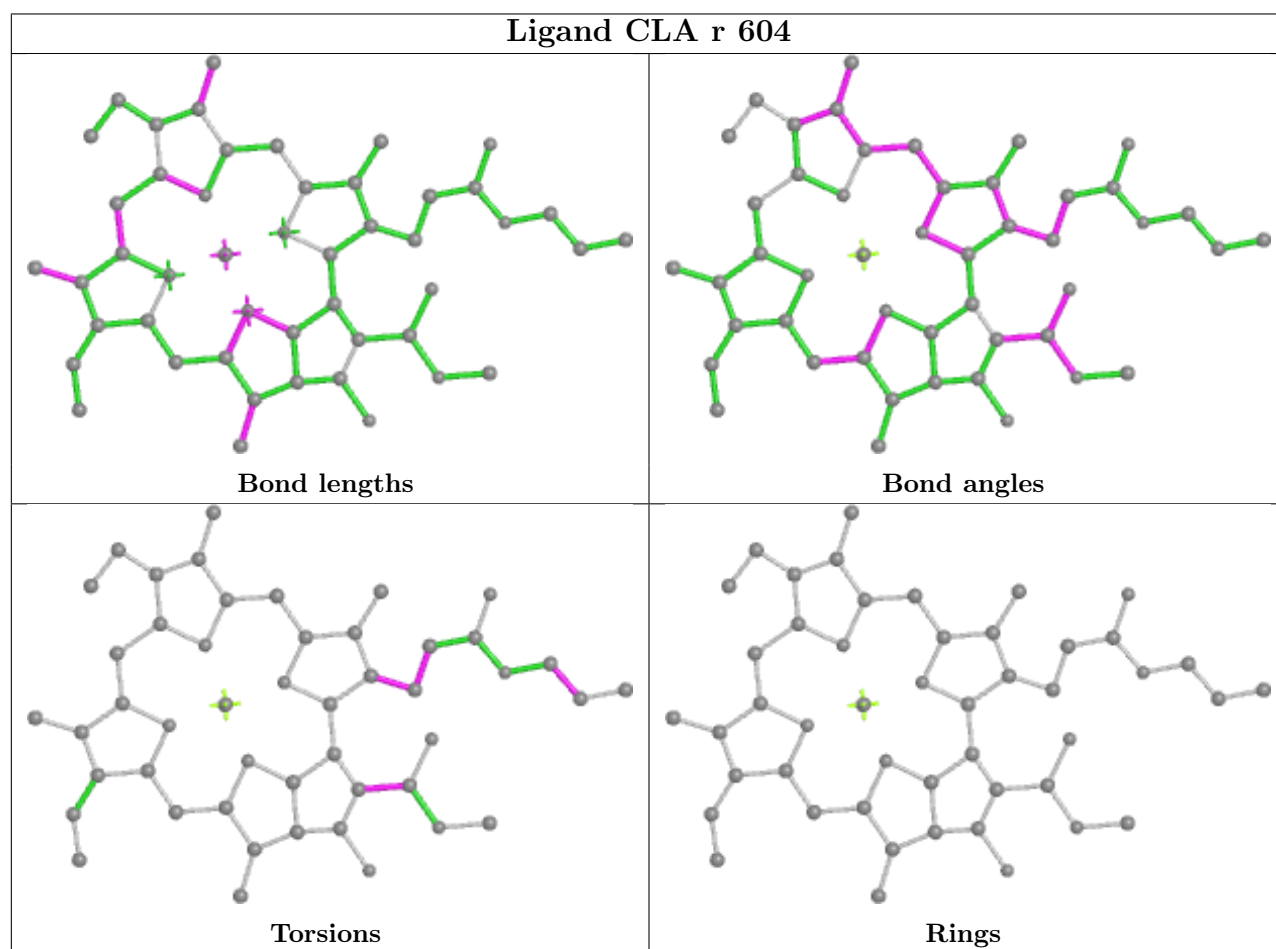
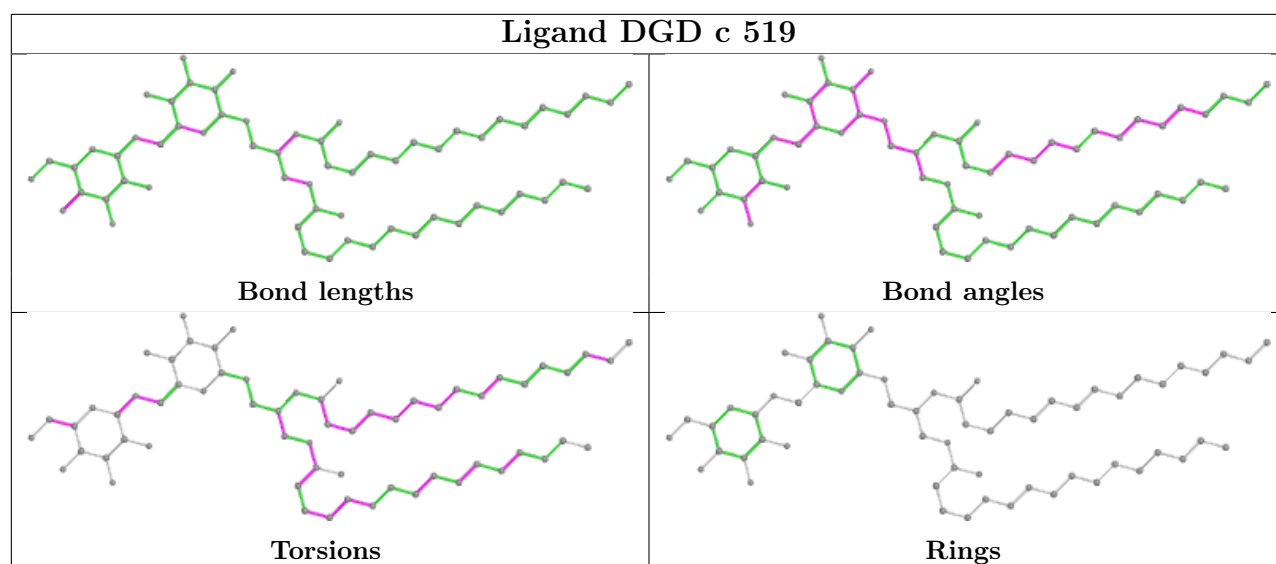


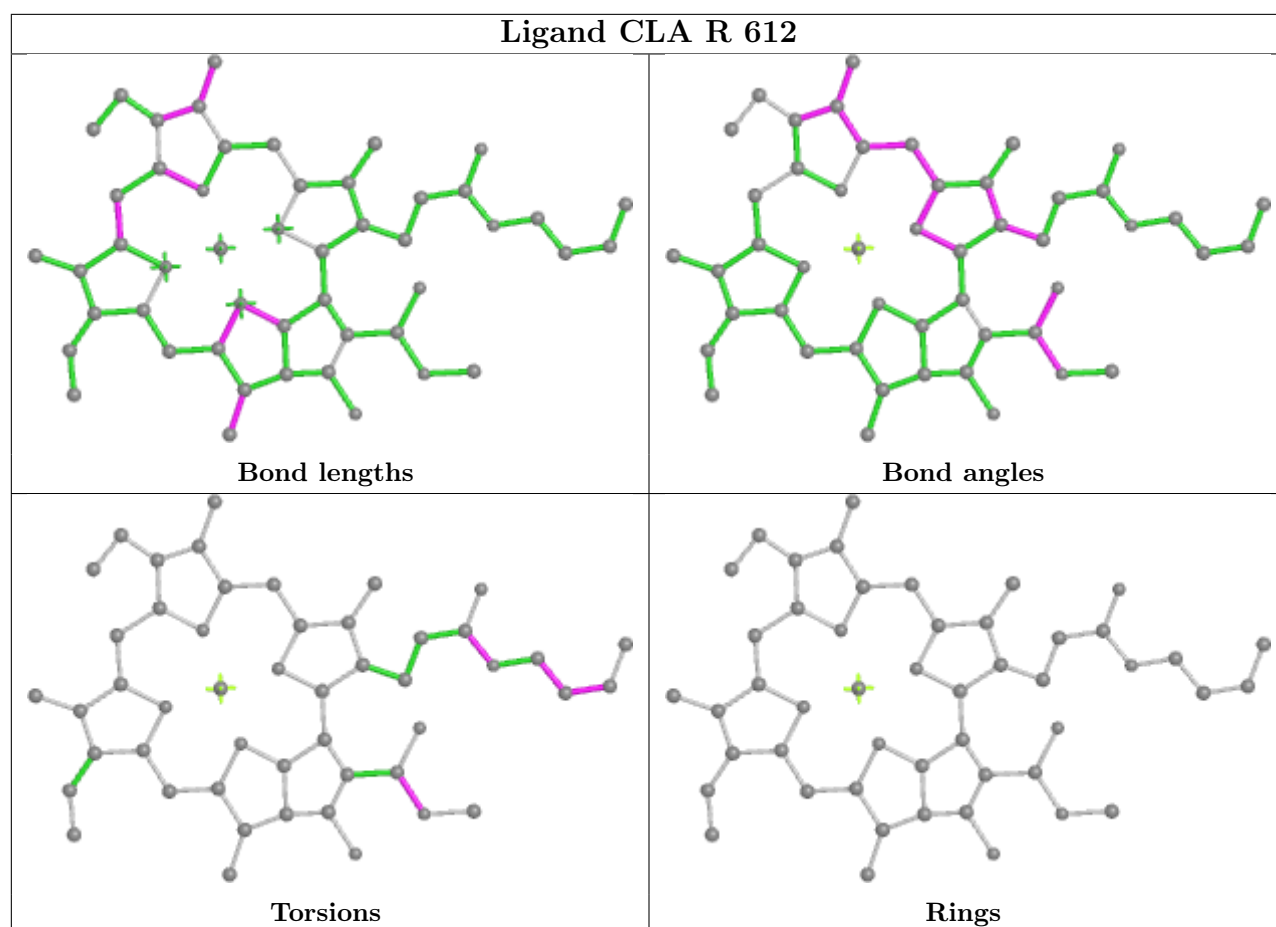
Ligand CLA s 613



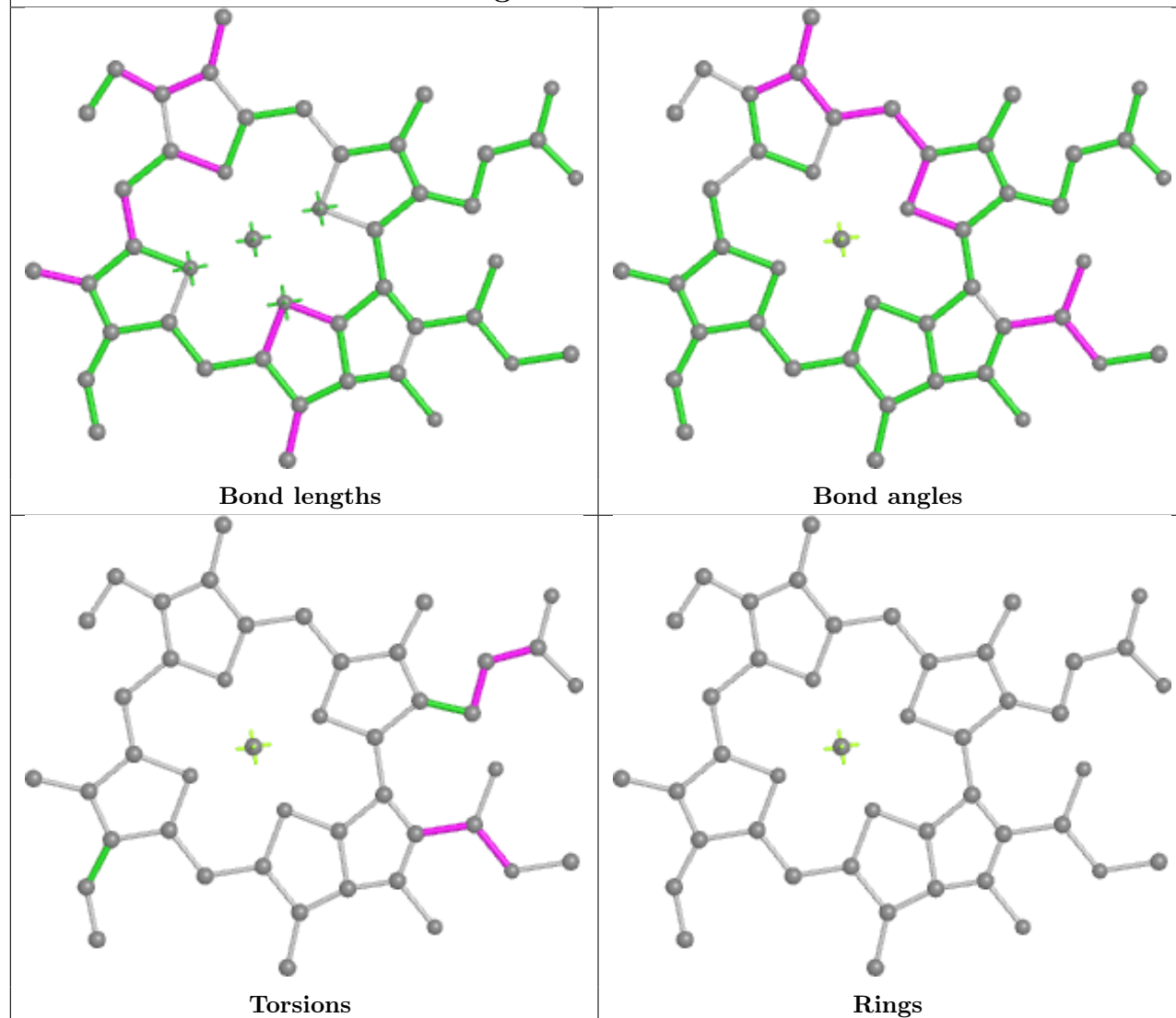
Ligand LHG D 408



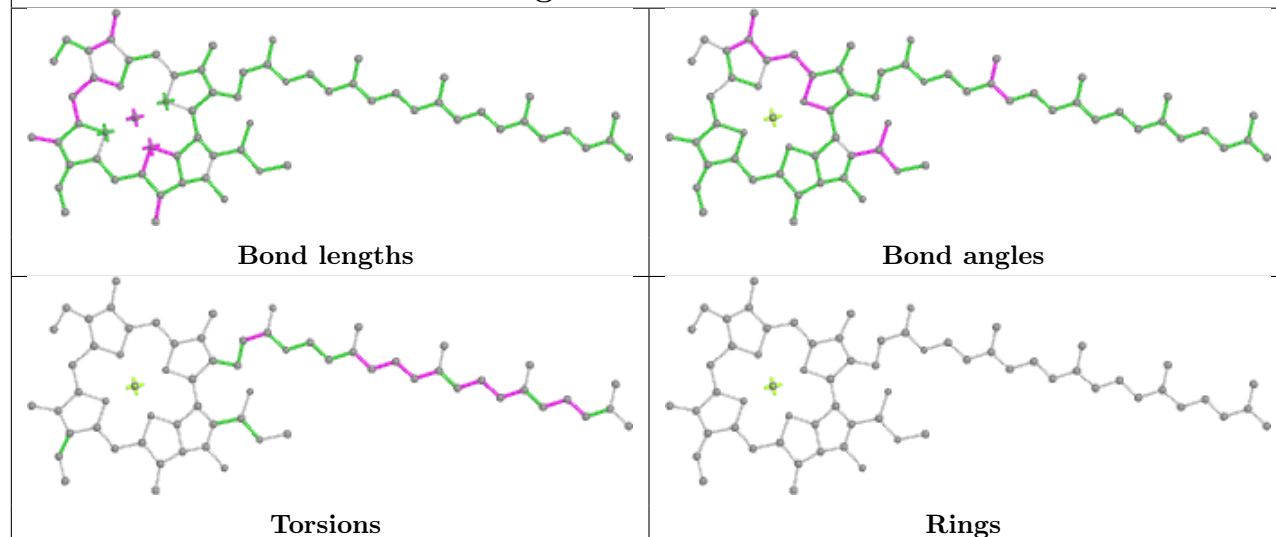




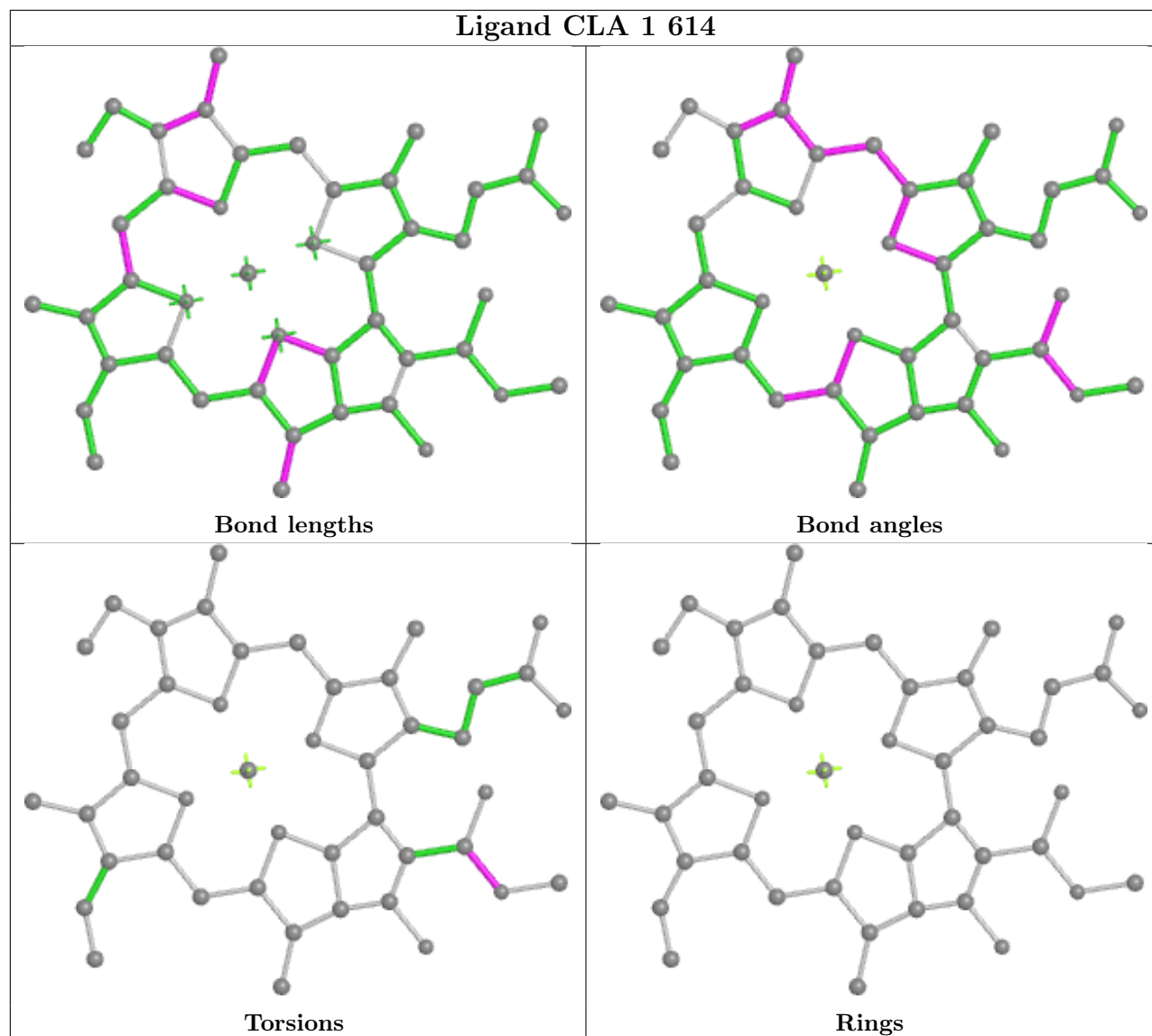
Ligand CLA 8 602



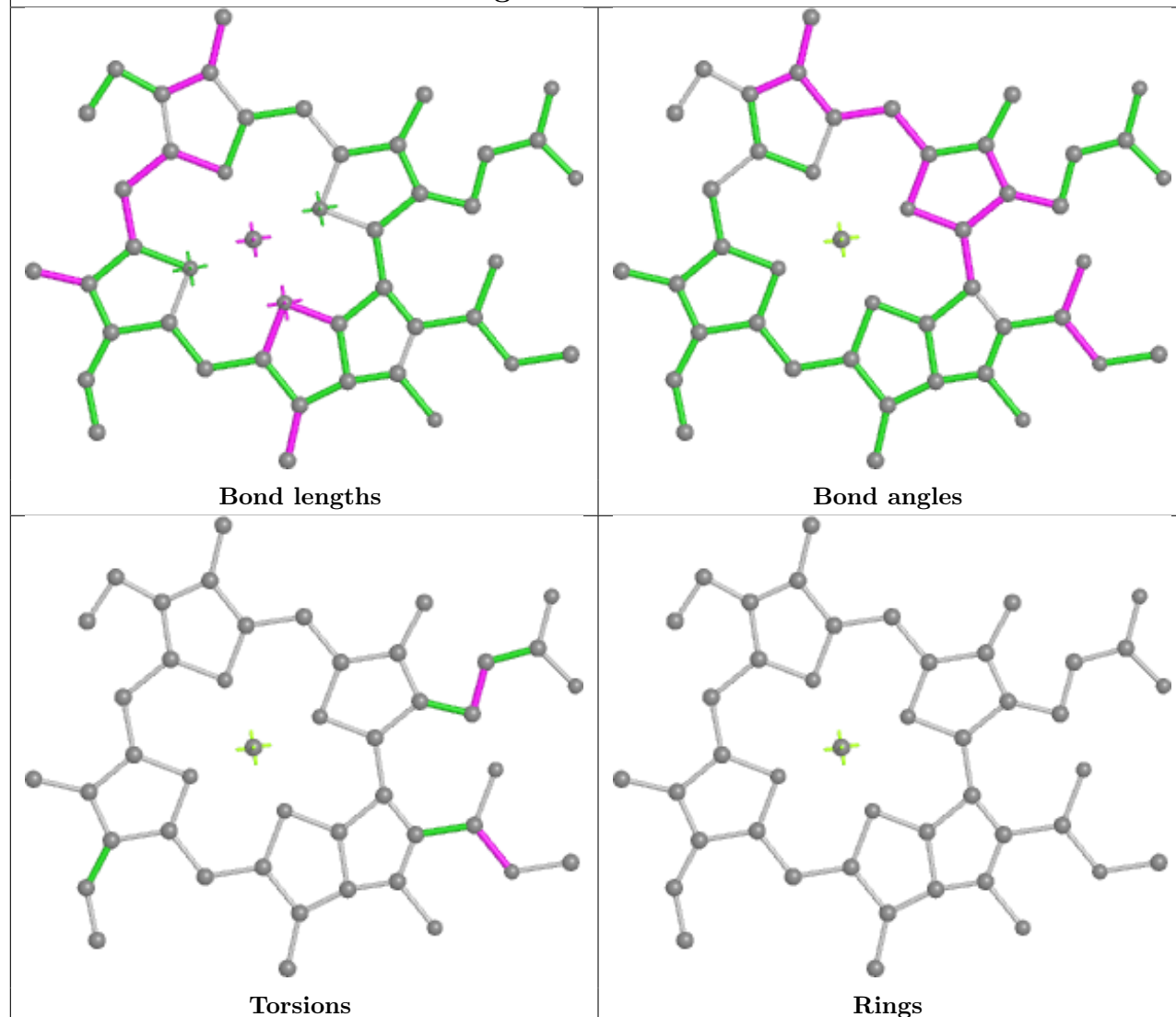
Ligand CLA b 614



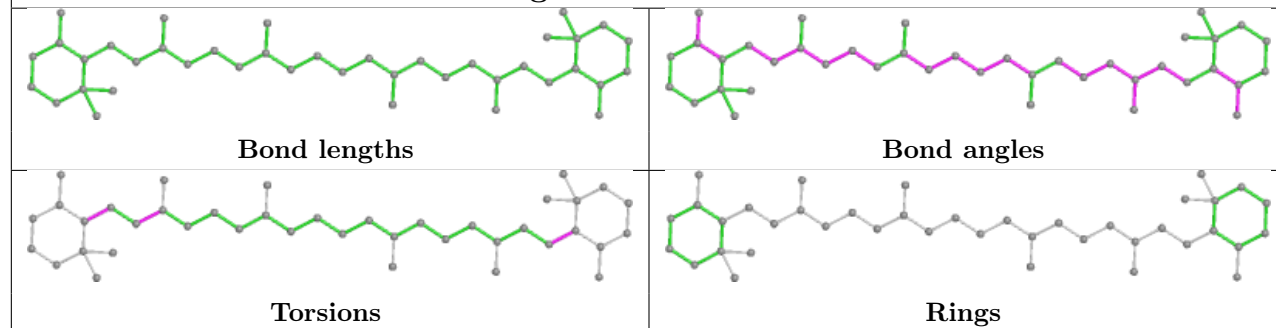
Ligand CLA 1 614

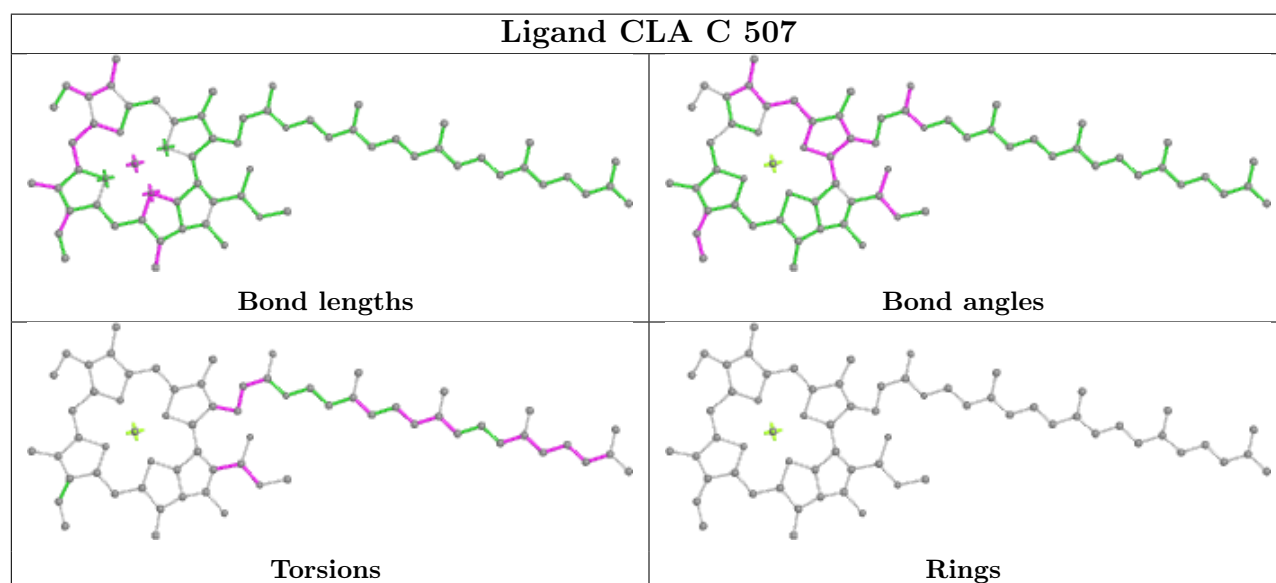
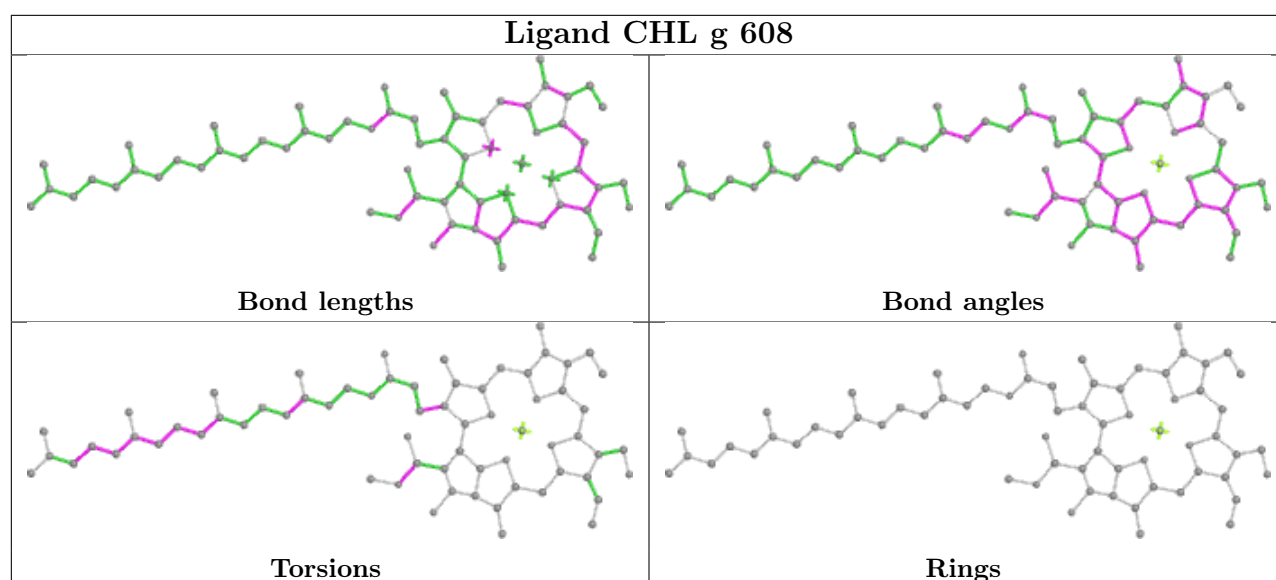
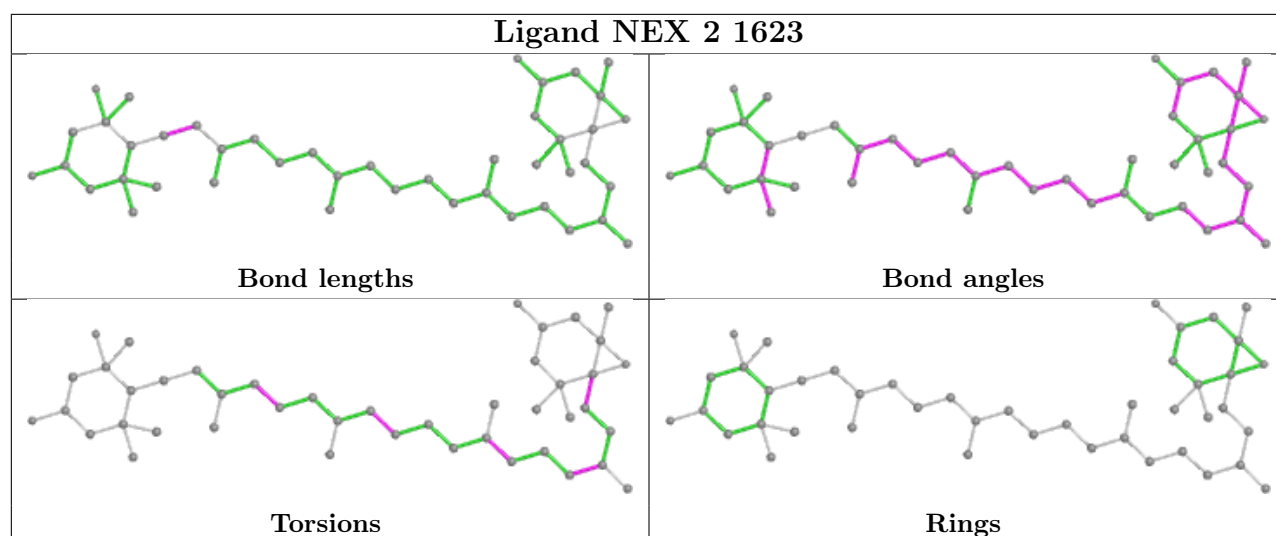


Ligand CLA 1 612

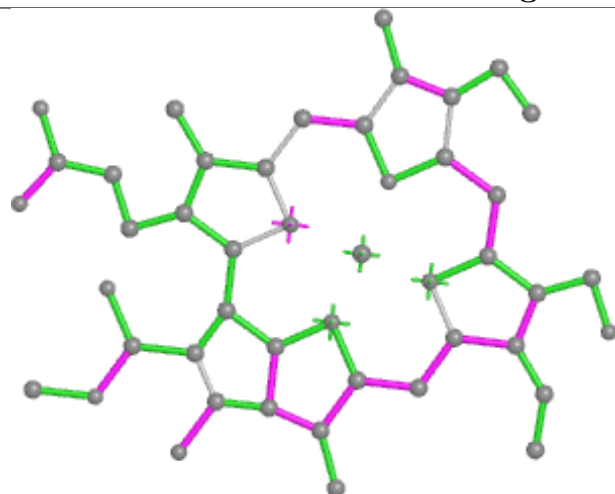


Ligand BCR A 411

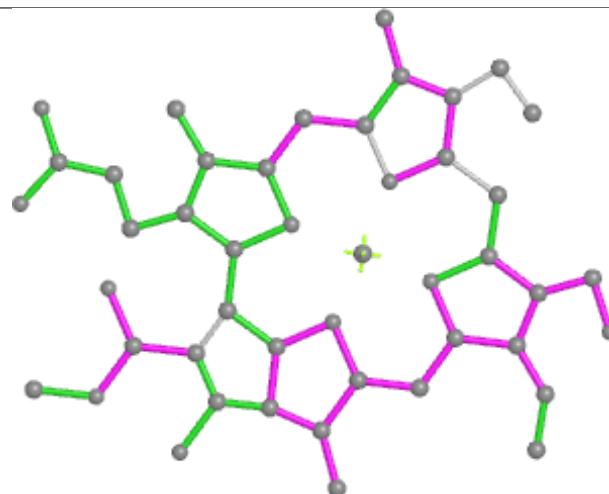




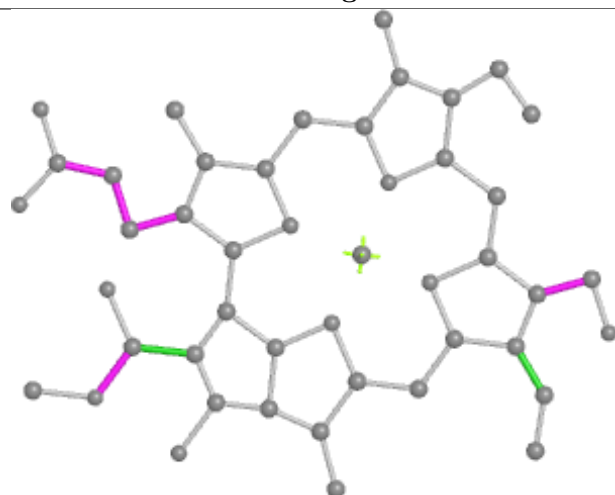
Ligand CHL 4 607



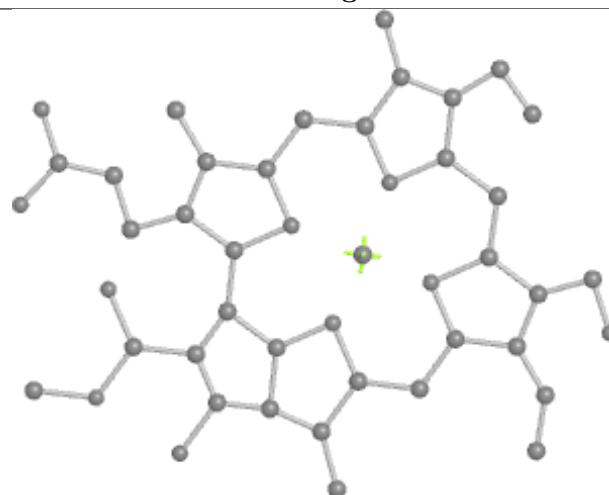
Bond lengths



Bond angles

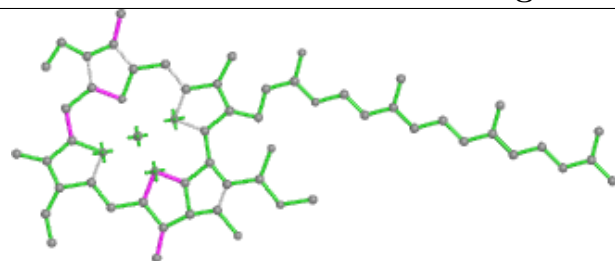


Torsions

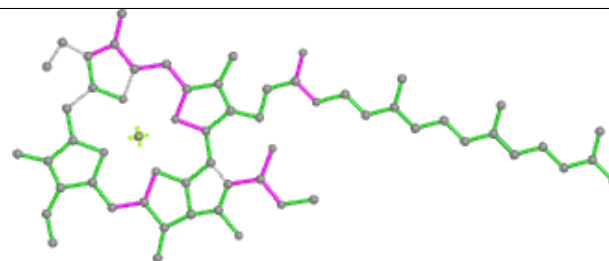


Rings

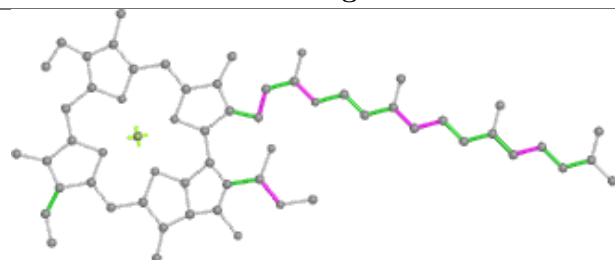
Ligand CLA R 602



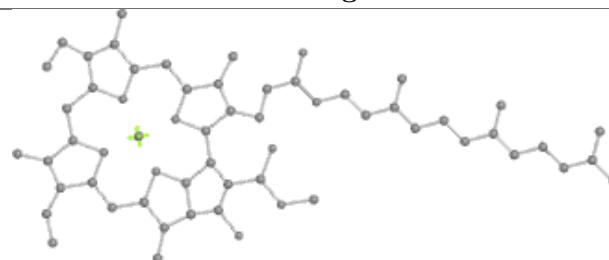
Bond lengths



Bond angles

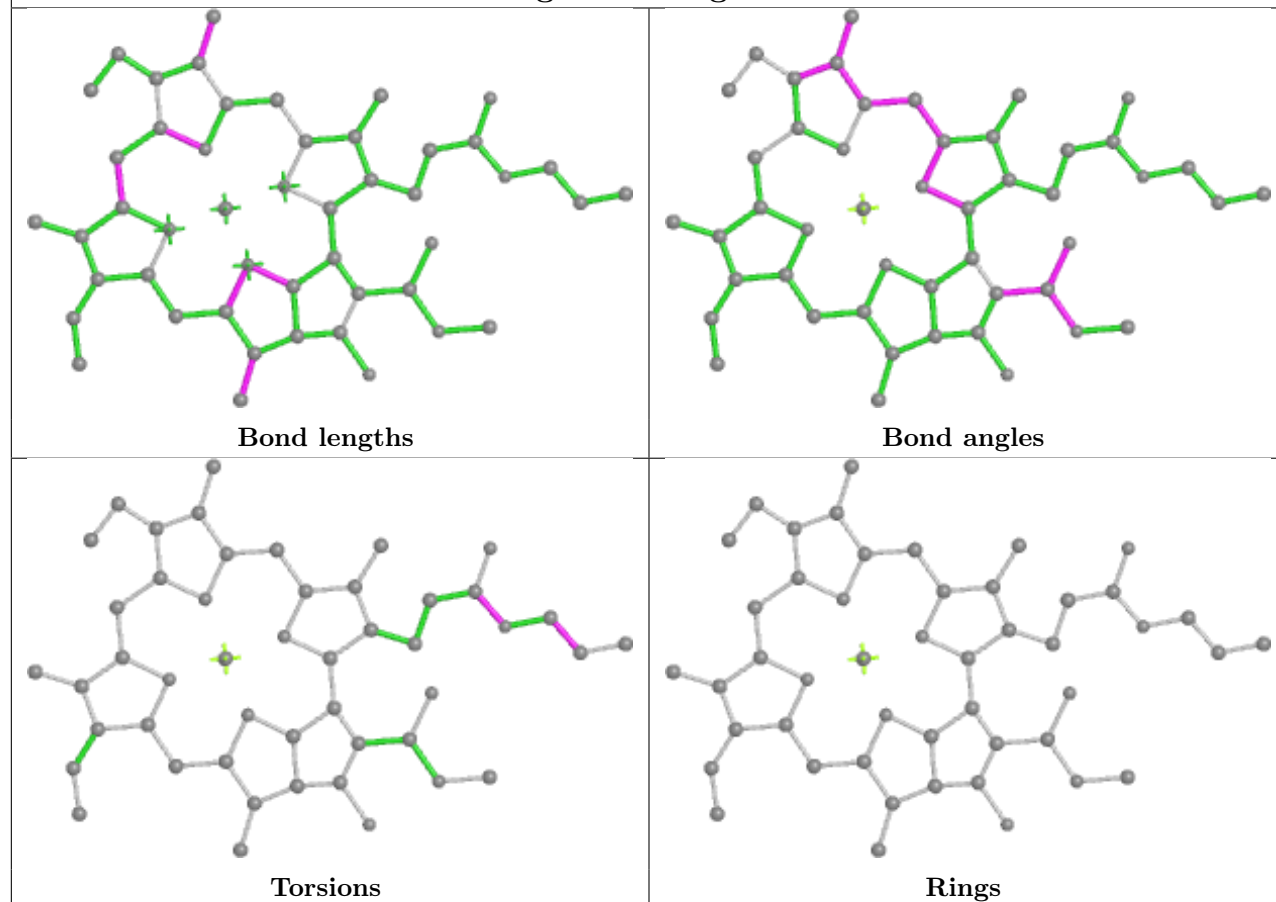


Torsions

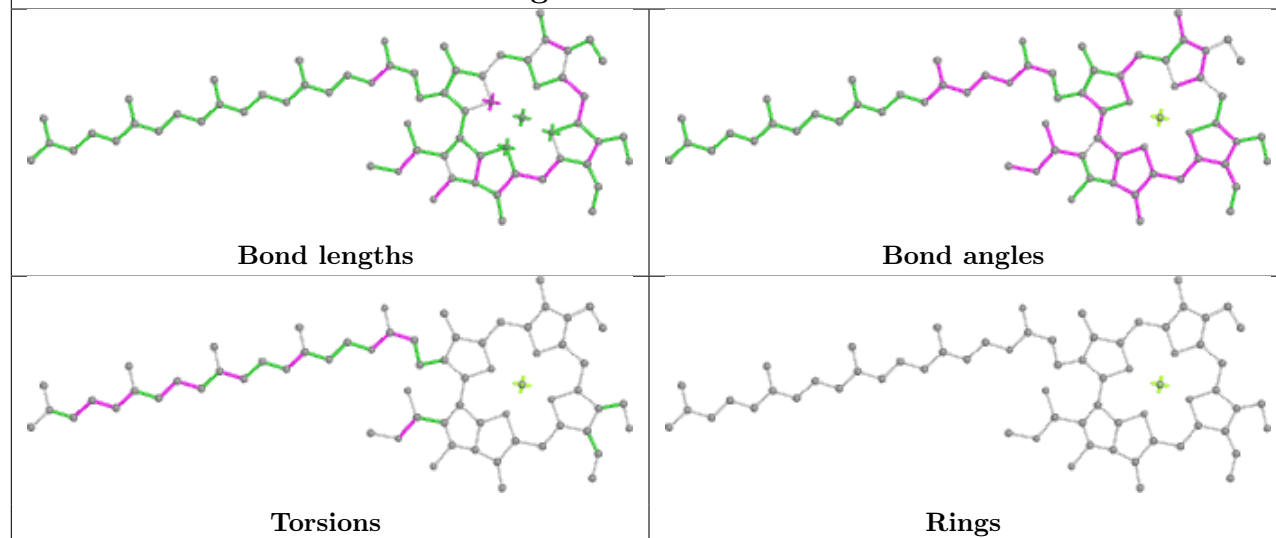


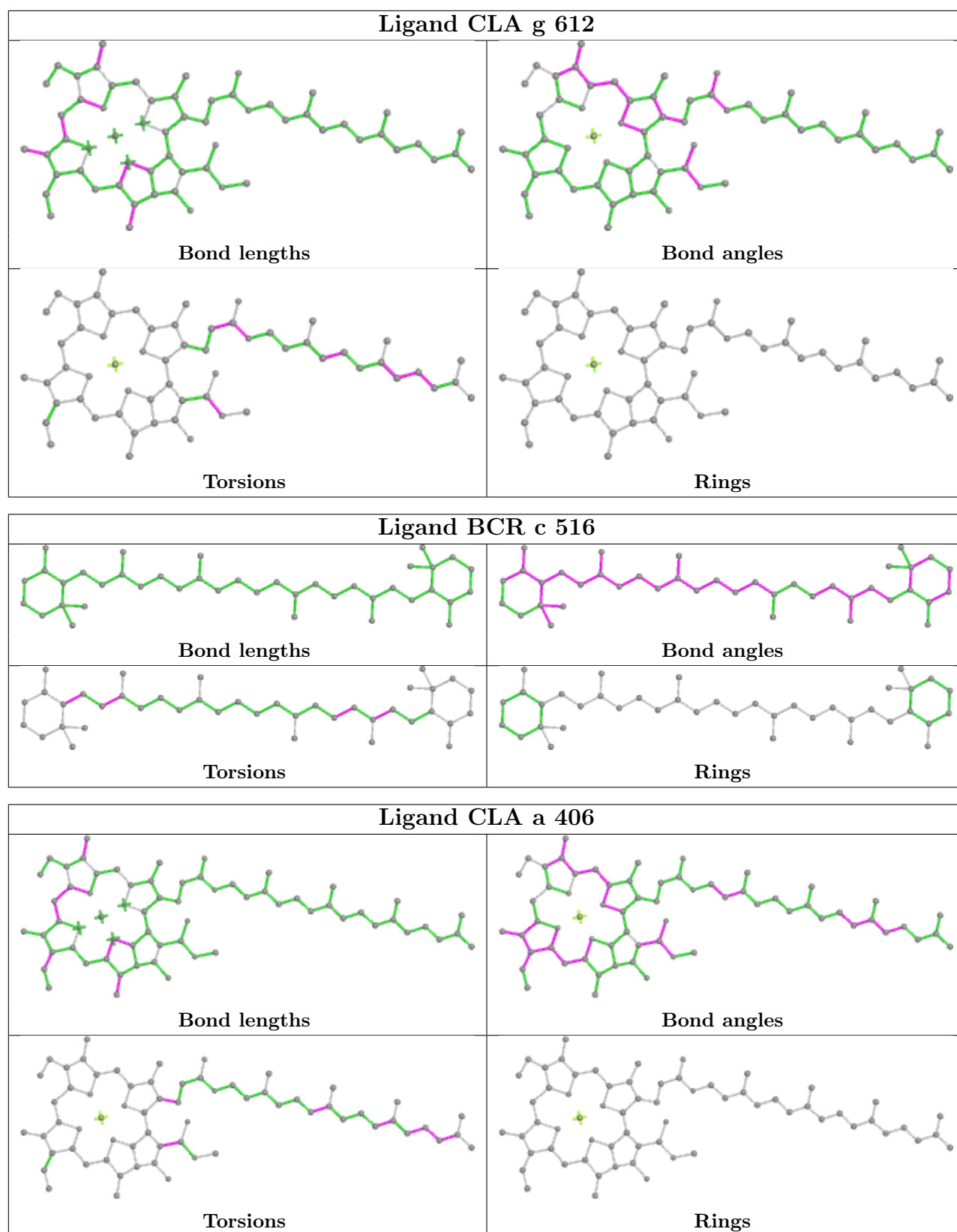
Rings

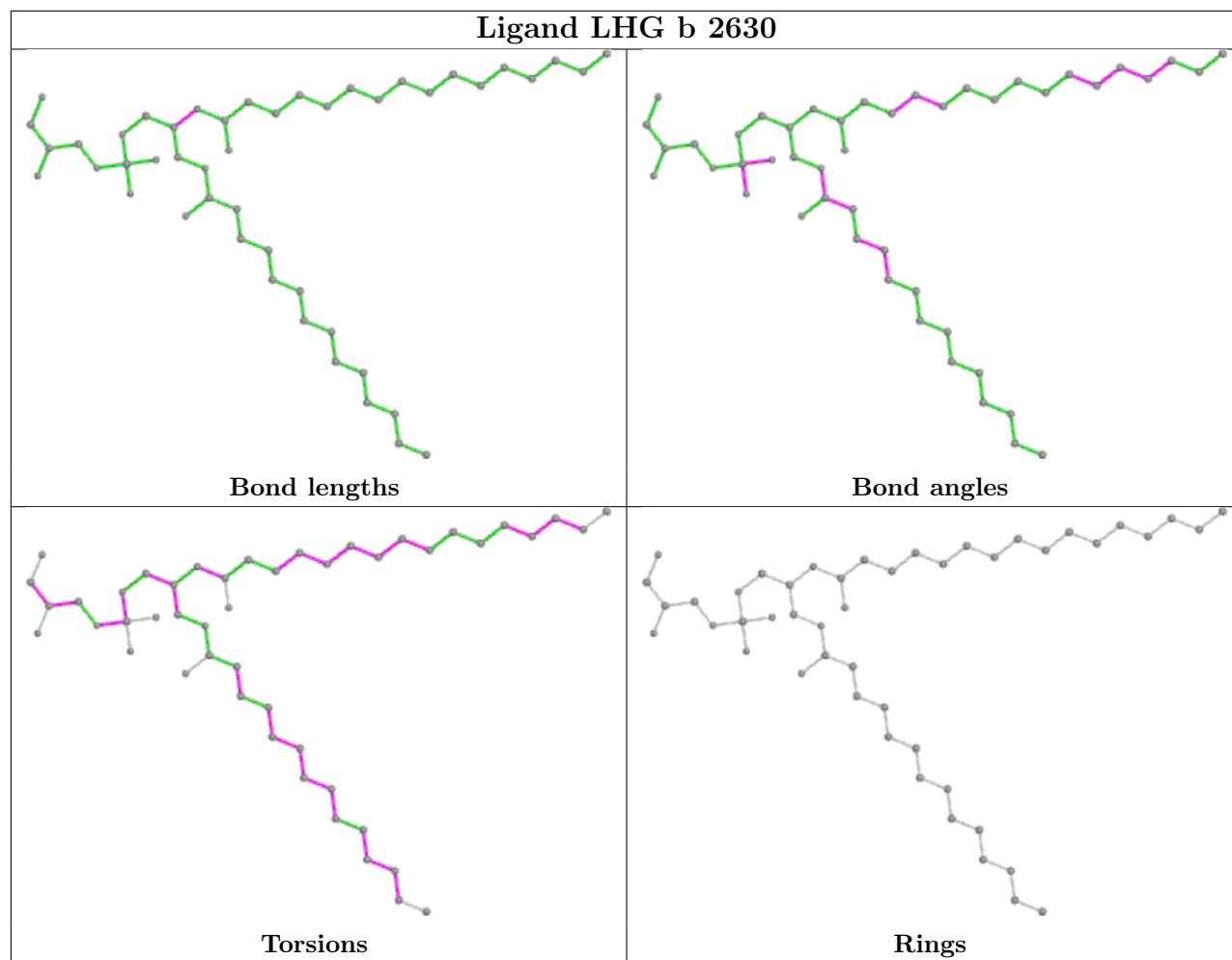
Ligand CLA g 614



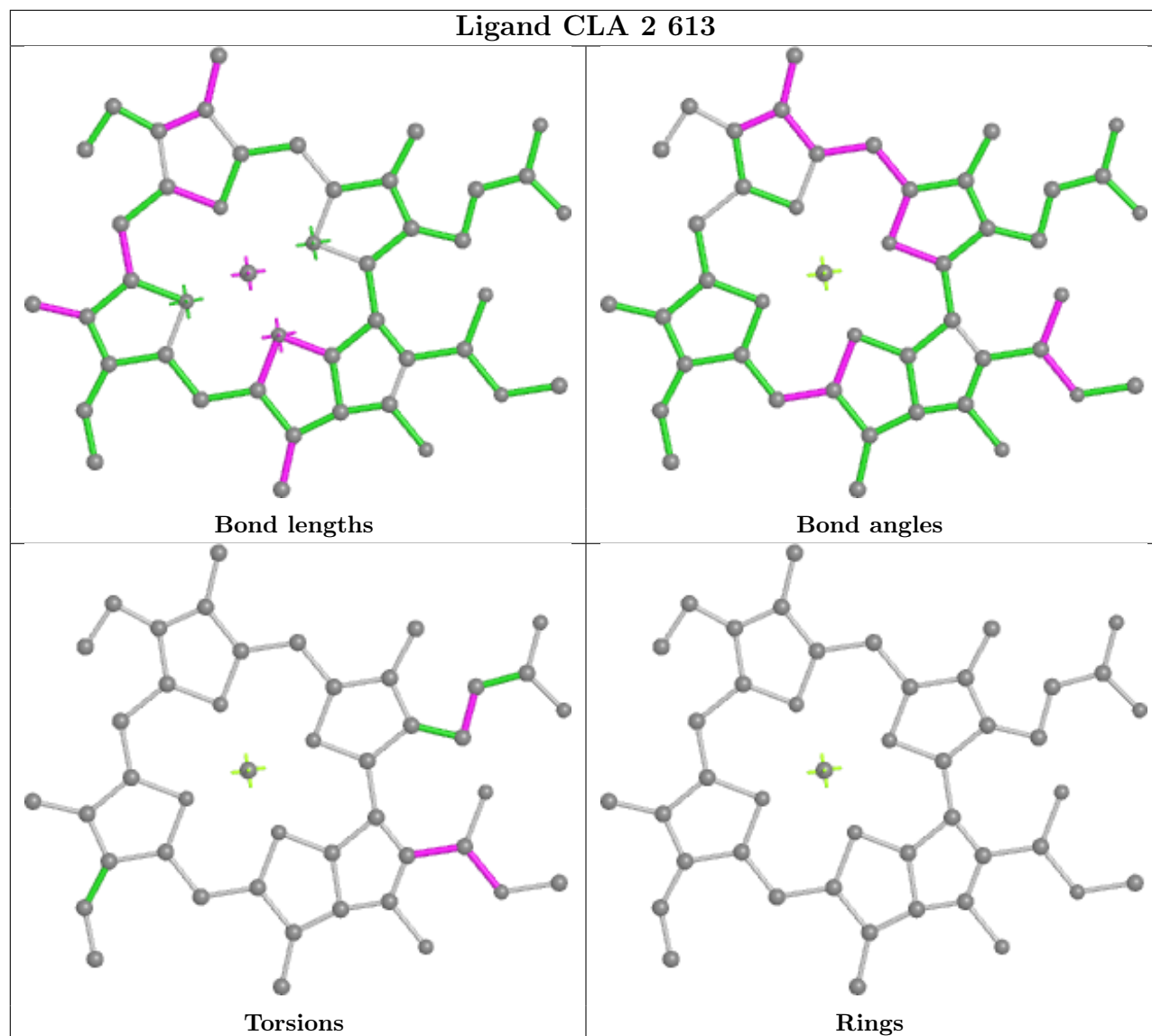
Ligand CHL G 601



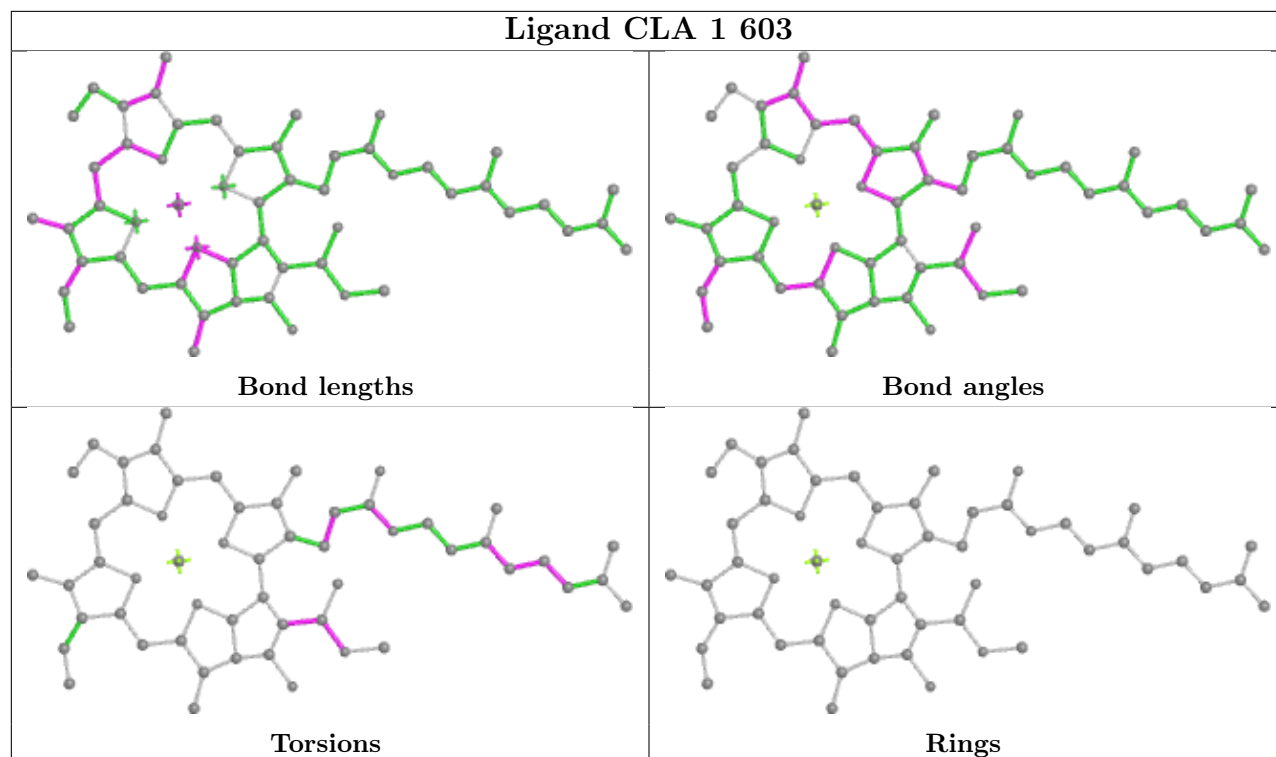




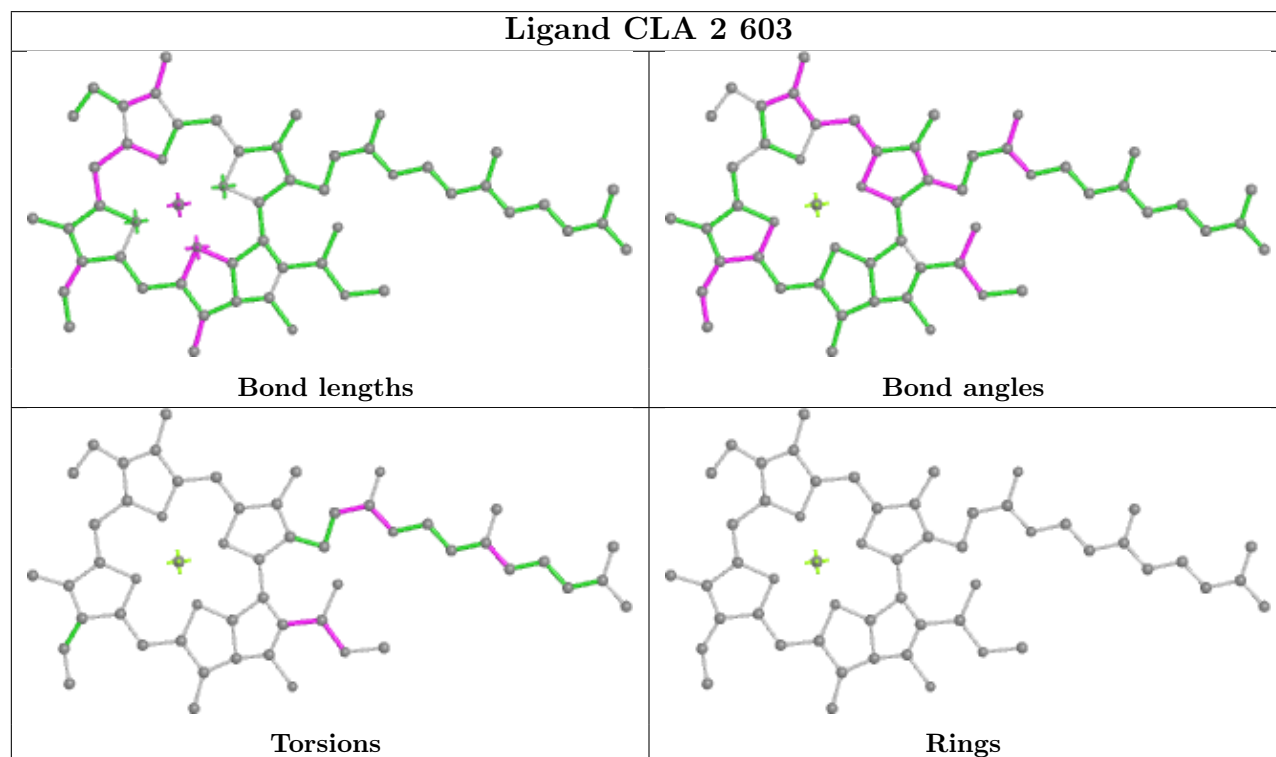
Ligand CLA 2 613

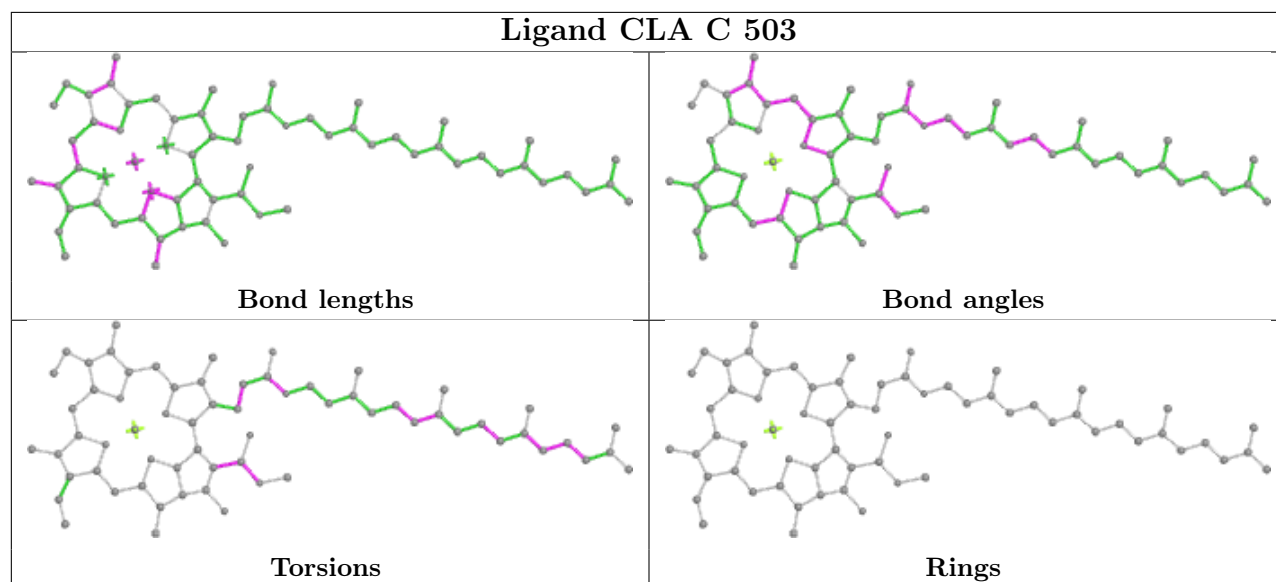
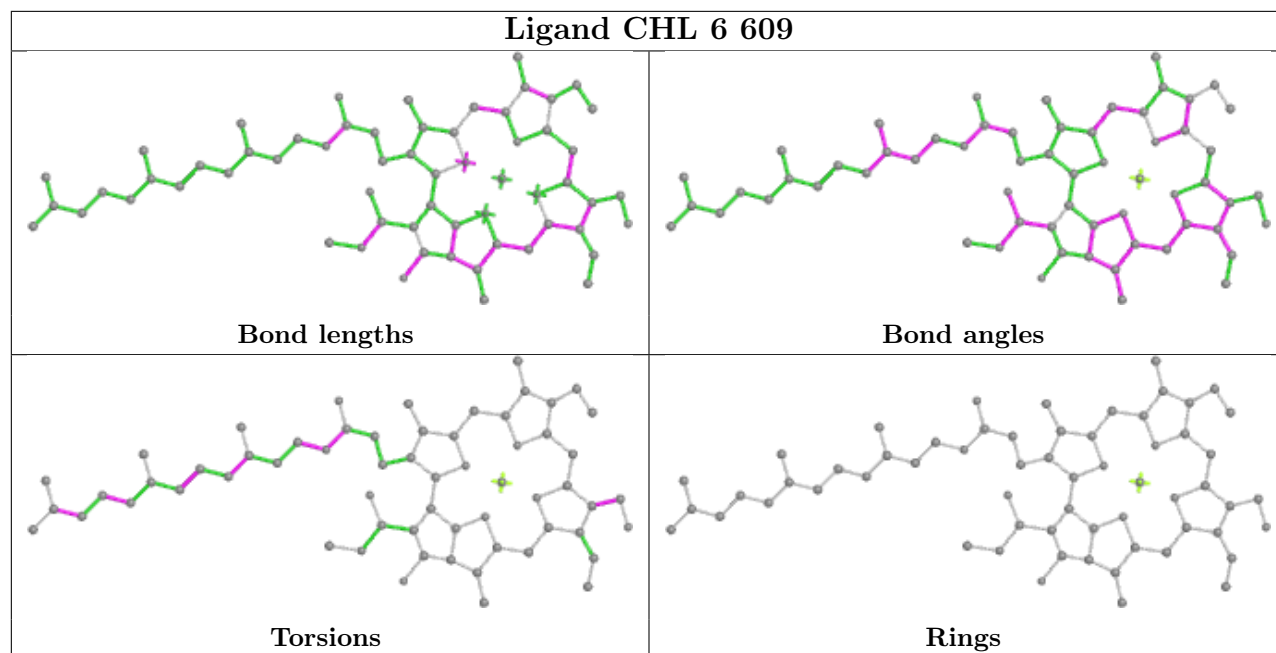


Ligand CLA 1 603

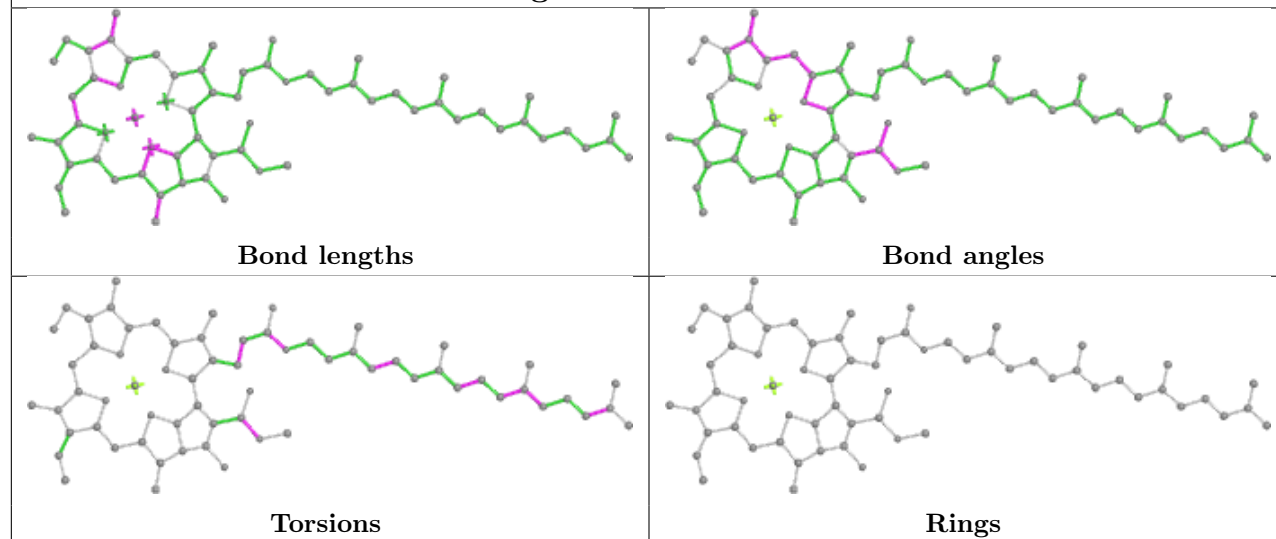


Ligand CLA 2 603

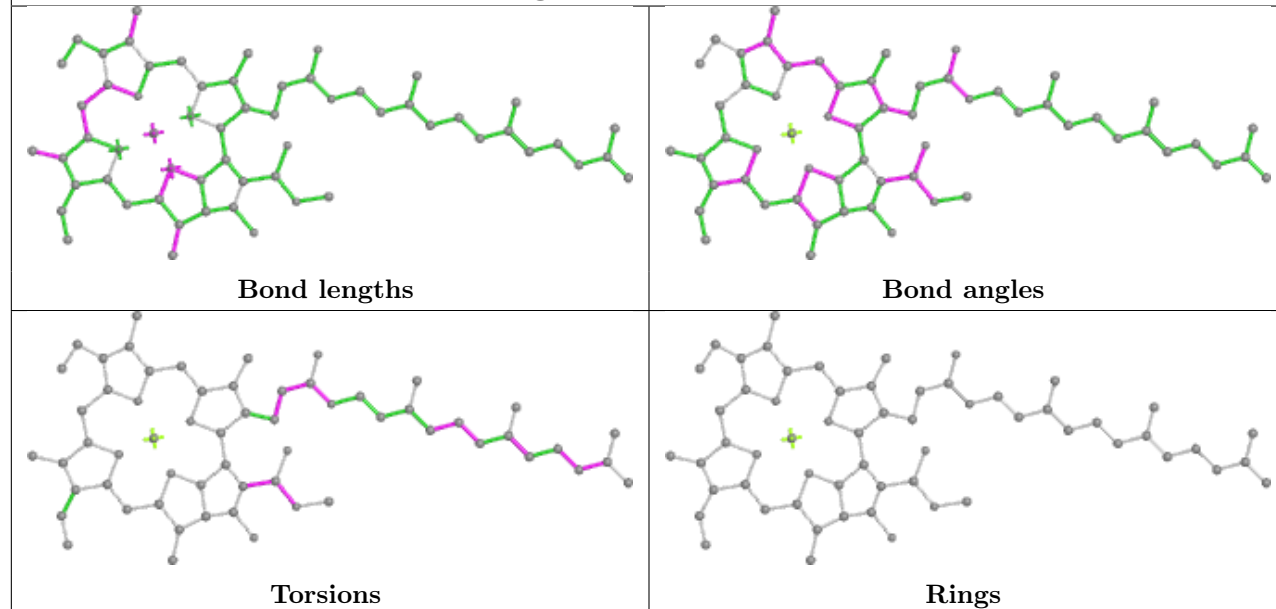


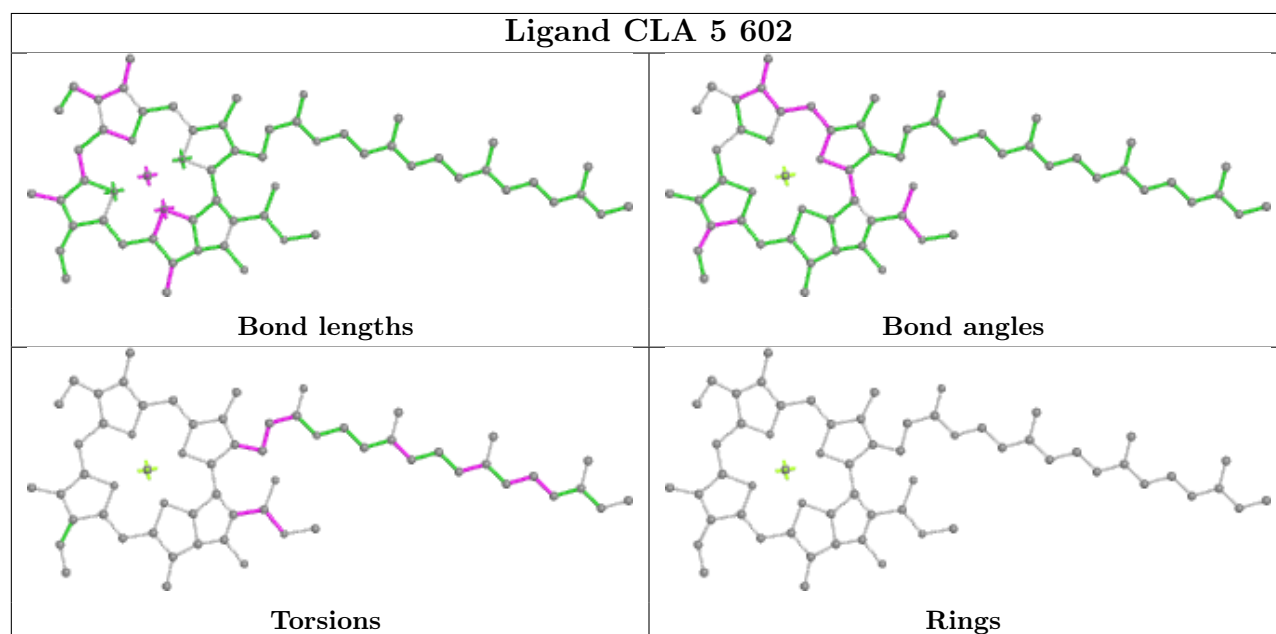
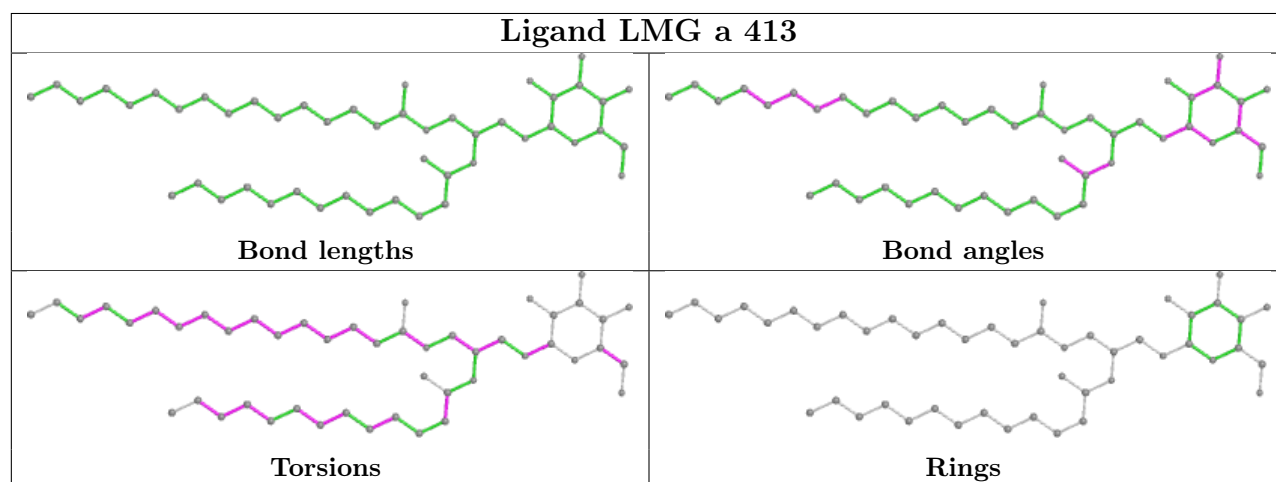
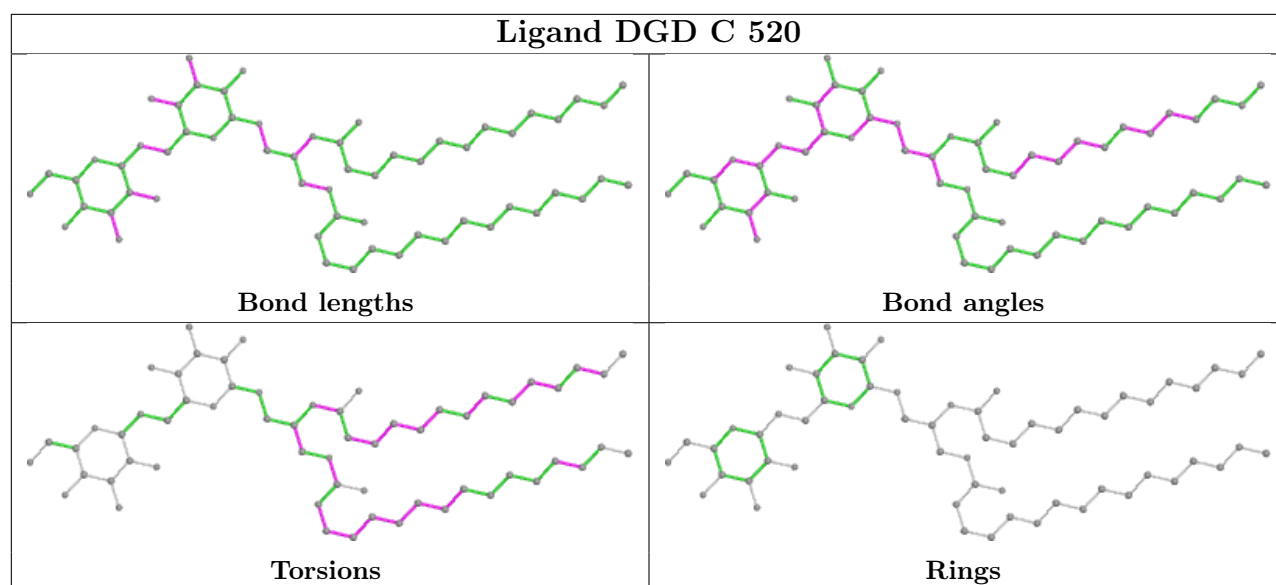


Ligand CLA G 613

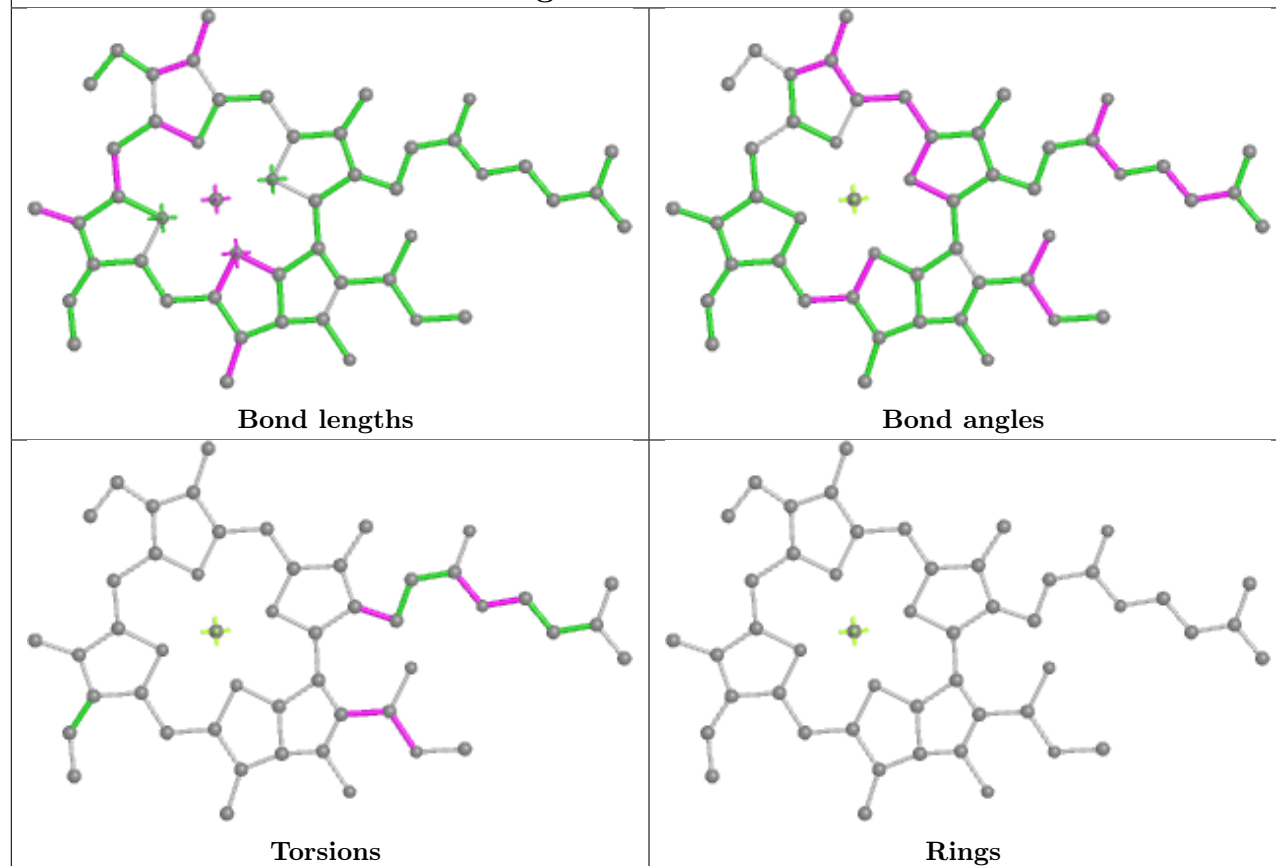


Ligand CLA R 603

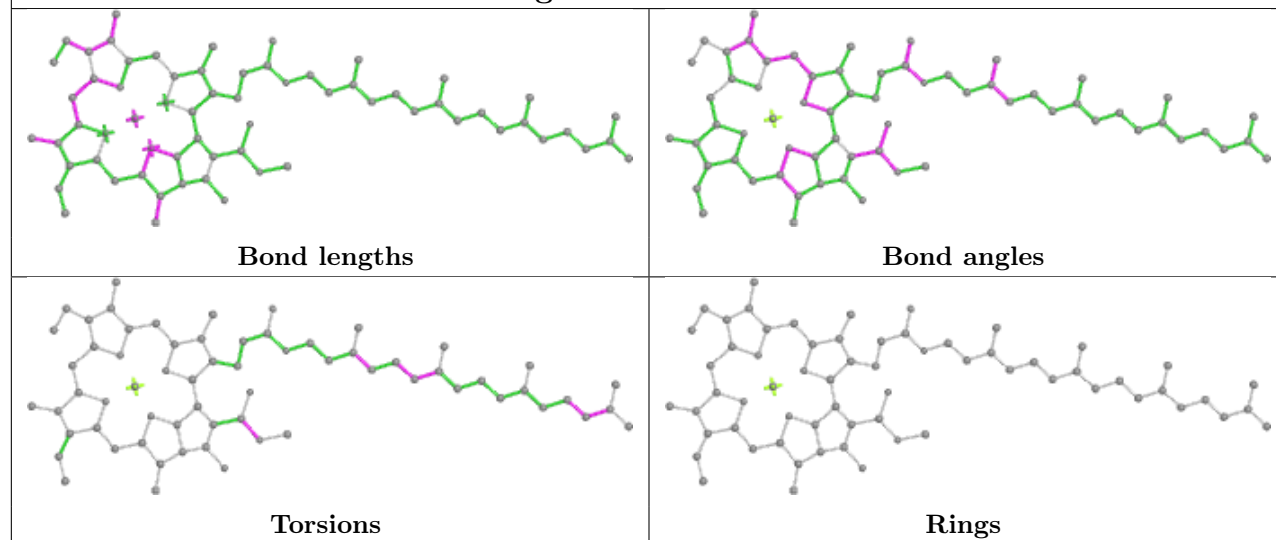




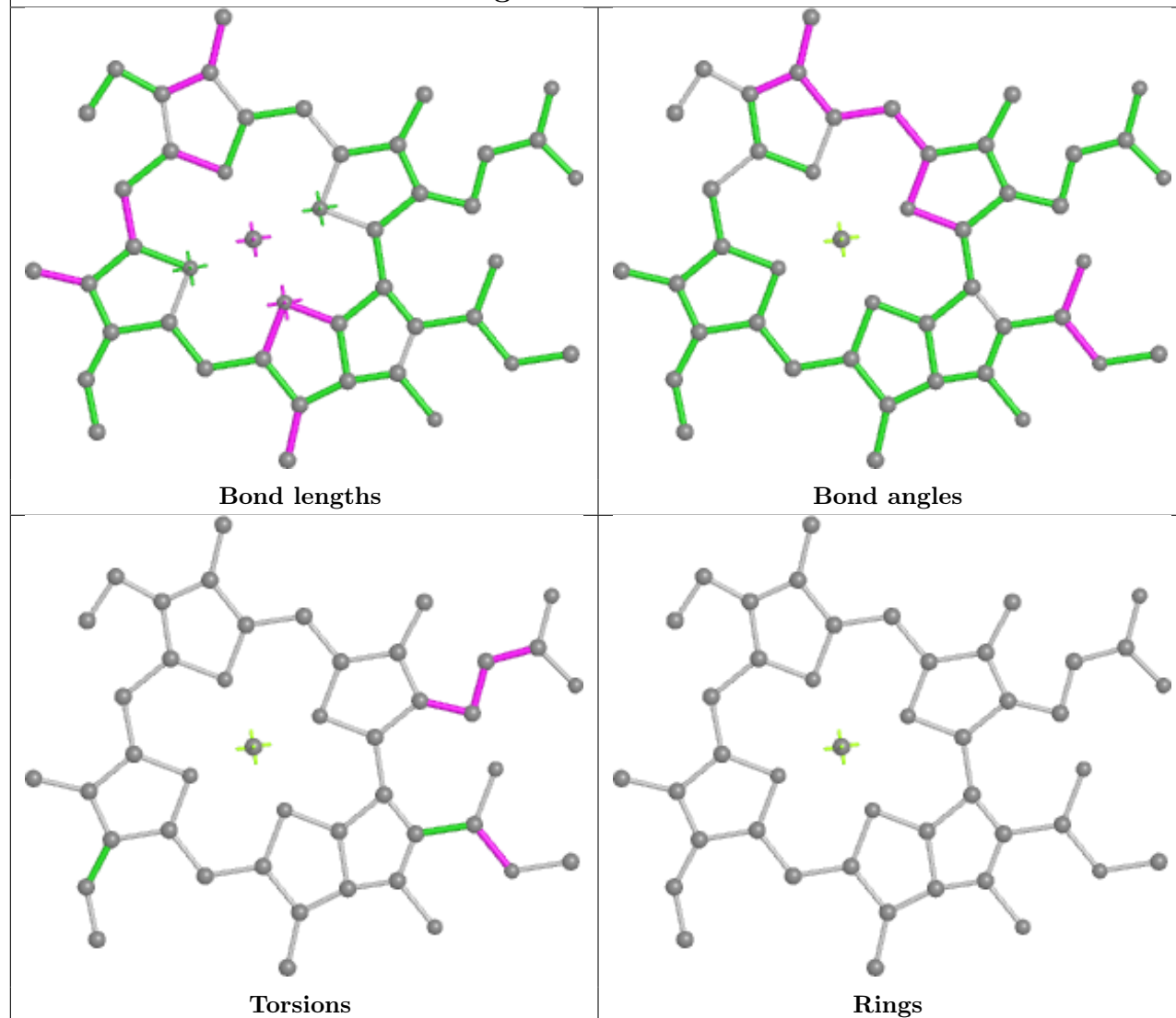
Ligand CLA 5 604



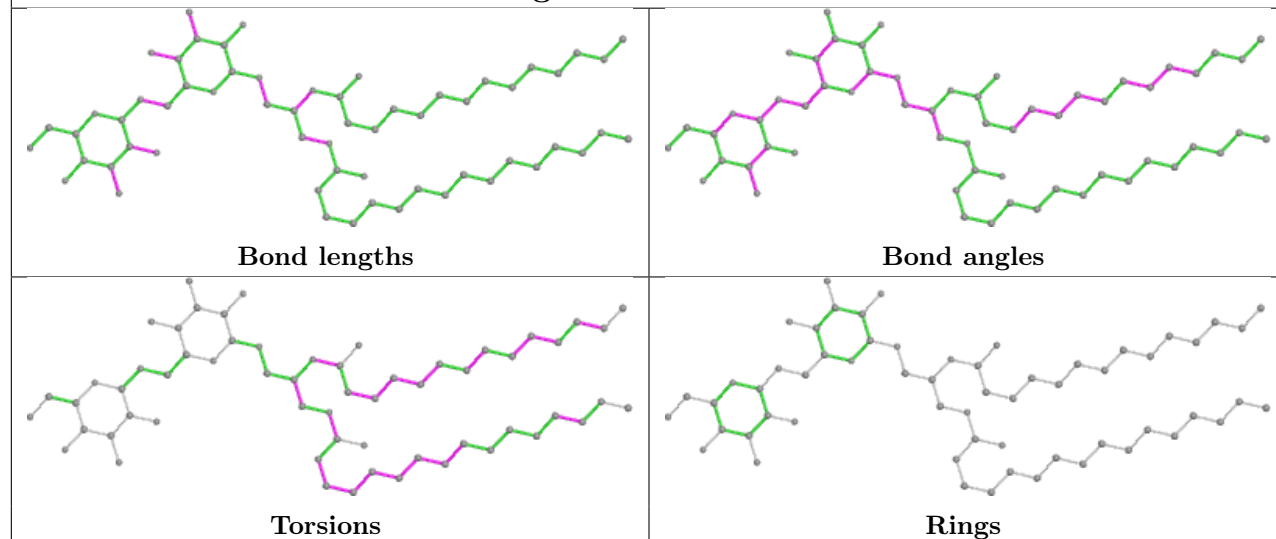
Ligand CLA b 604



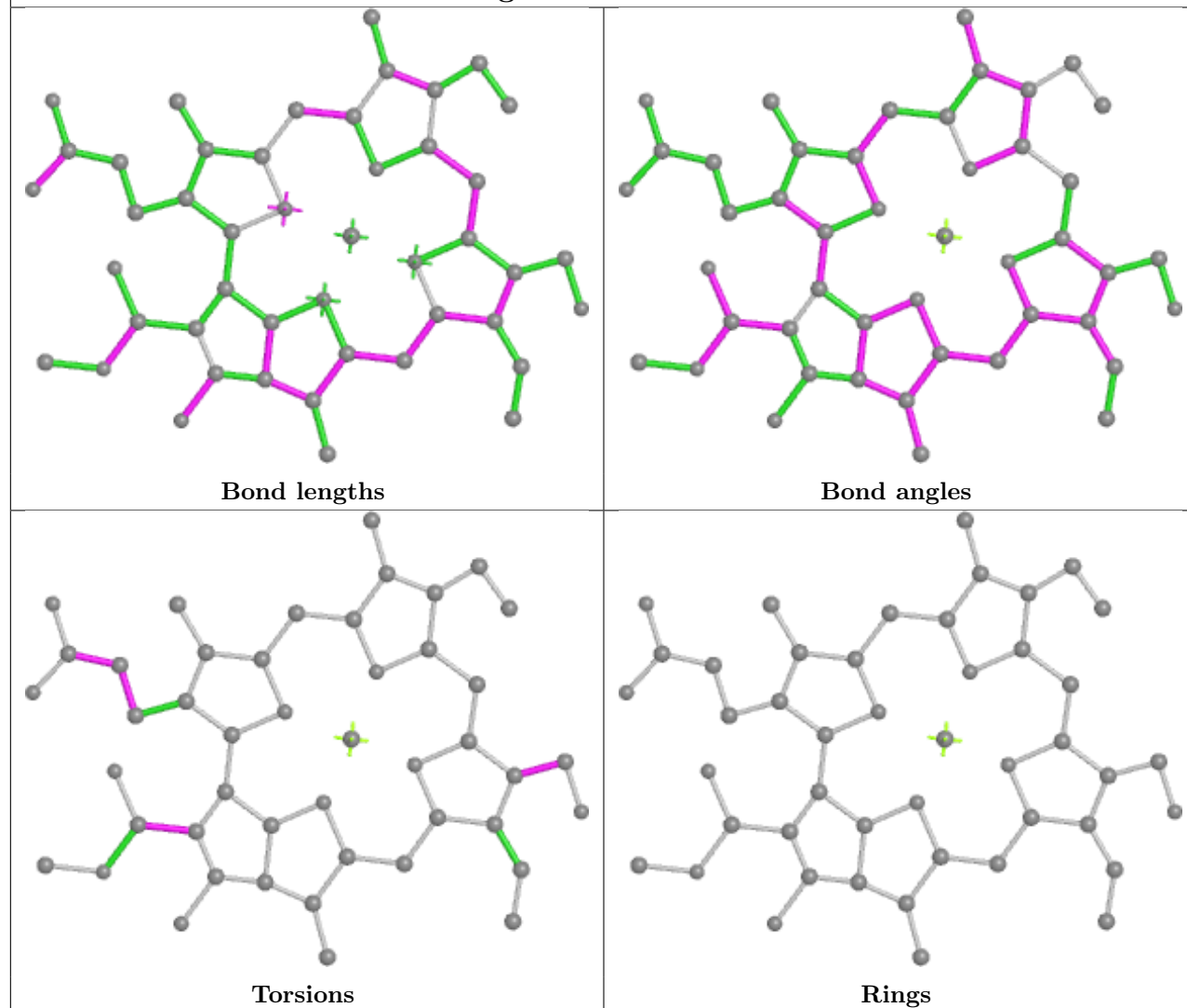
Ligand CLA 1 611



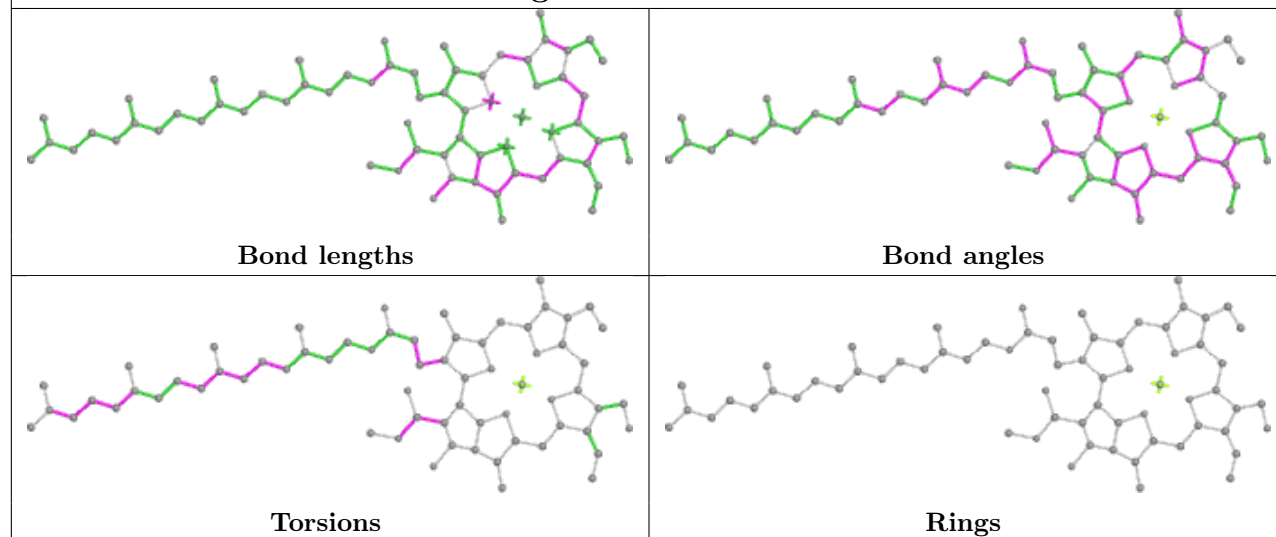
Ligand DGD c 520

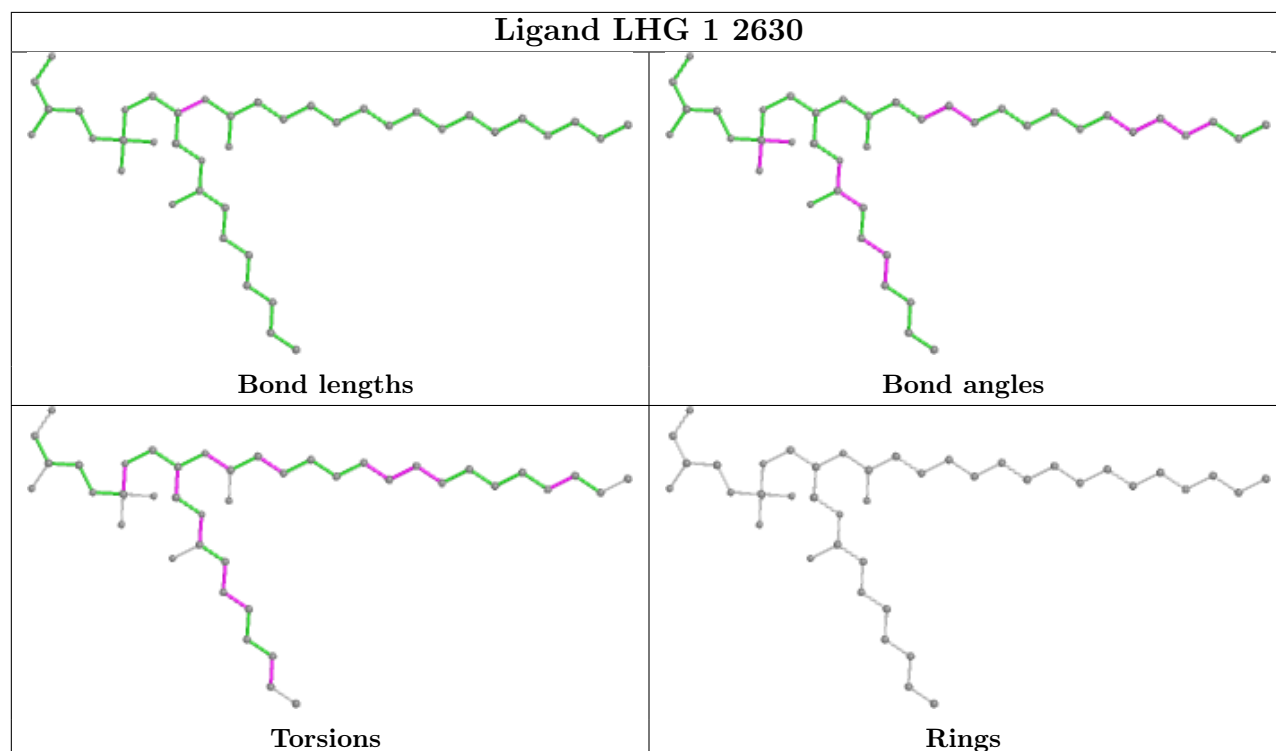
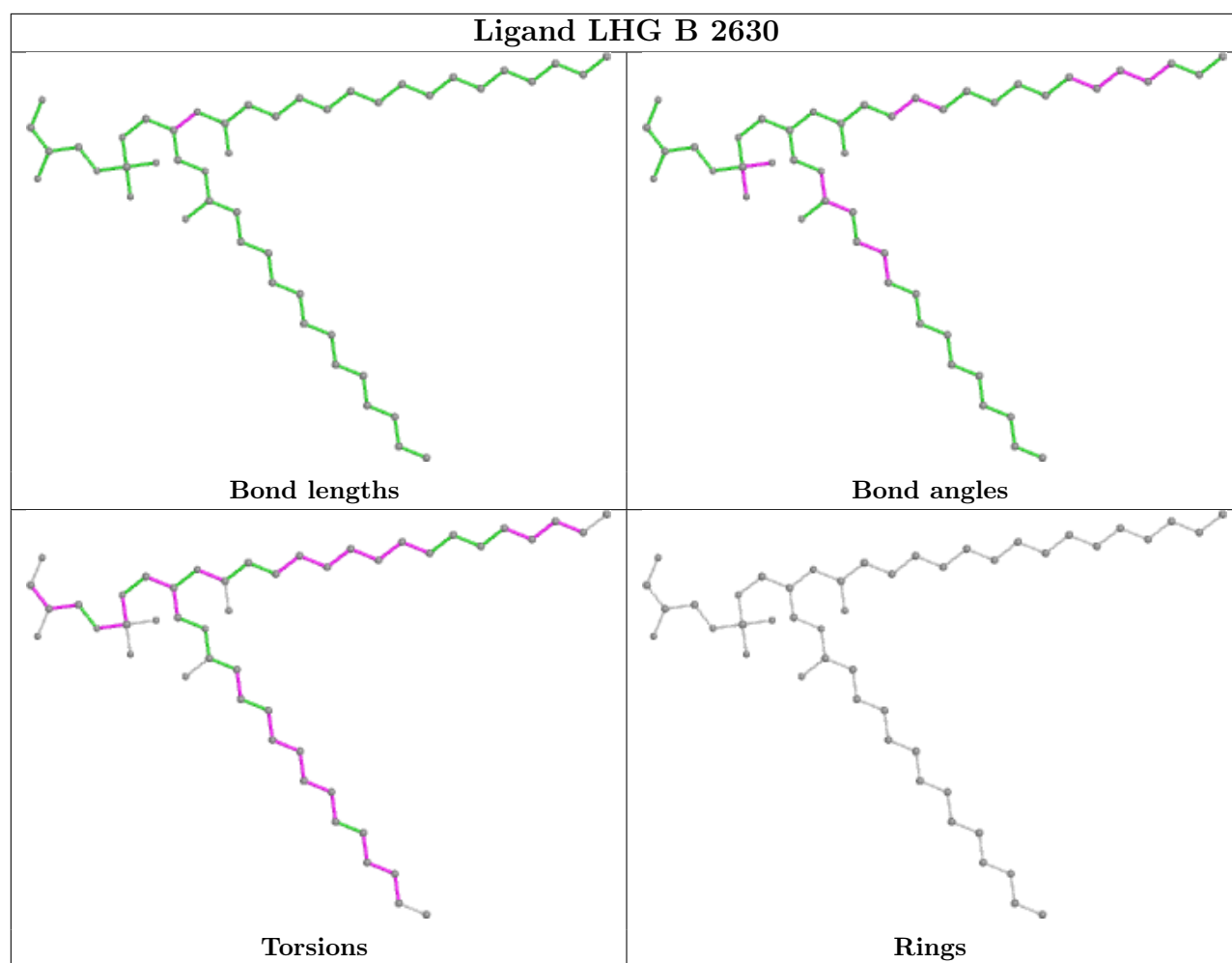


Ligand CHL 2 606

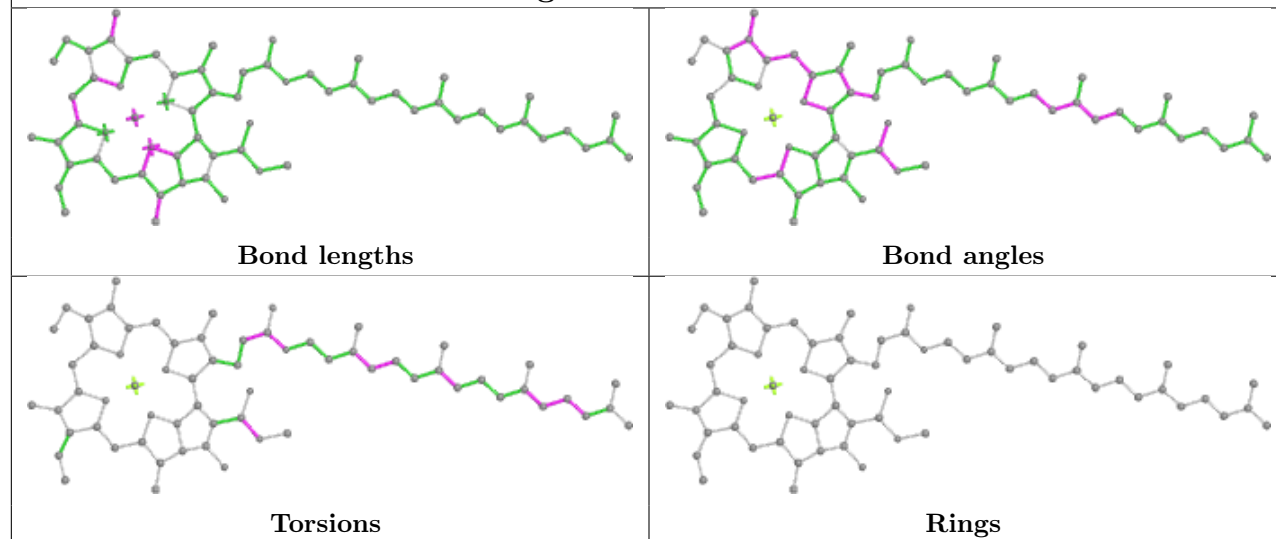


Ligand CHL R 606

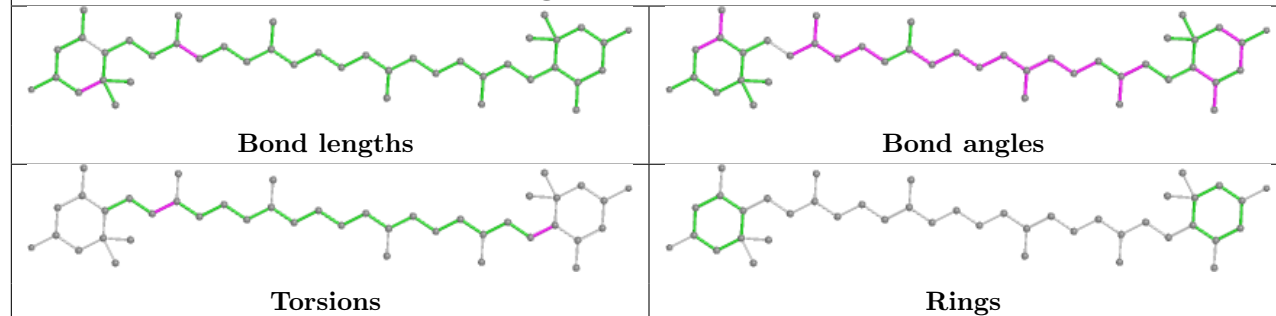




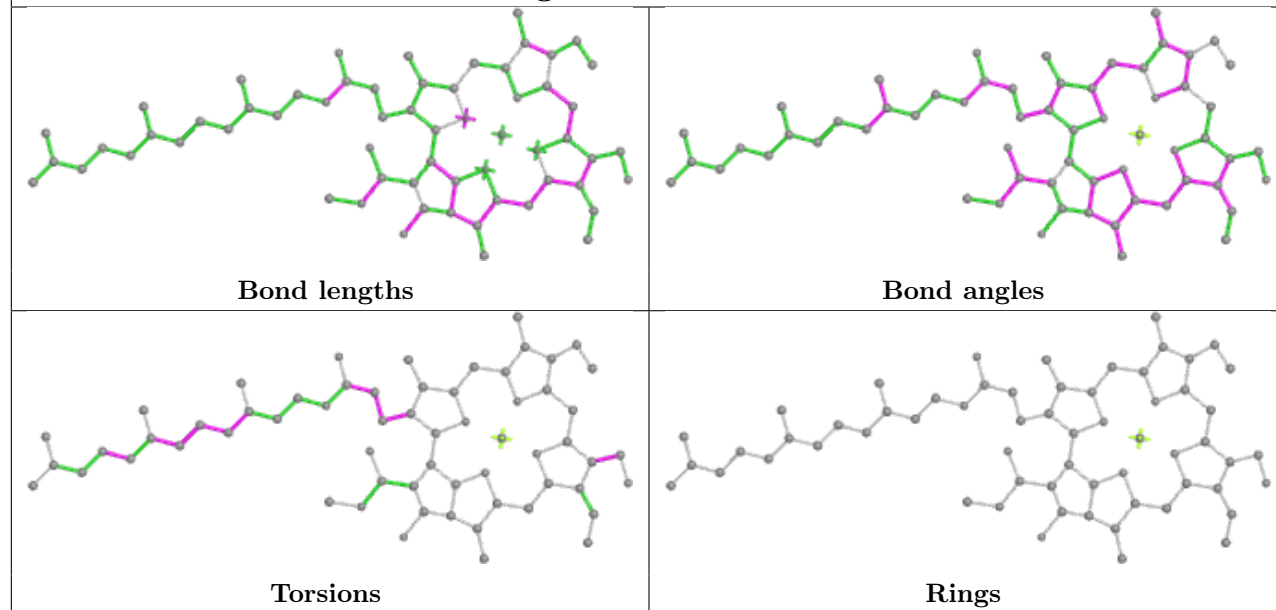
Ligand CLA c 510



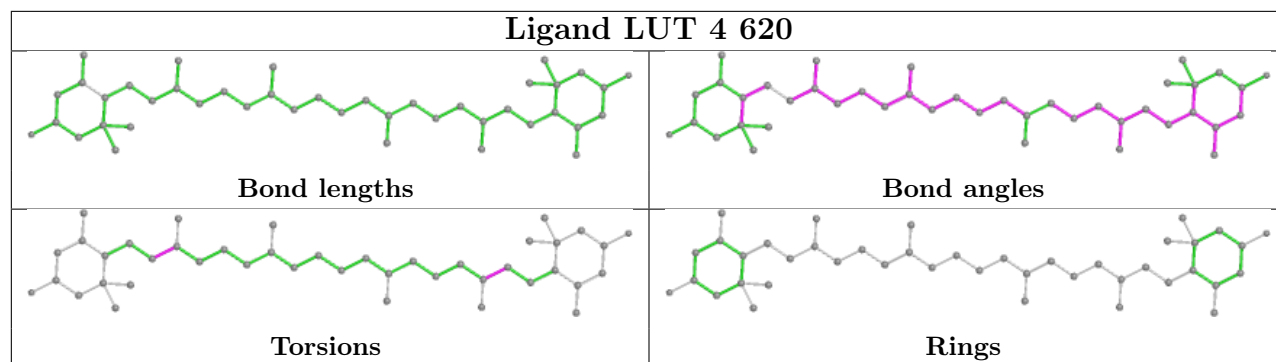
Ligand LUT r 620



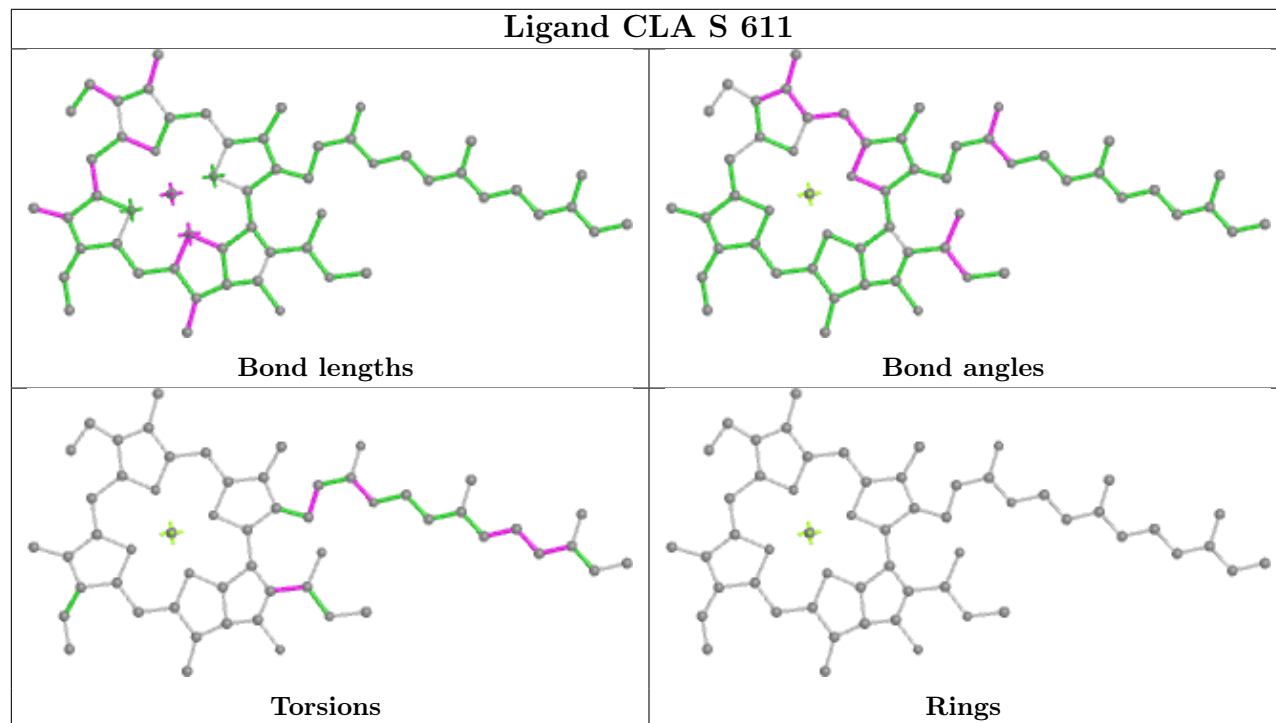
Ligand CHL 6 607



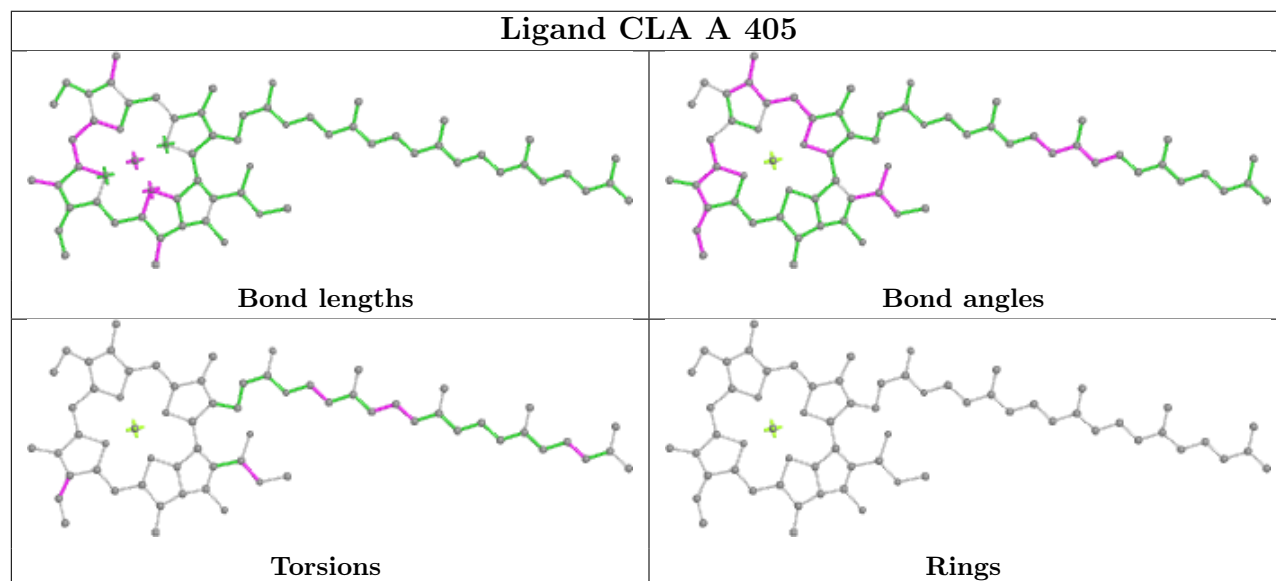
Ligand LUT 4 620

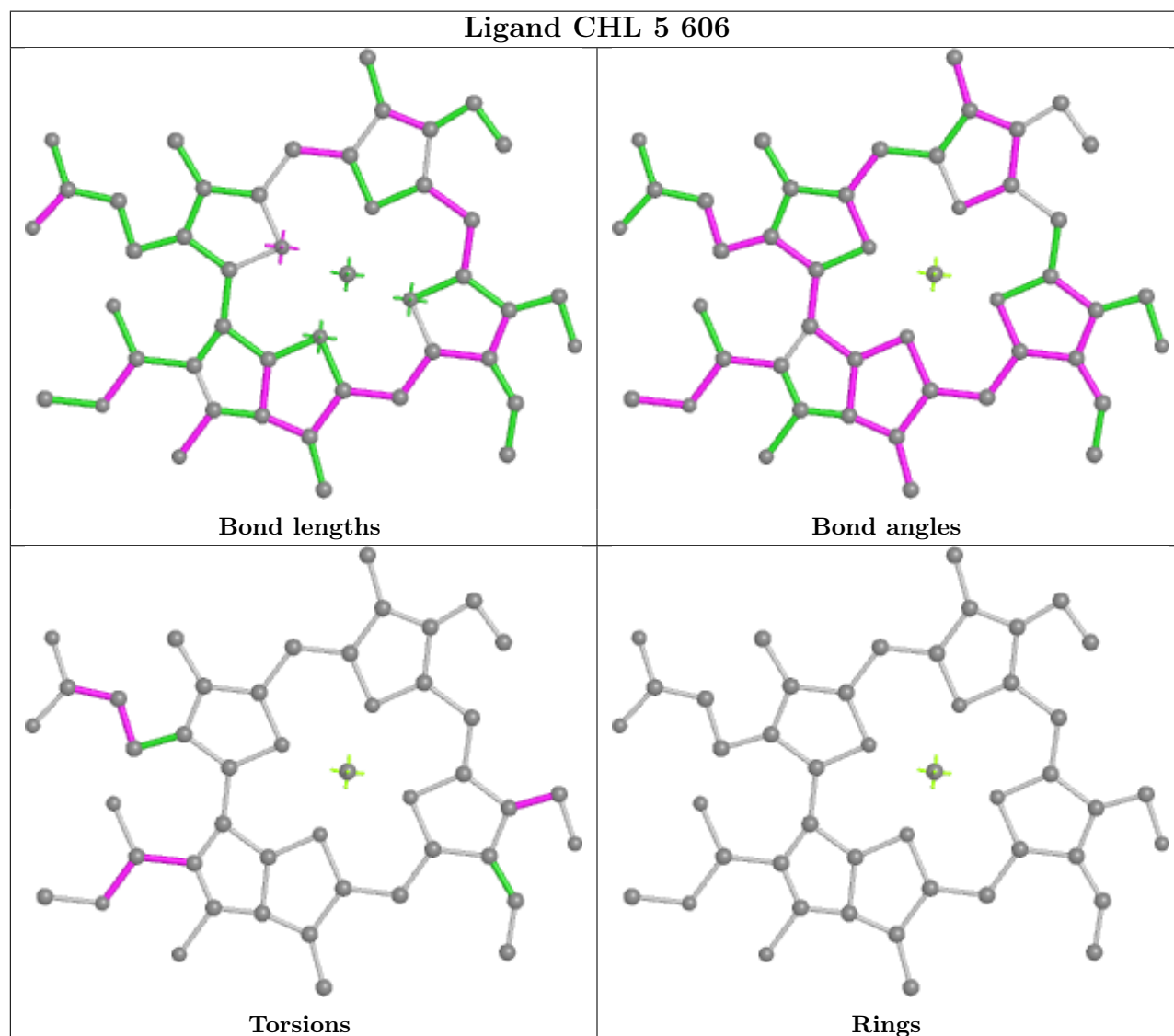
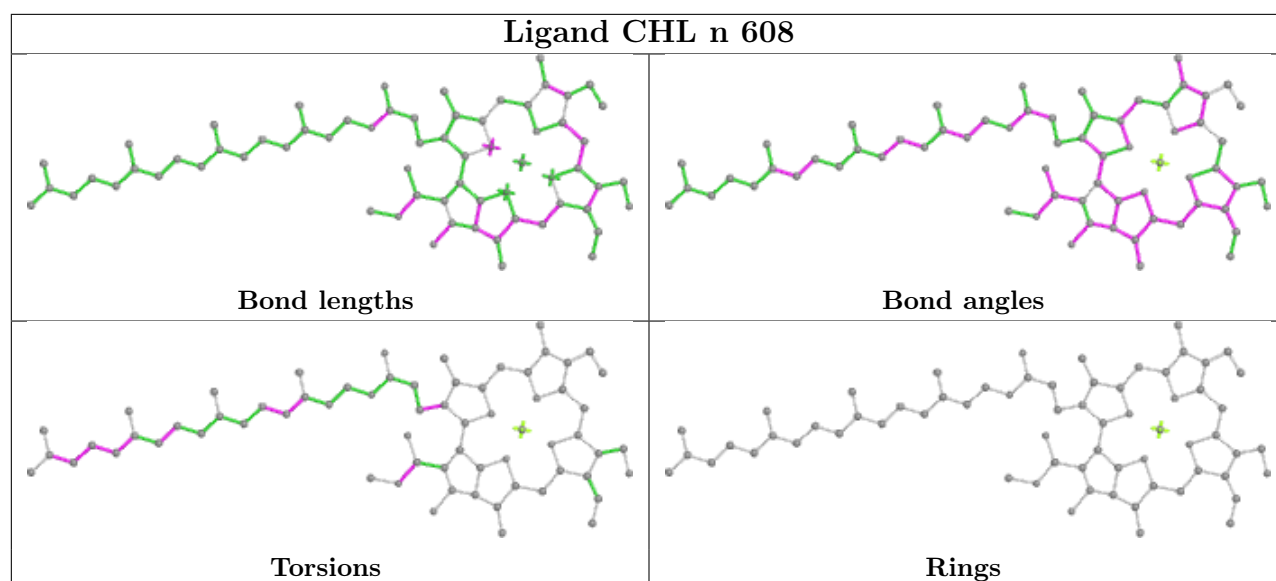


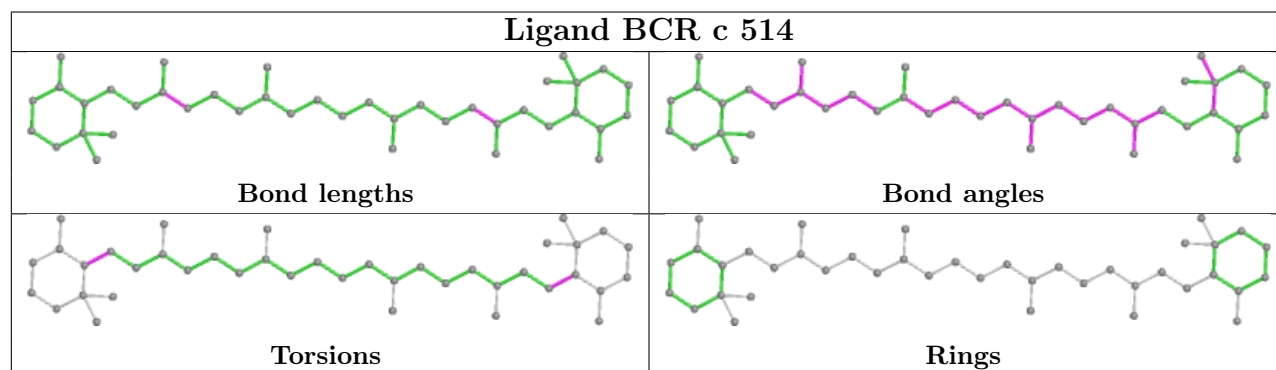
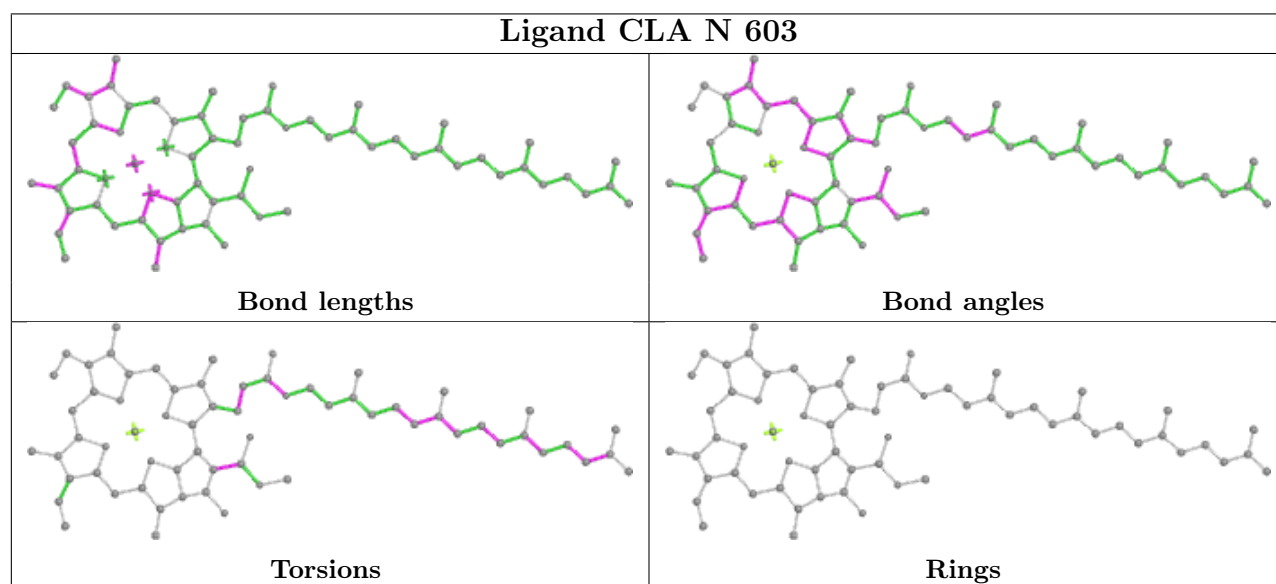
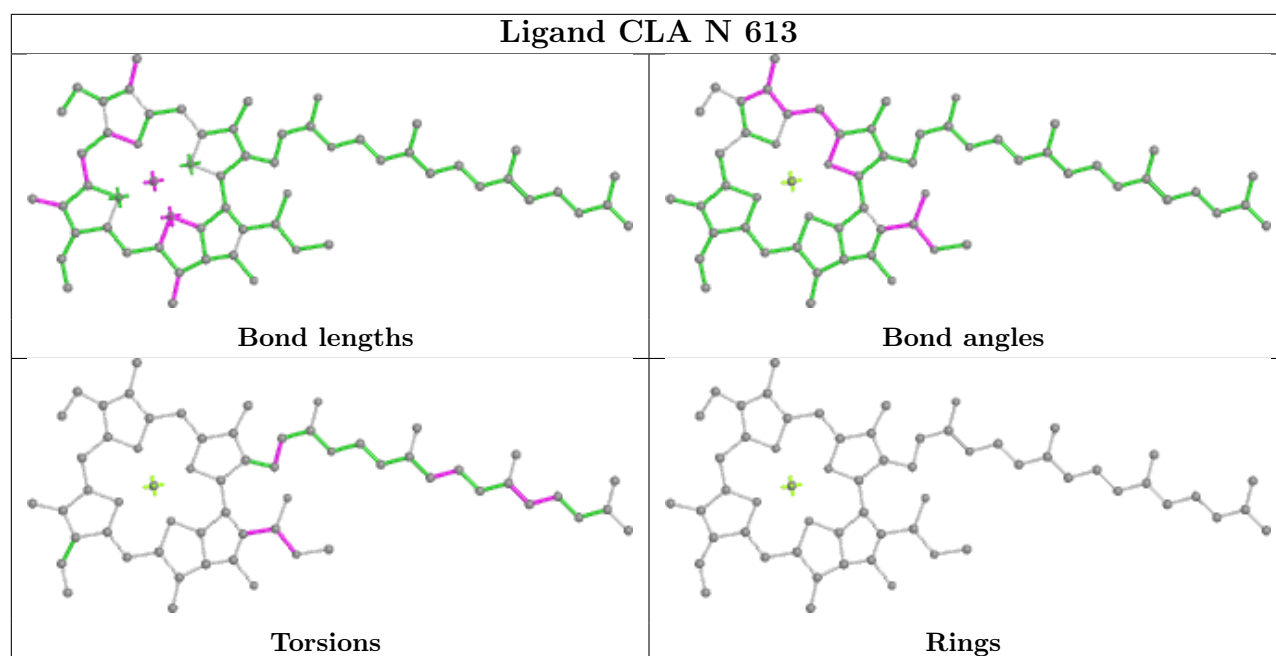
Ligand CLA S 611



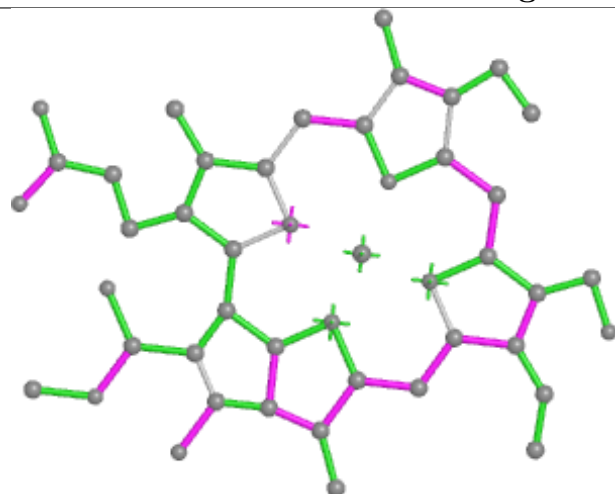
Ligand CLA A 405



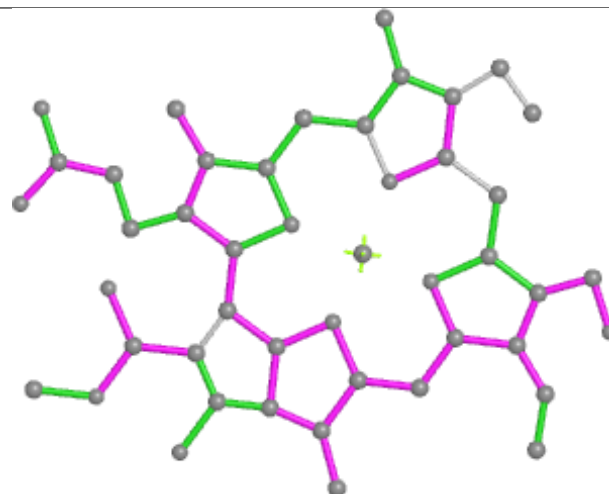




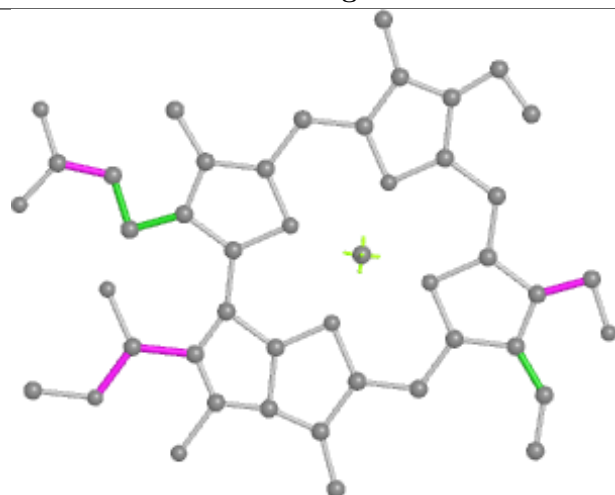
Ligand CHL S 606



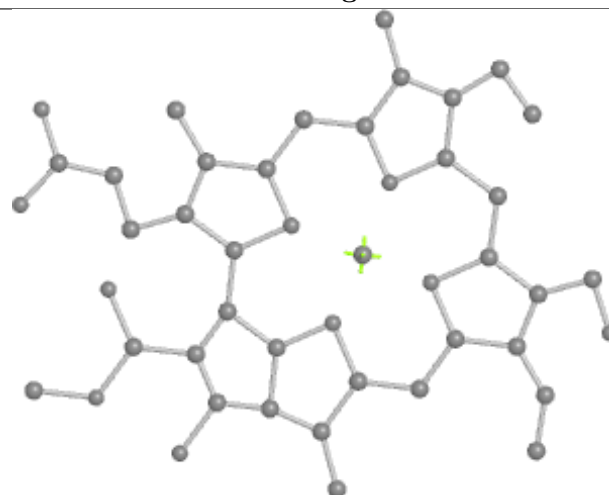
Bond lengths



Bond angles

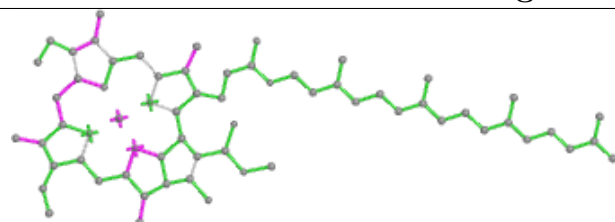


Torsions

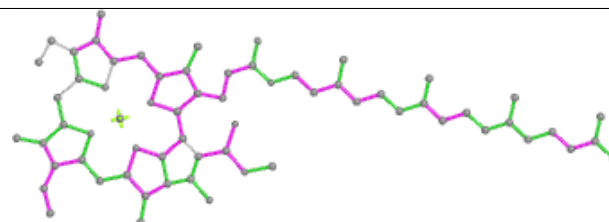


Rings

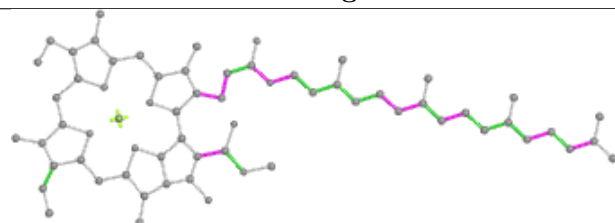
Ligand CLA B 605



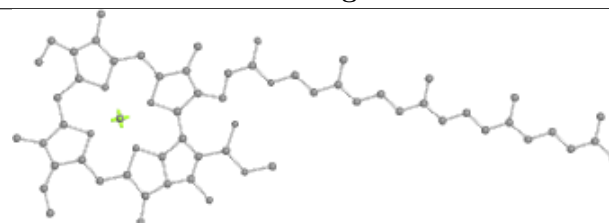
Bond lengths



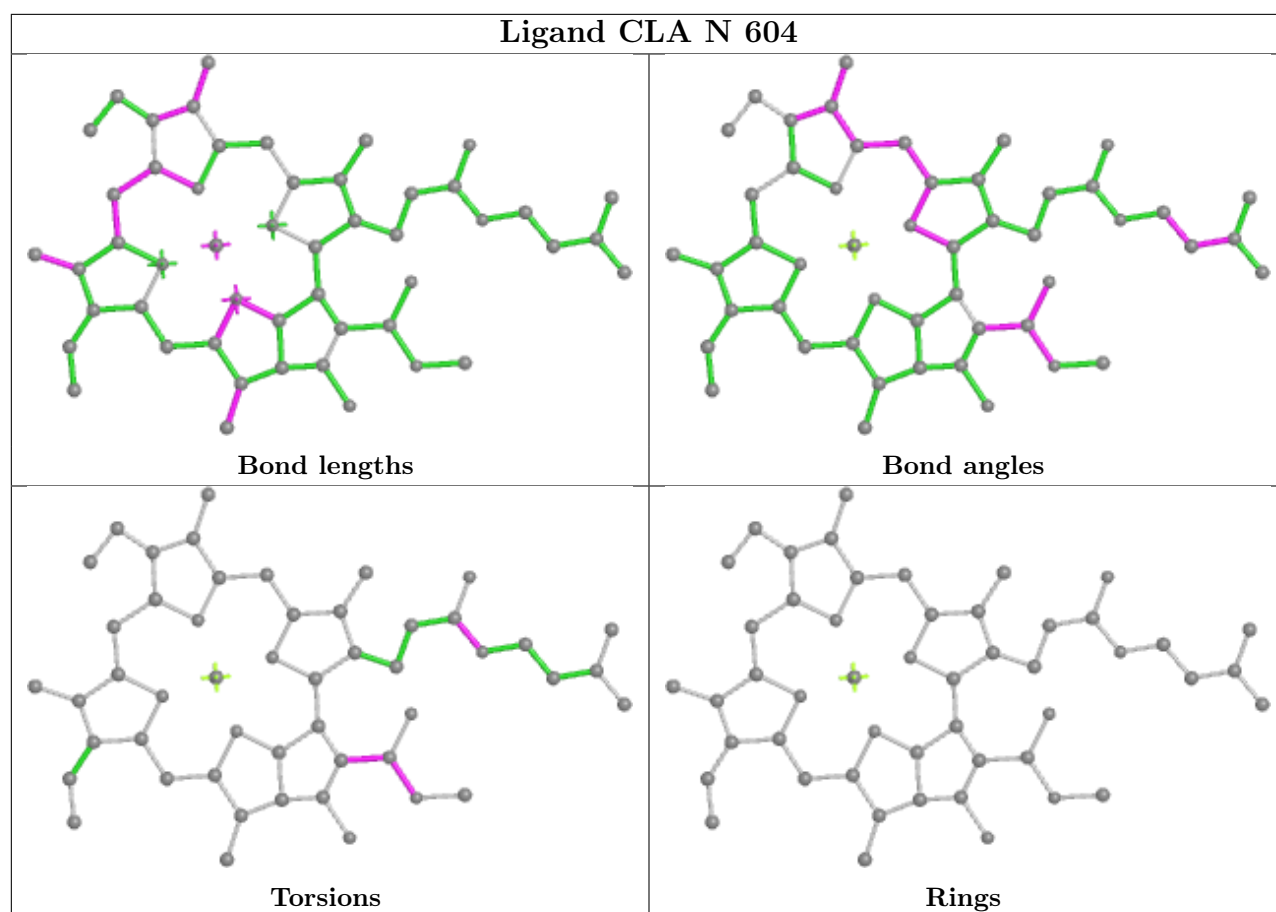
Bond angles



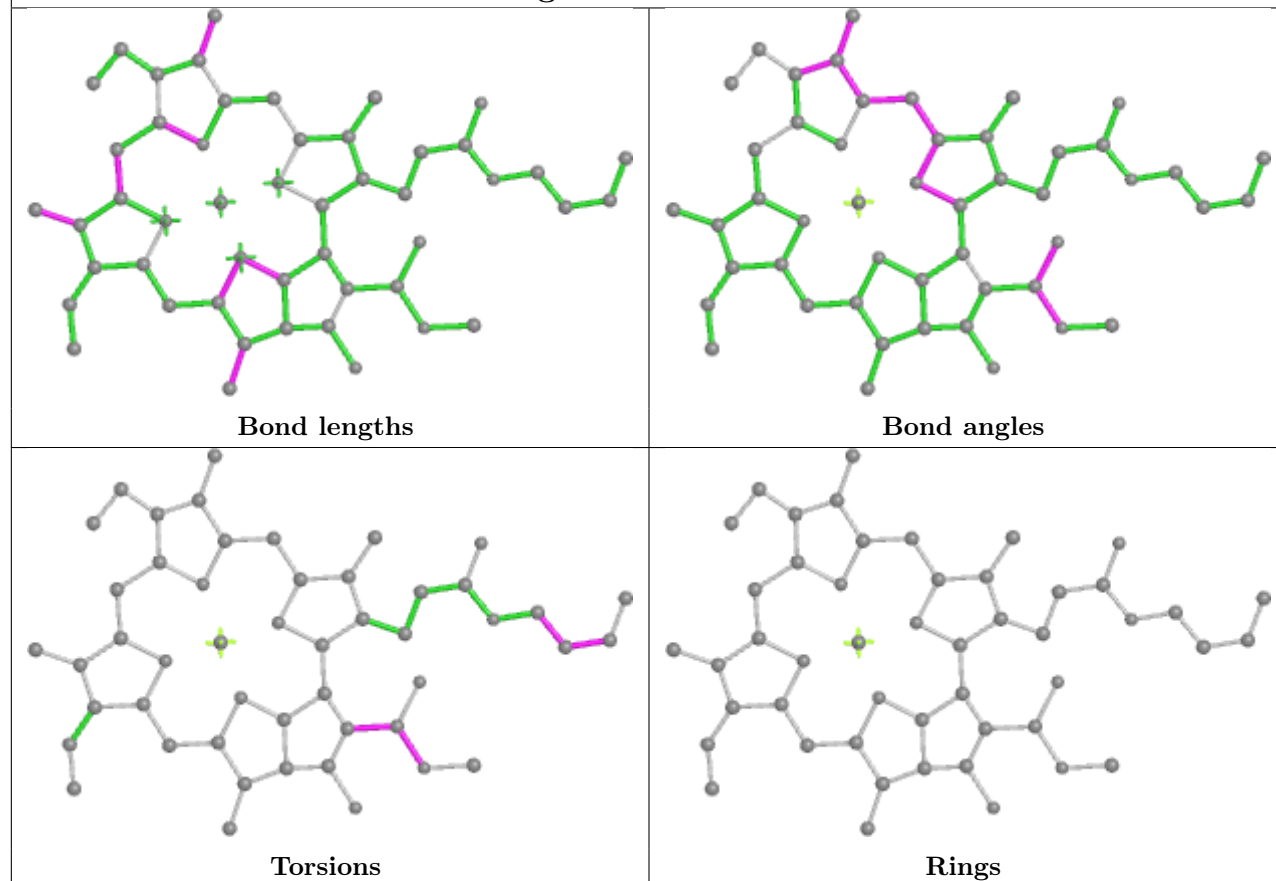
Torsions



Rings

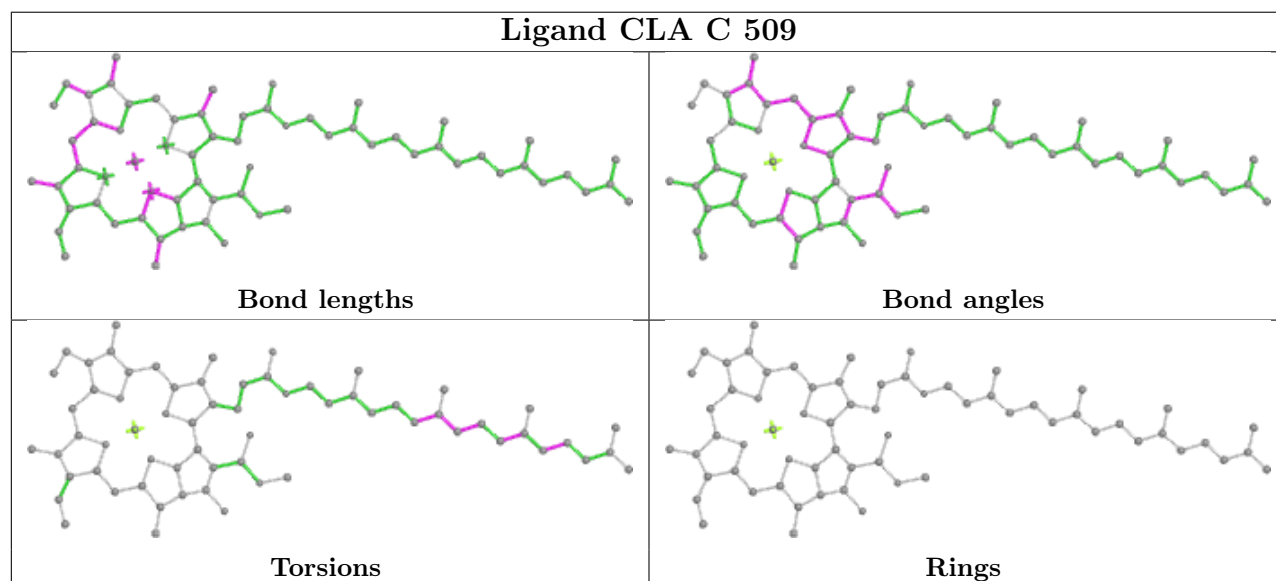
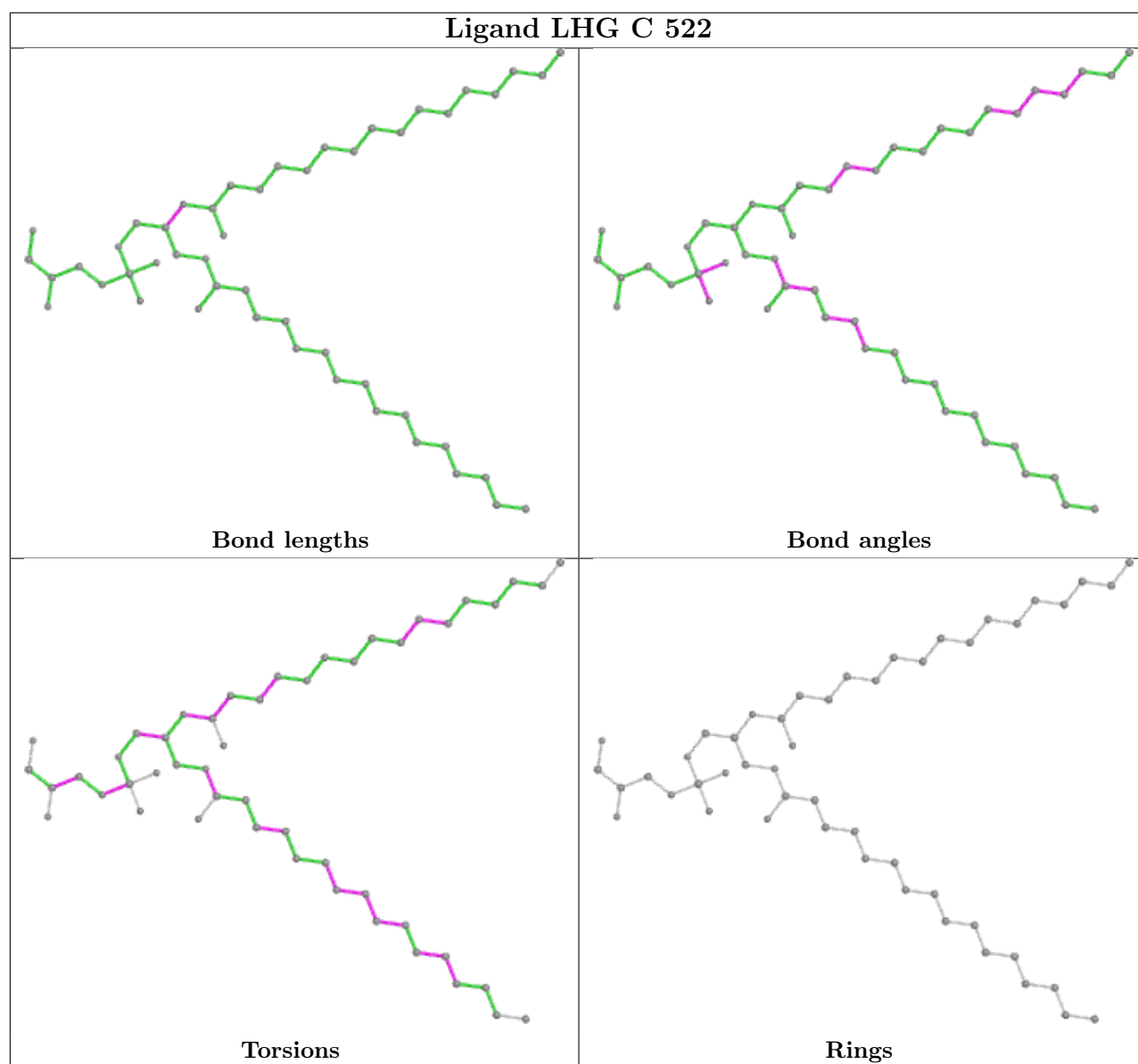


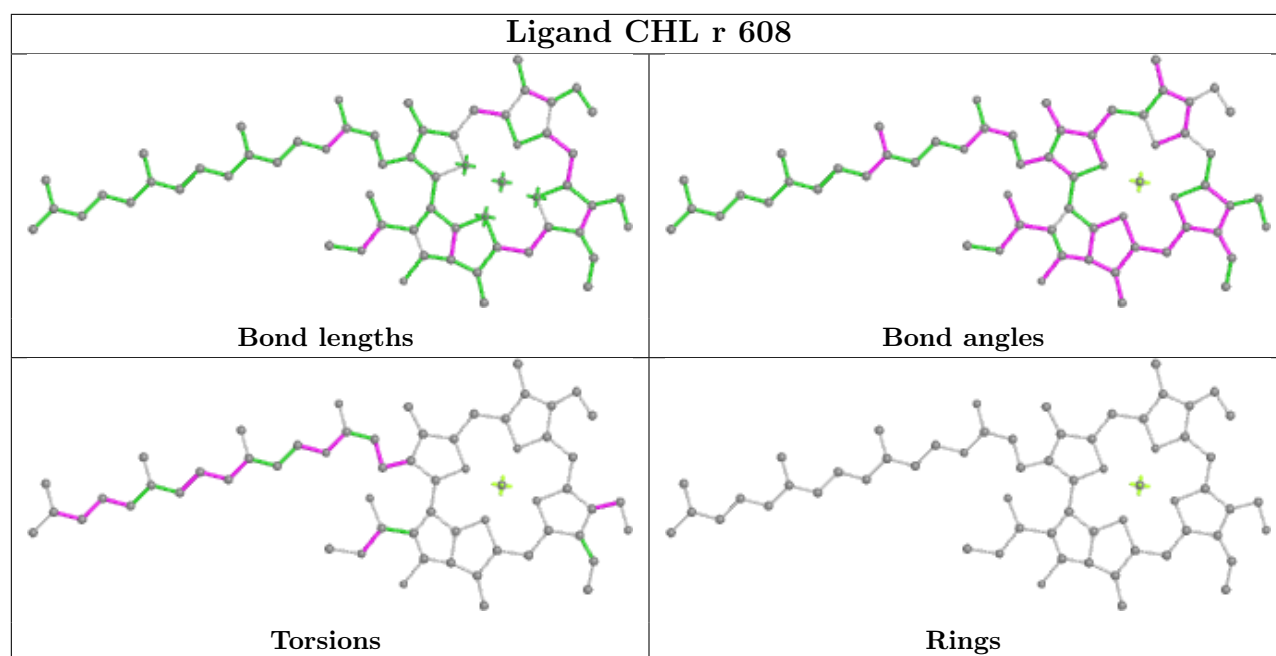
Ligand CLA s 612

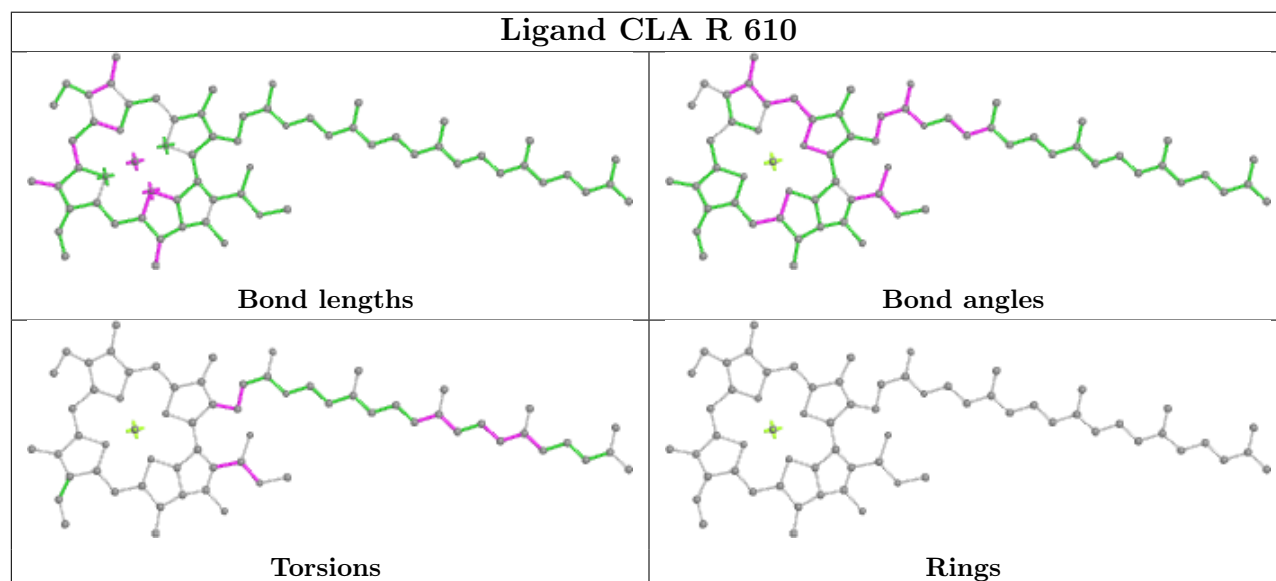
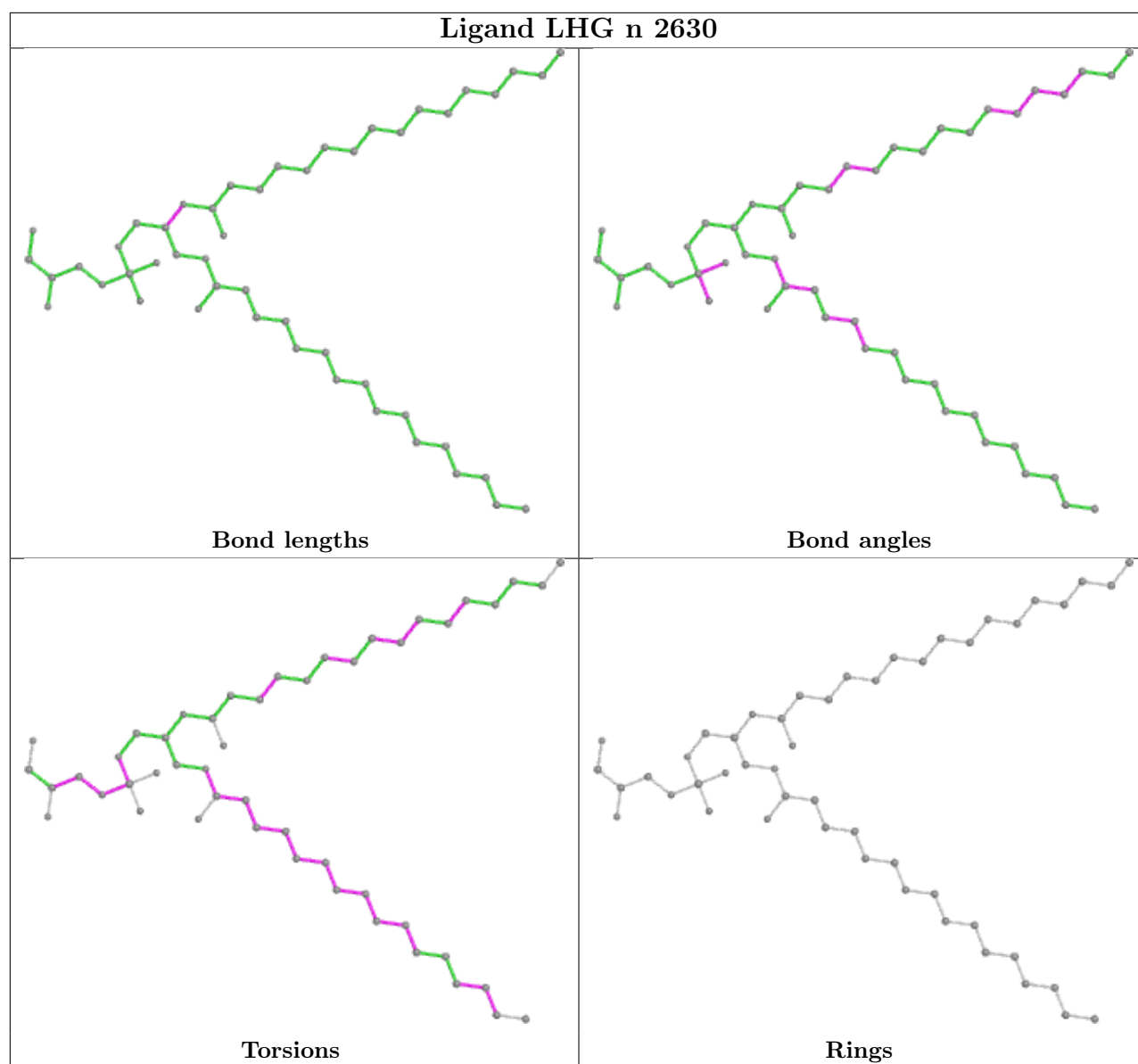


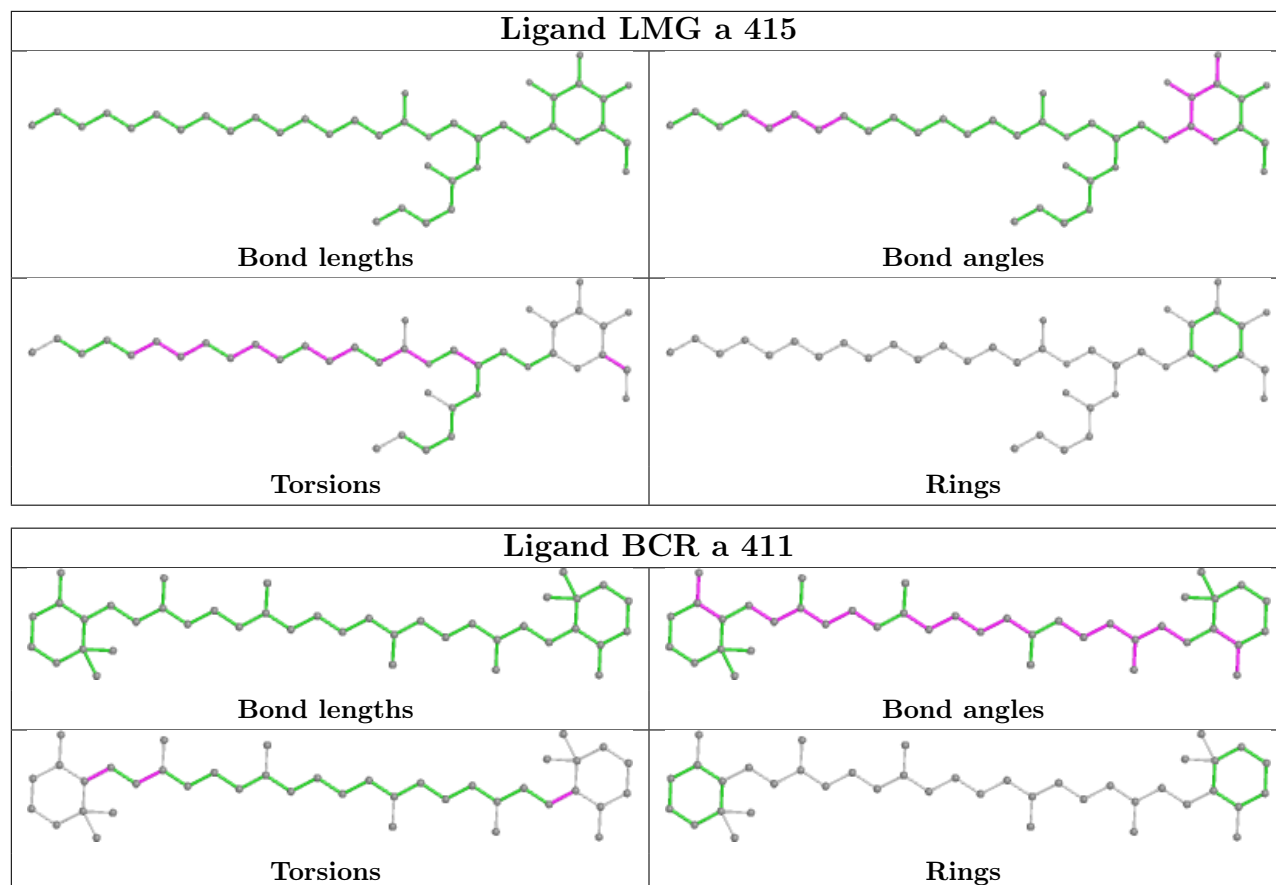
Ligand LMG A 413



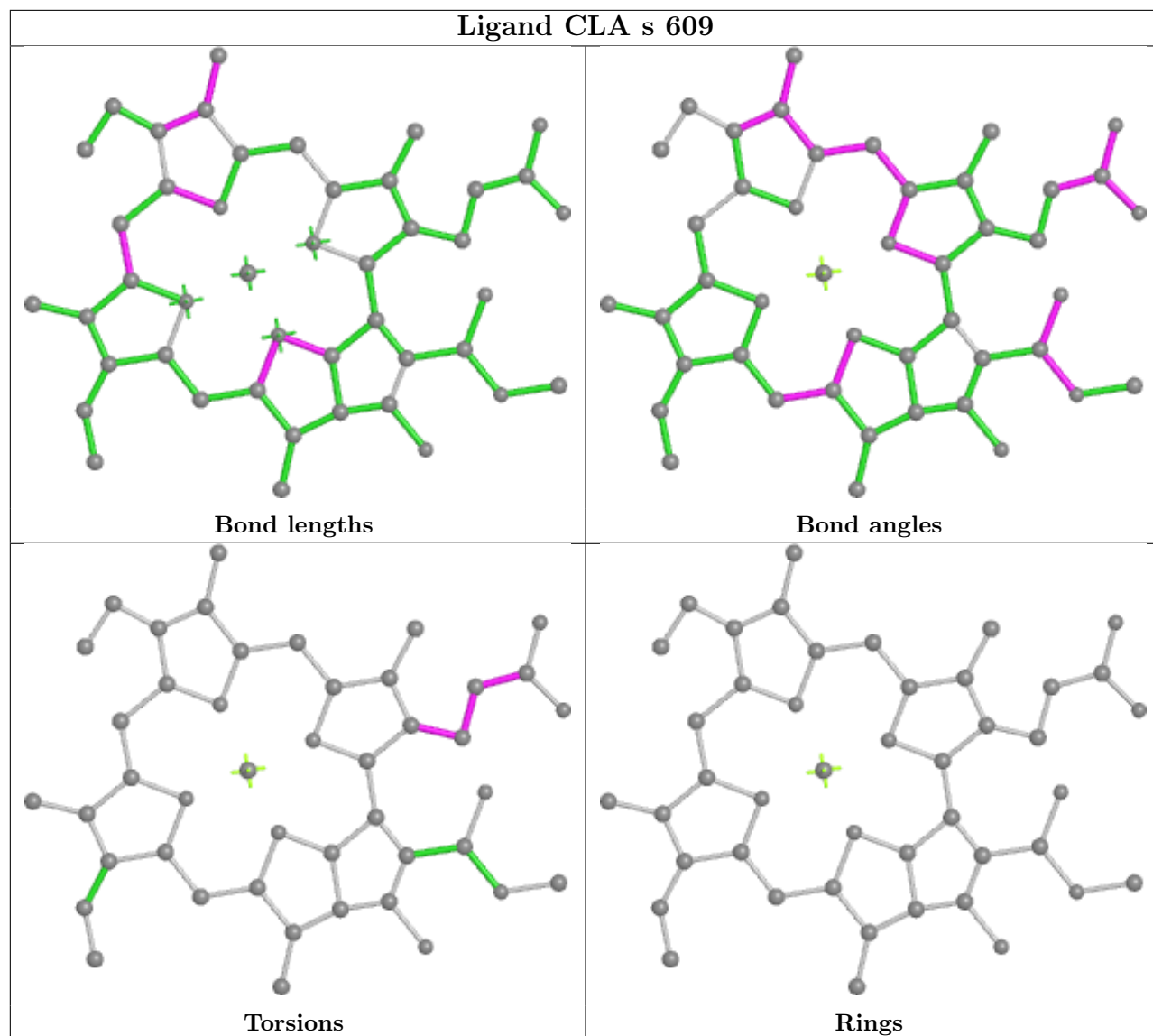


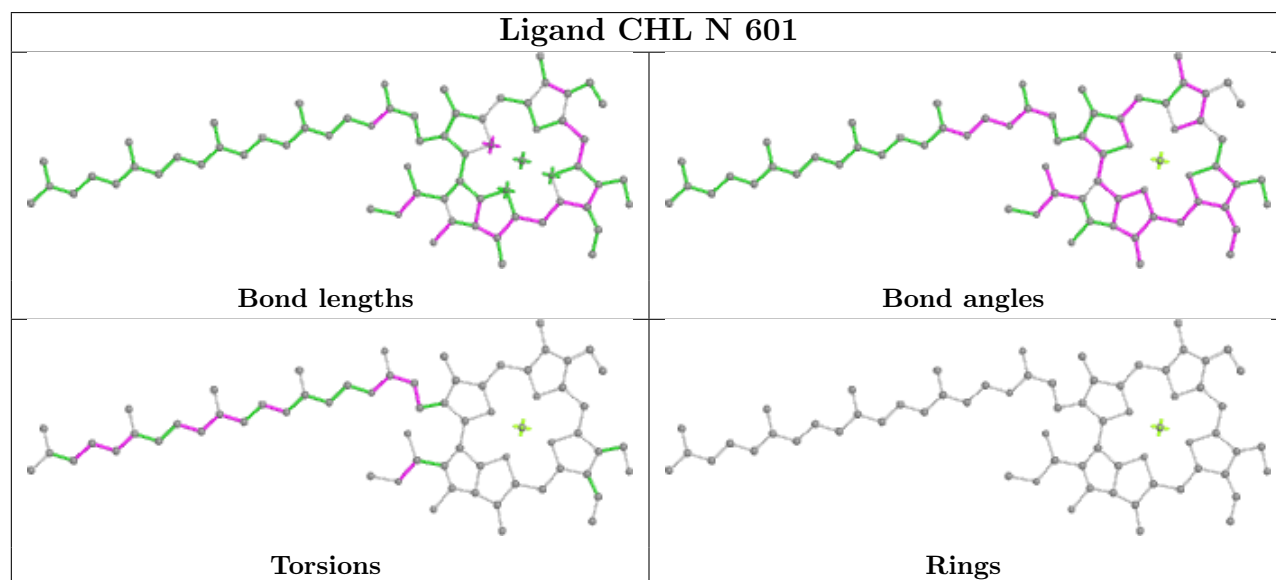
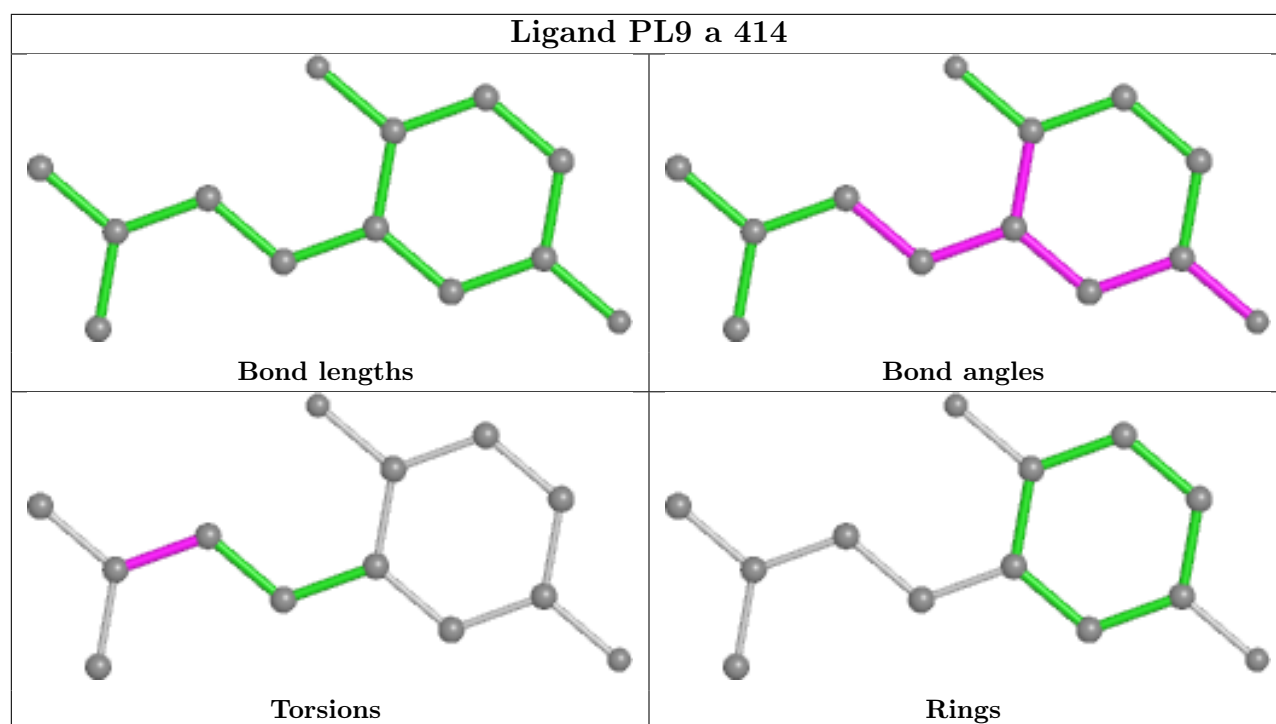


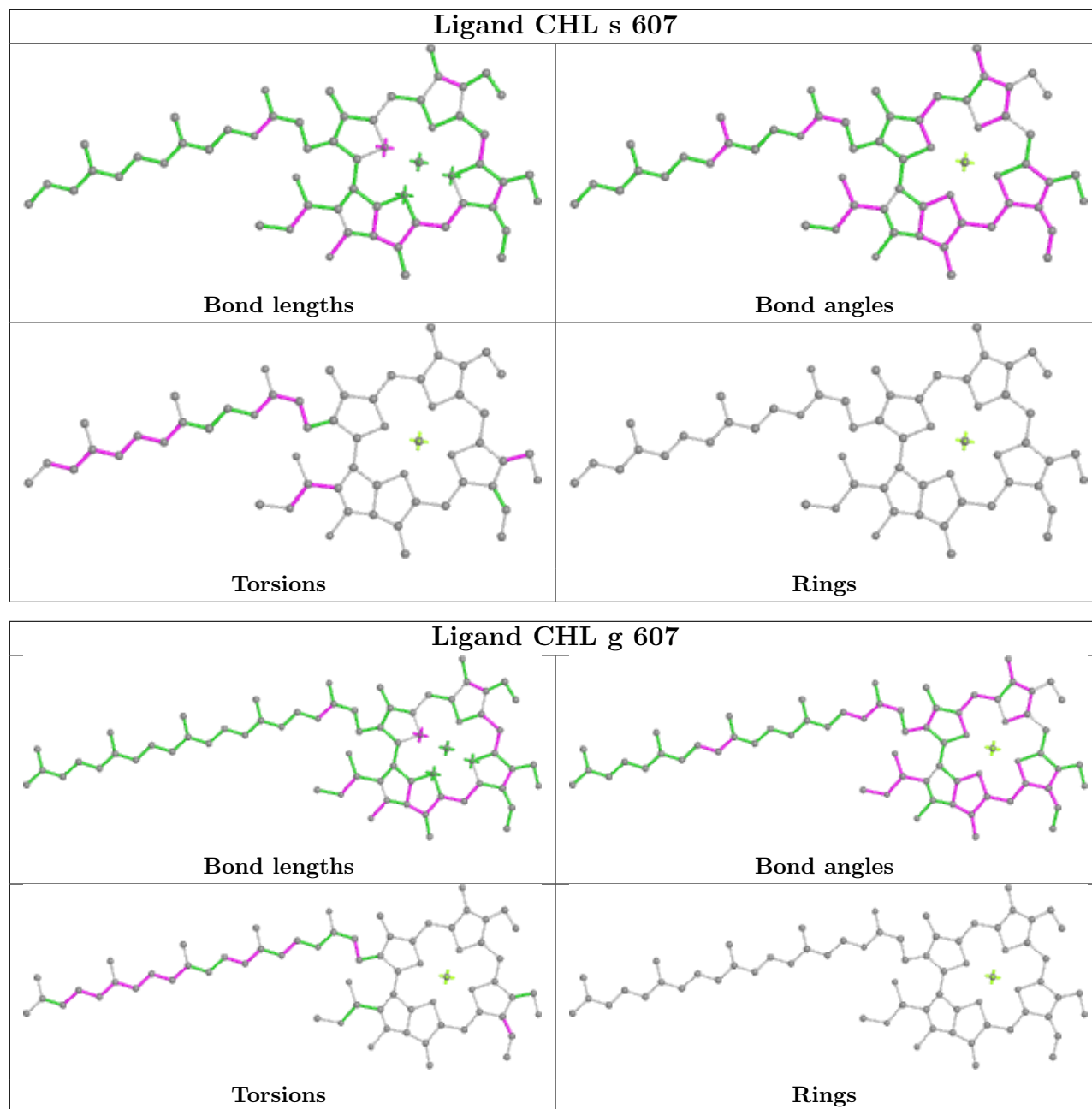


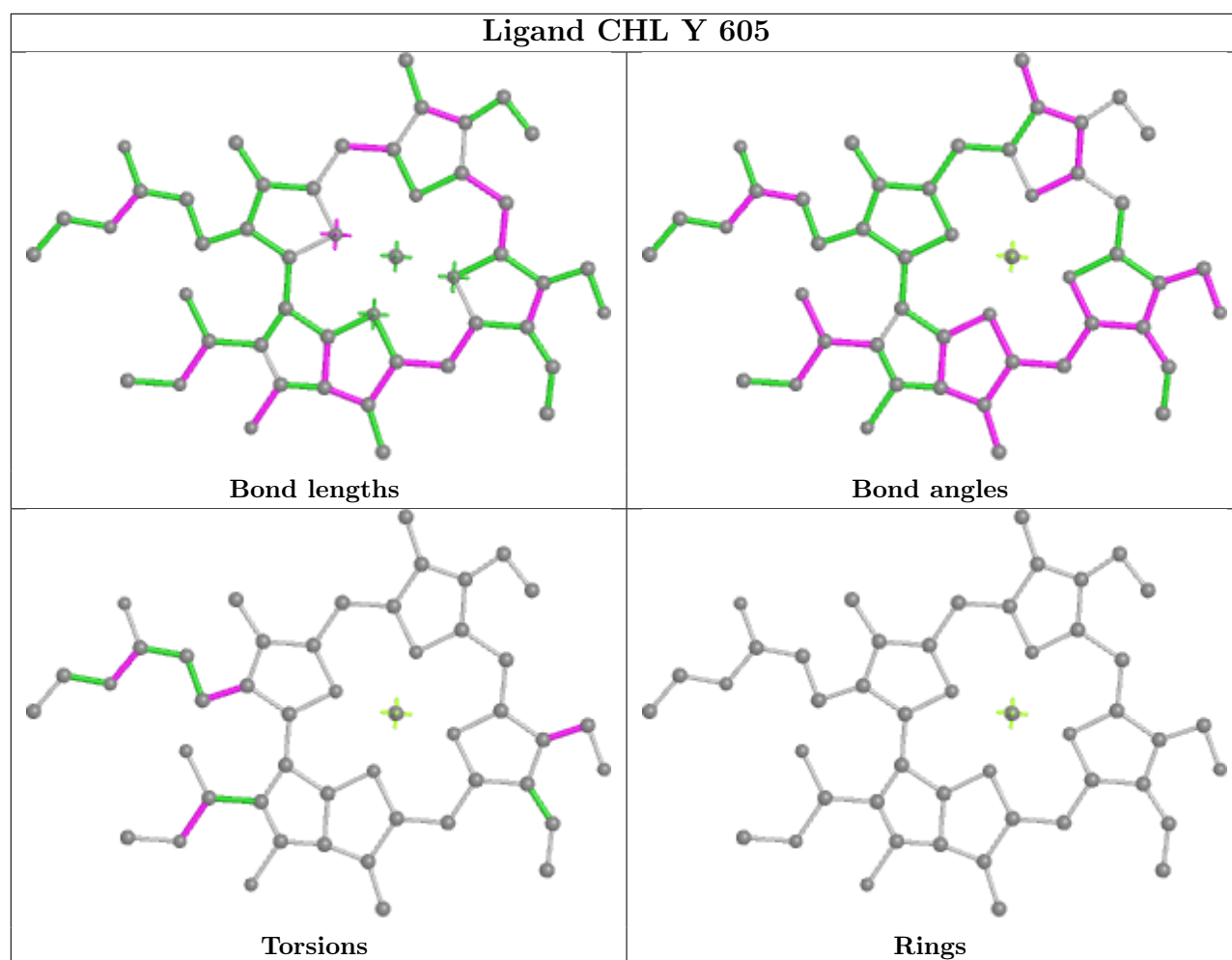


Ligand CLA s 609

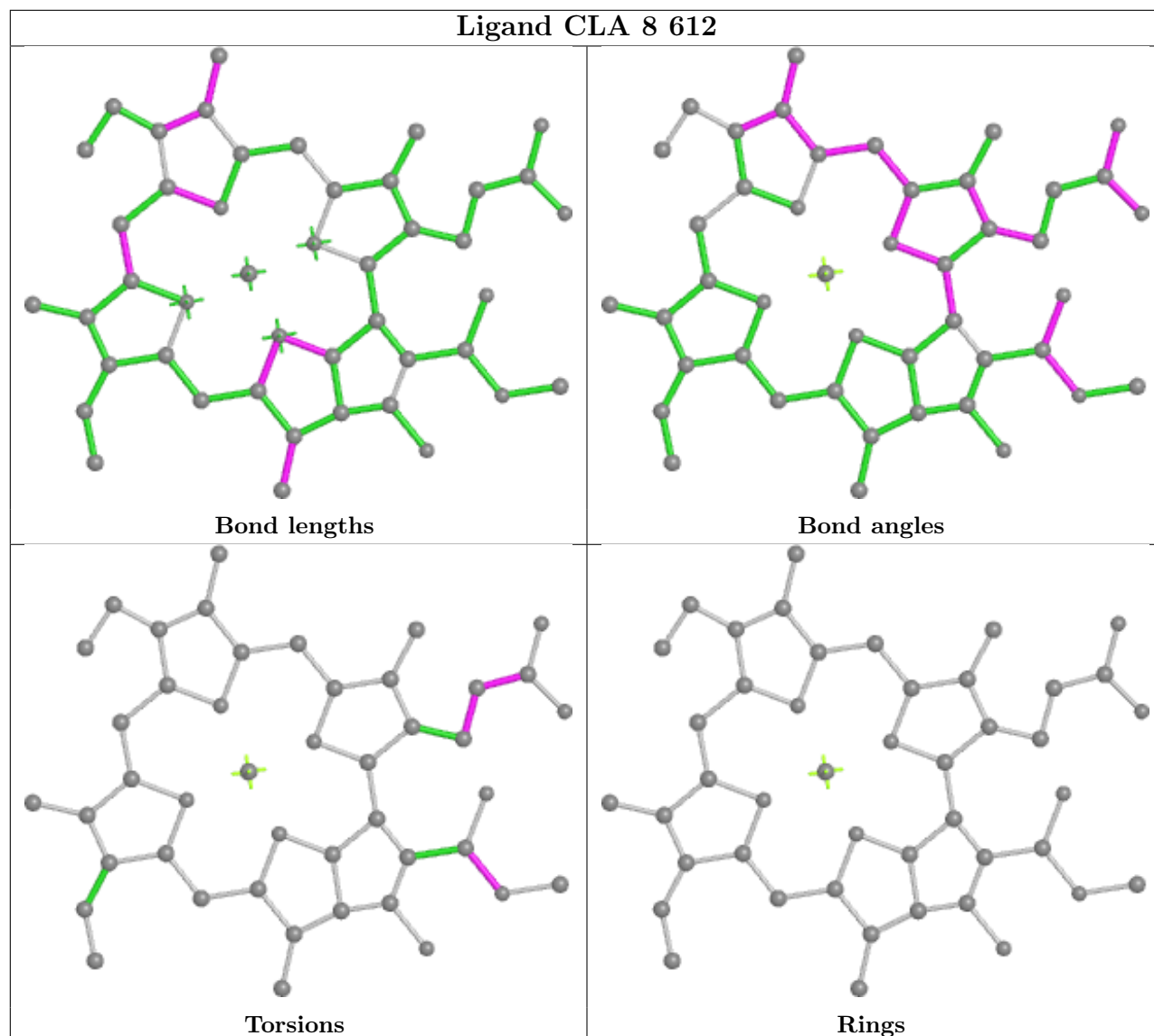


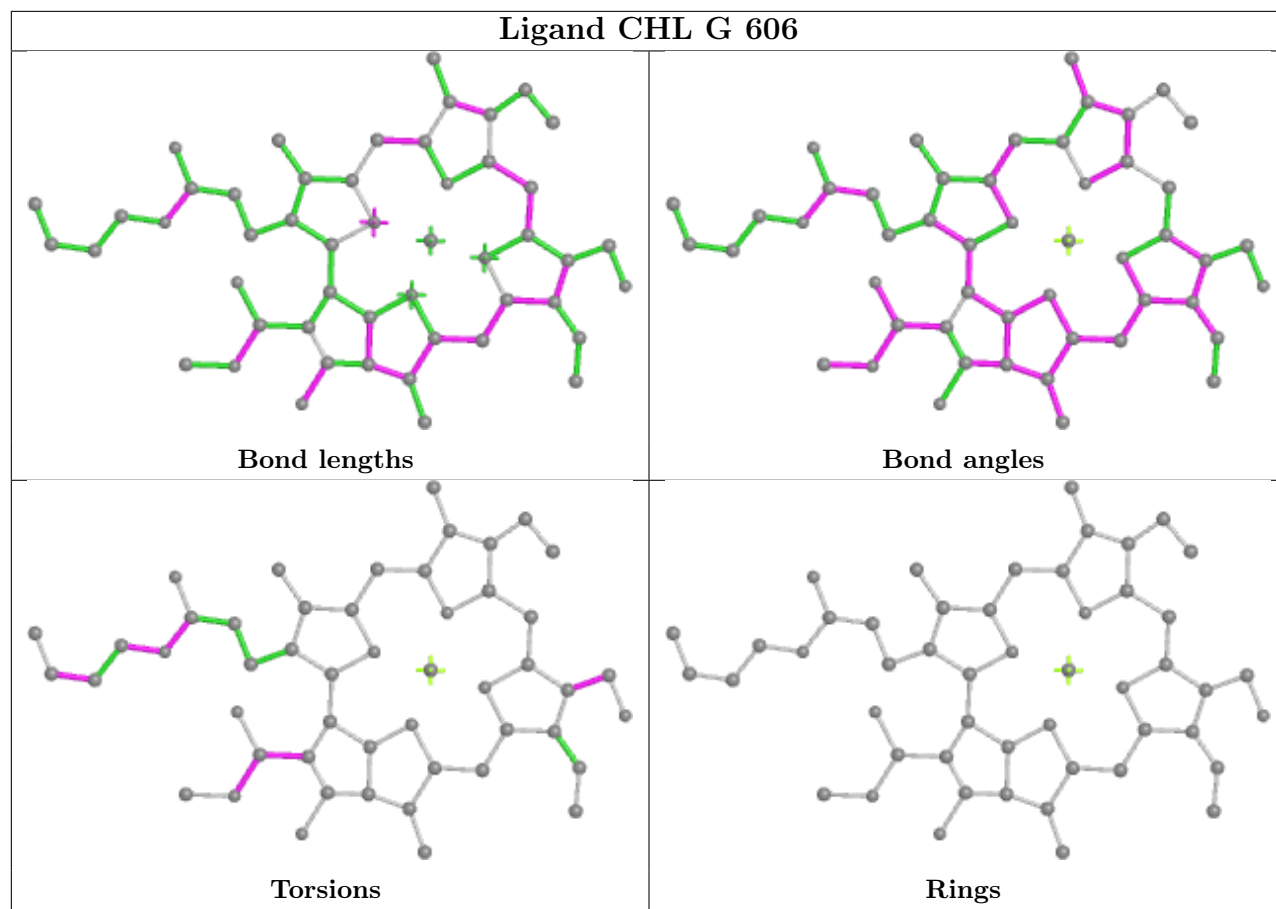




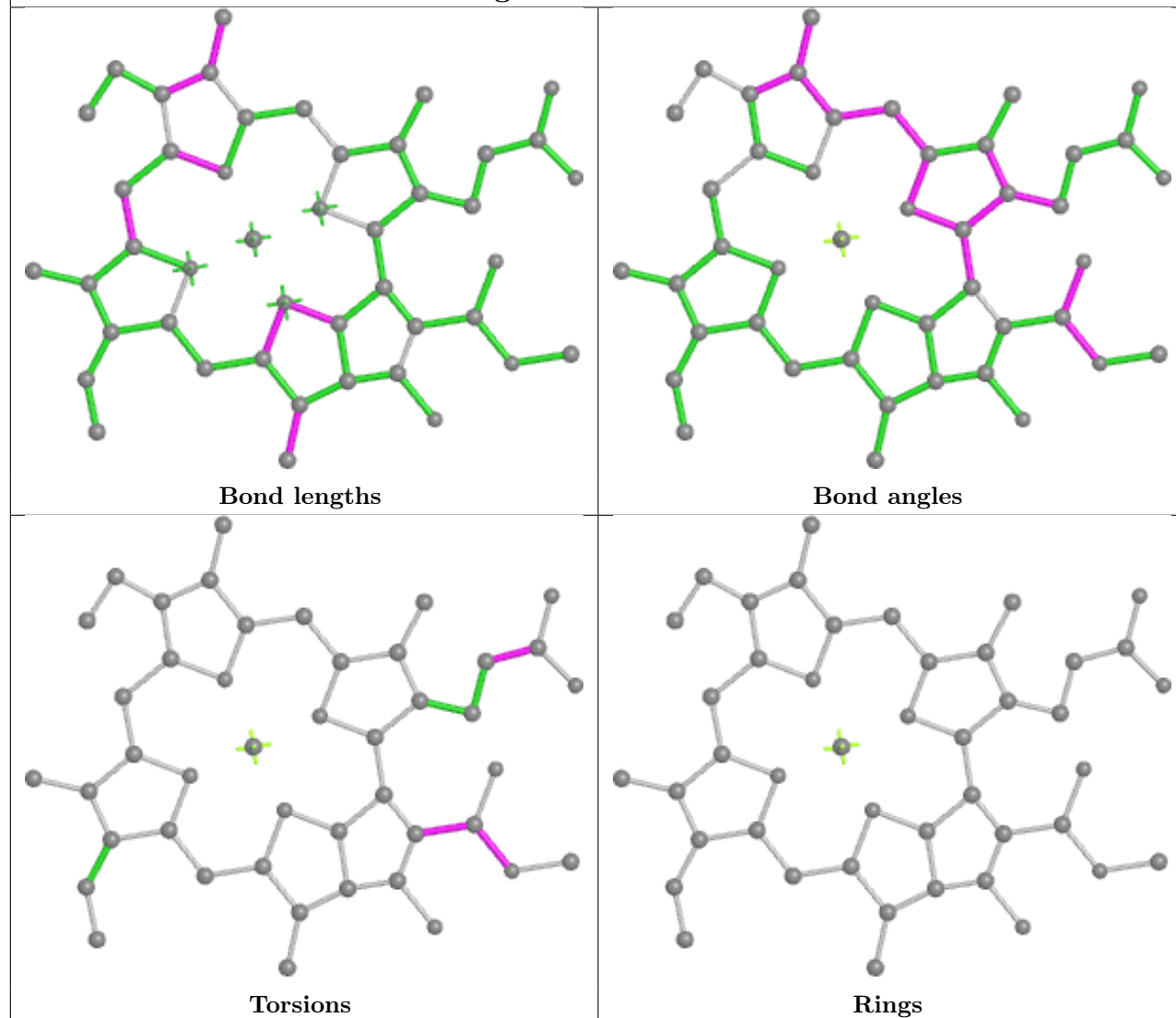


Ligand CLA 8 612

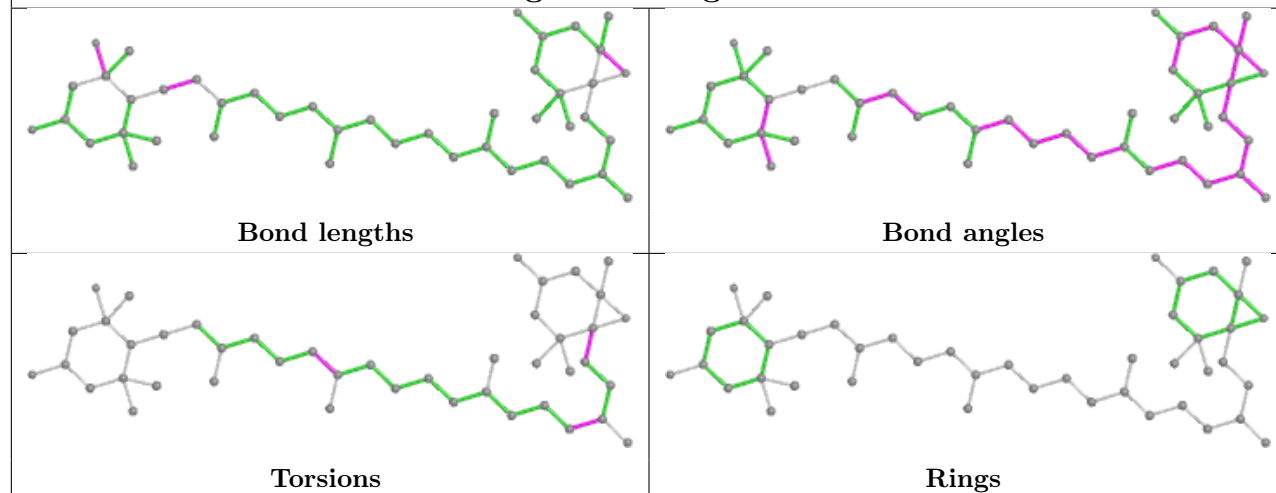


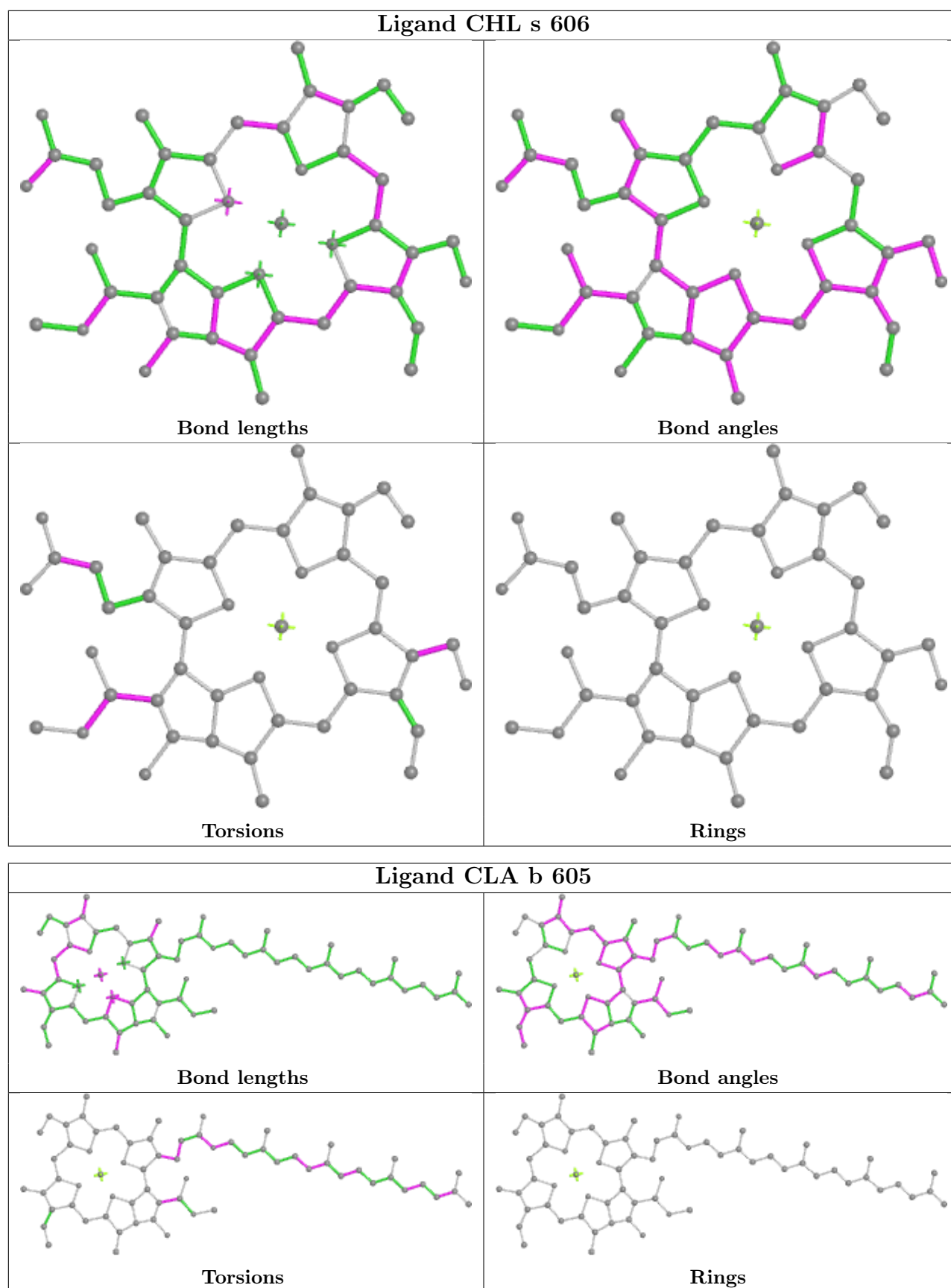


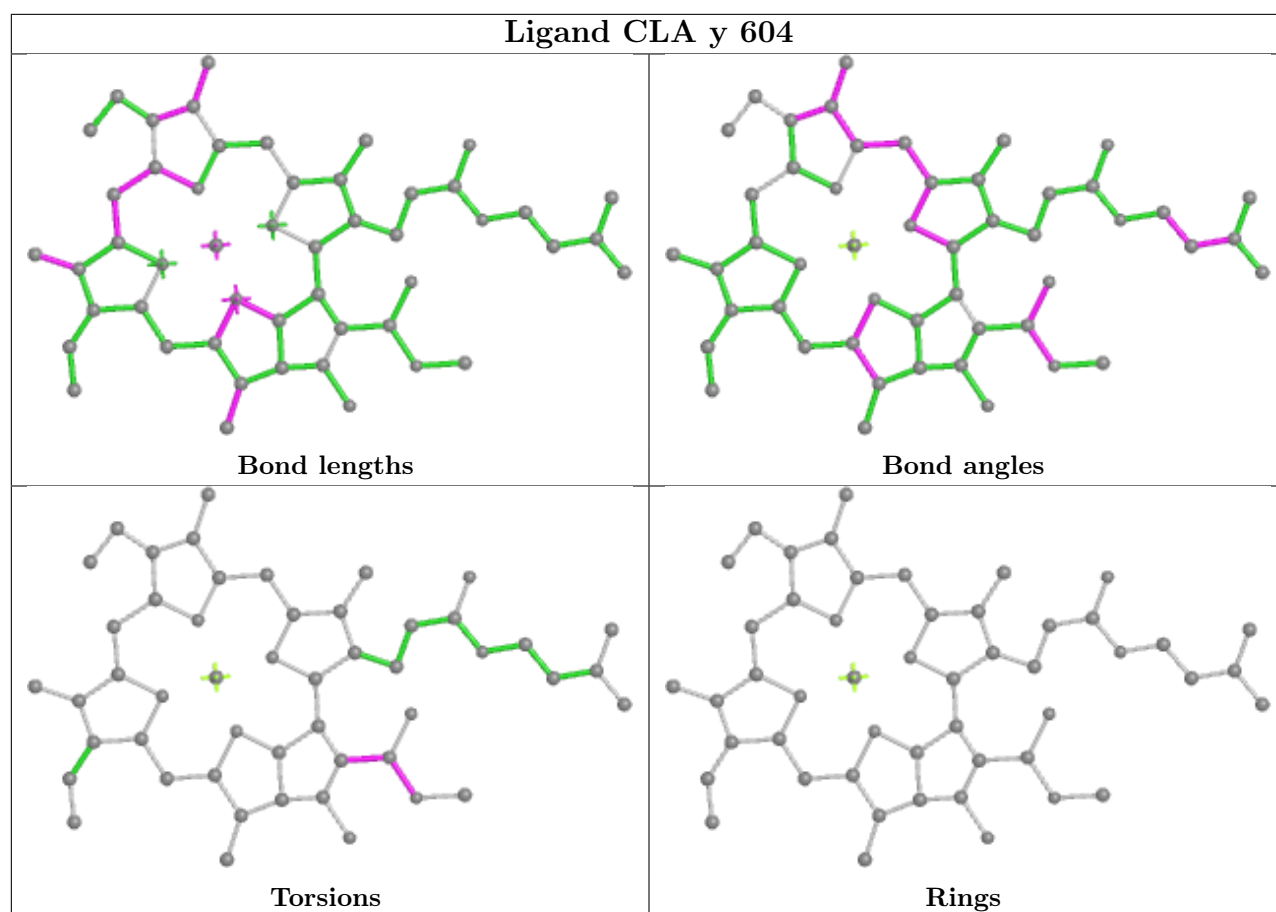
Ligand CLA 2 612



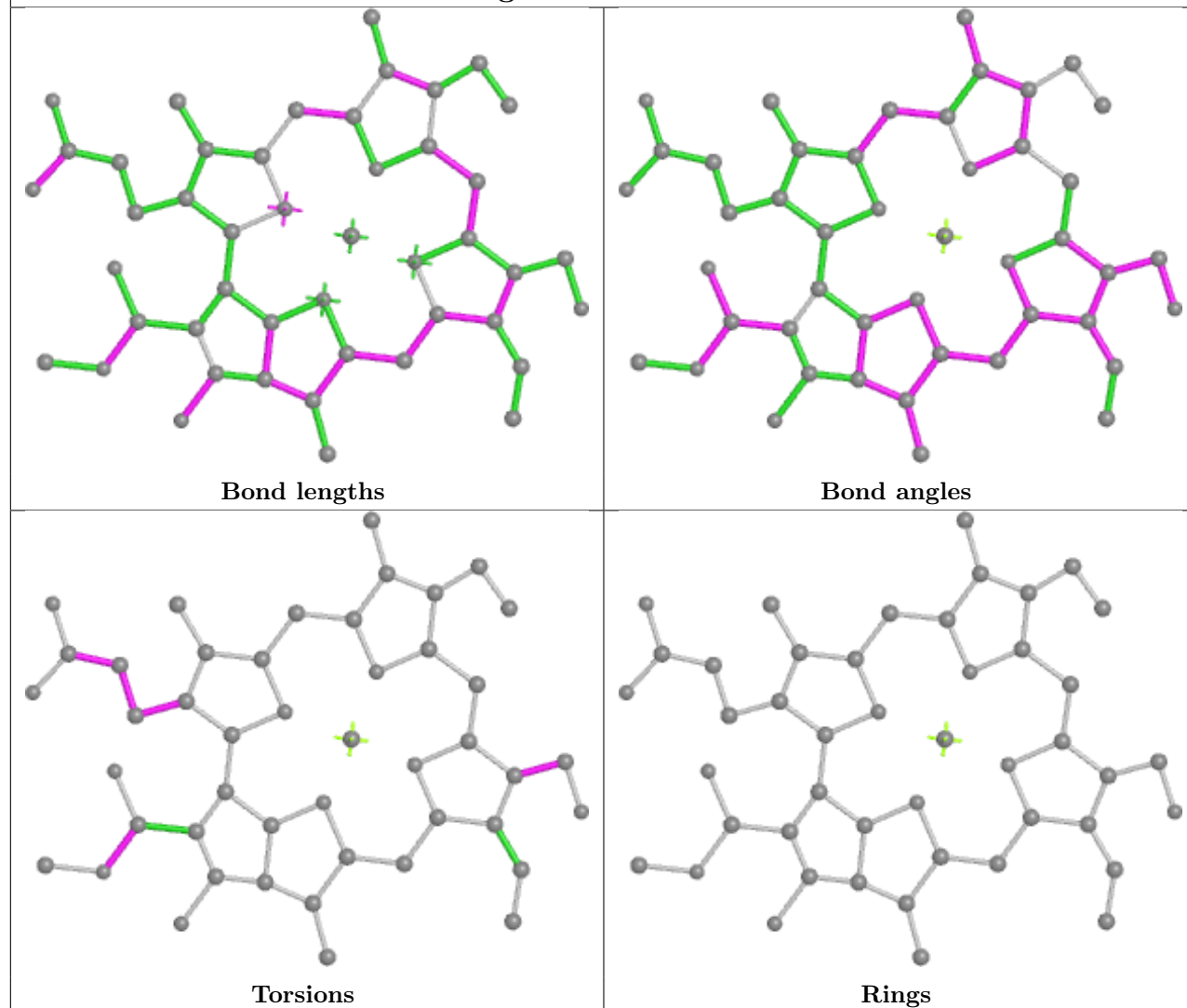
Ligand NEX g 1623



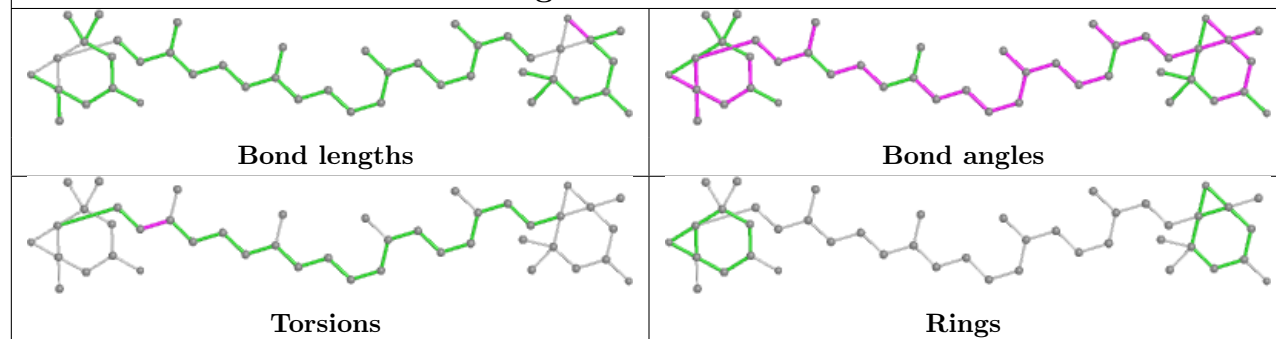




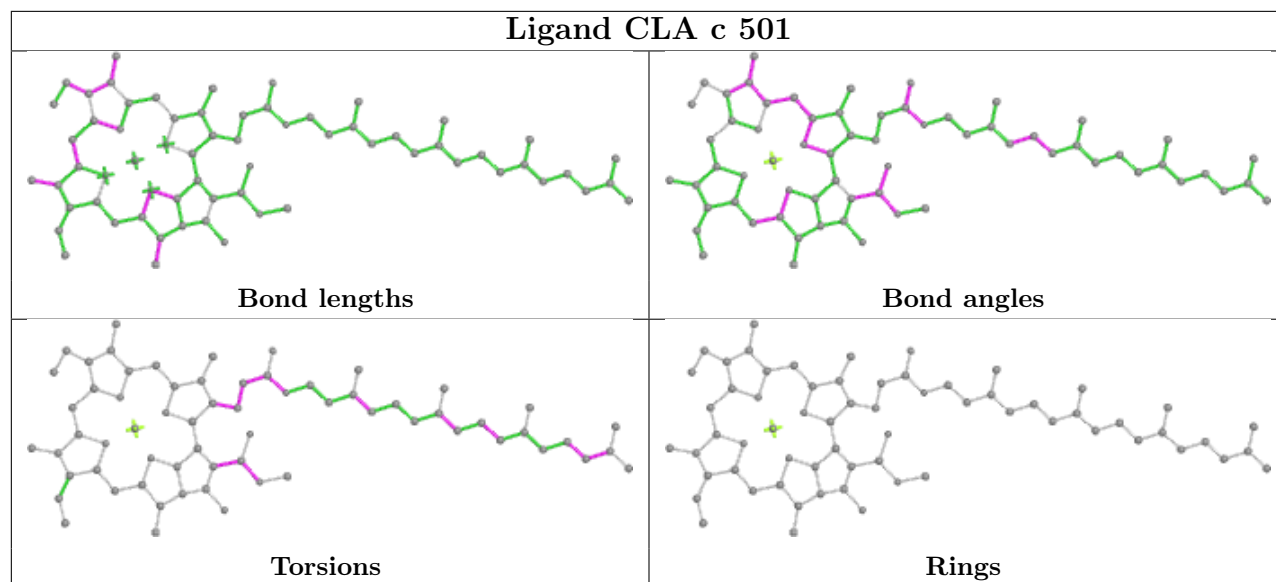
Ligand CHL 8 607



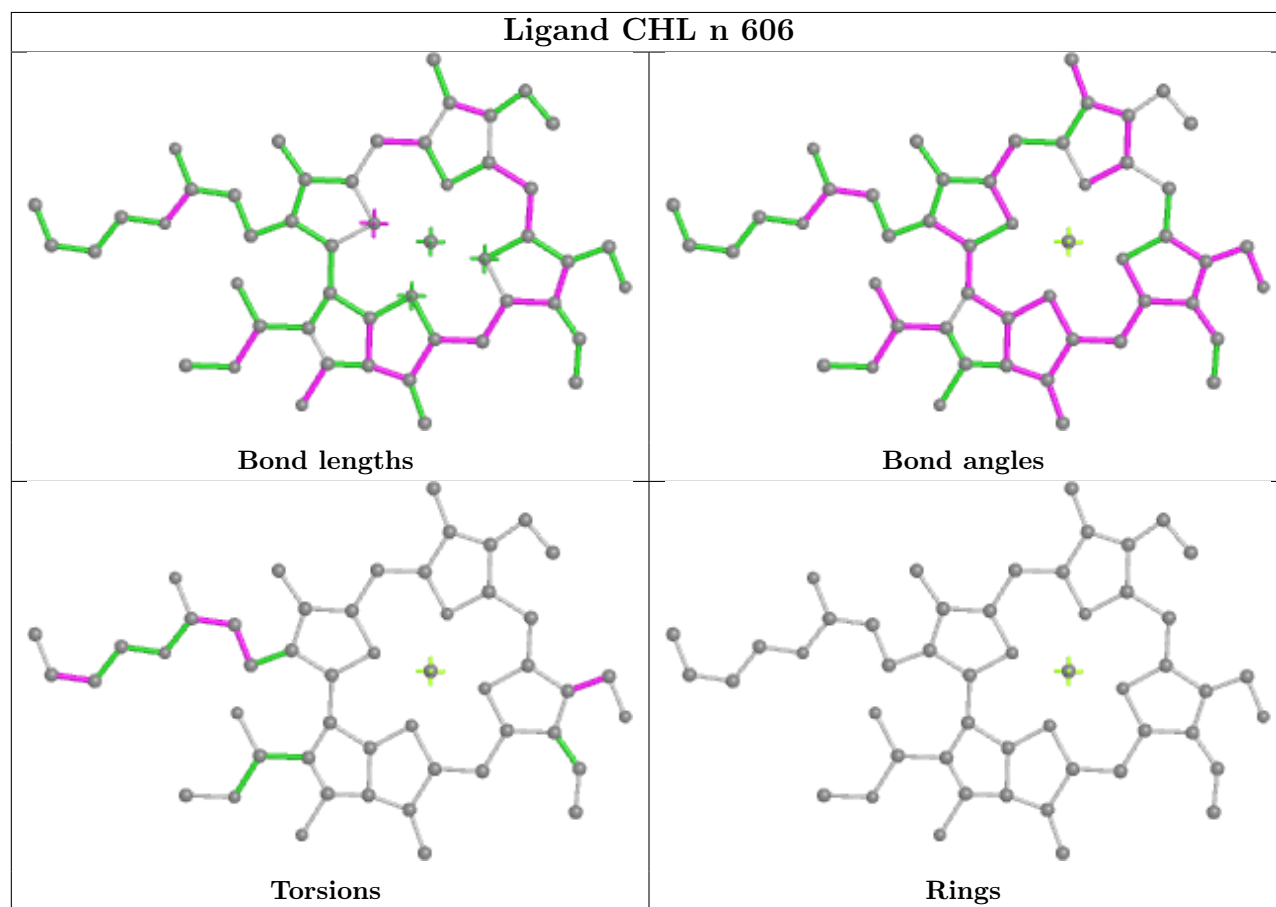
Ligand XAT 8 622

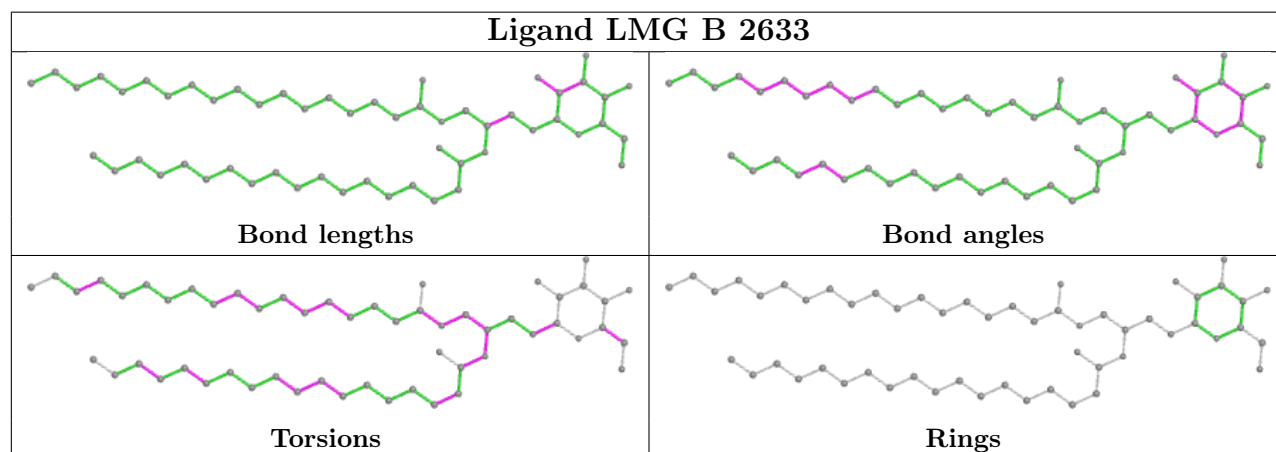
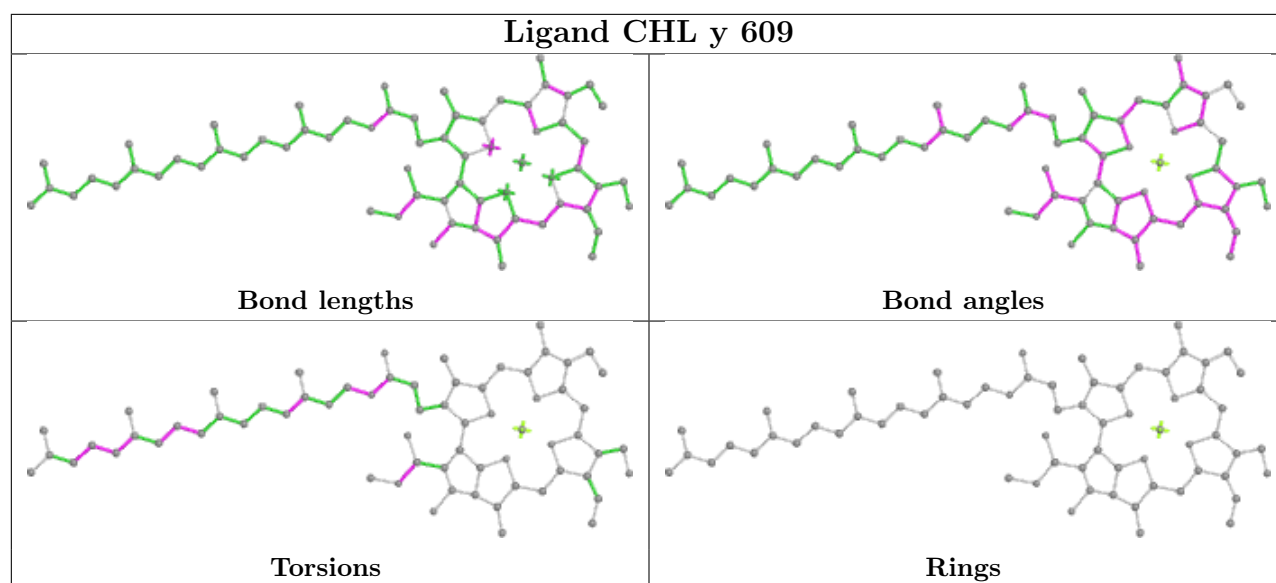


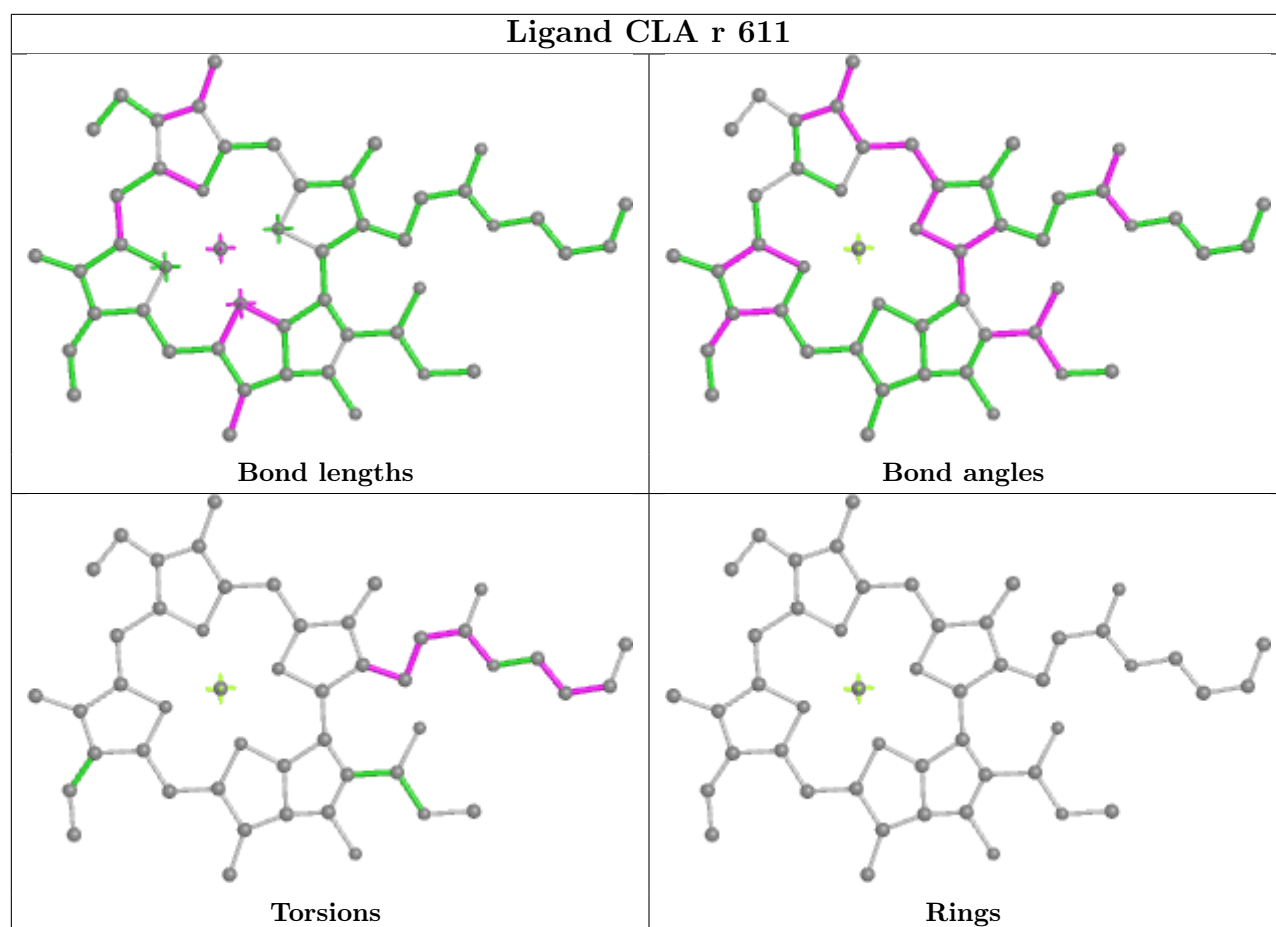
Ligand CLA c 501



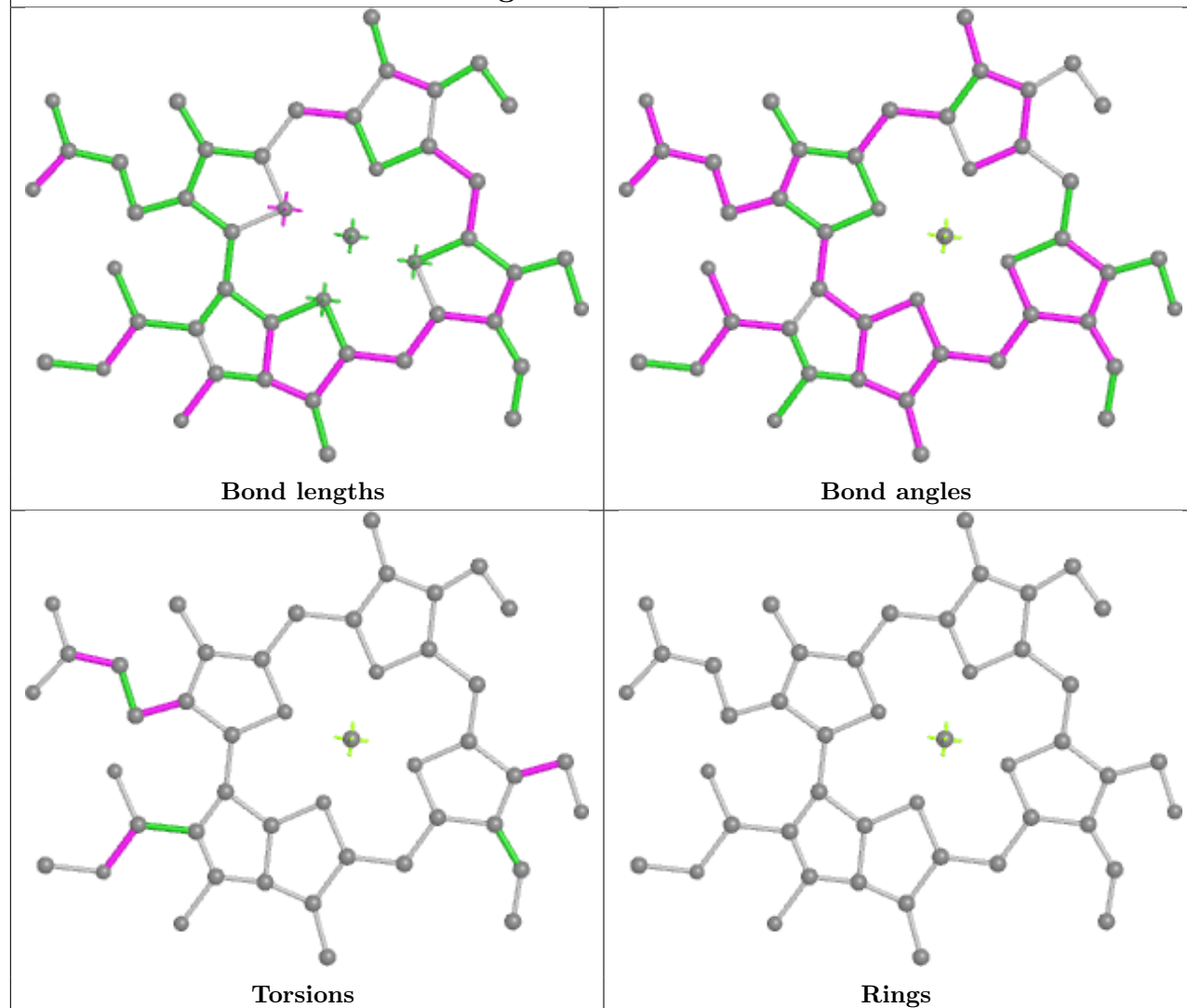
Ligand CHL n 606



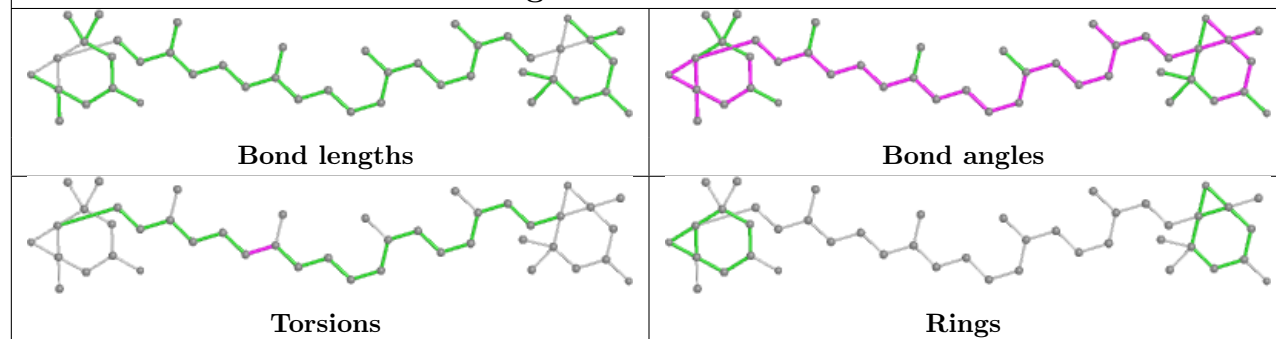


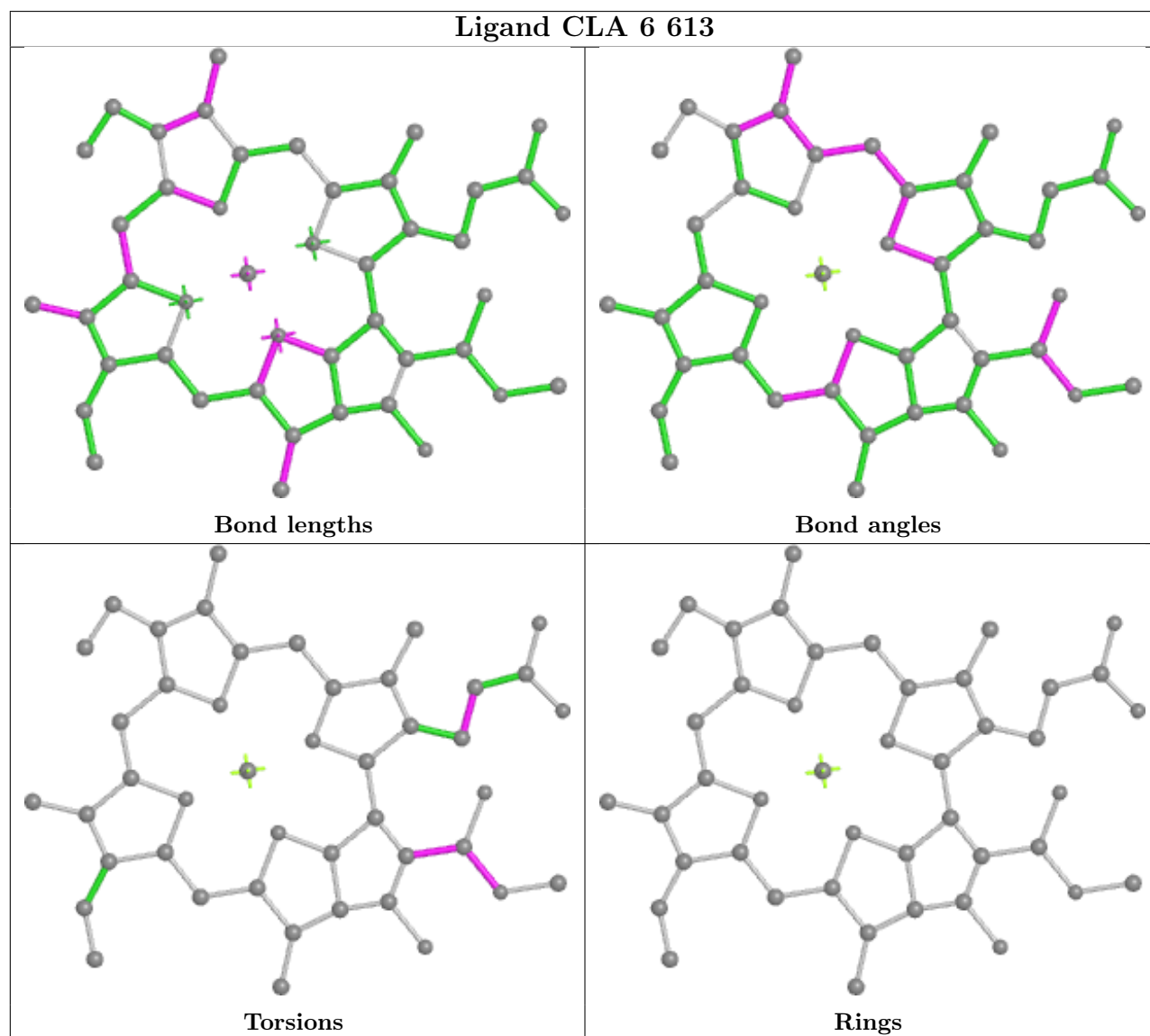
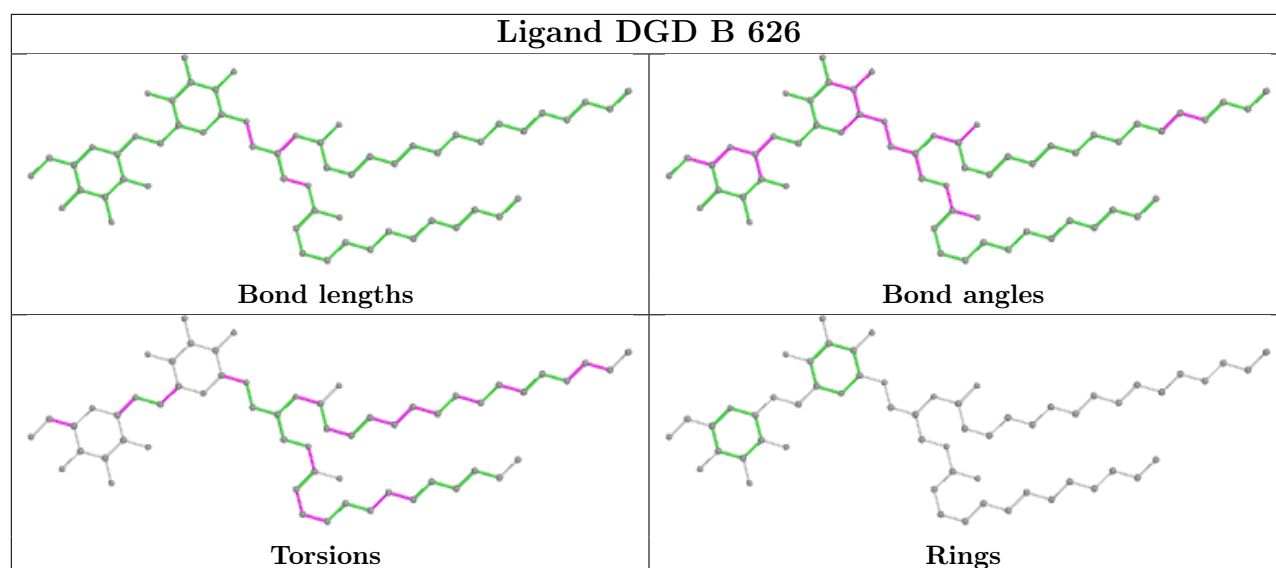


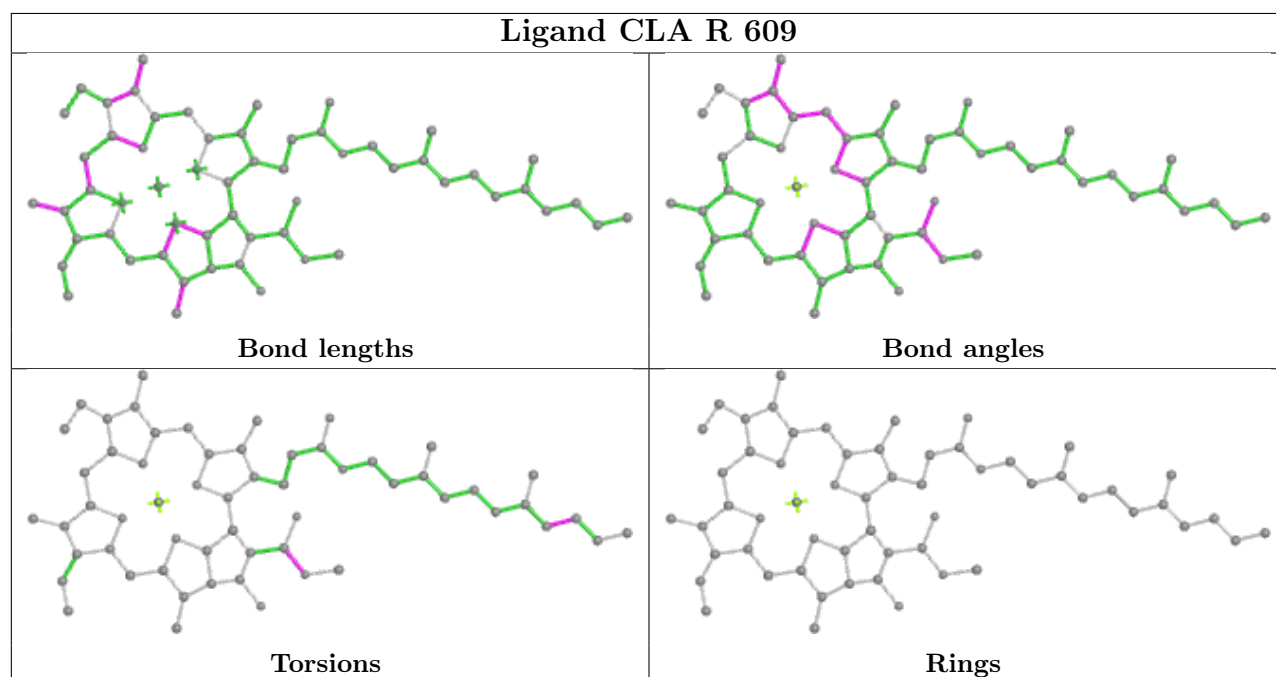
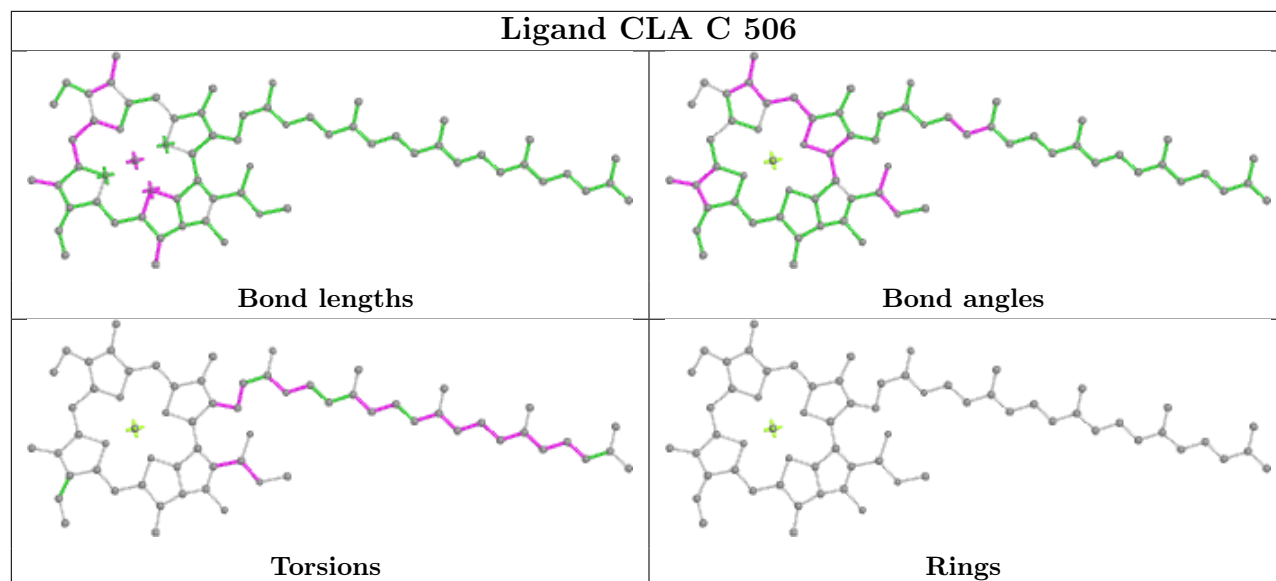
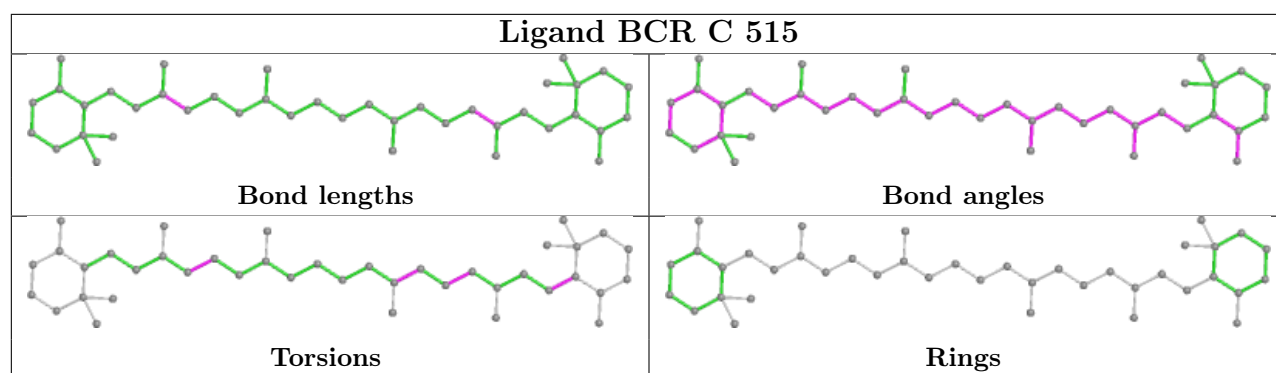
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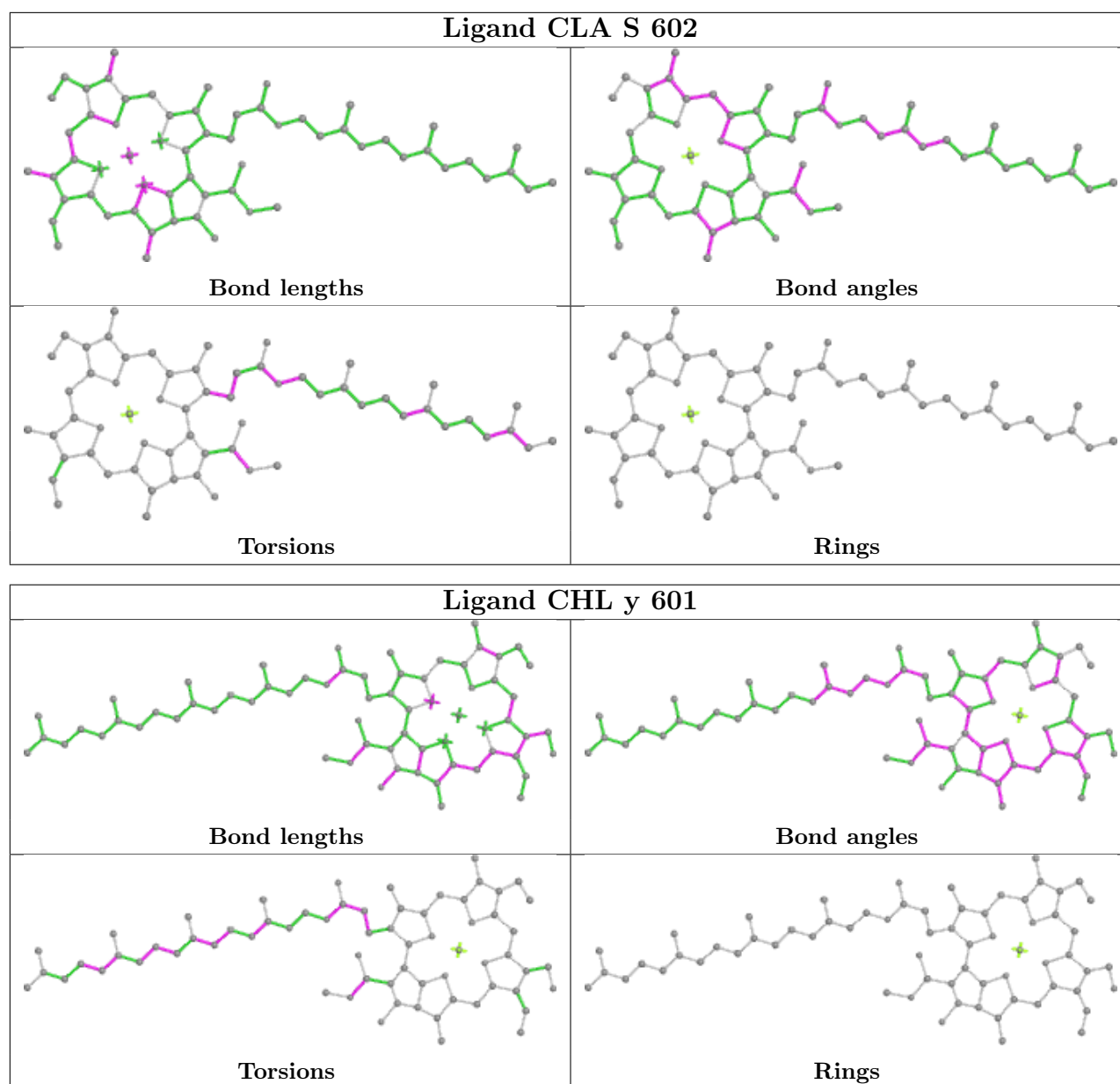


Ligand XAT 5 1622

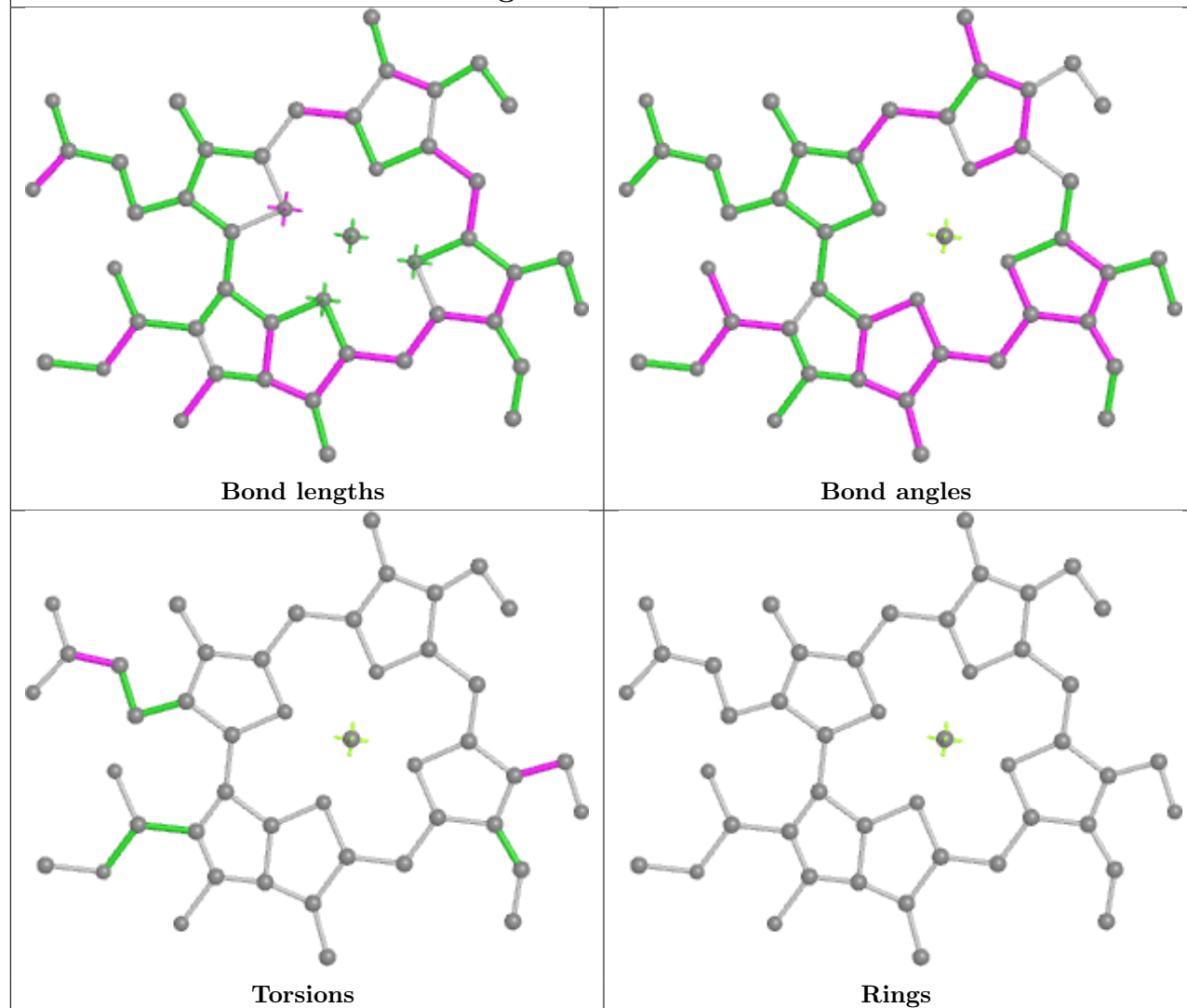




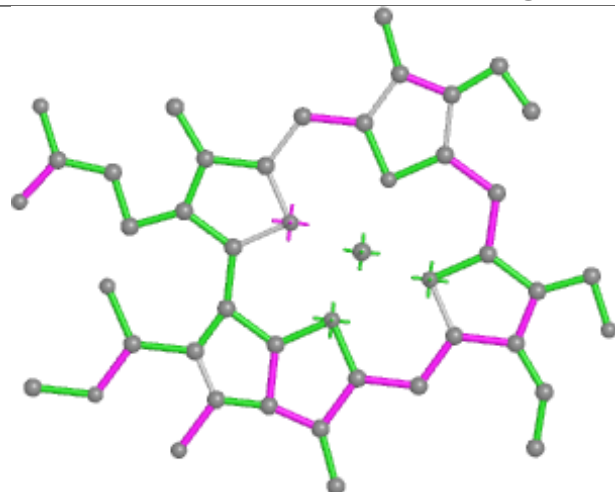




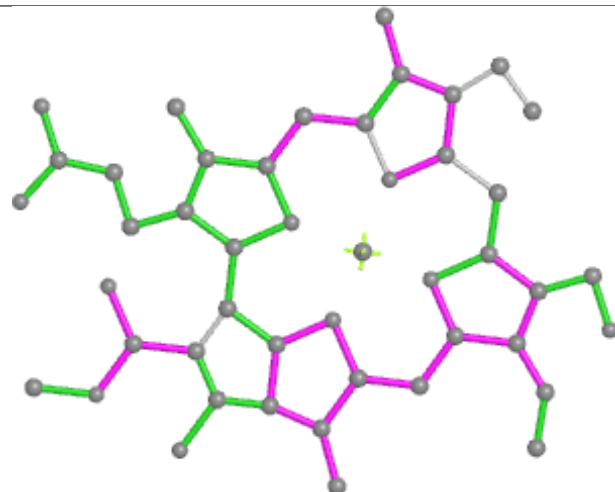
Ligand CHL 4 609



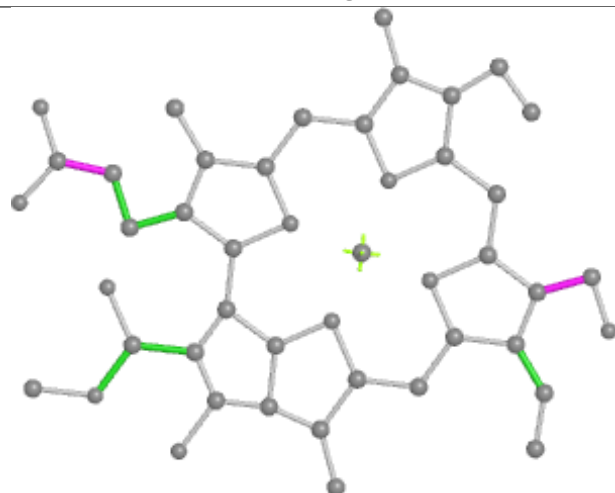
Ligand CHL 8 609



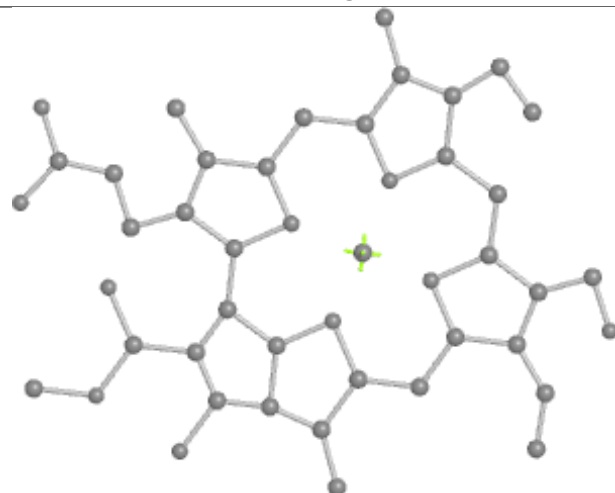
Bond lengths



Bond angles

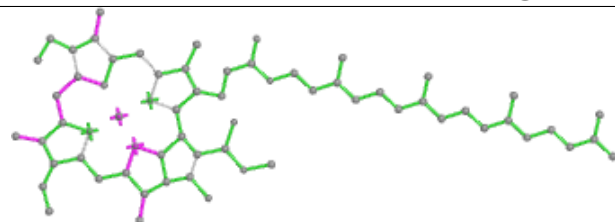


Torsions

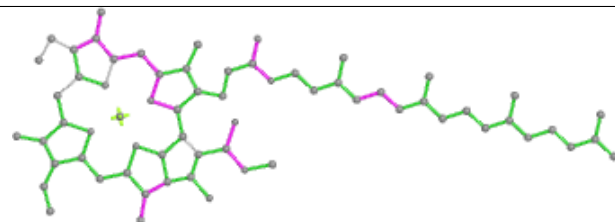


Rings

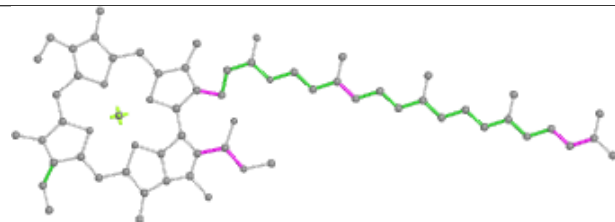
Ligand CLA B 610



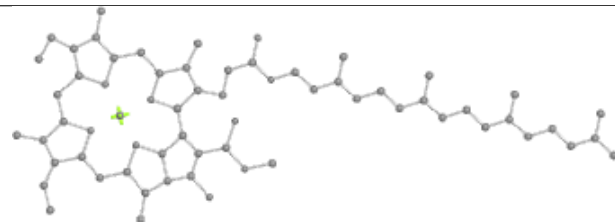
Bond lengths



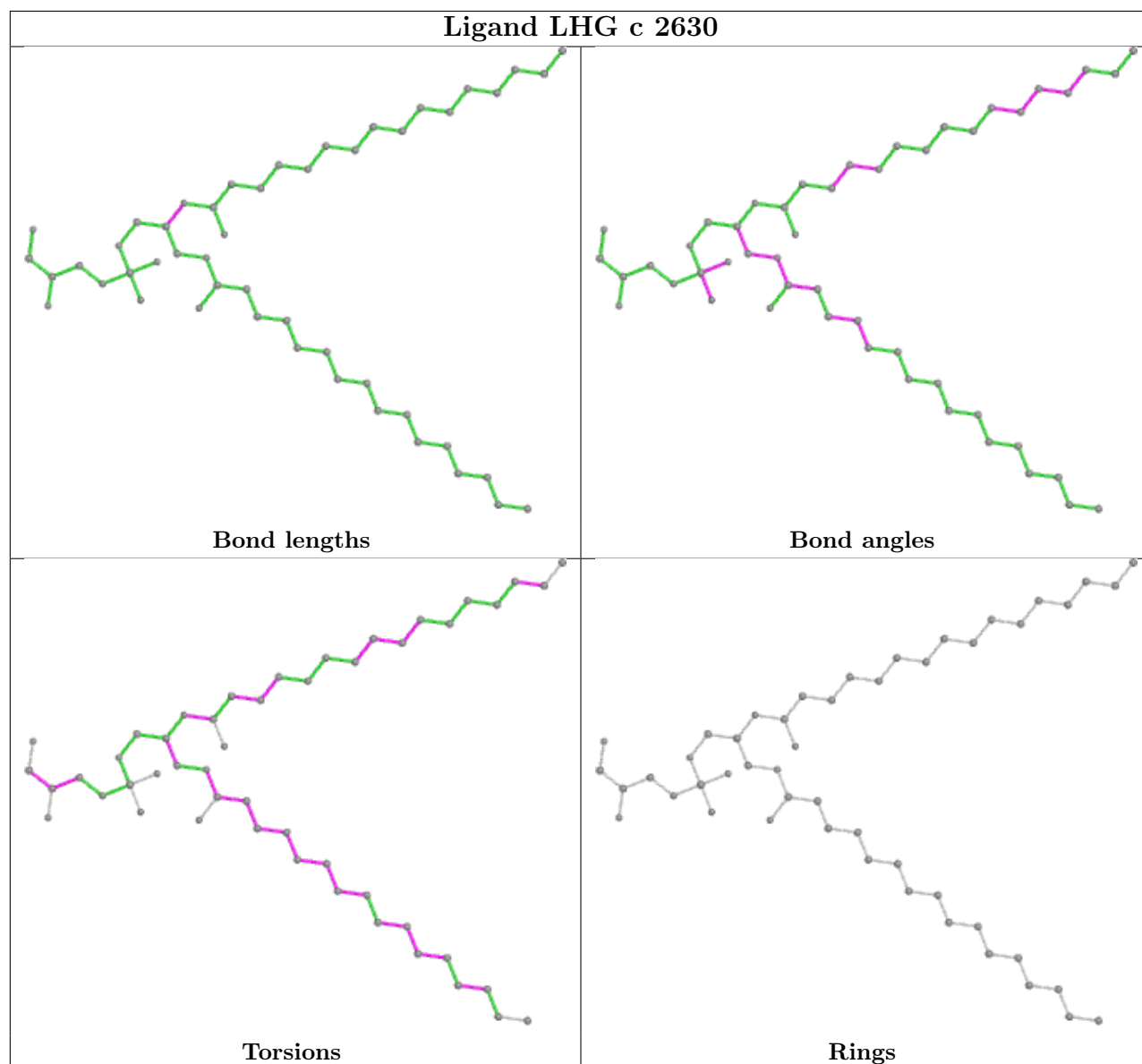
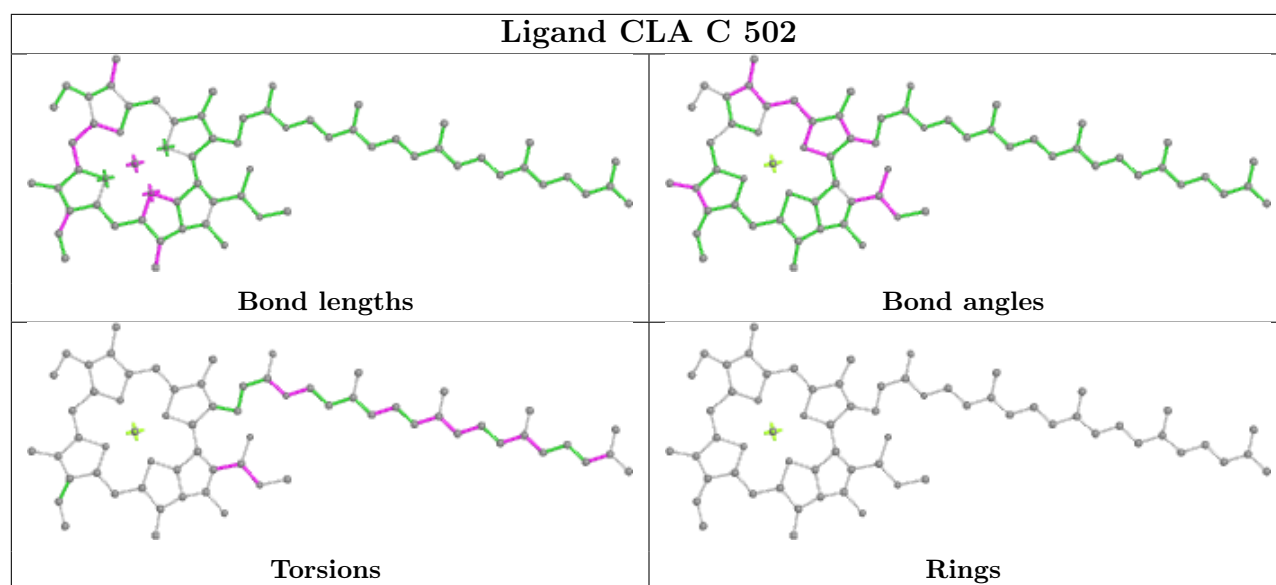
Bond angles

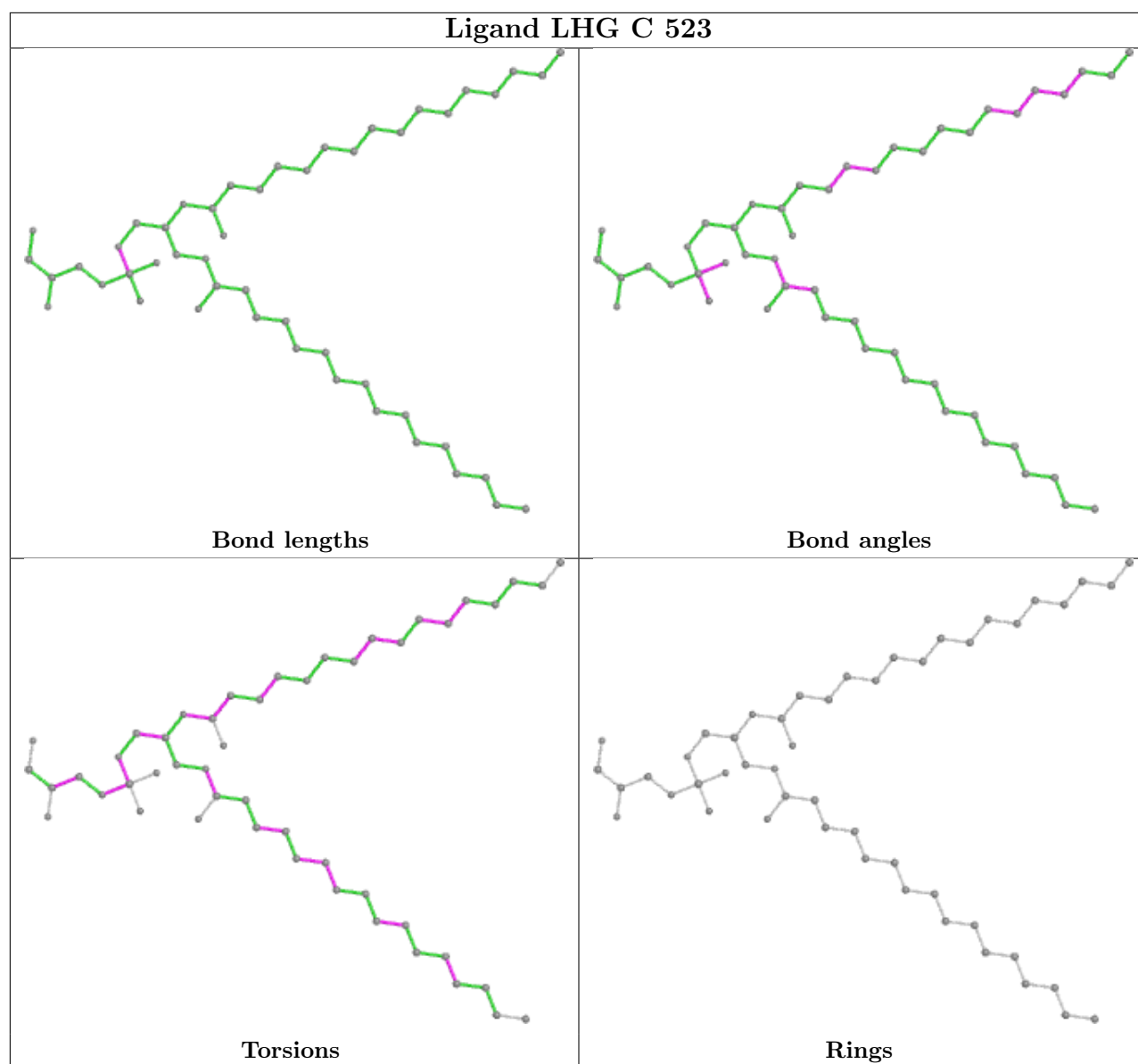


Torsions

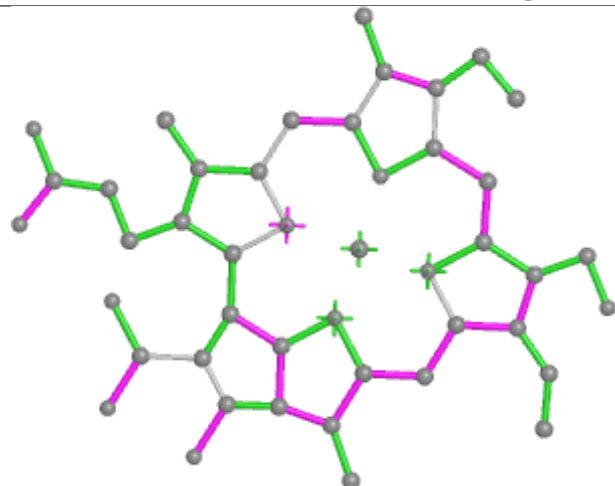


Rings

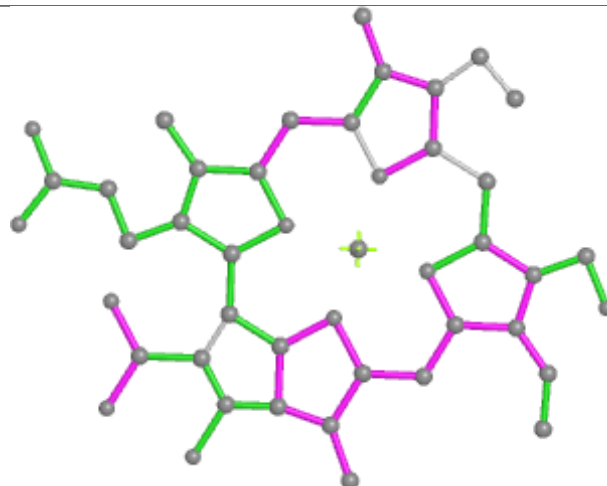




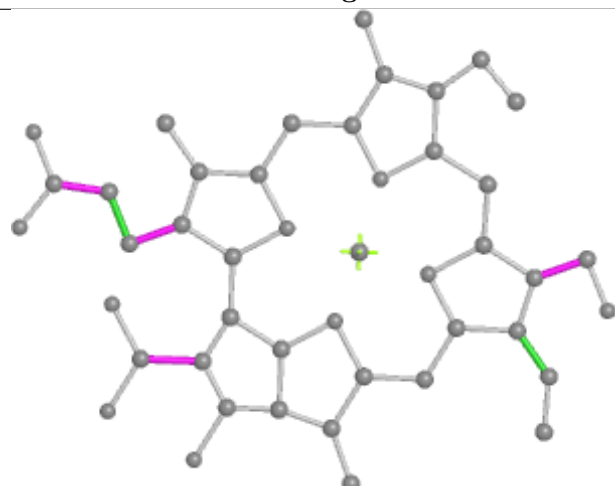
Ligand CHL 8 601



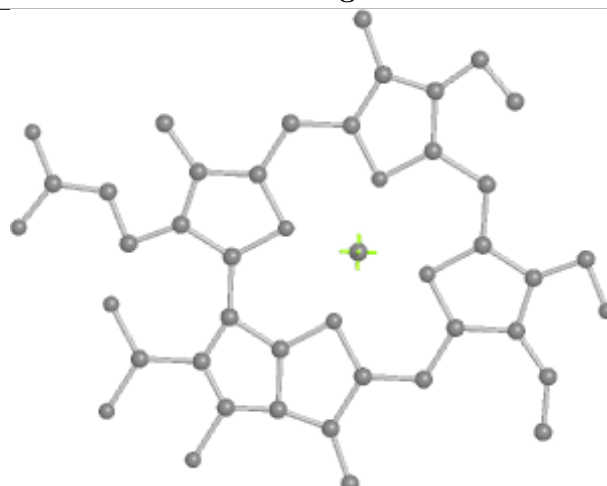
Bond lengths



Bond angles

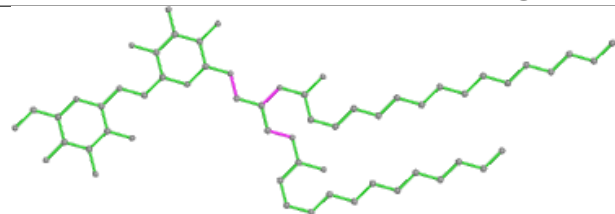


Torsions

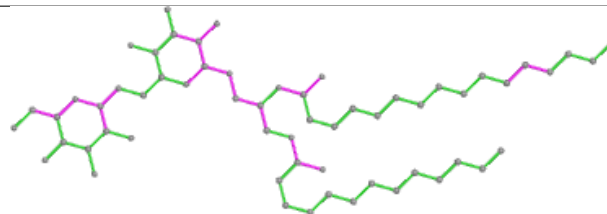


Rings

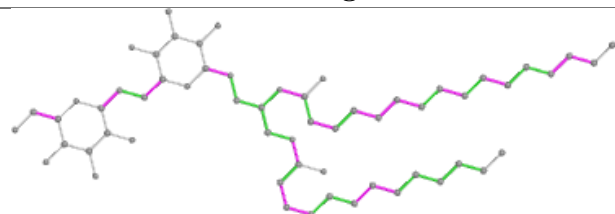
Ligand DGD b 626



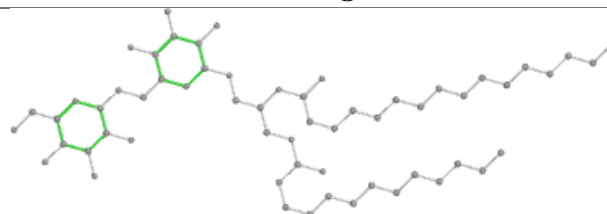
Bond lengths



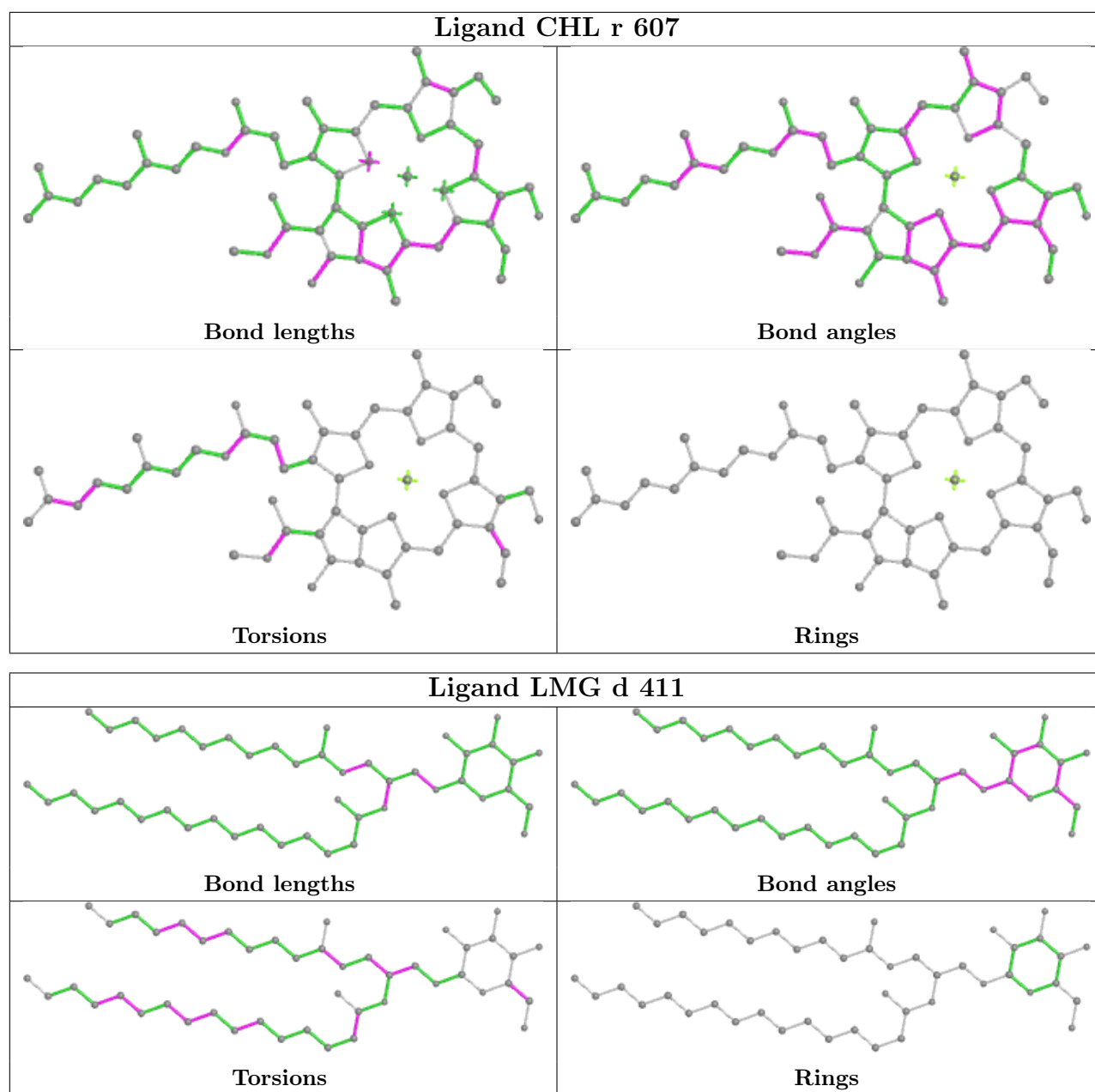
Bond angles

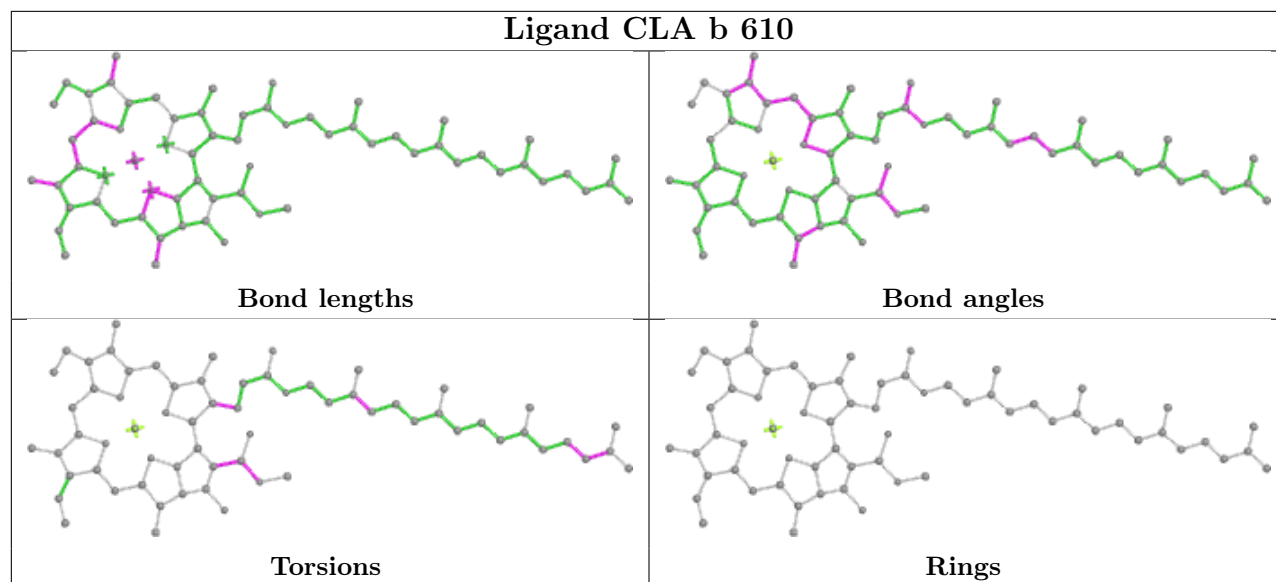
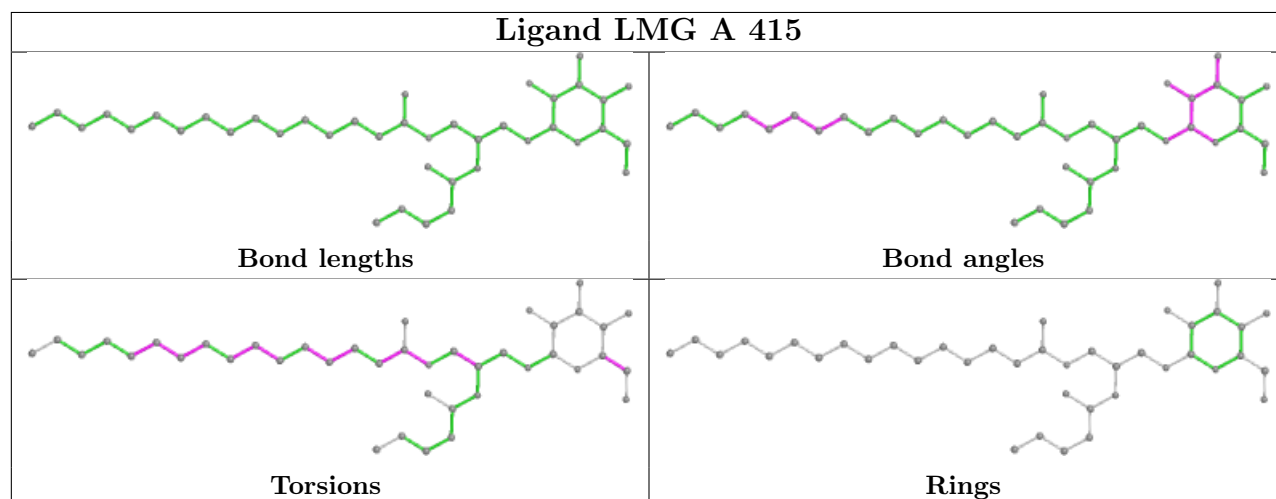


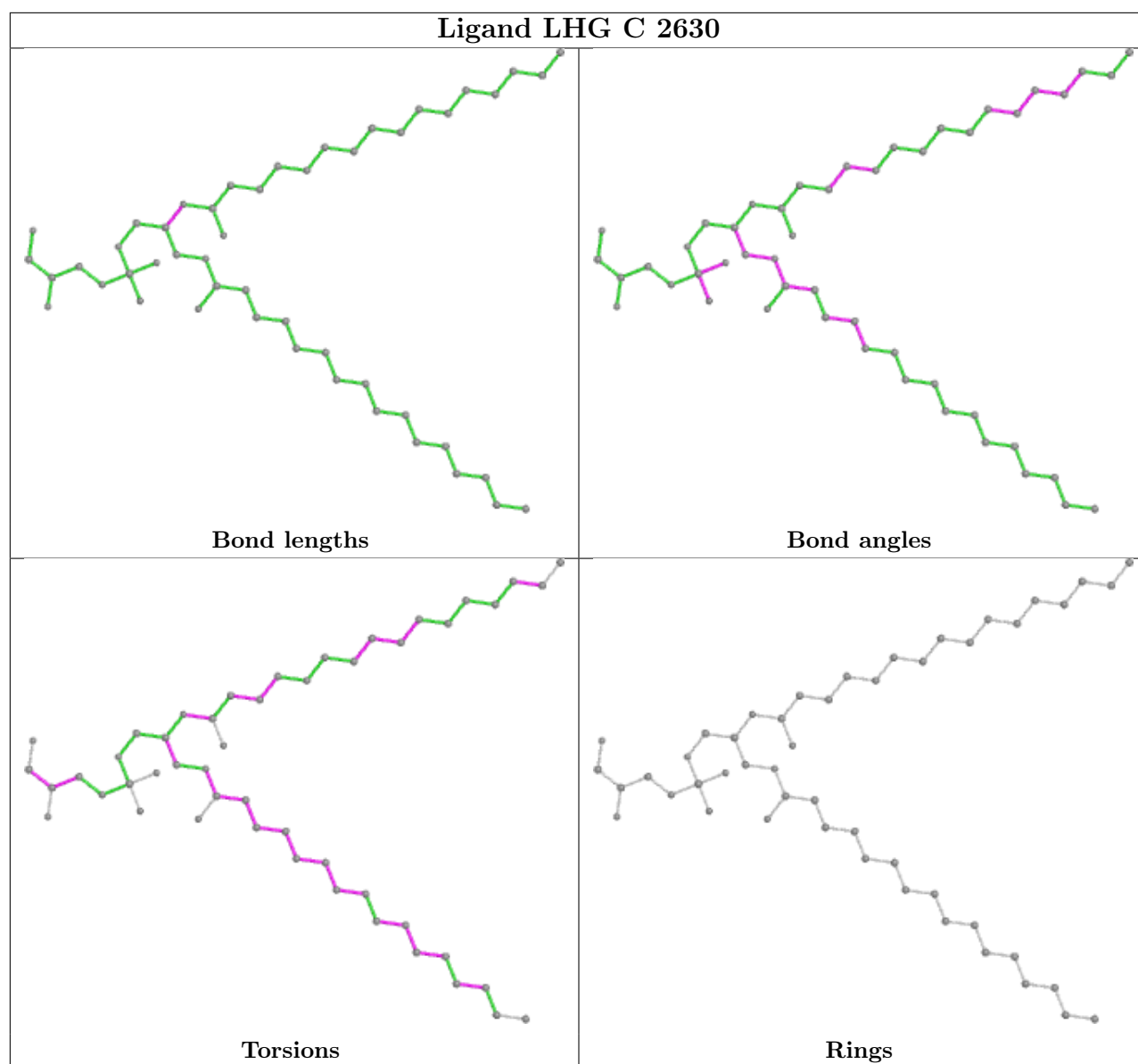
Torsions

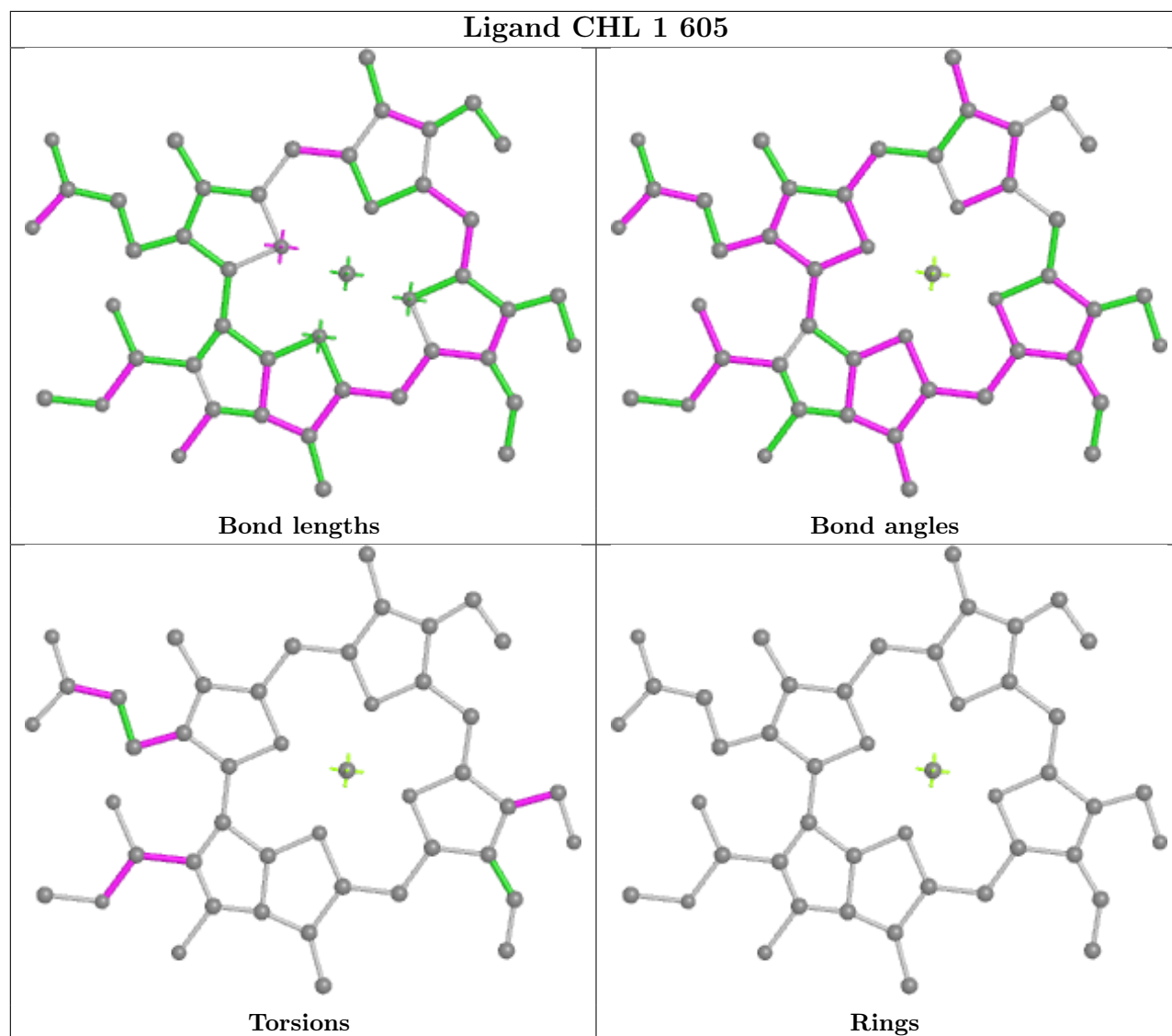
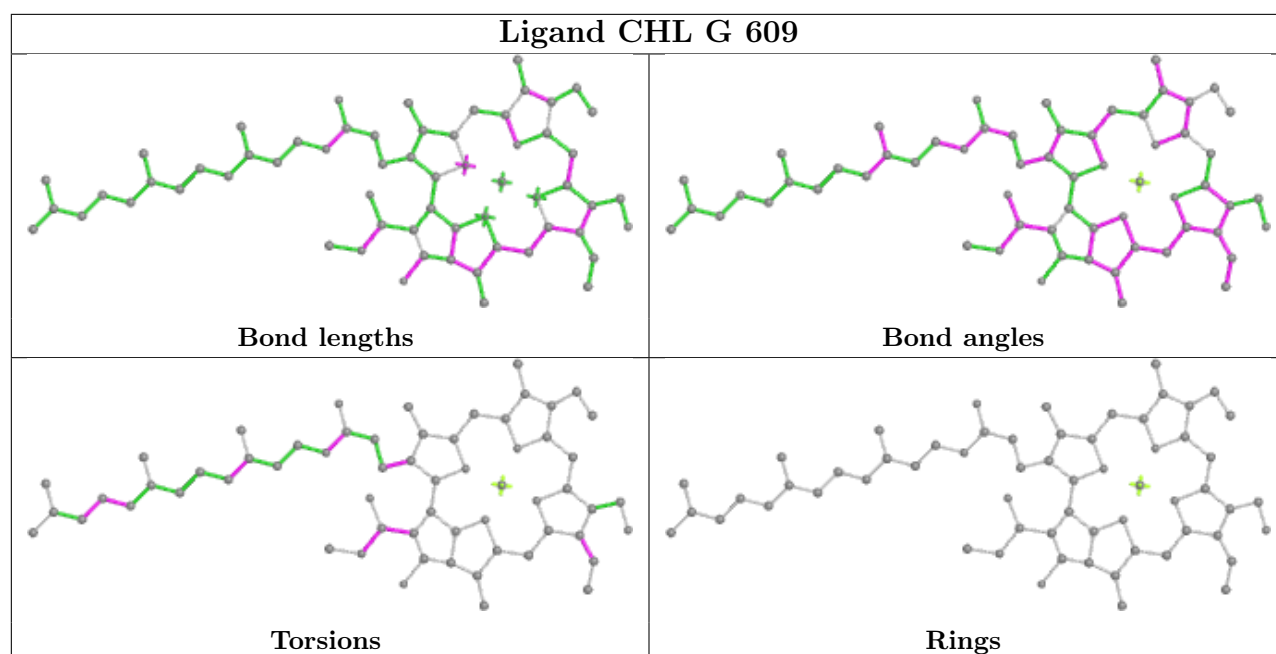


Rings

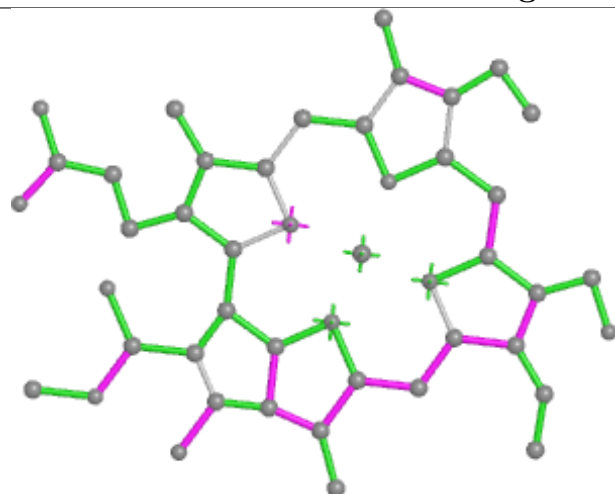


Ligand CLA b 610**Ligand LMG A 415**

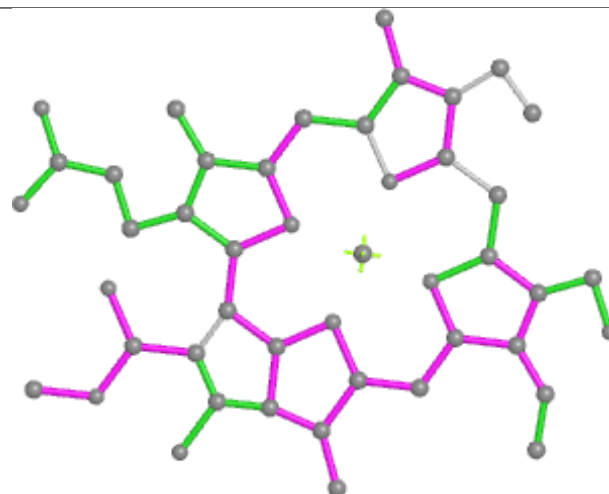




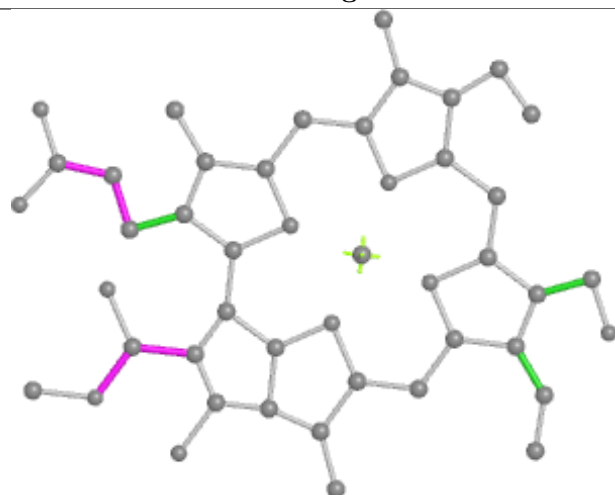
Ligand CHL S 601



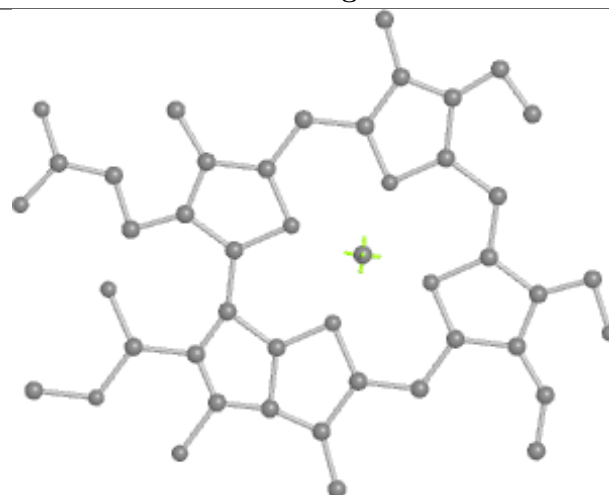
Bond lengths



Bond angles

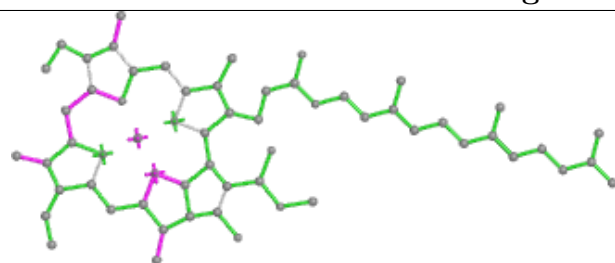


Torsions

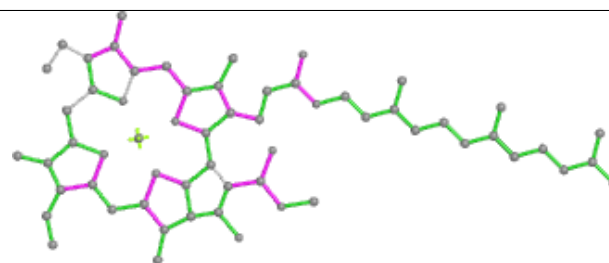


Rings

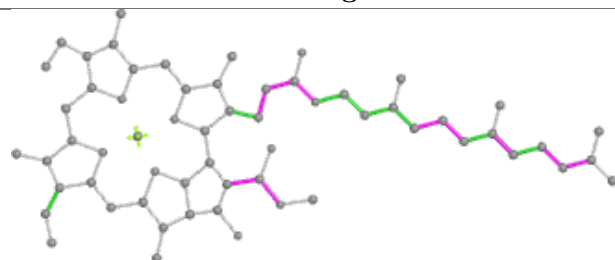
Ligand CLA r 603



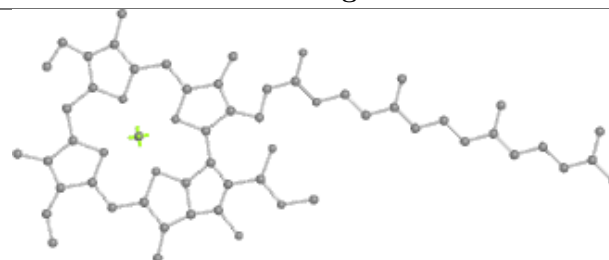
Bond lengths



Bond angles

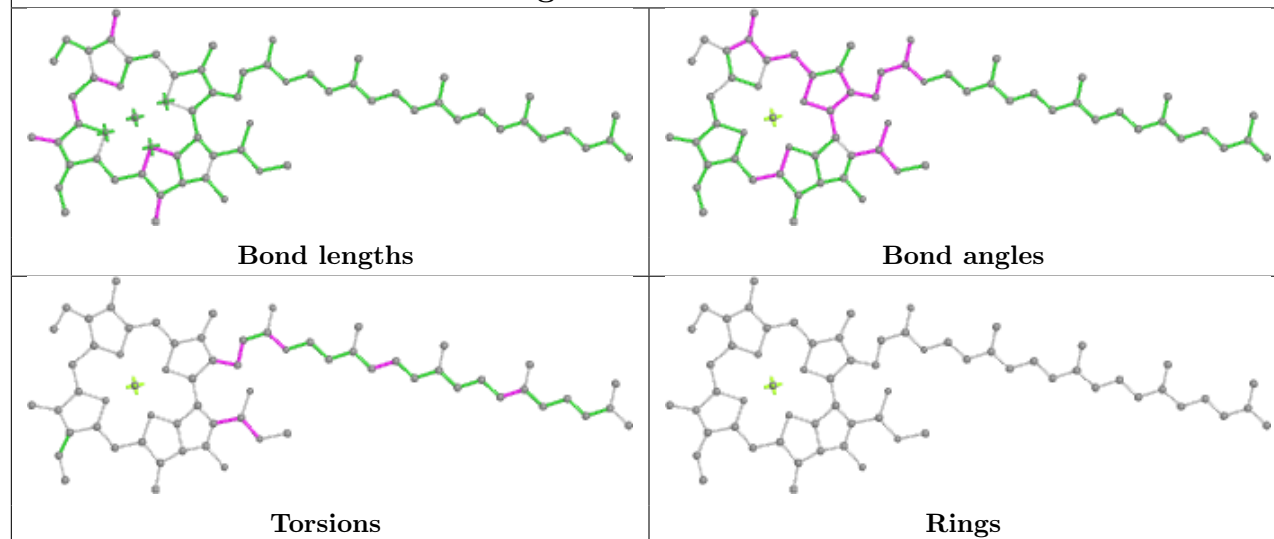


Torsions

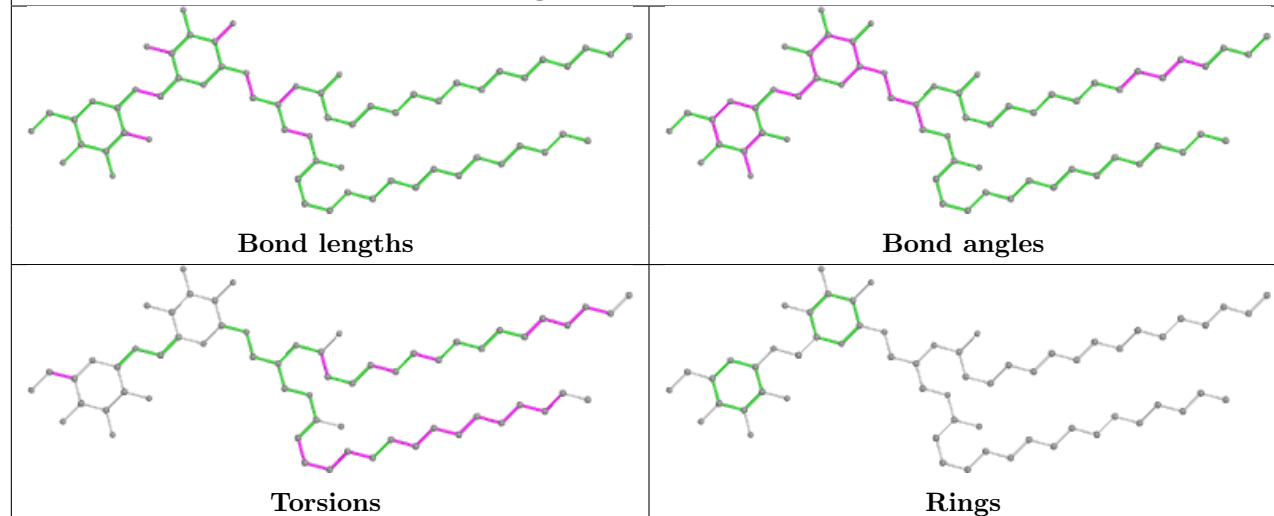


Rings

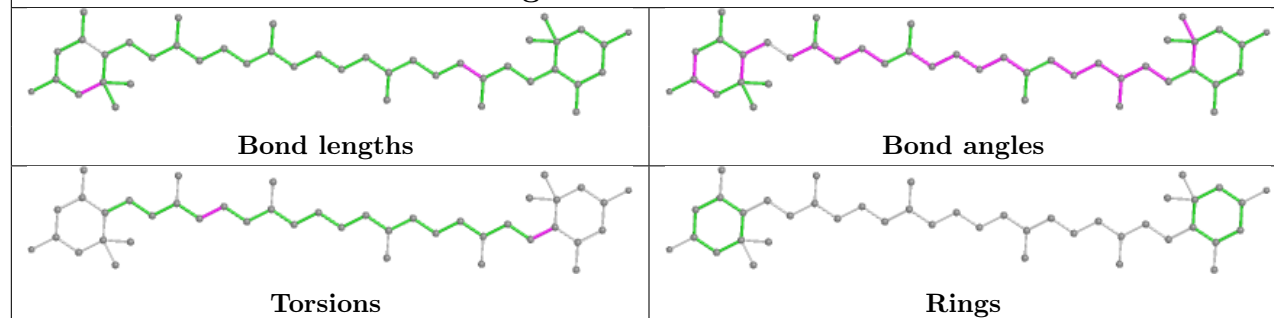
Ligand CLA c 513



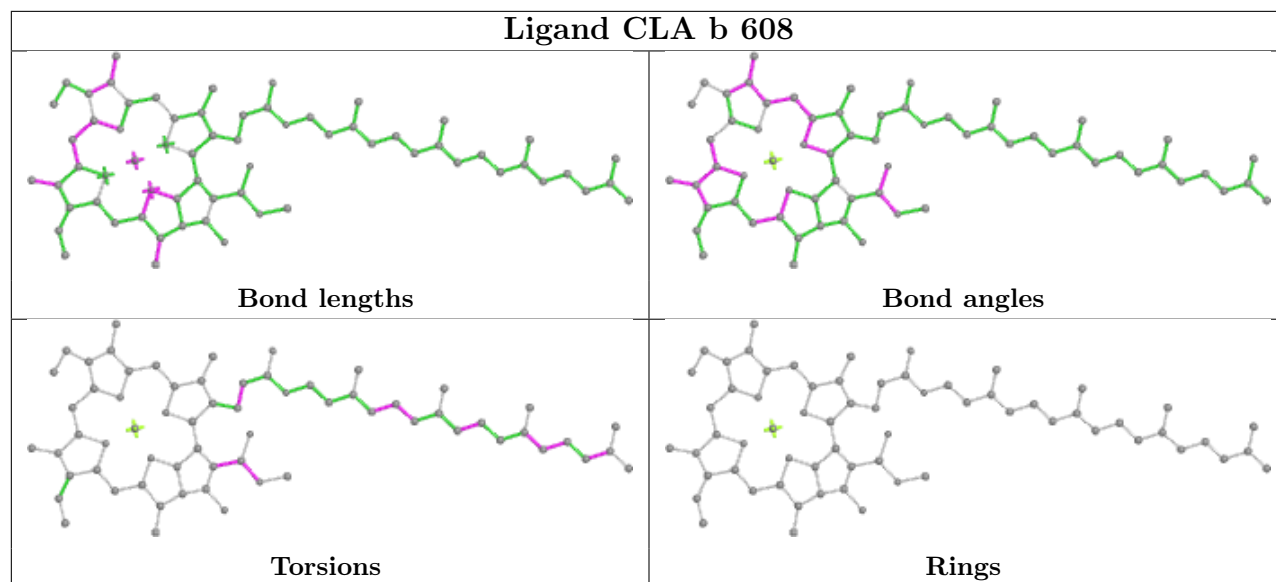
Ligand DGD h 102



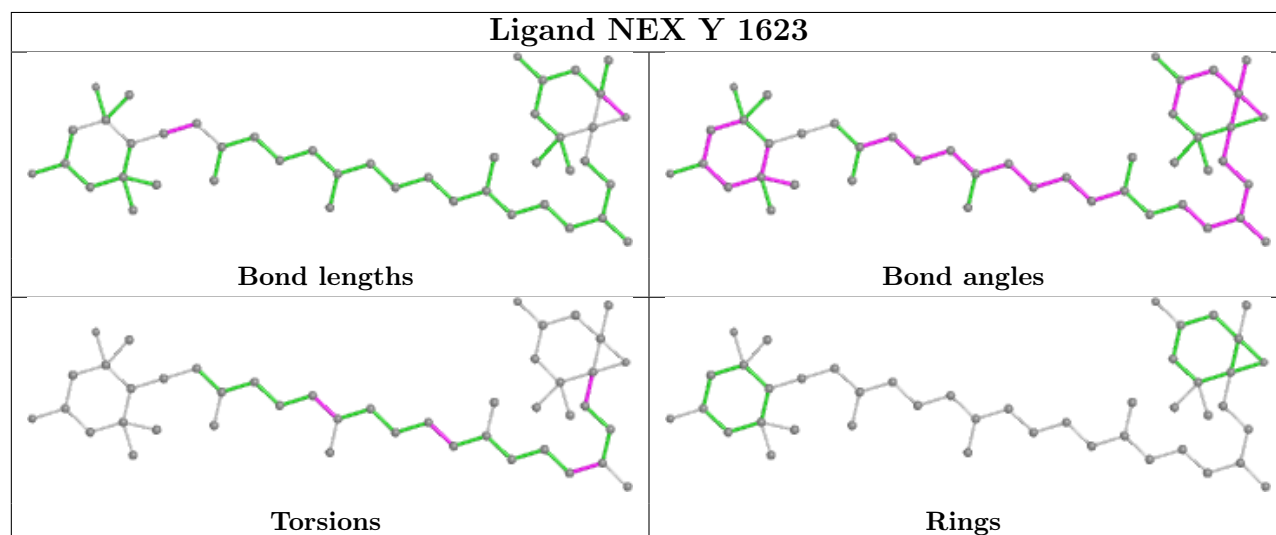
Ligand LUT N 1621



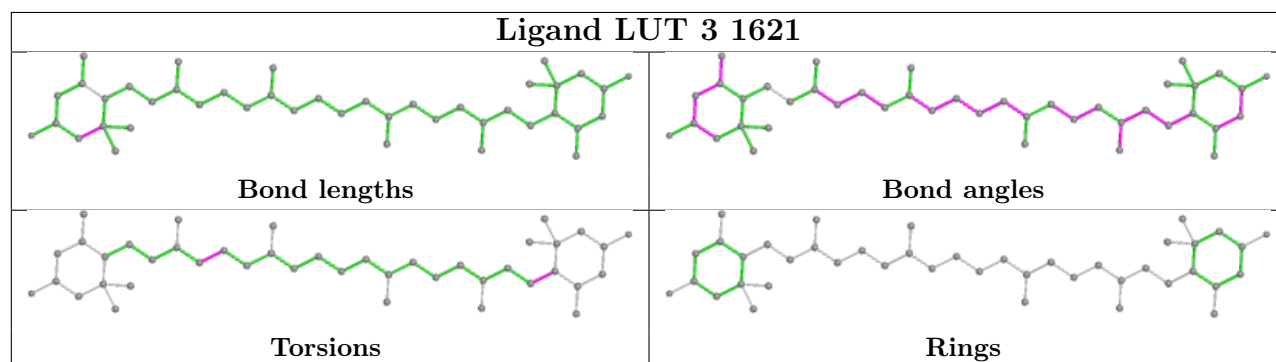
Ligand CLA b 608

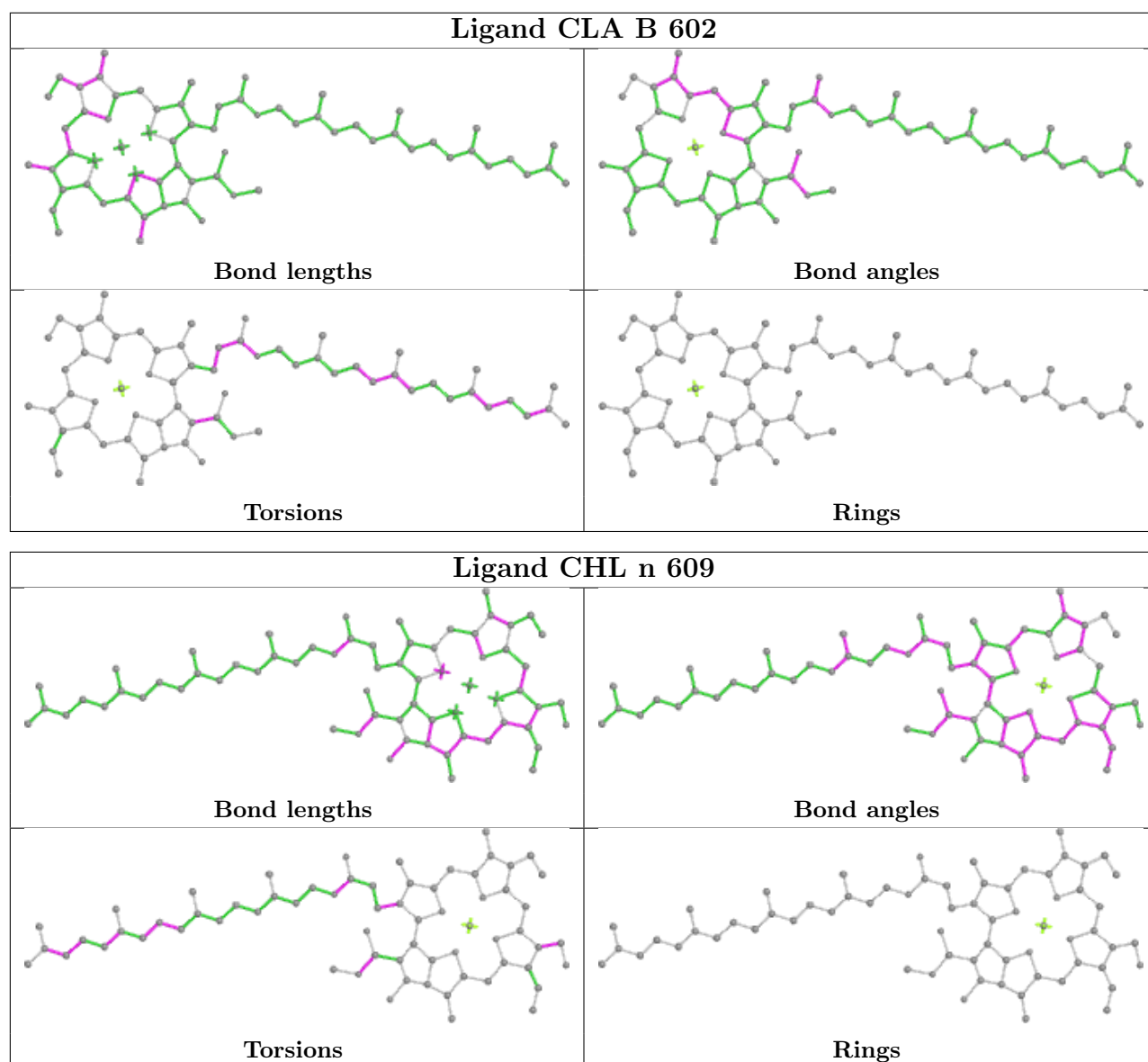


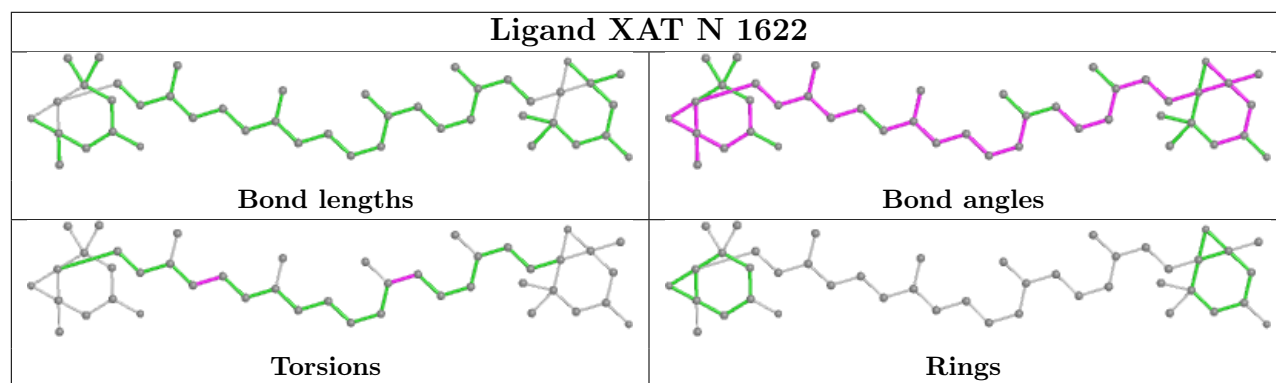
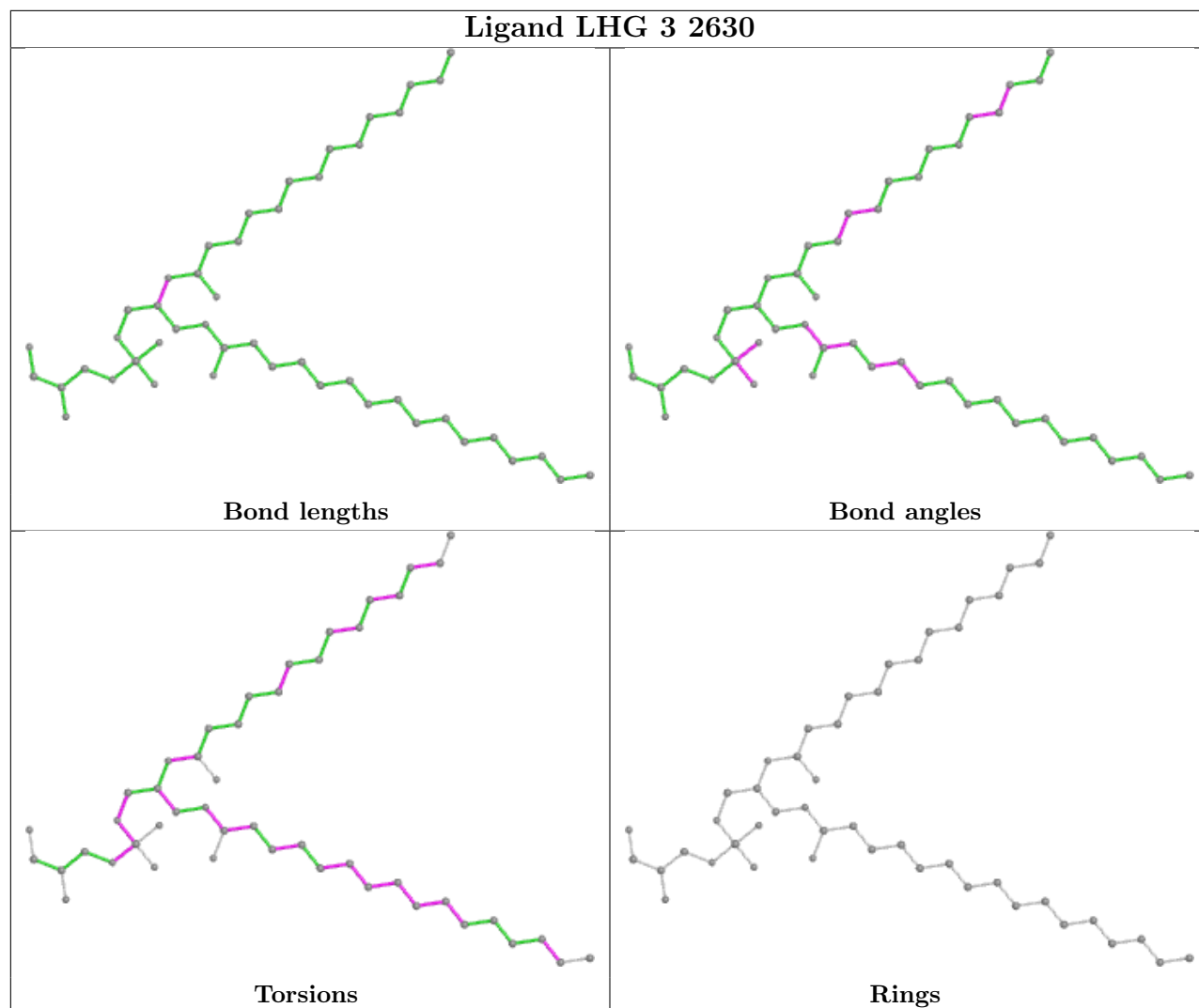
Ligand NEX Y 1623

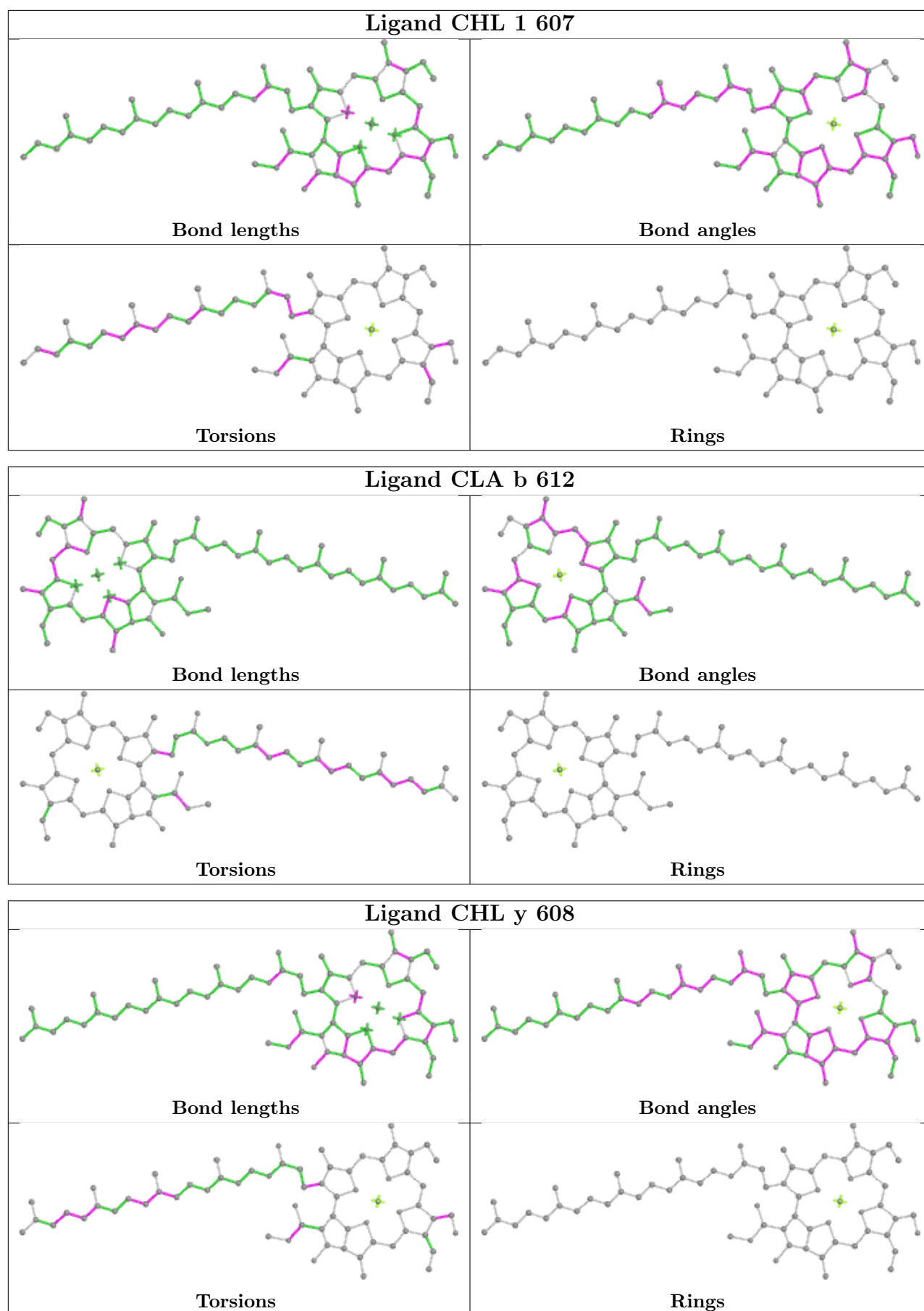


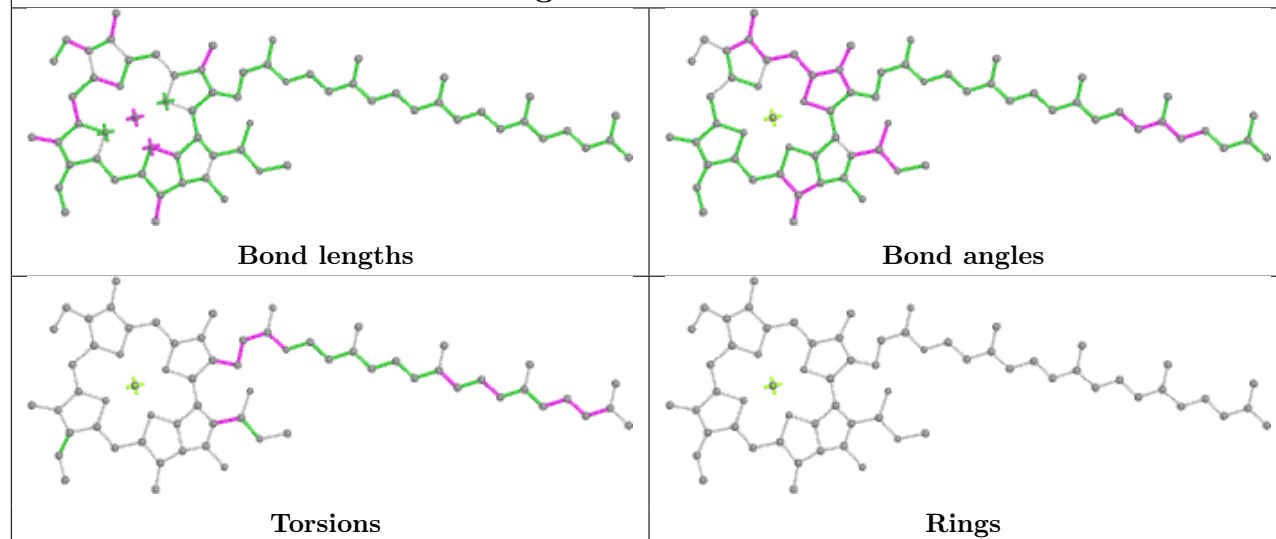
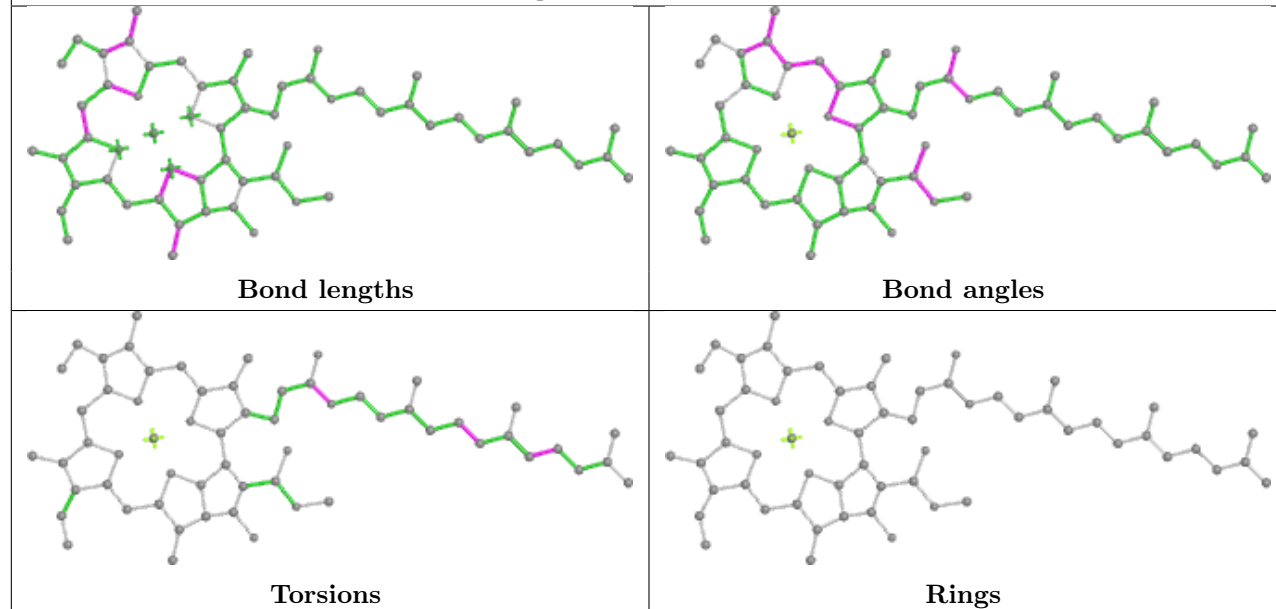
Ligand LUT 3 1621

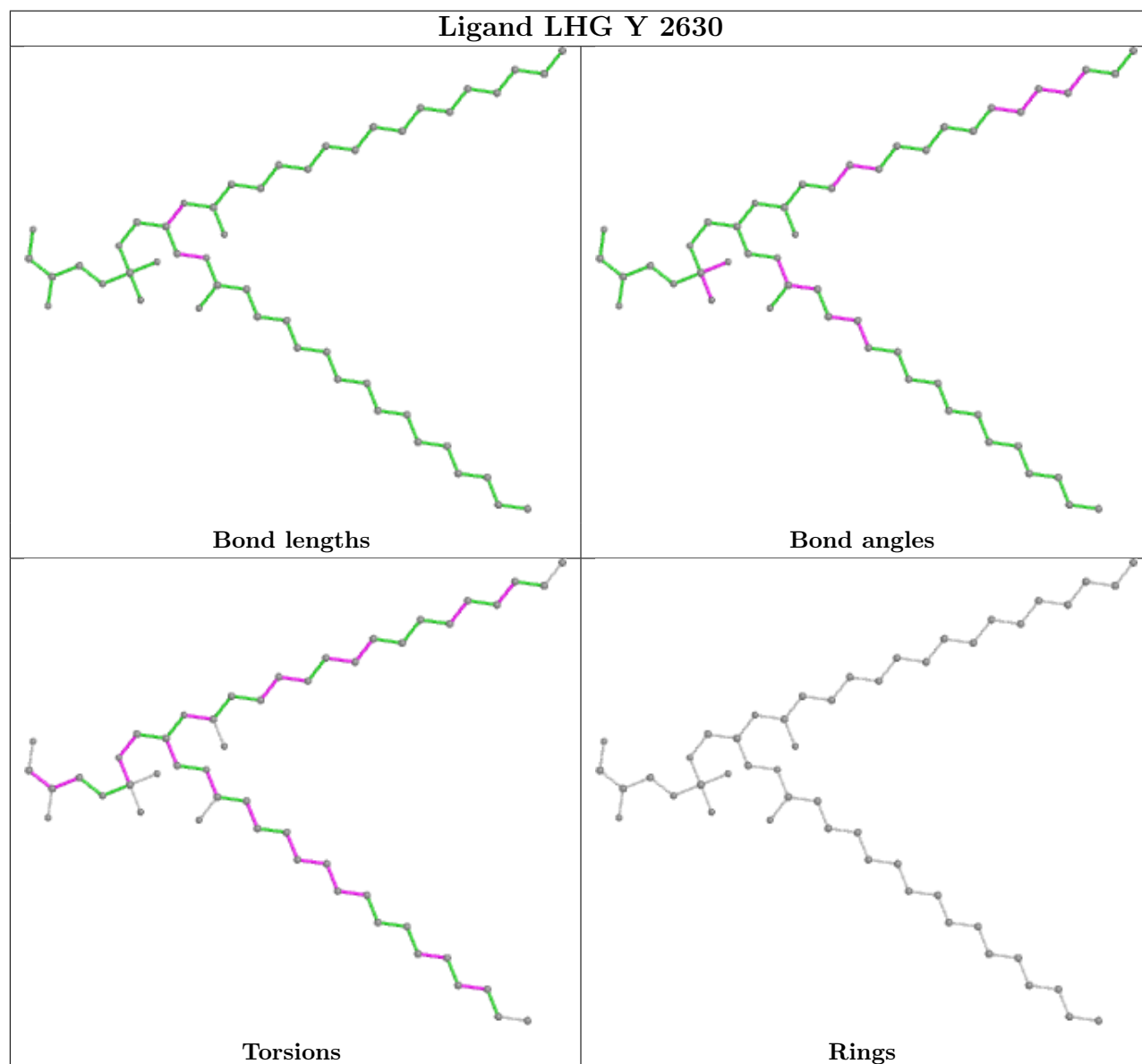
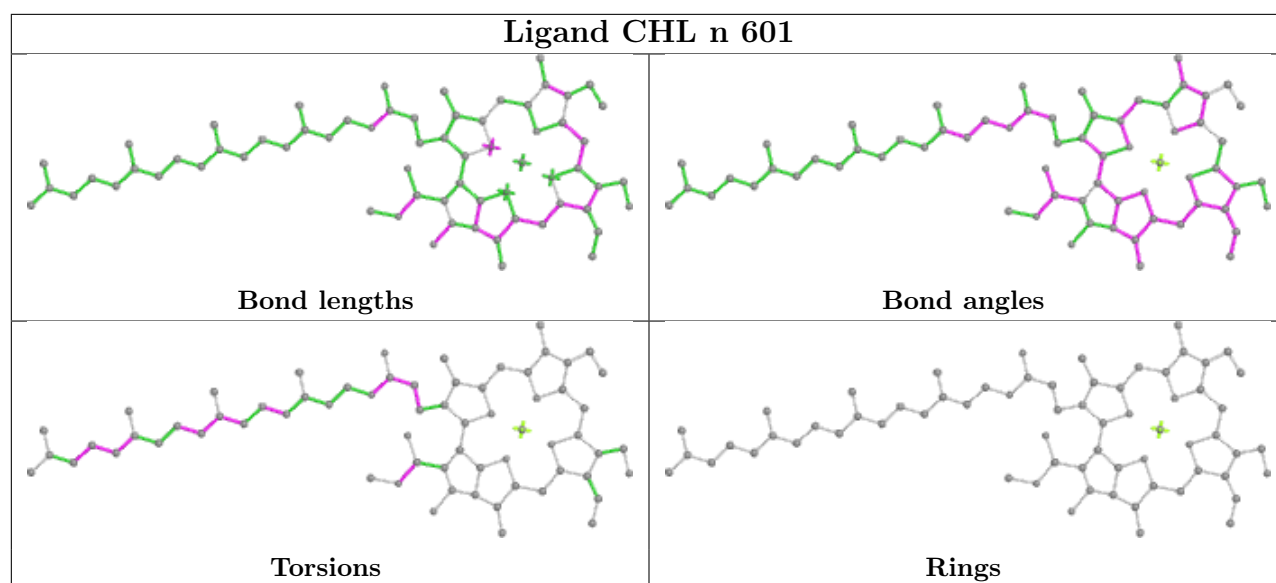


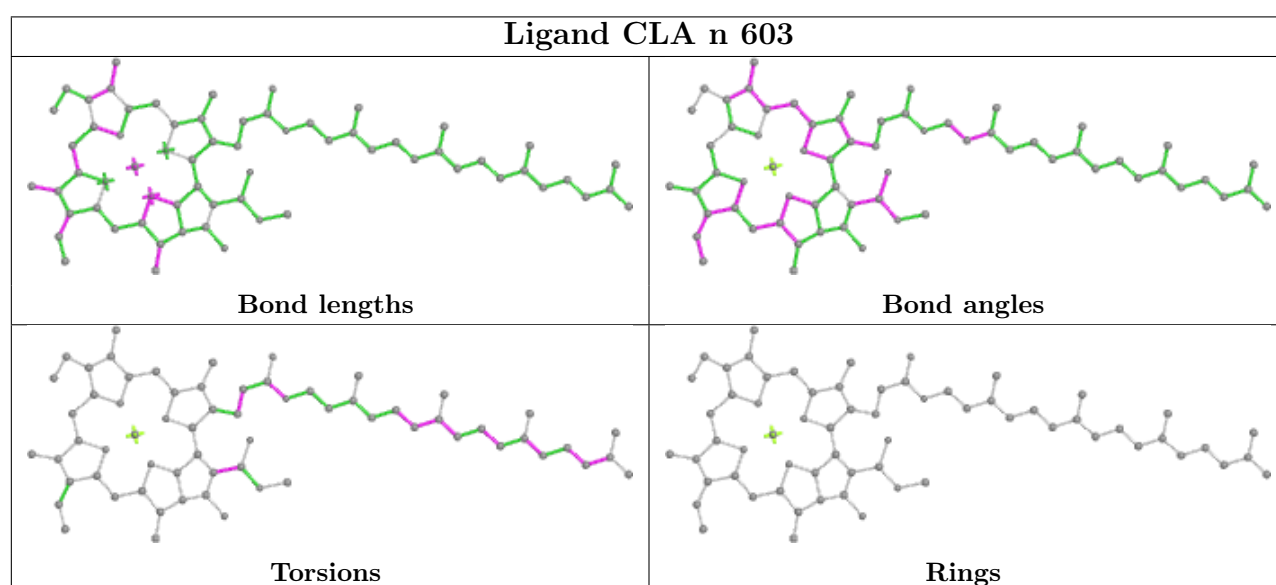
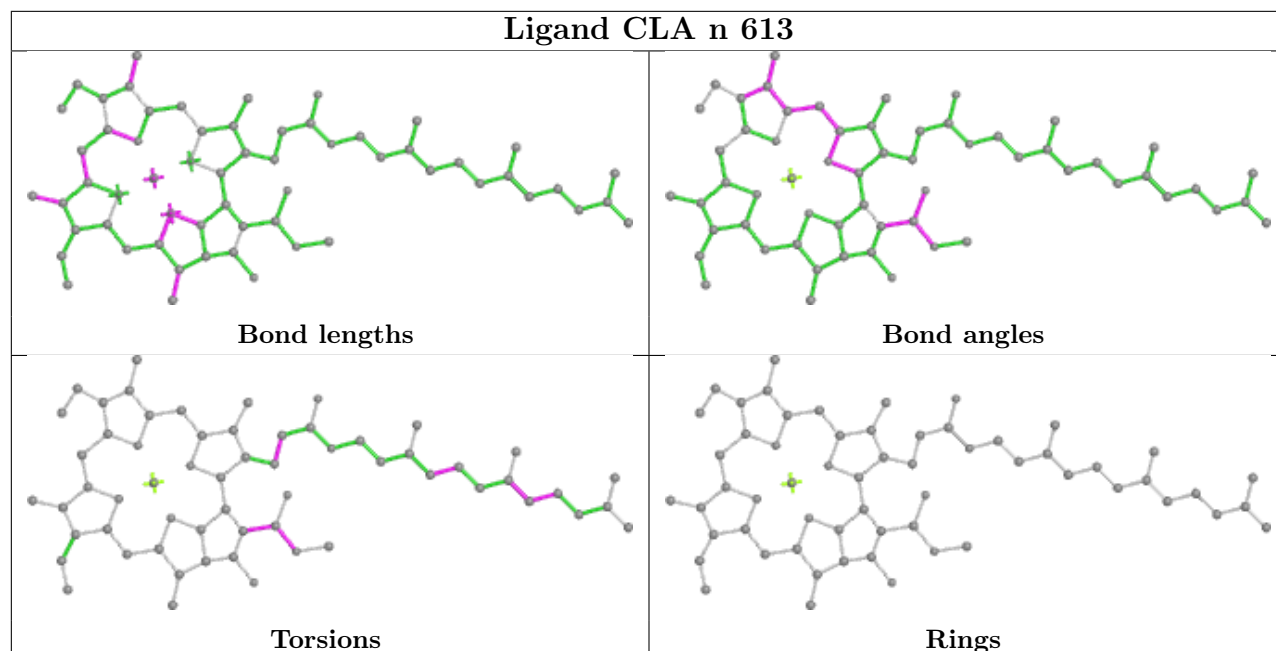
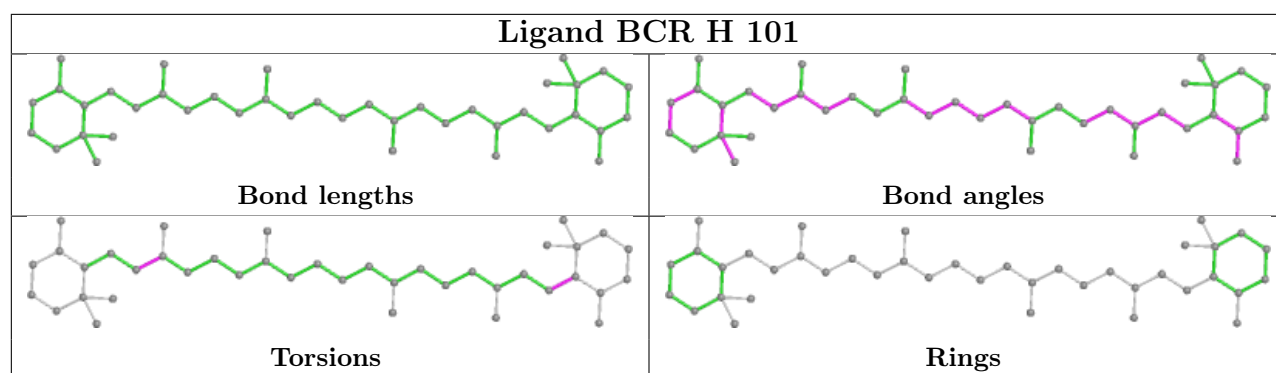




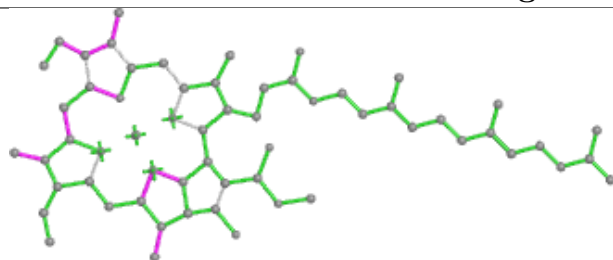


Ligand CLA b 613**Ligand CLA N 611**

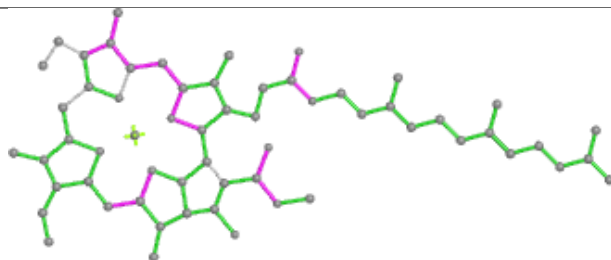




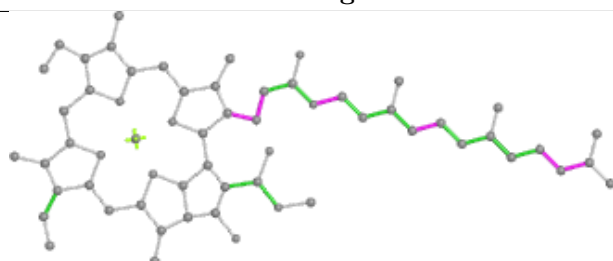
Ligand CLA 3 610



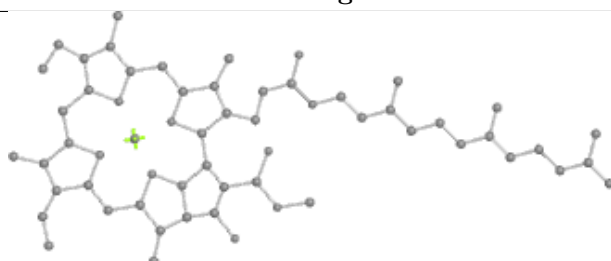
Bond lengths



Bond angles

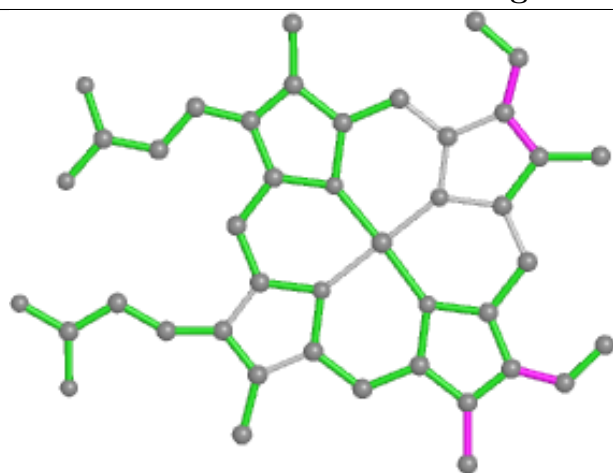


Torsions

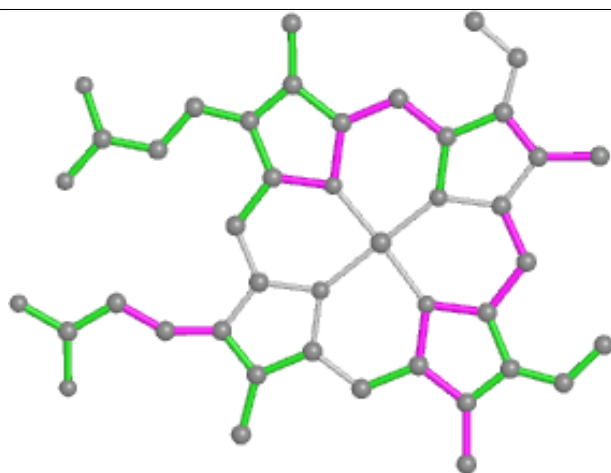


Rings

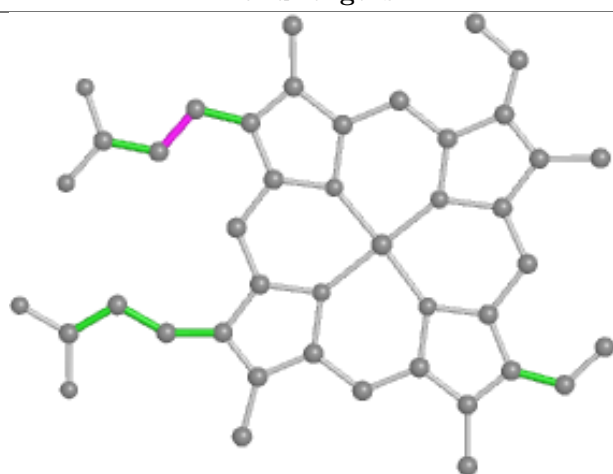
Ligand HEM F 101



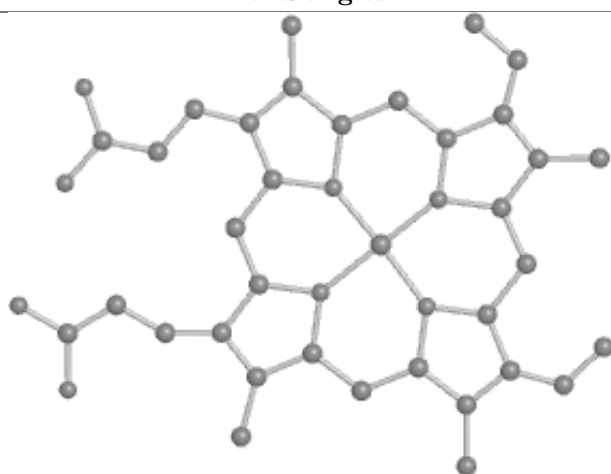
Bond lengths



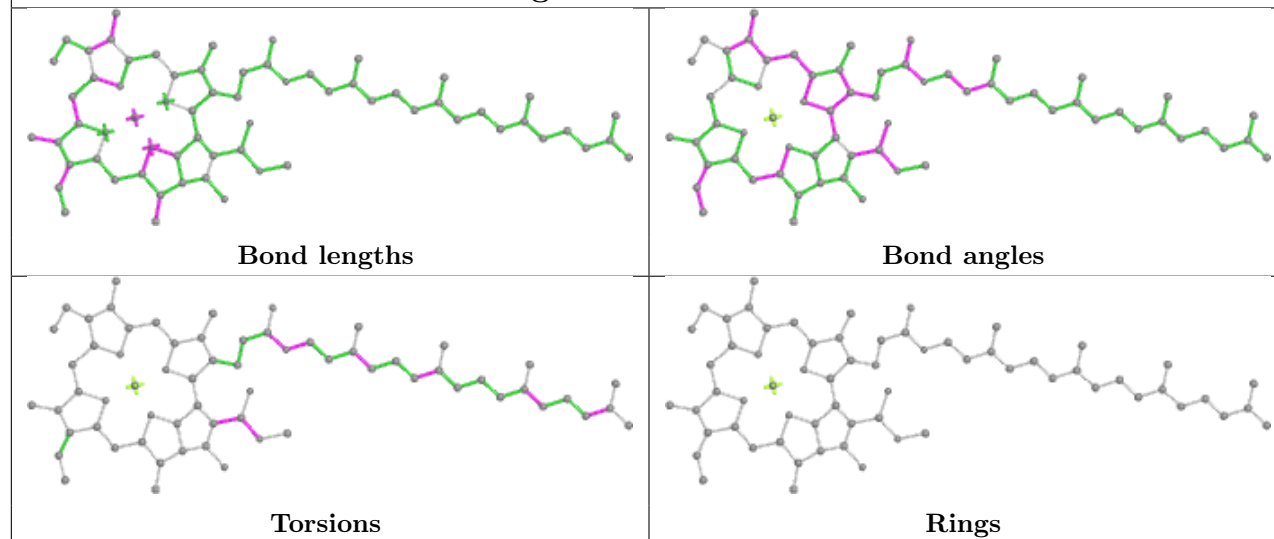
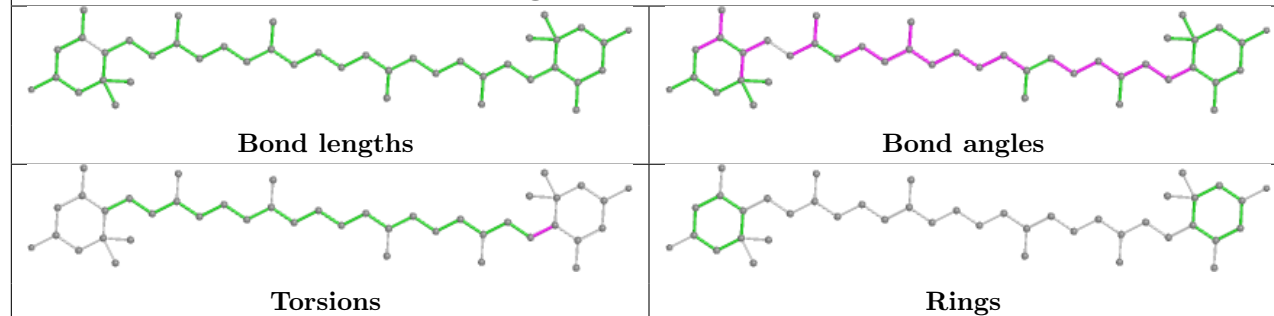
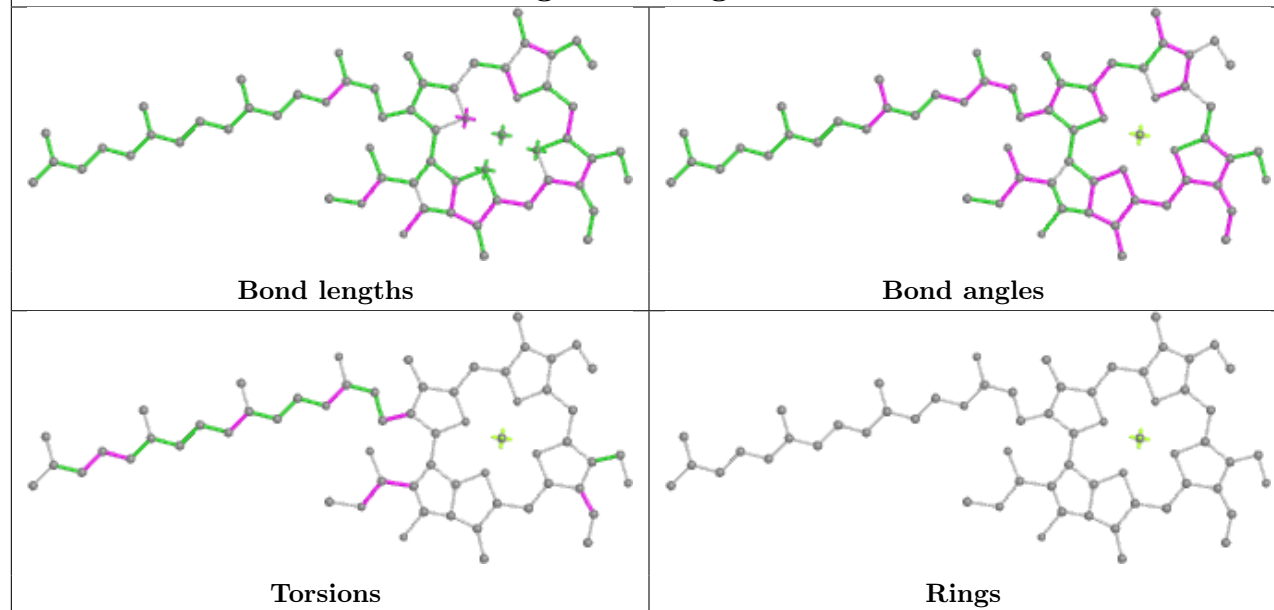
Bond angles

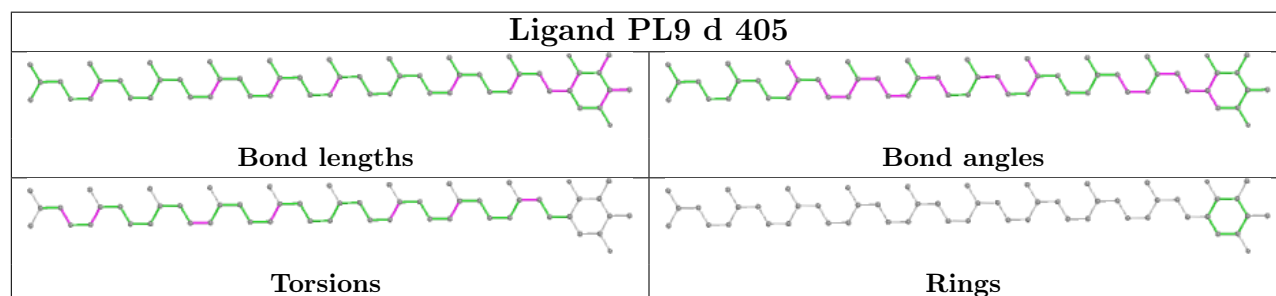
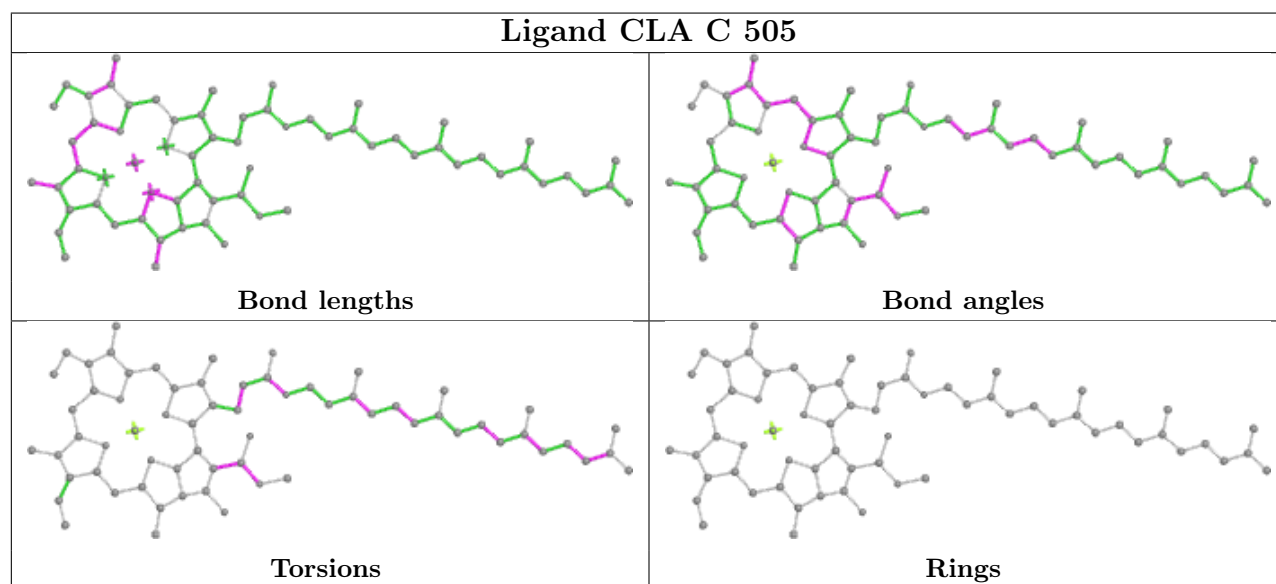
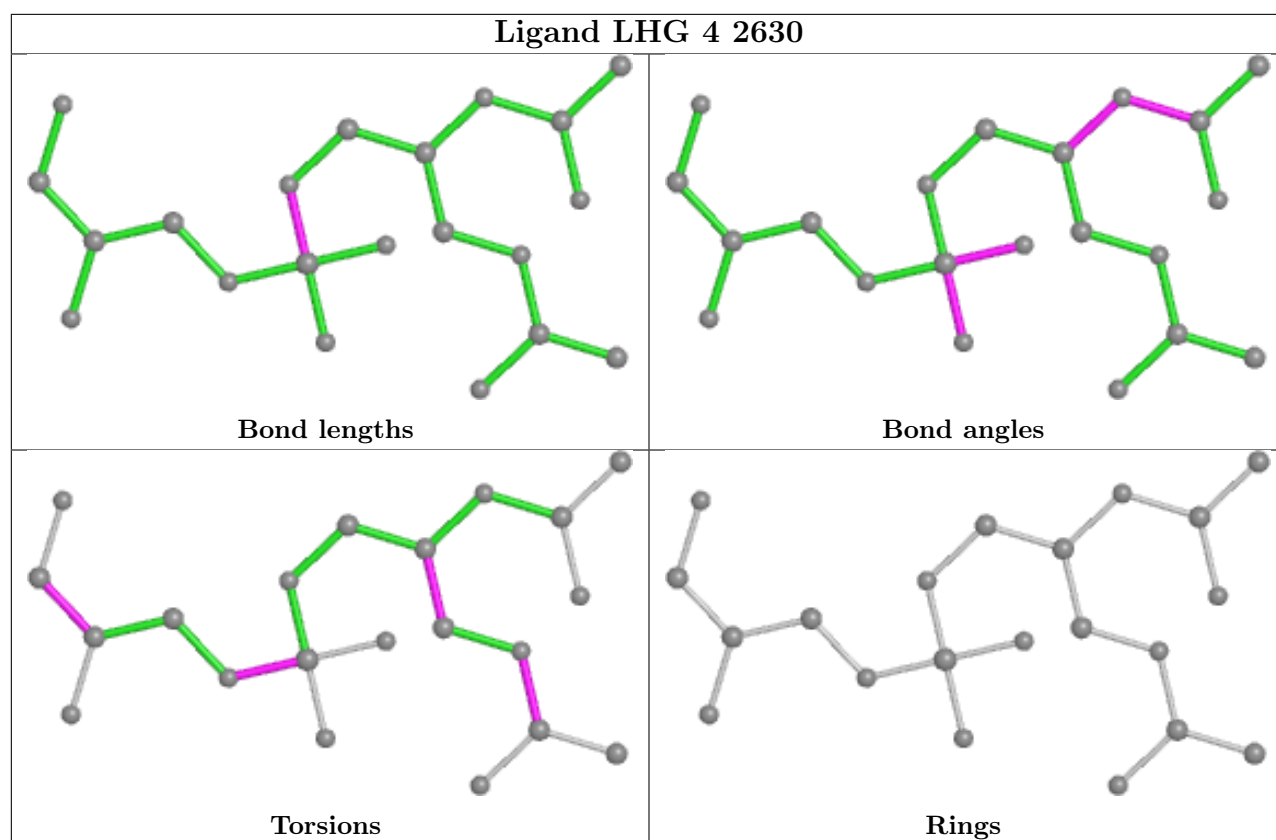


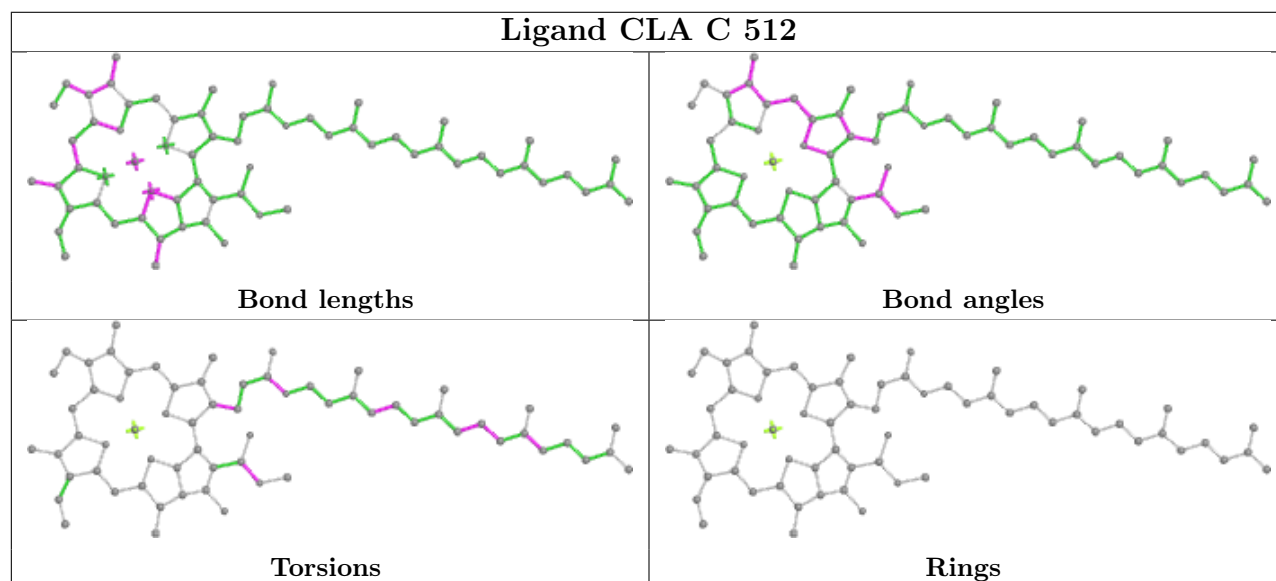
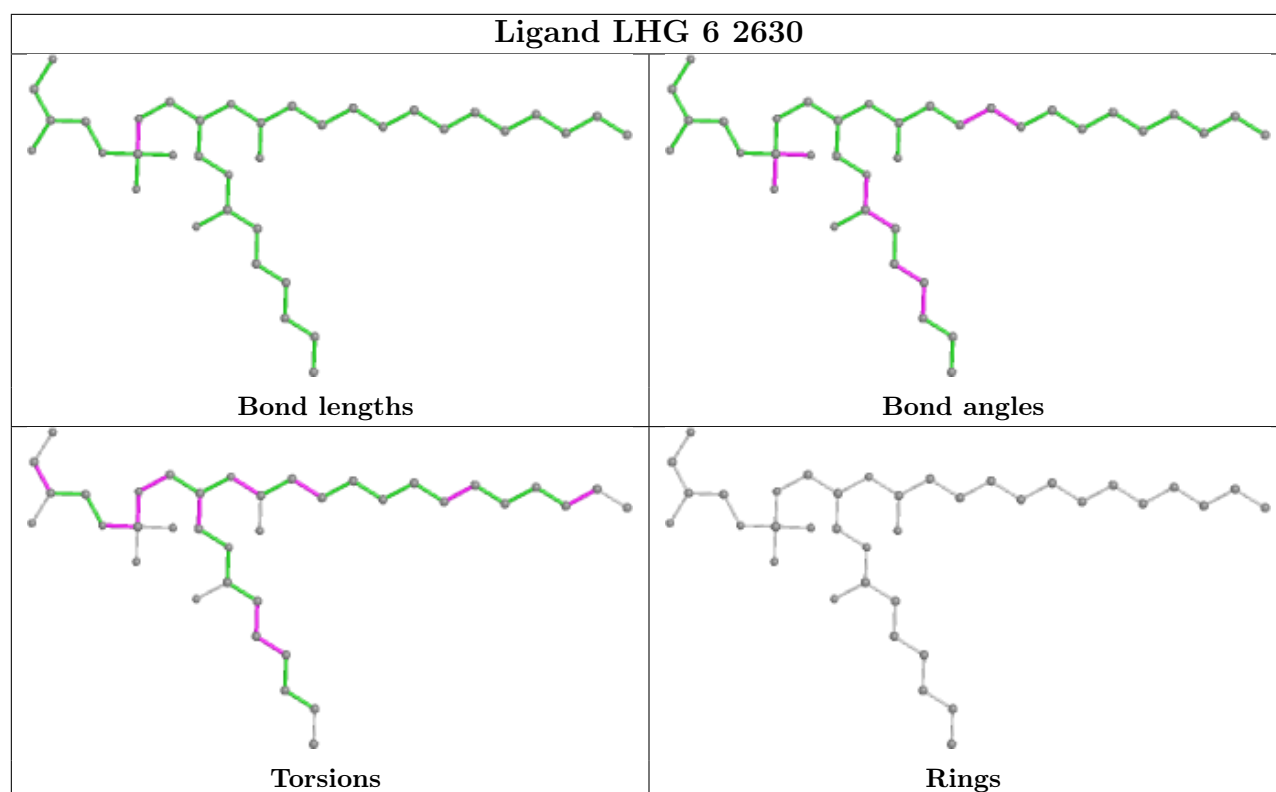
Torsions



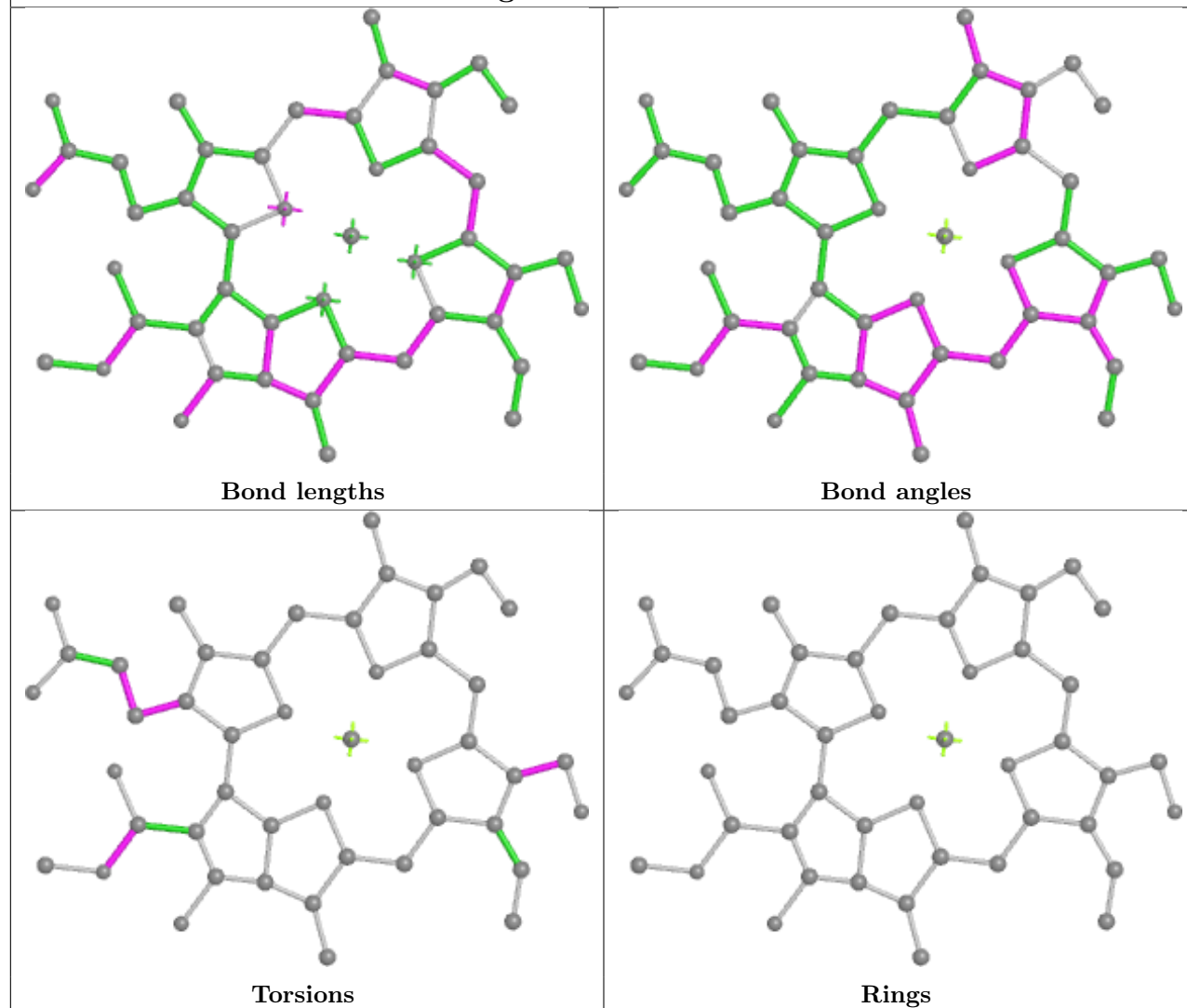
Rings

Ligand CLA Y 603**Ligand LUT S 1620****Ligand CHL g 609**

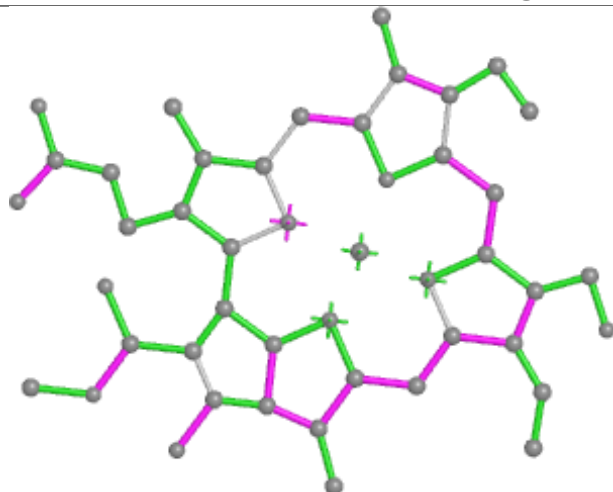




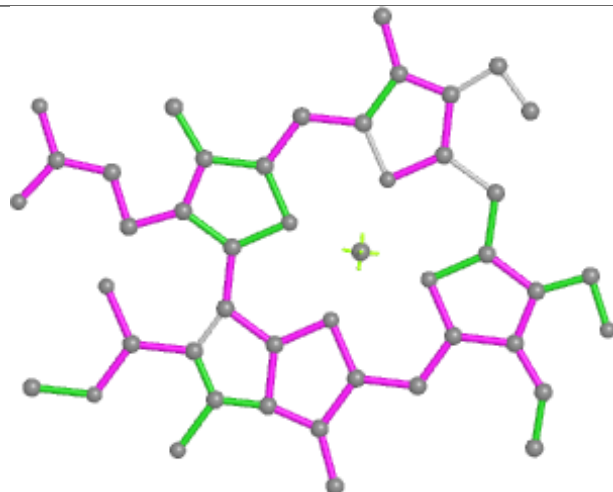
Ligand CHL 1 608



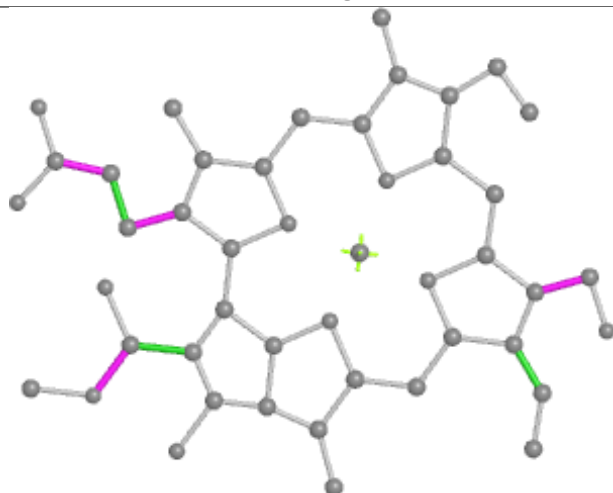
Ligand CHL 4 606



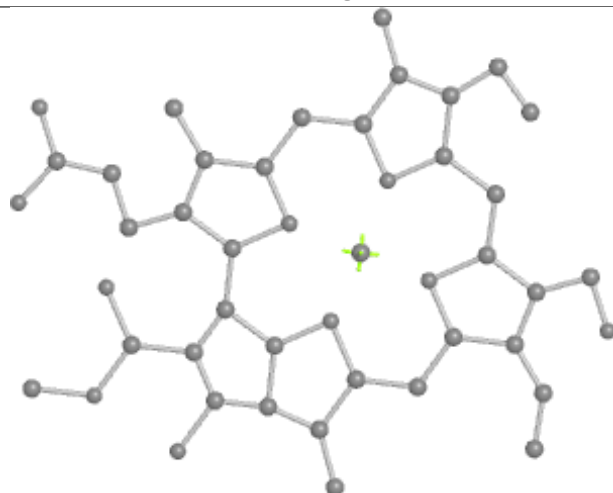
Bond lengths



Bond angles

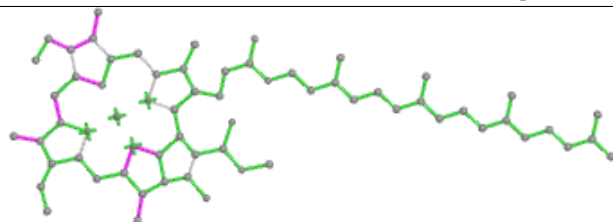


Torsions

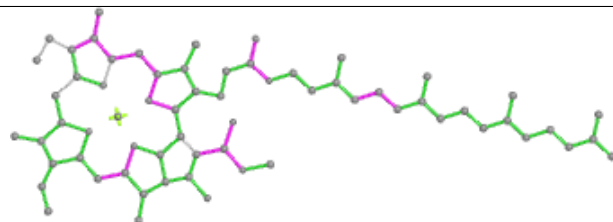


Rings

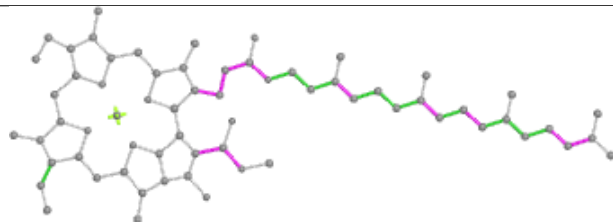
Ligand CLA C 501



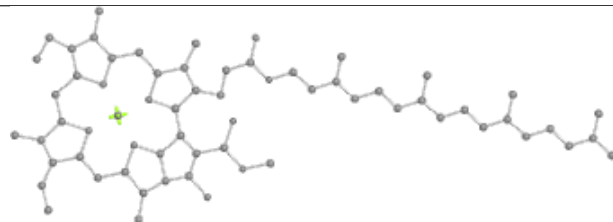
Bond lengths



Bond angles

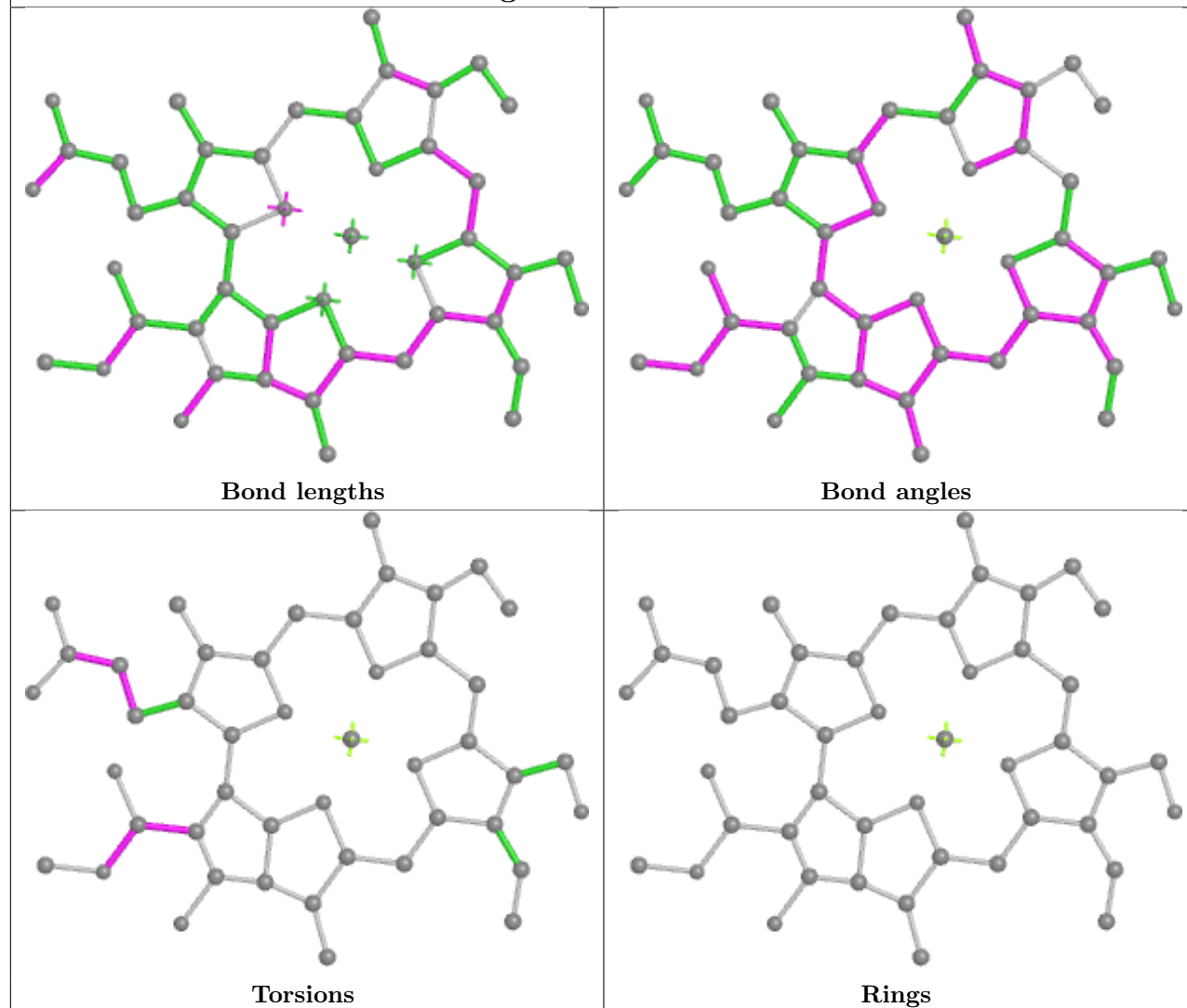


Torsions

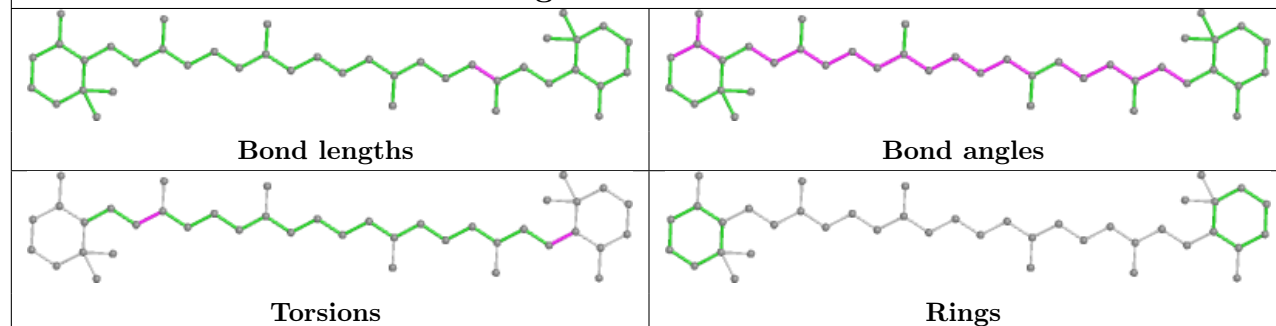


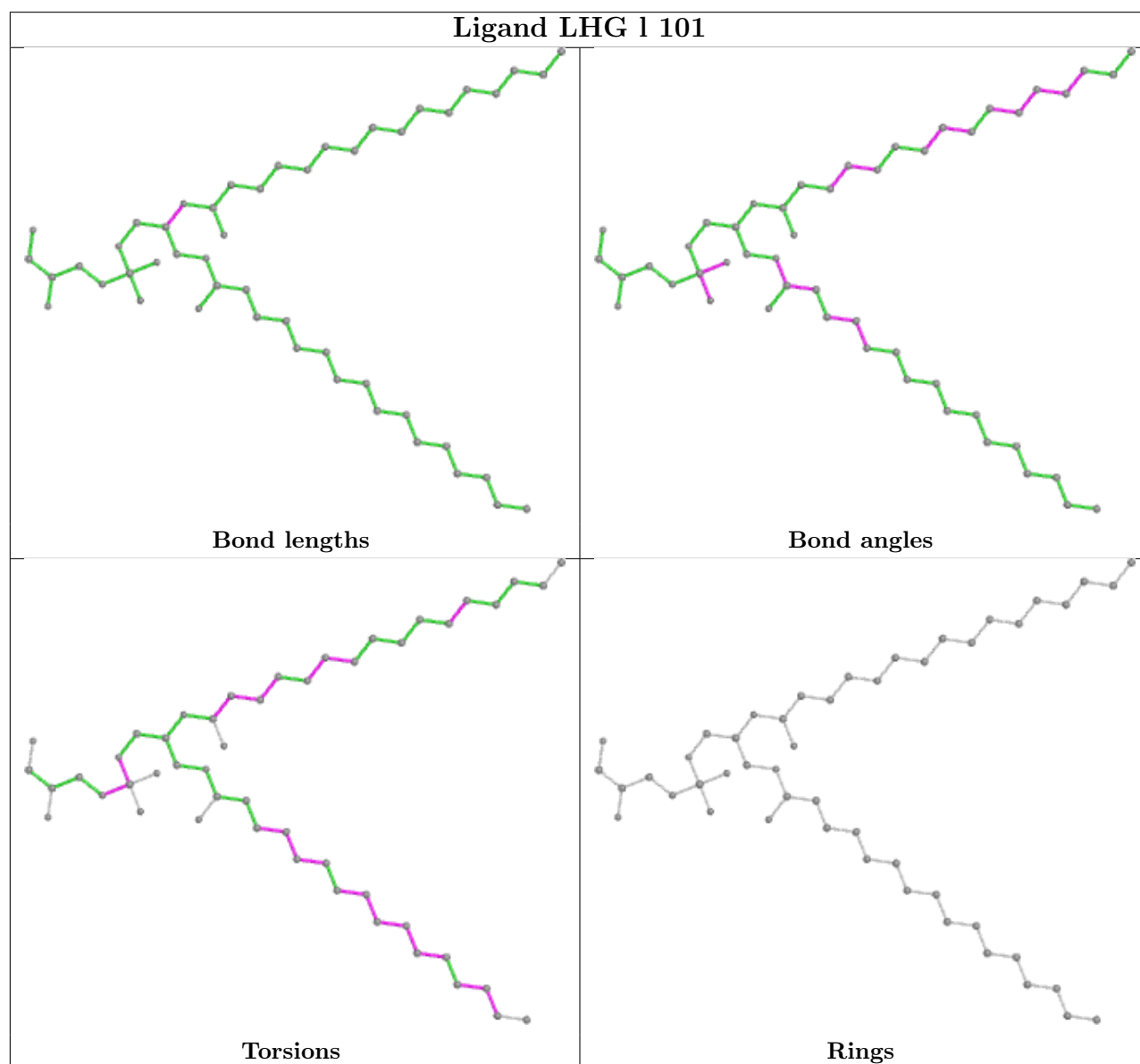
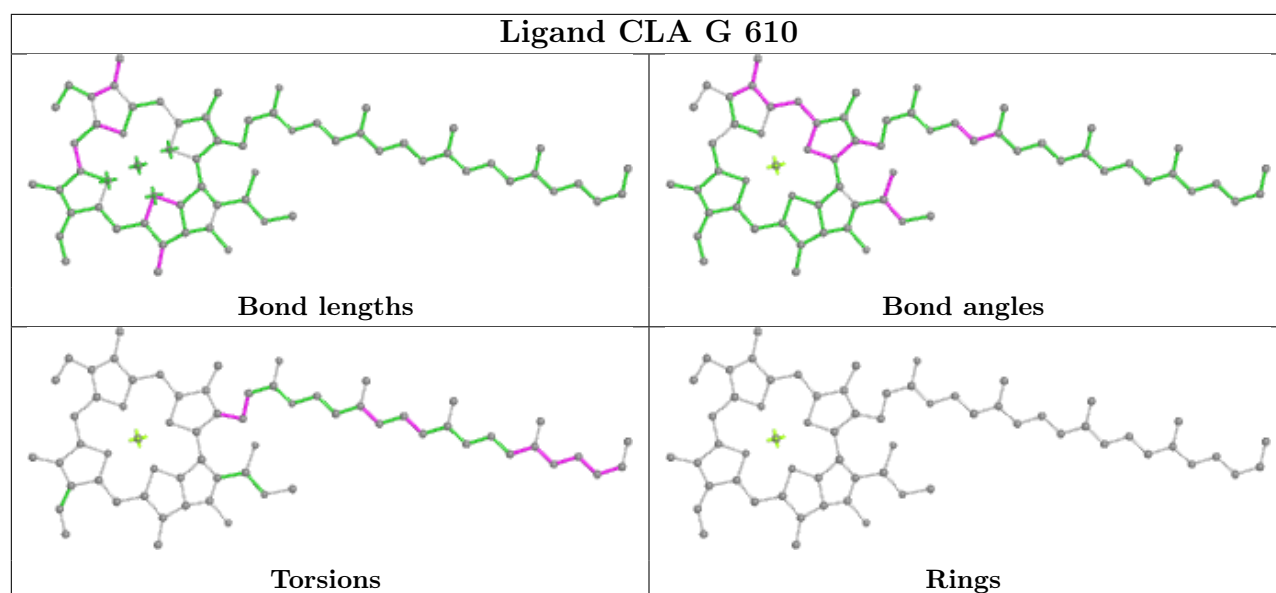
Rings

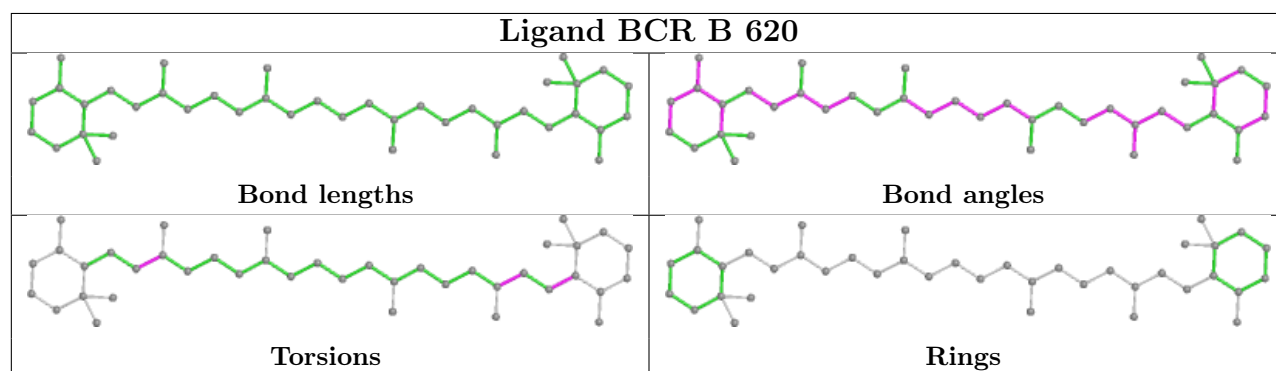
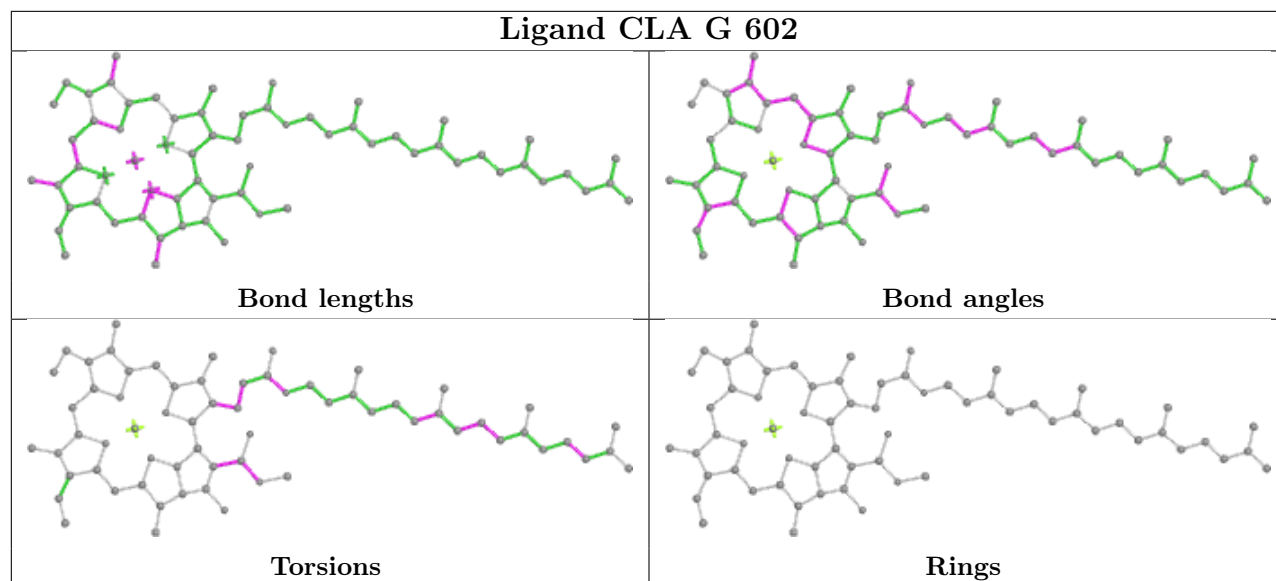
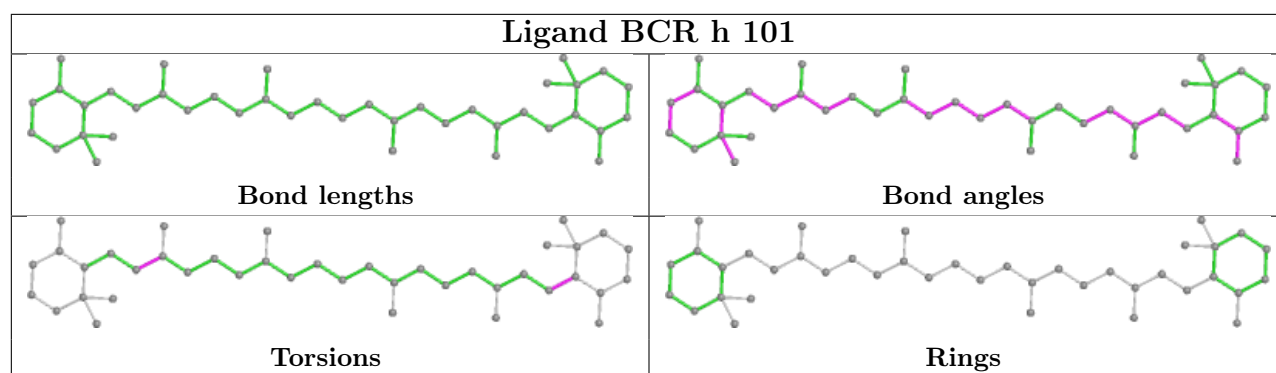
Ligand CHL s 601



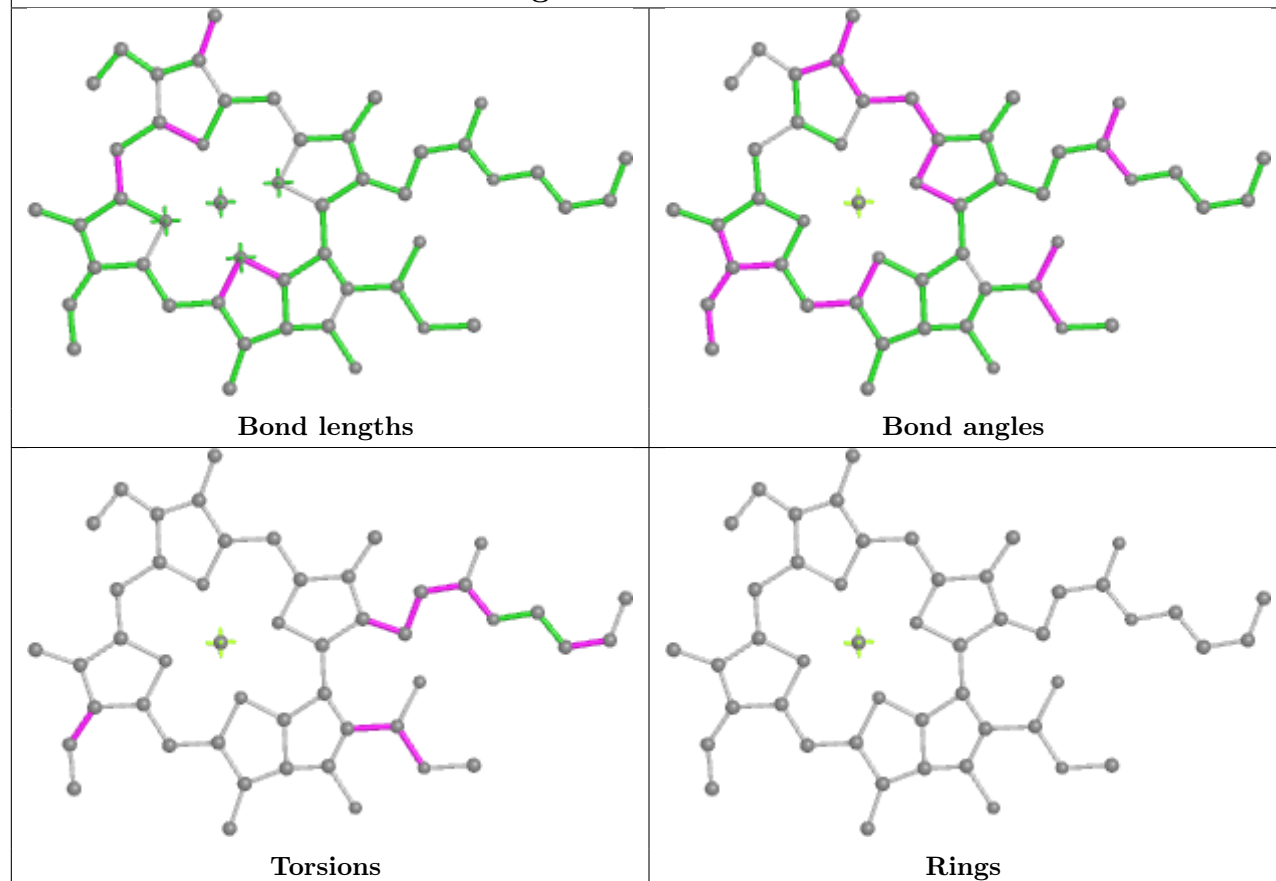
Ligand BCR c 517



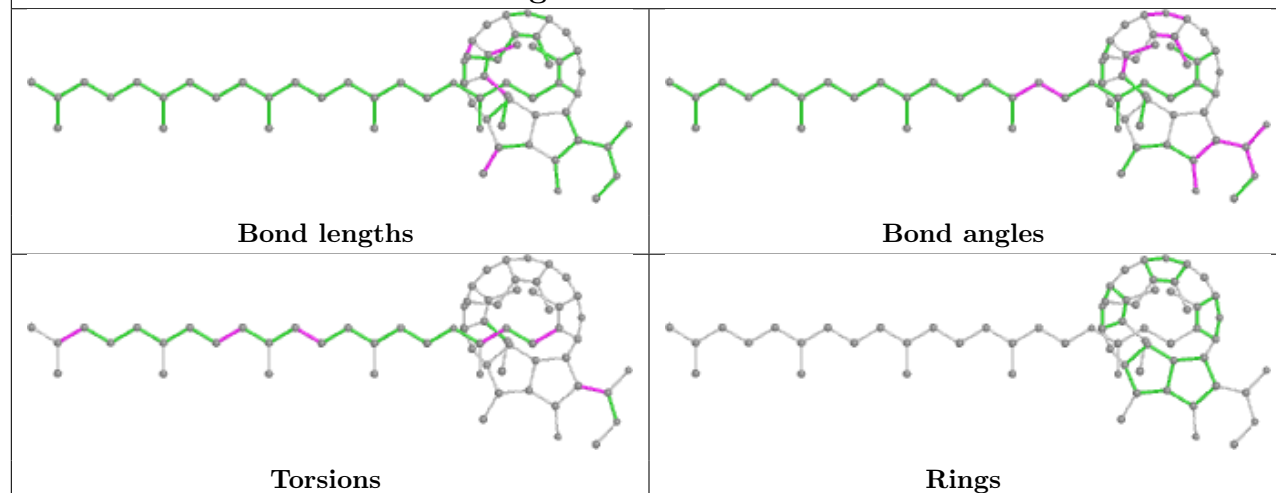


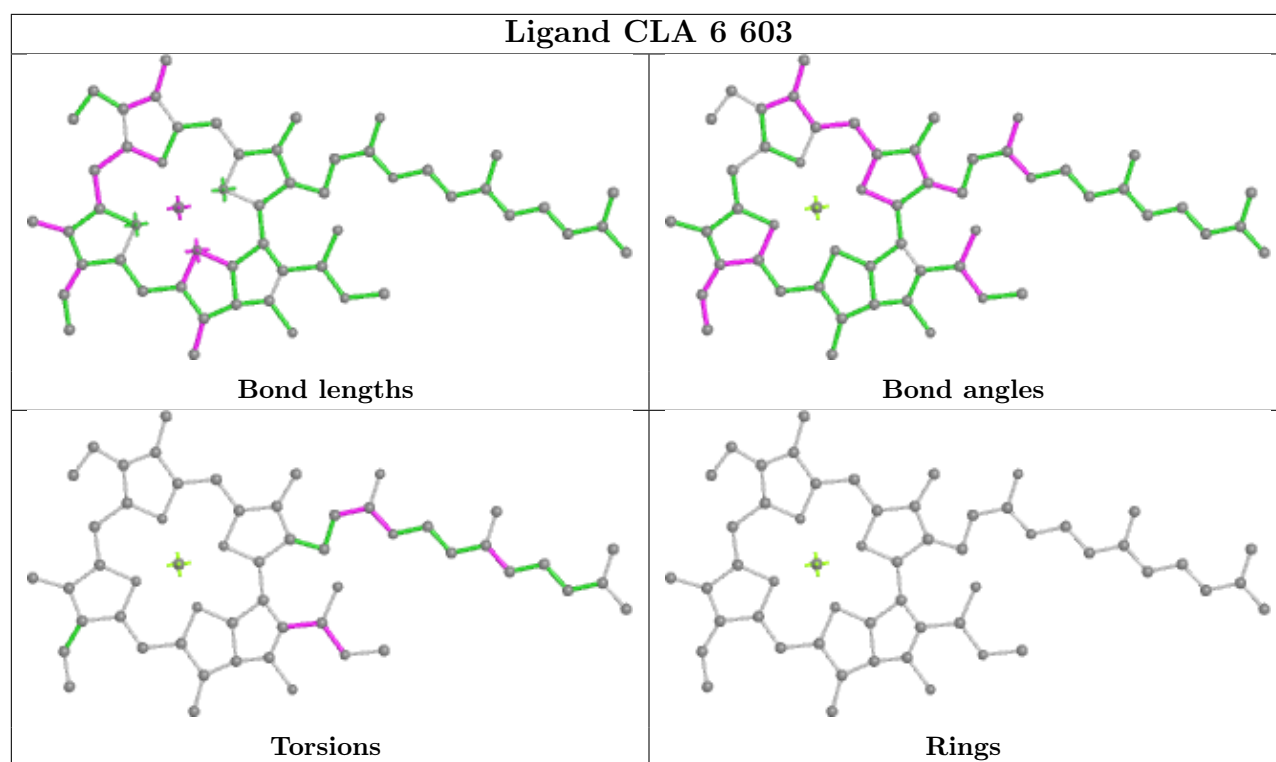


Ligand CLA R 601

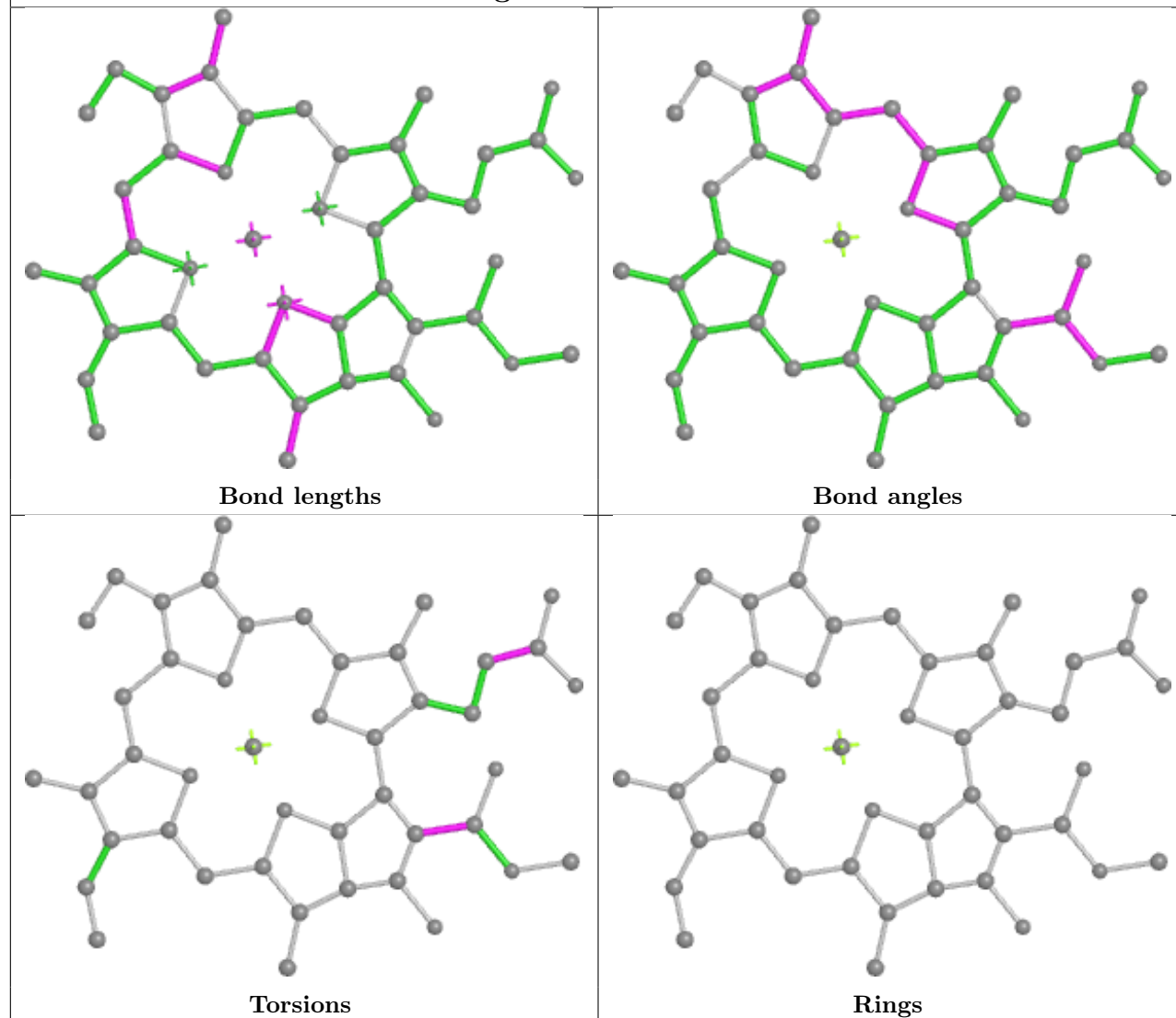


Ligand PHO A 409

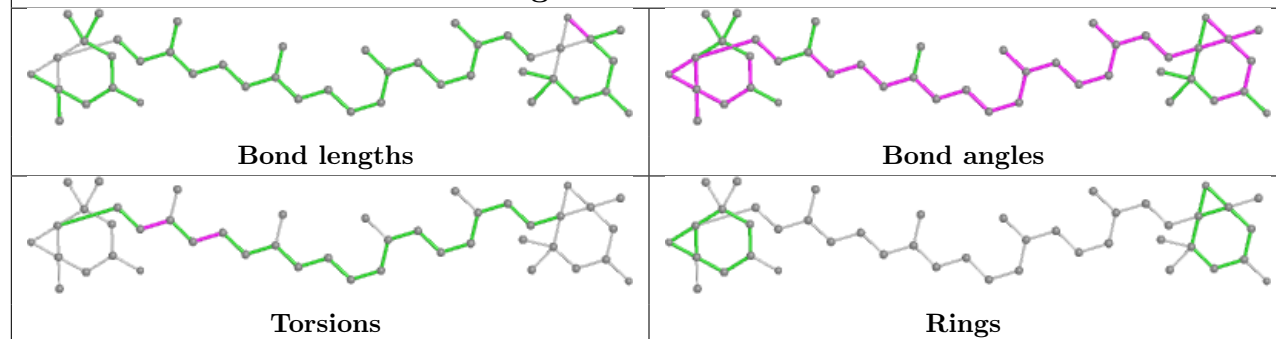


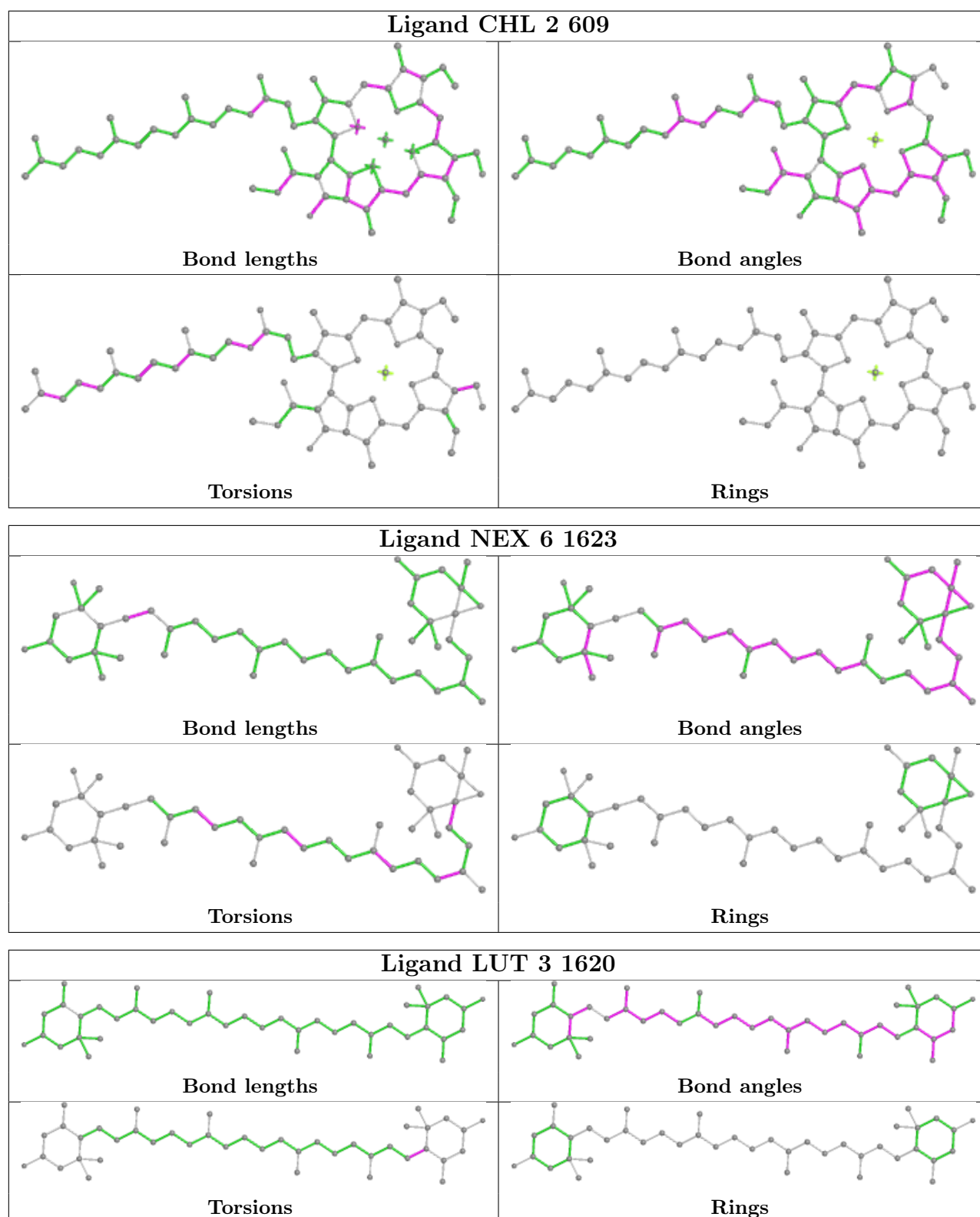


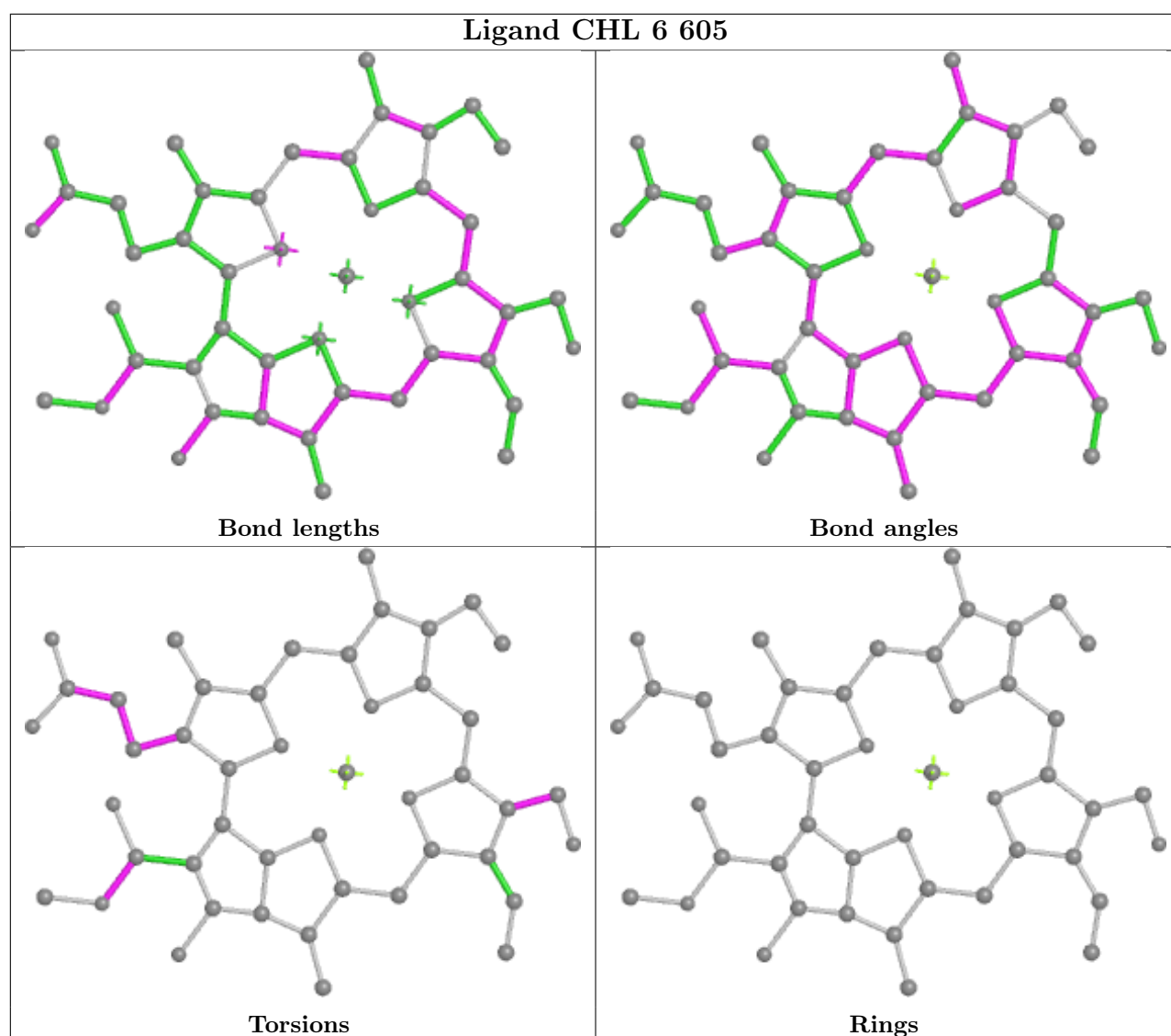
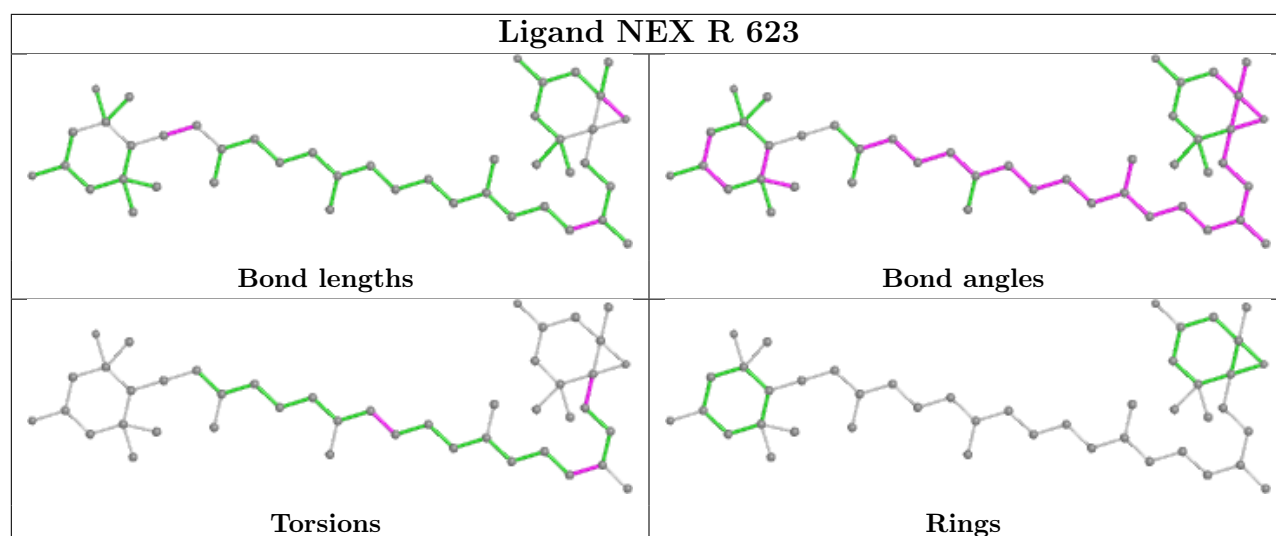
Ligand CLA 6 611

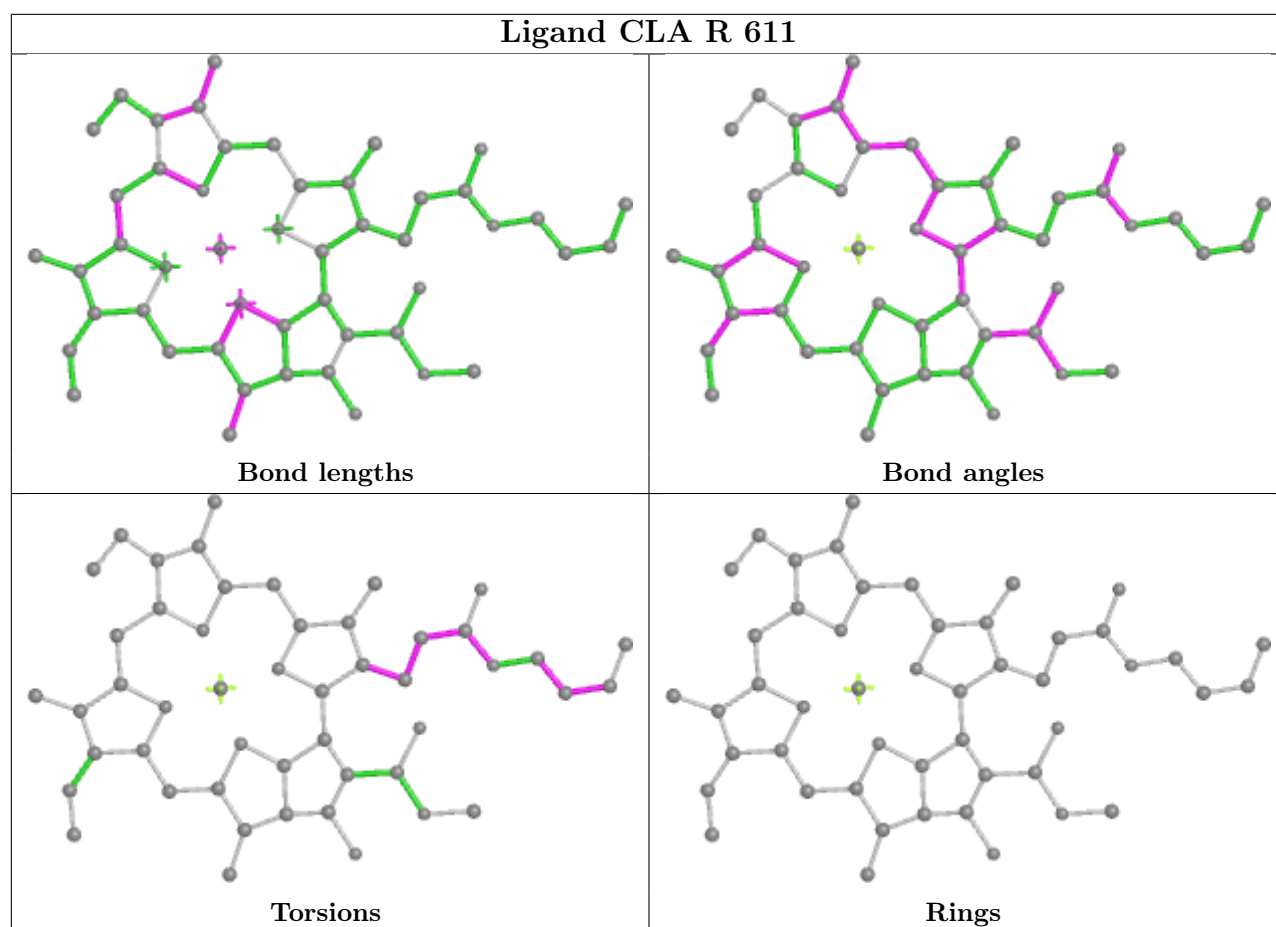


Ligand XAT R 622

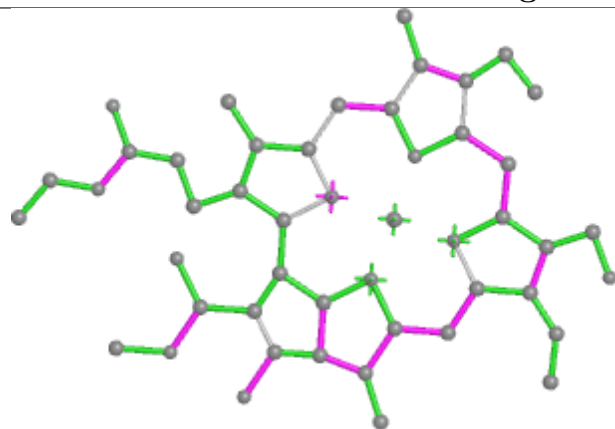




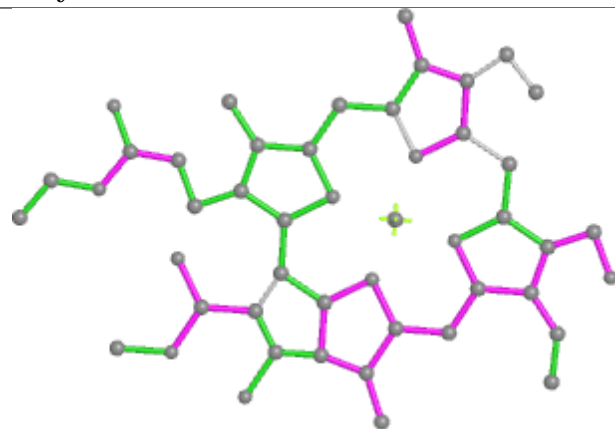




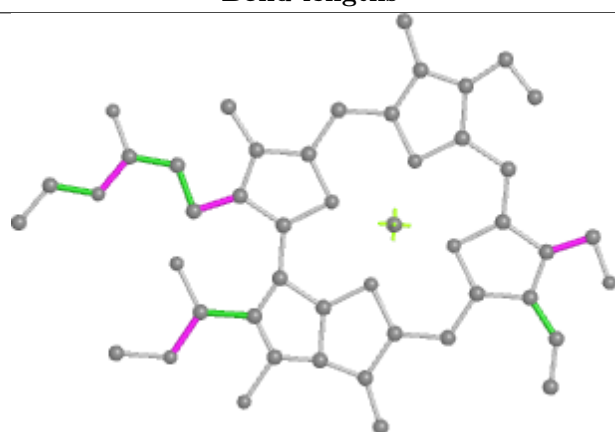
Ligand CHL y 605



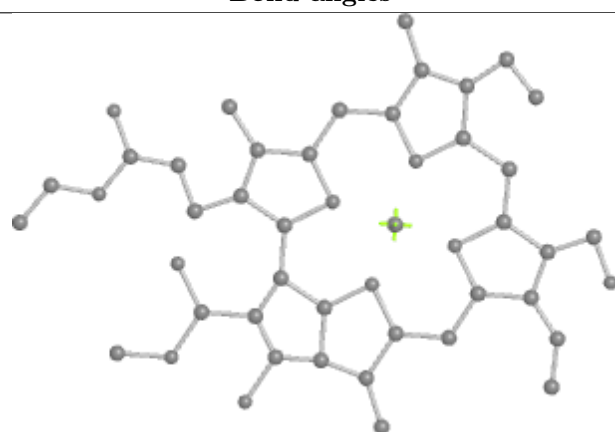
Bond lengths



Bond angles

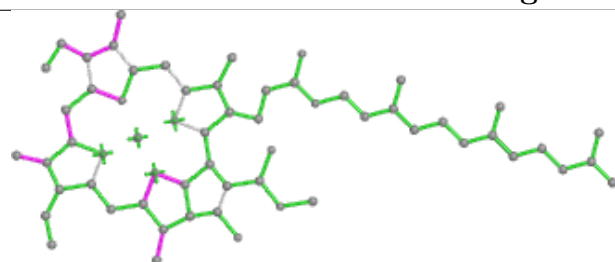


Torsions

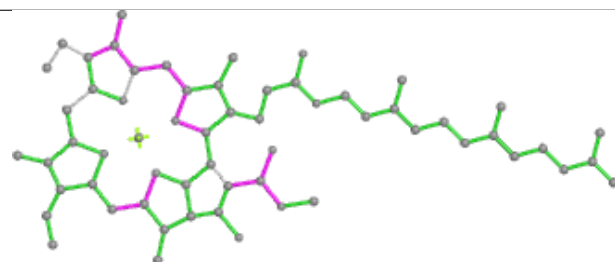


Rings

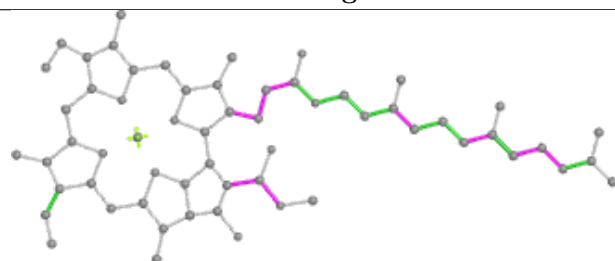
Ligand CLA 3 602



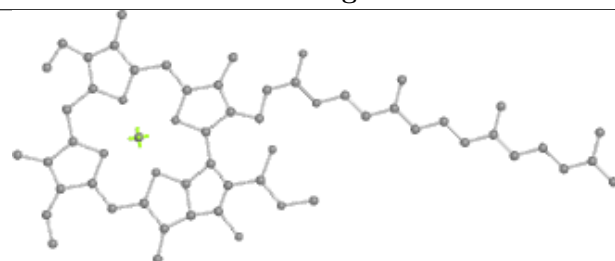
Bond lengths



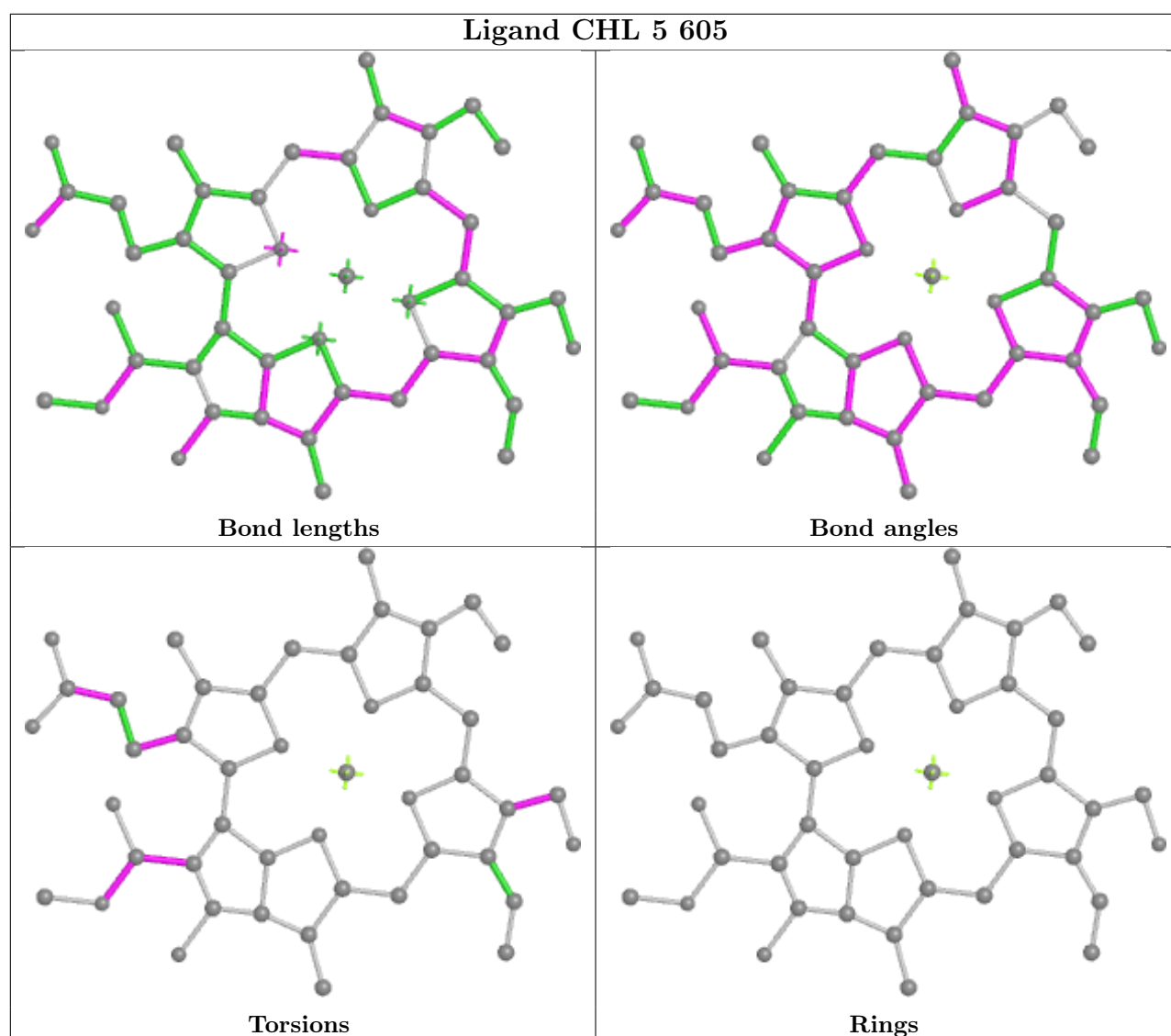
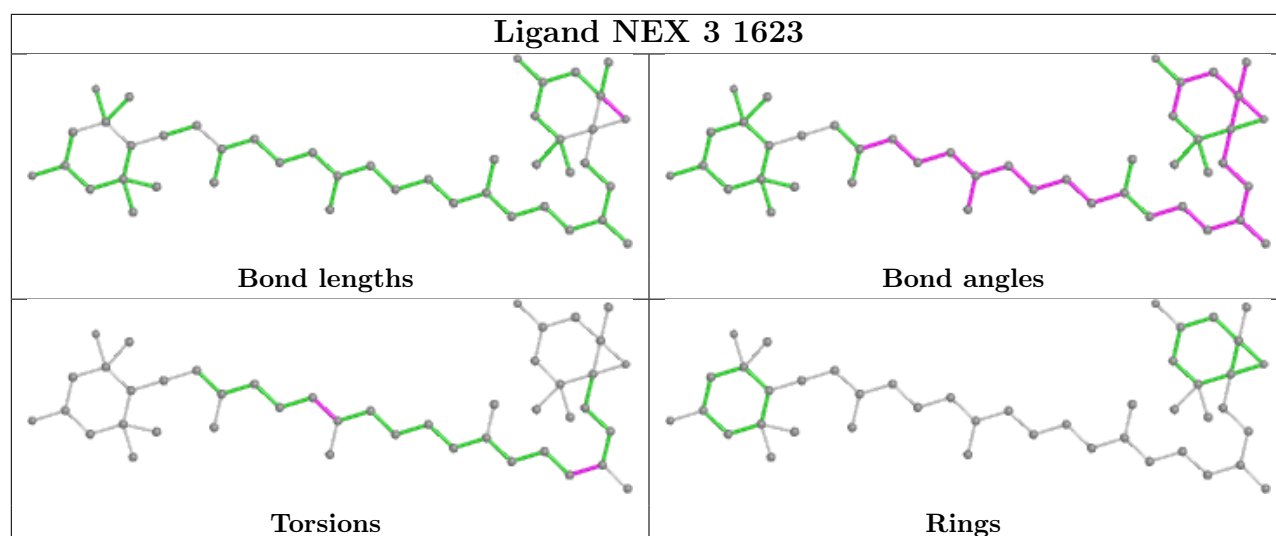
Bond angles

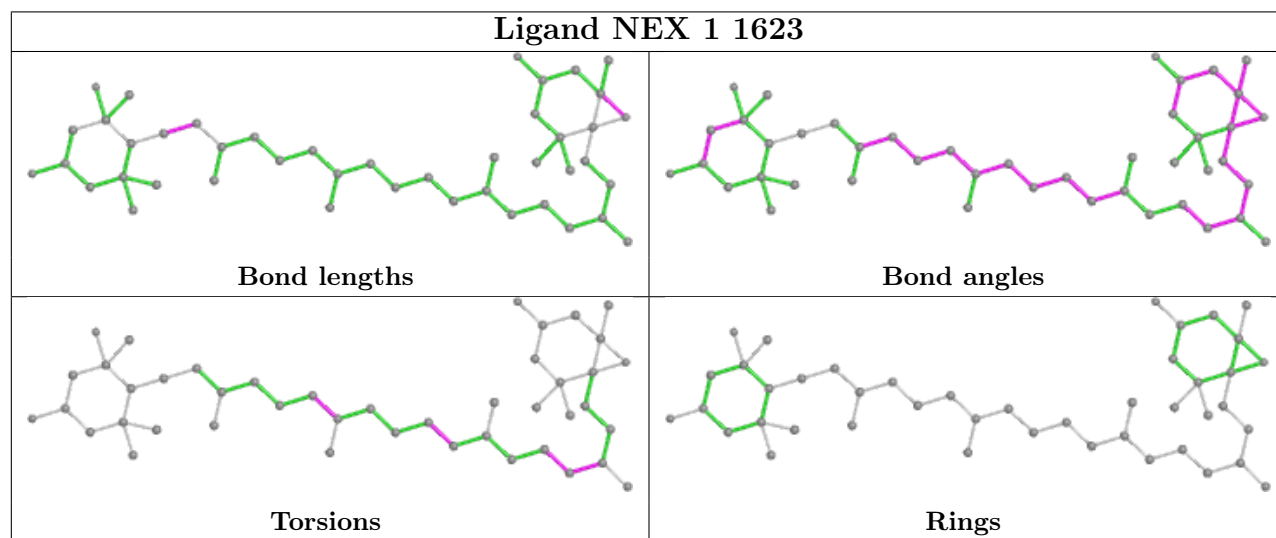
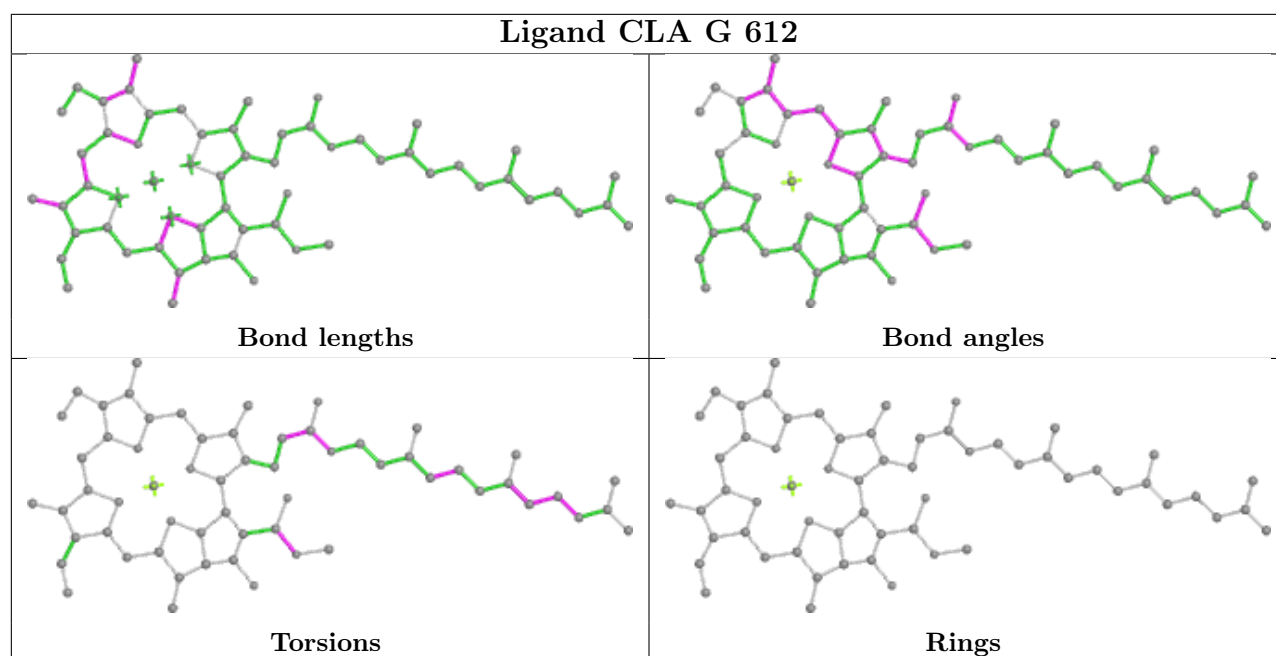


Torsions

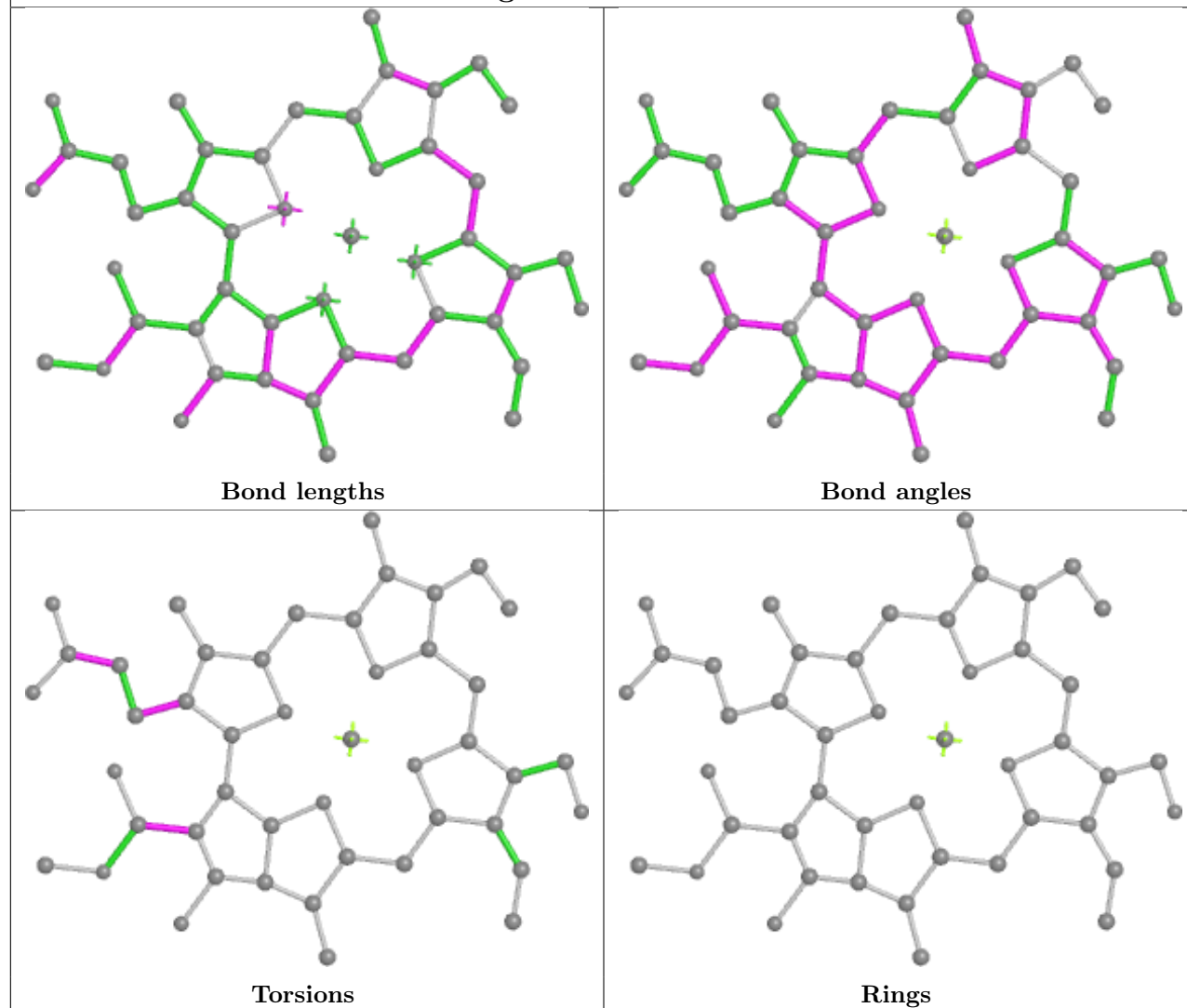


Rings

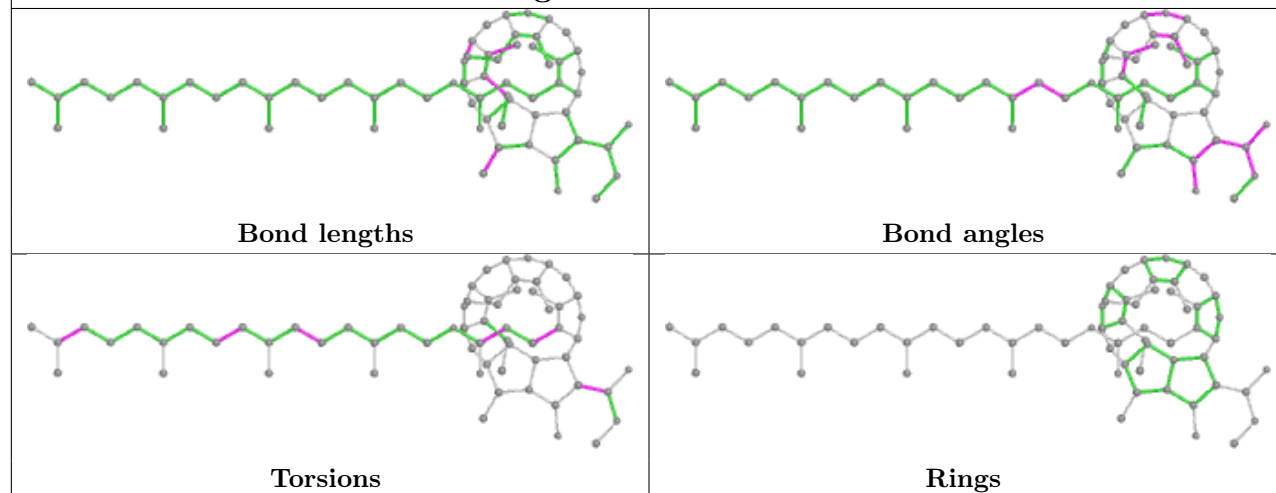


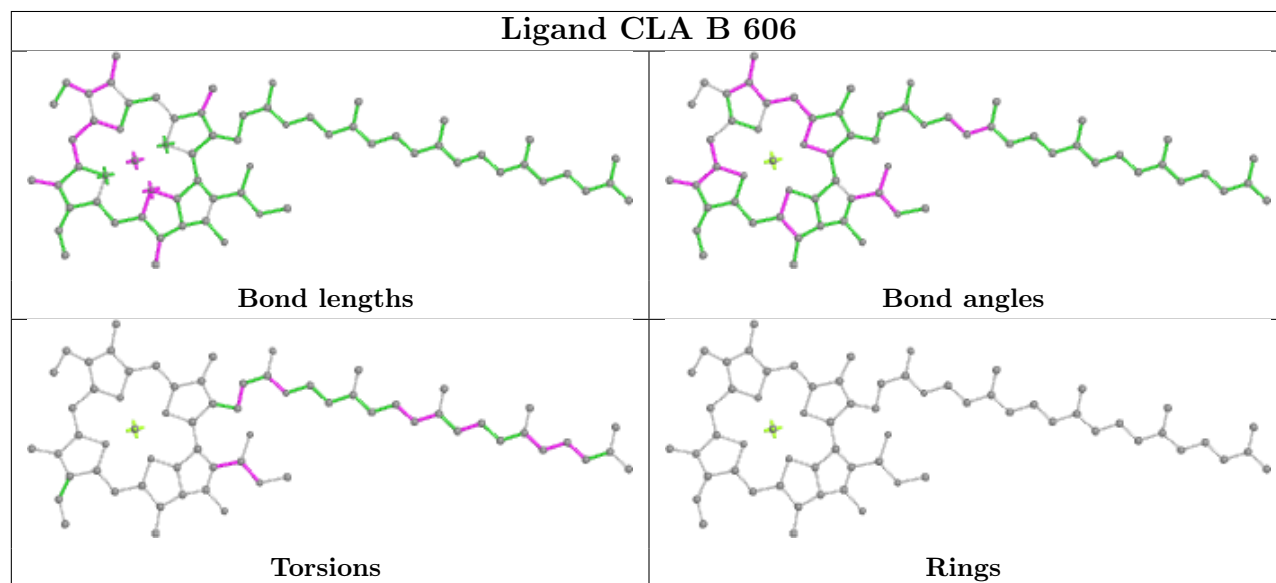
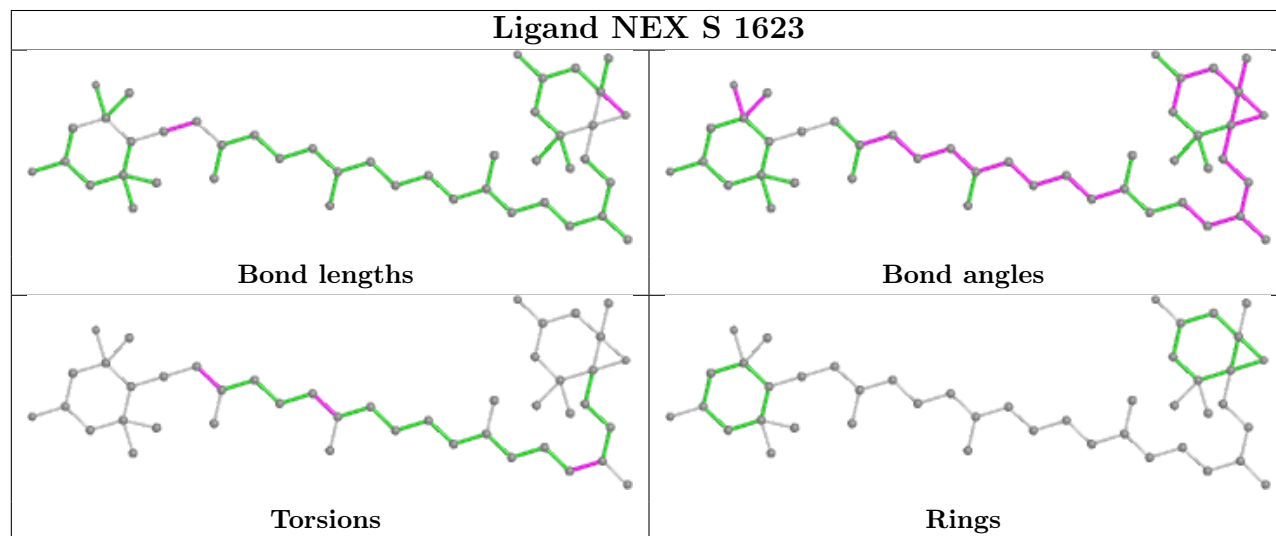
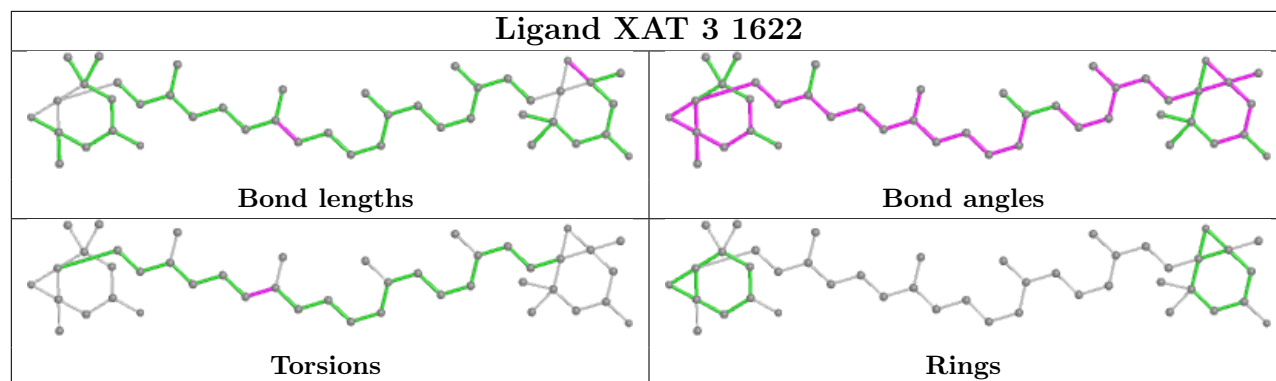


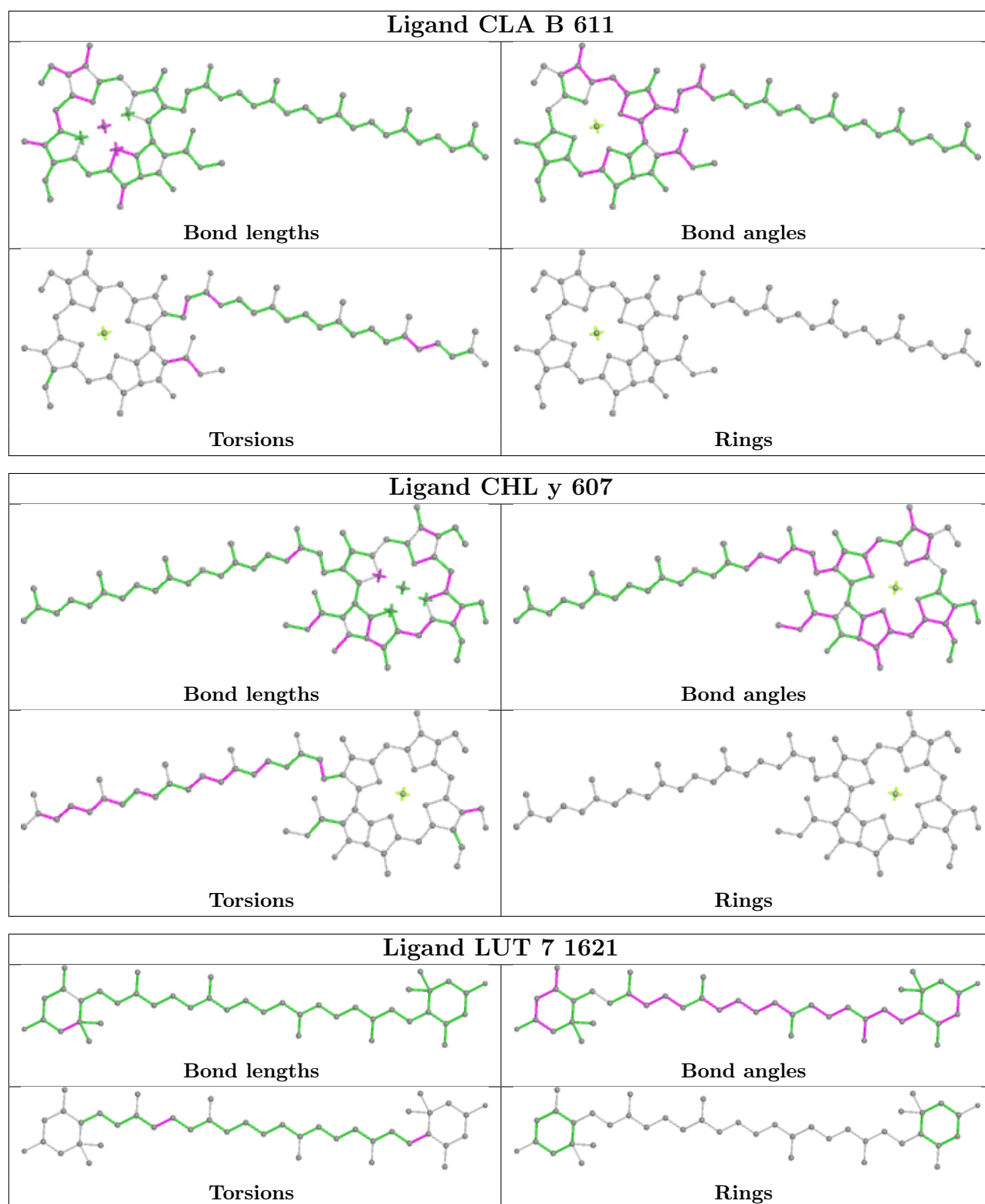
Ligand CHL 2 601

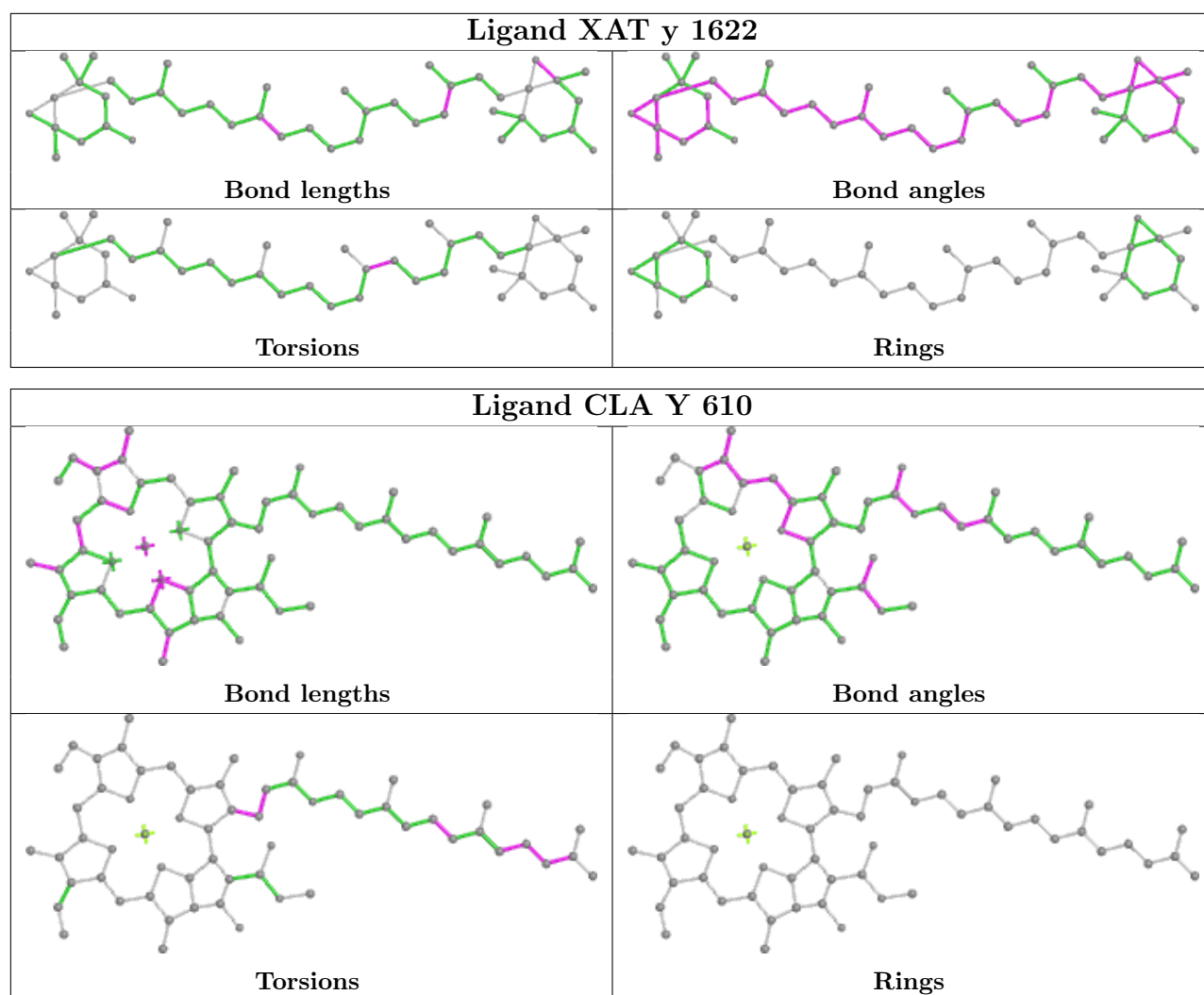


Ligand PHO a 409

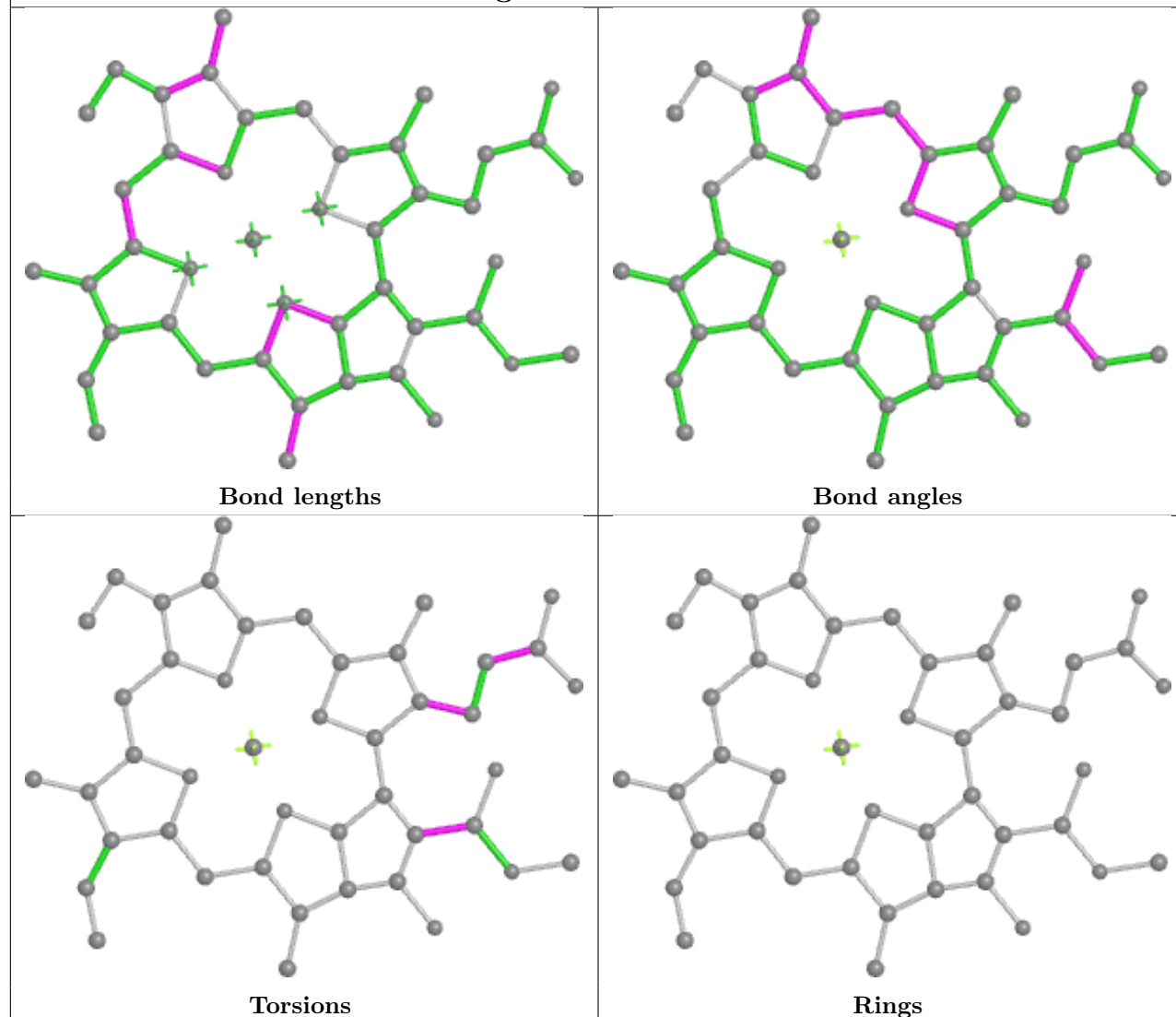




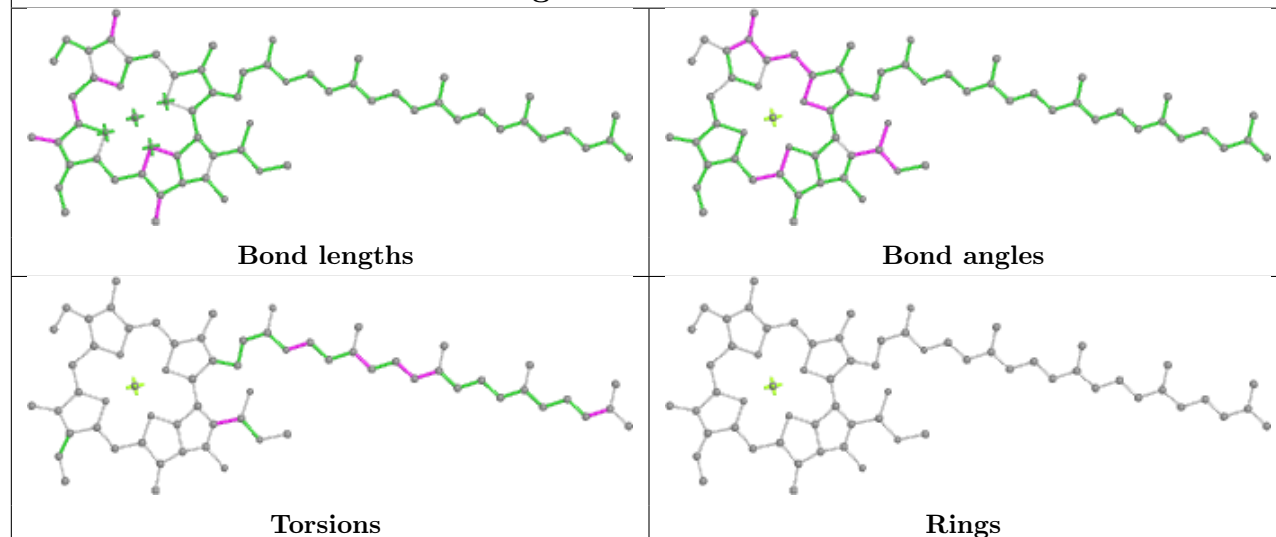


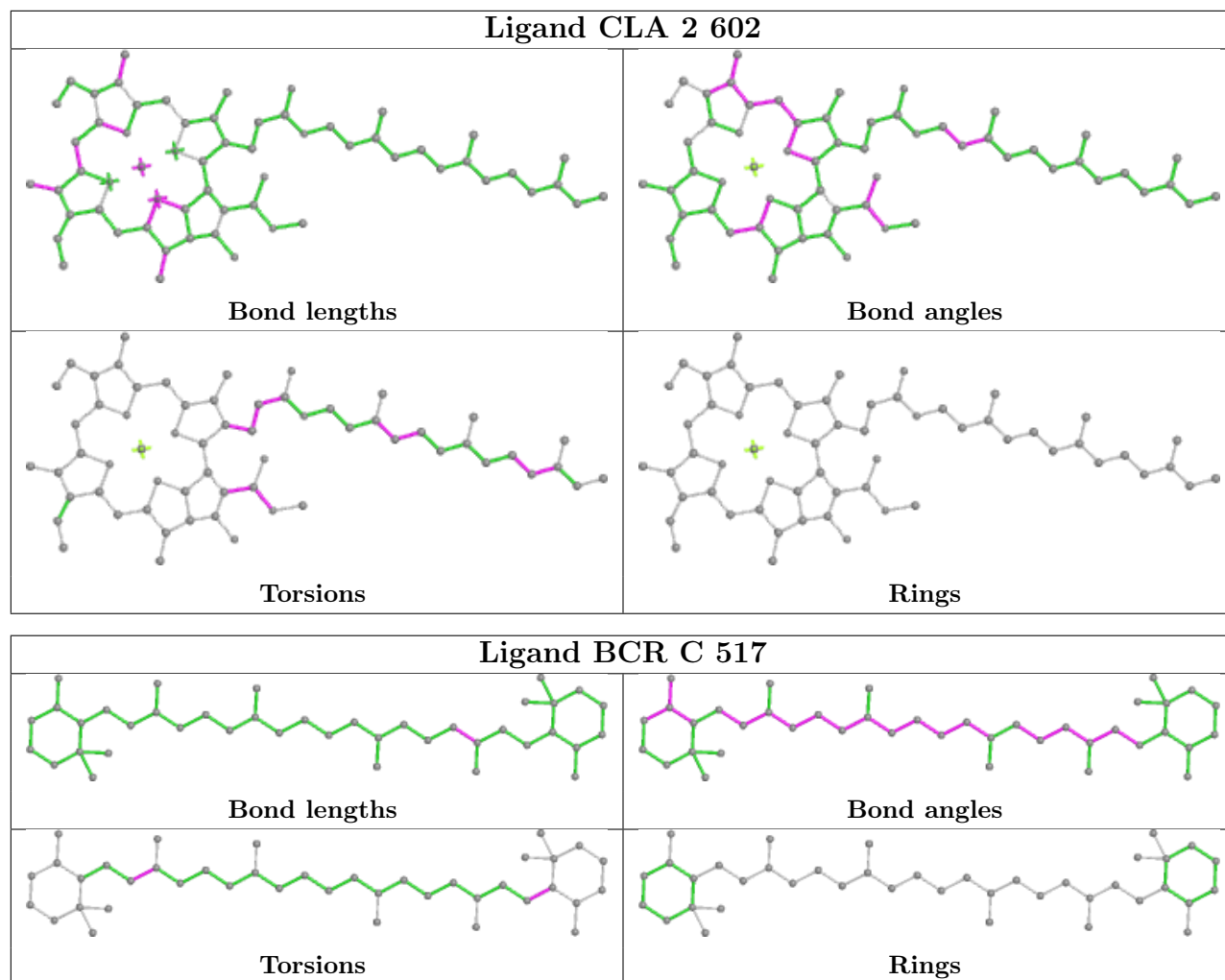


Ligand CLA r 616

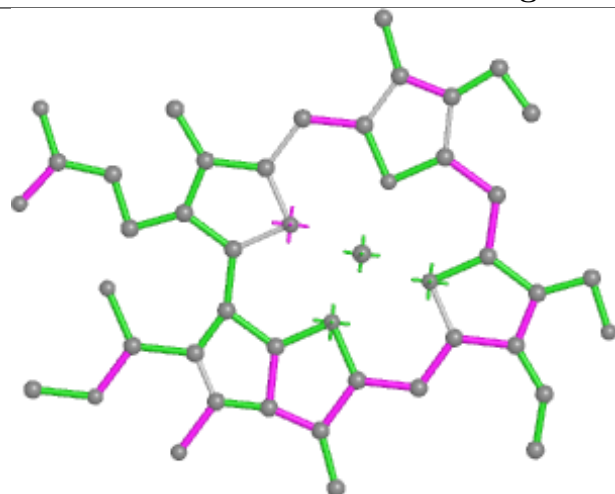


Ligand CLA B 603

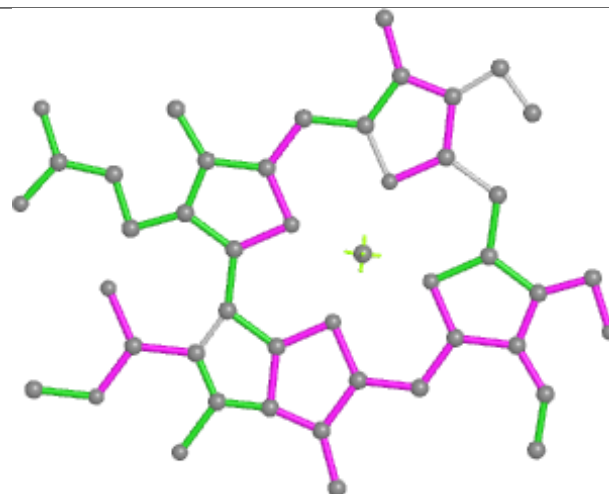




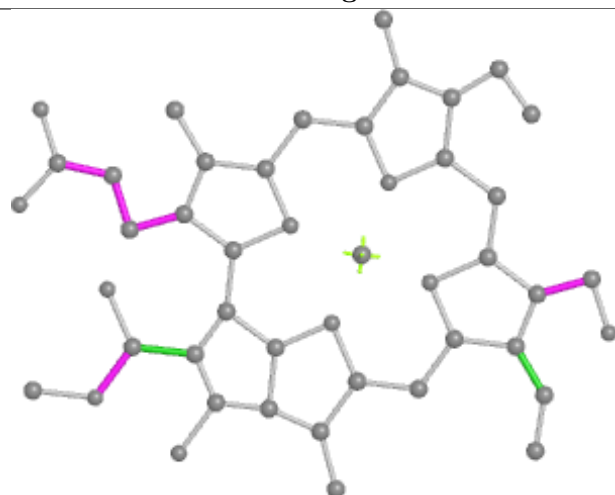
Ligand CHL 7 606



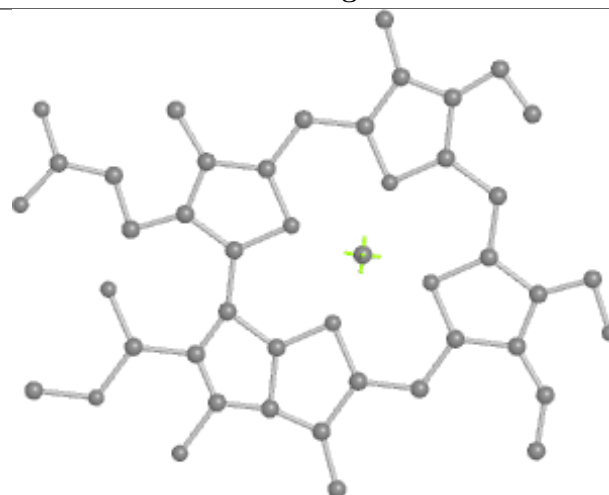
Bond lengths



Bond angles

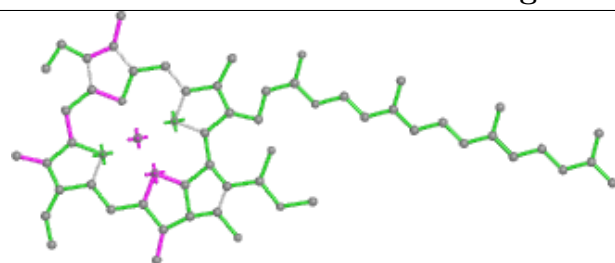


Torsions

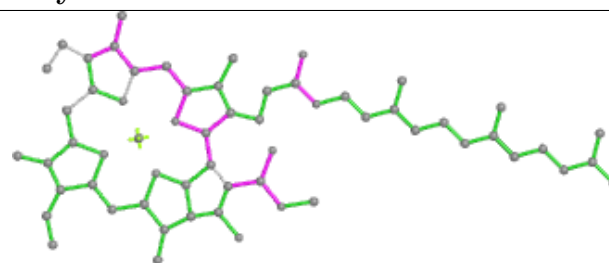


Rings

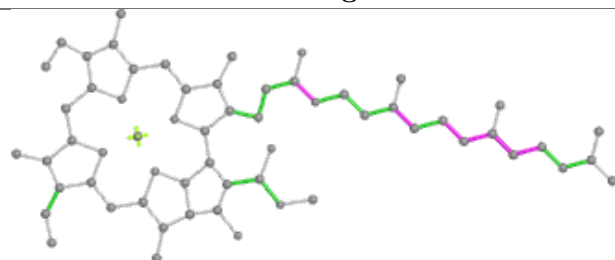
Ligand CLA y 611



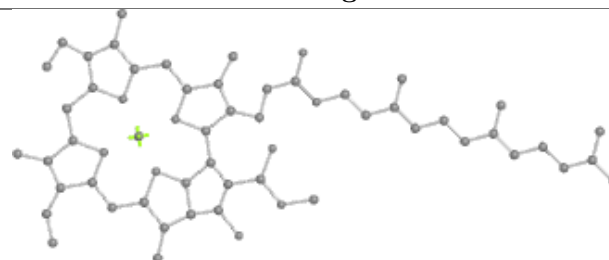
Bond lengths



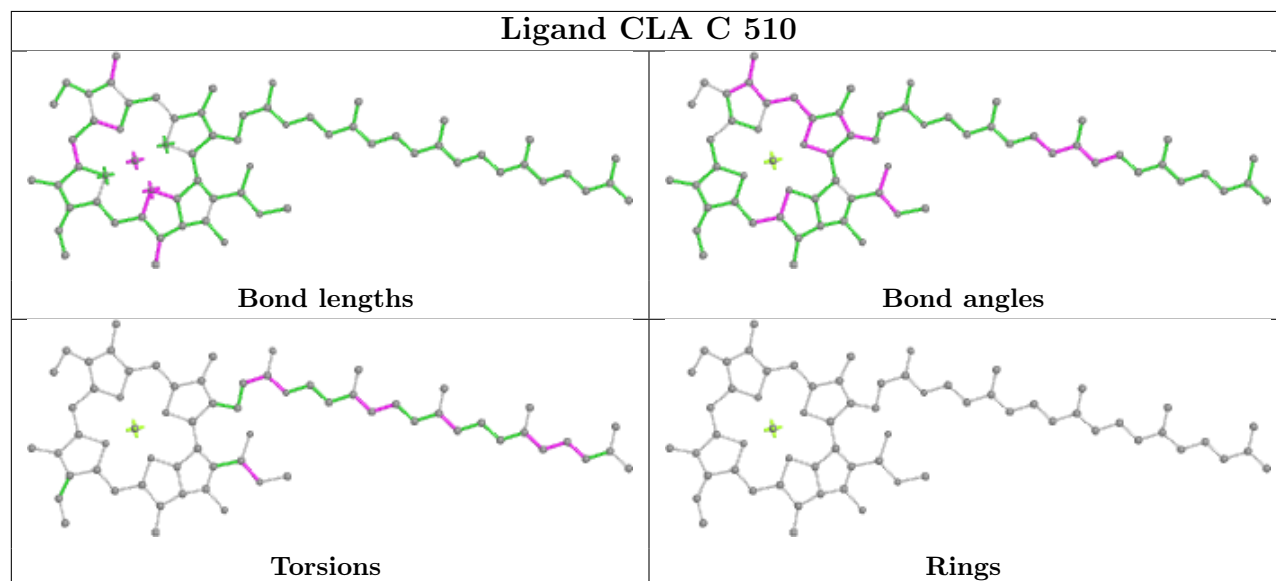
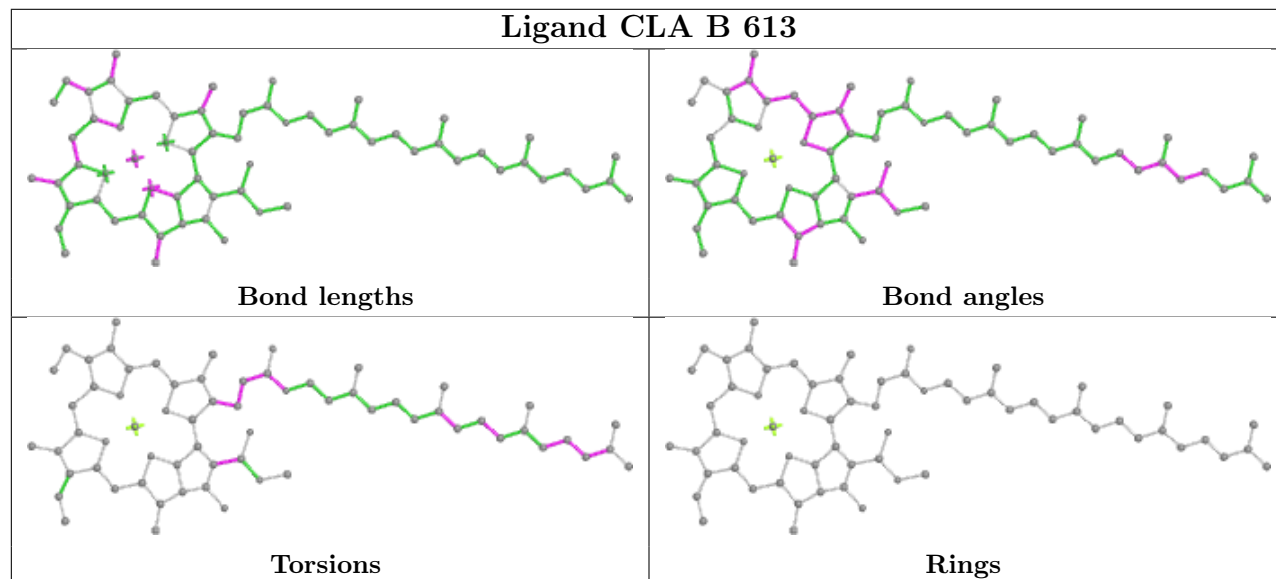
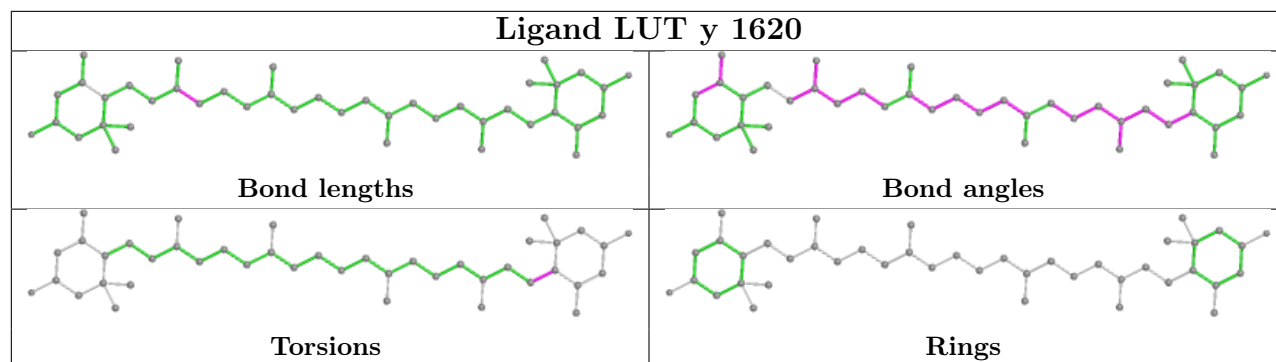
Bond angles

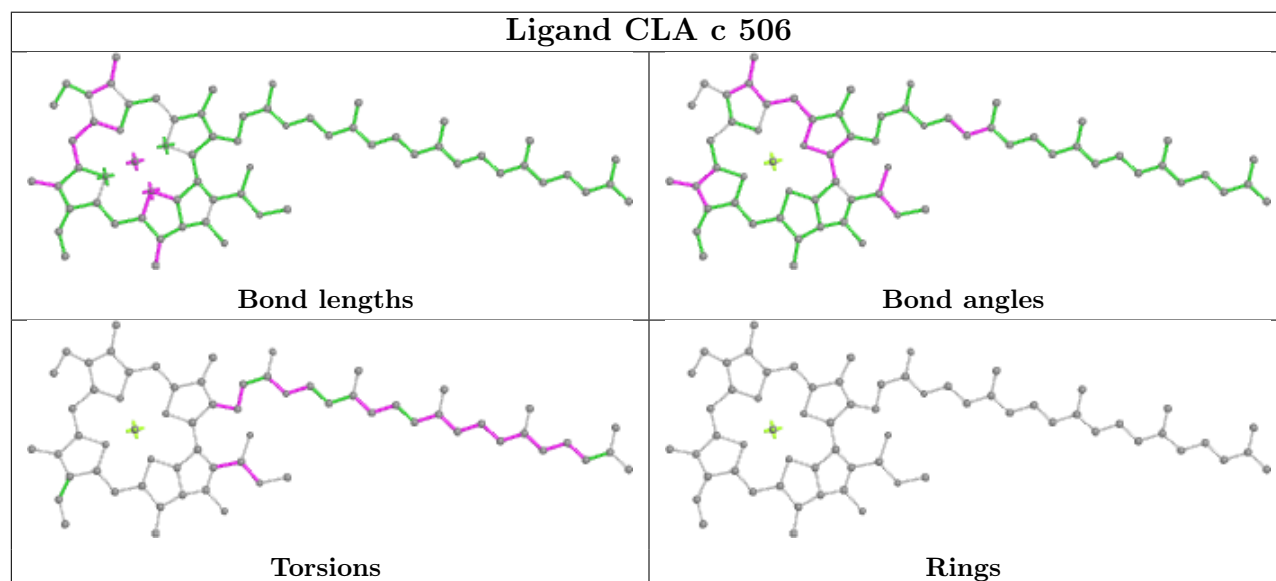
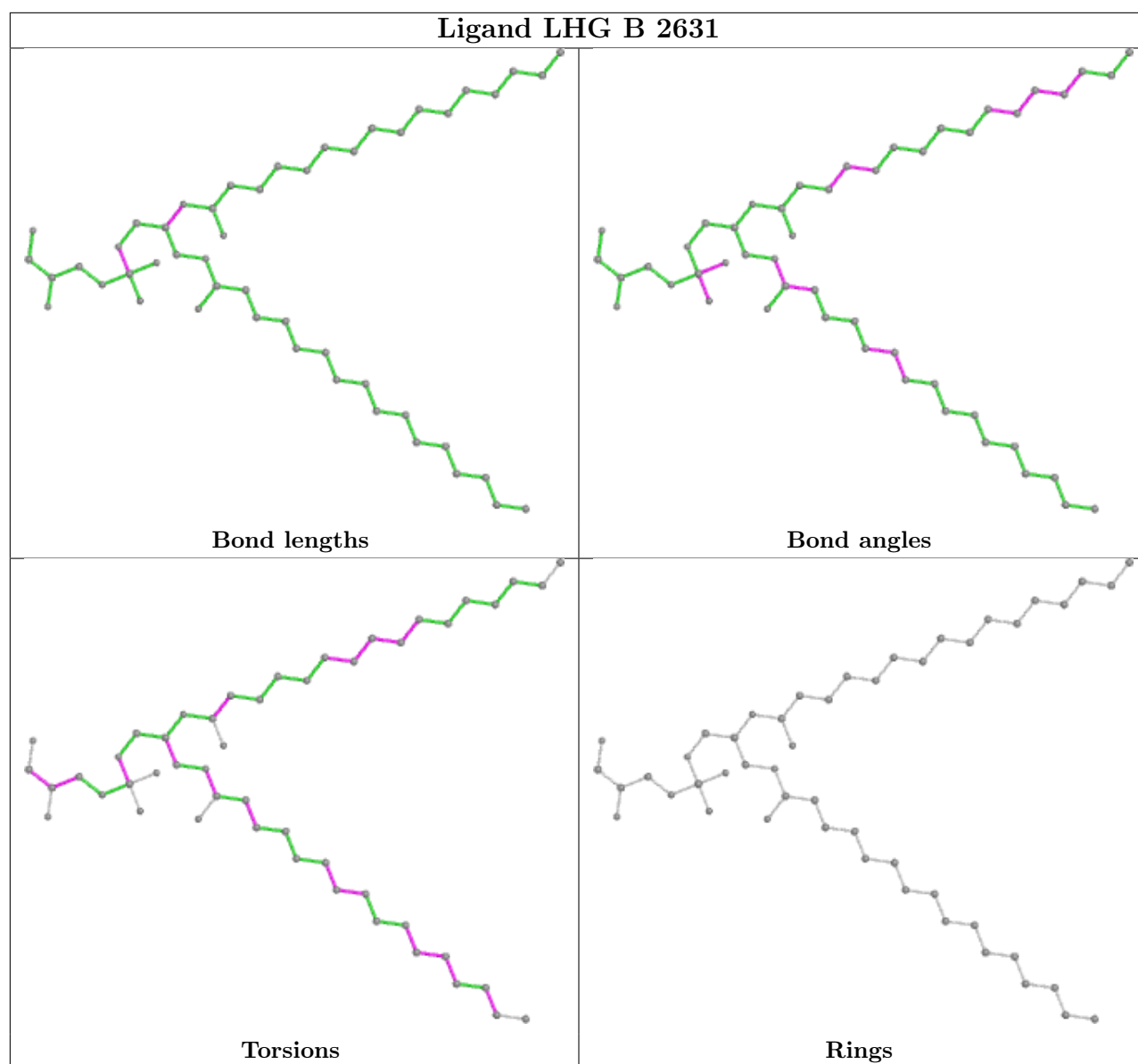


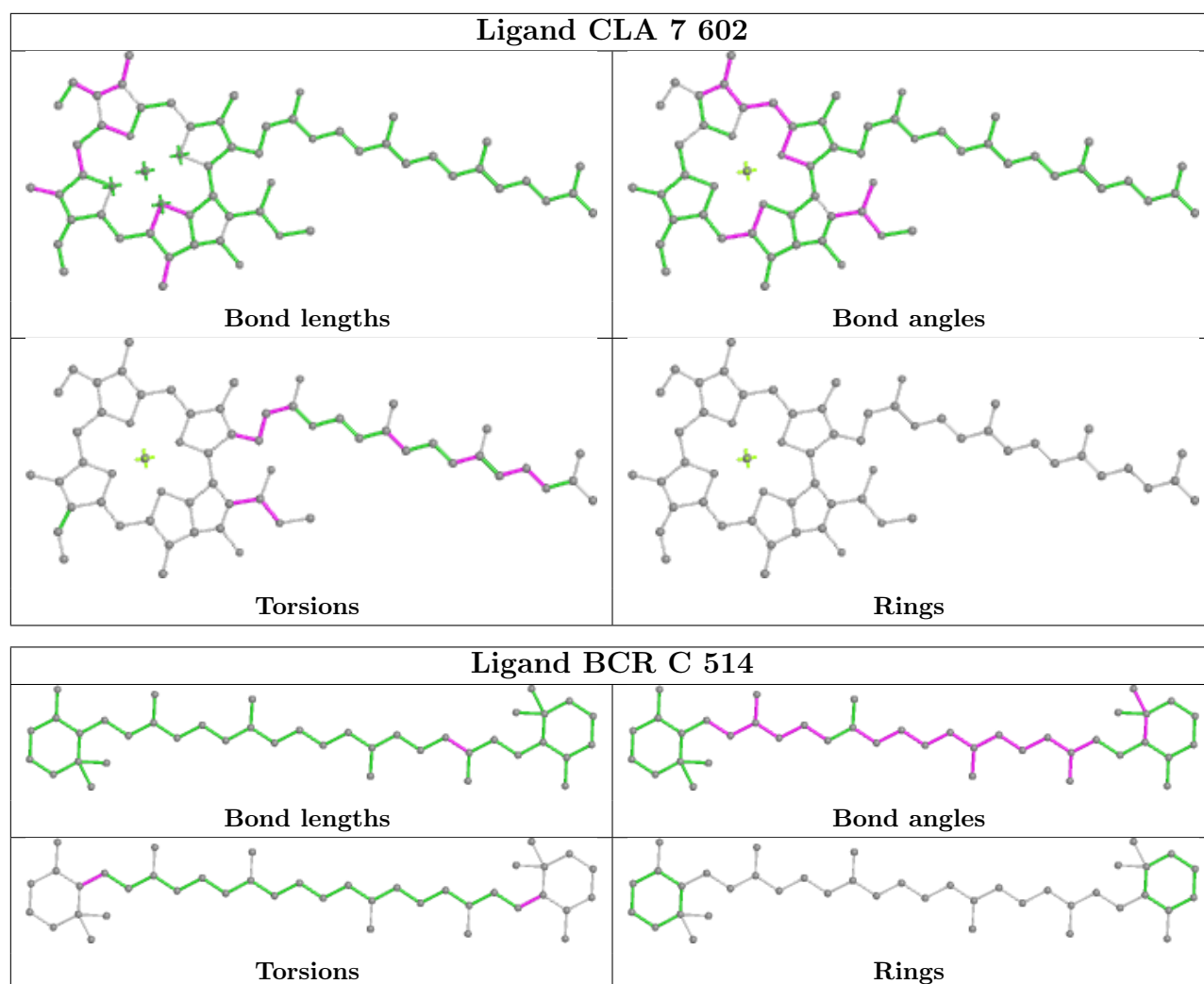
Torsions

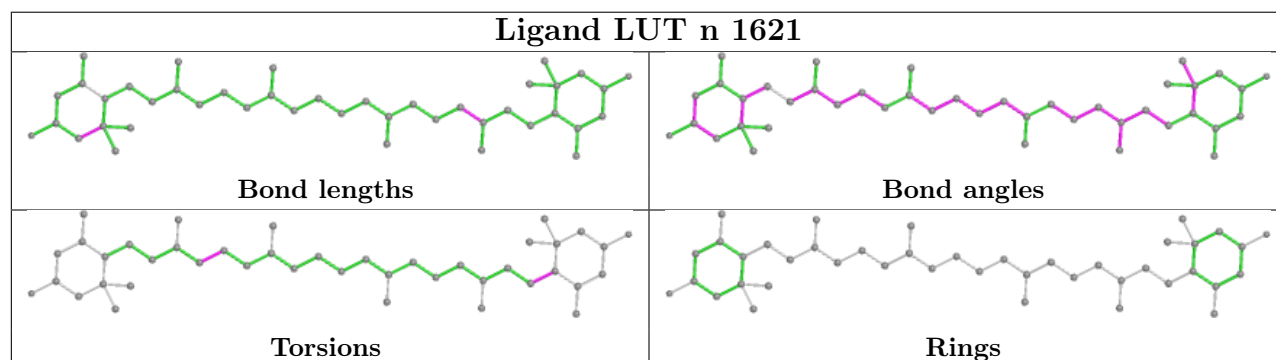
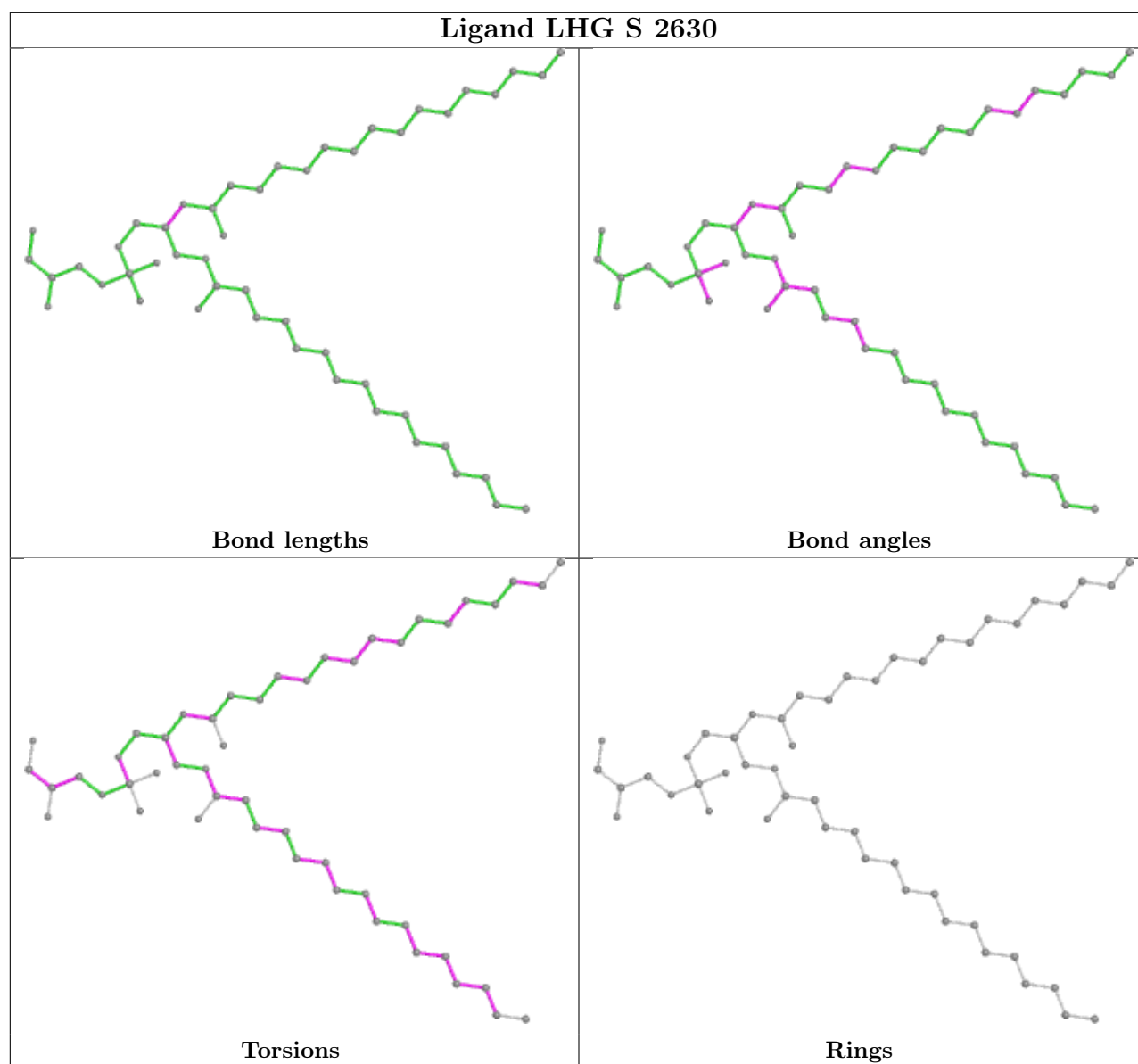


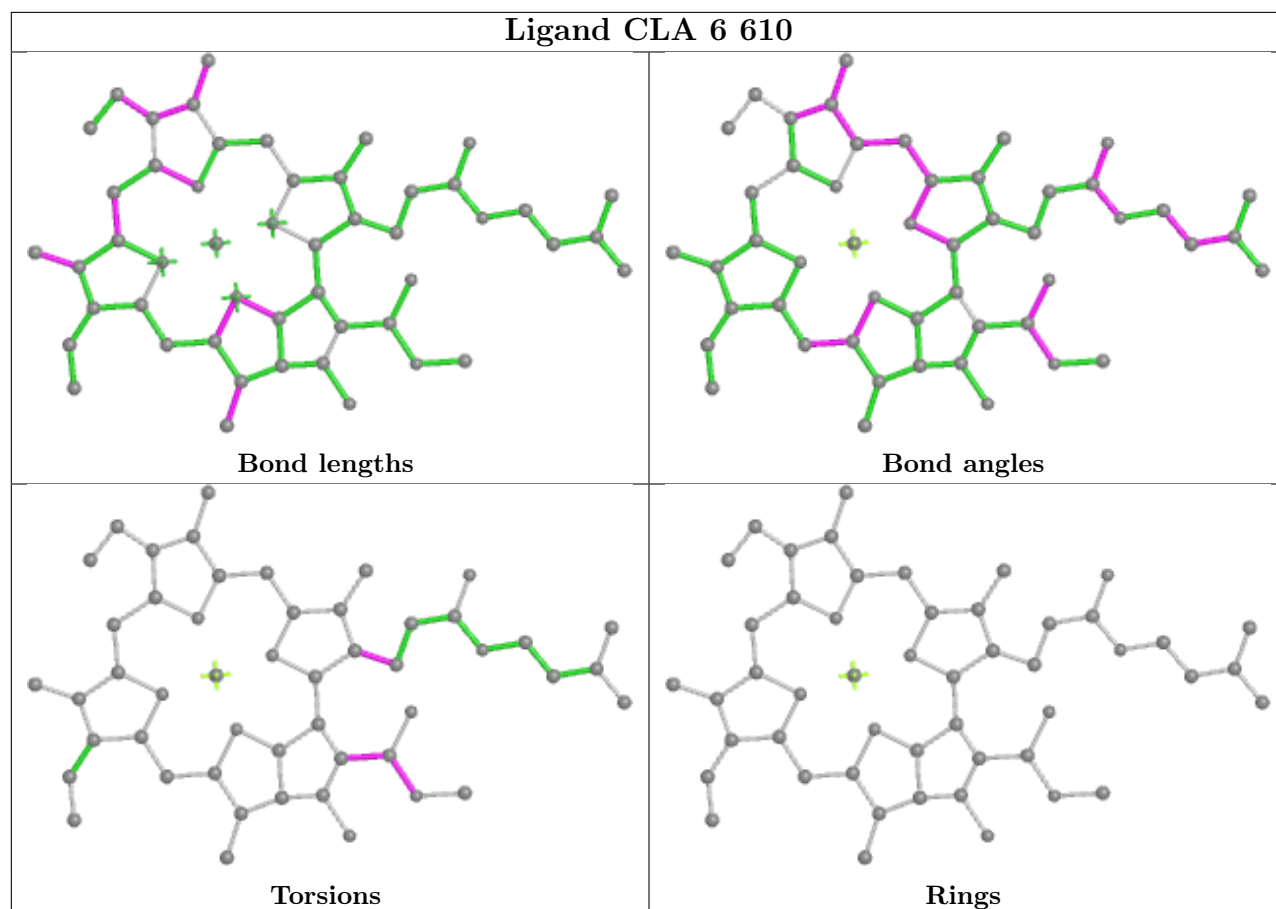
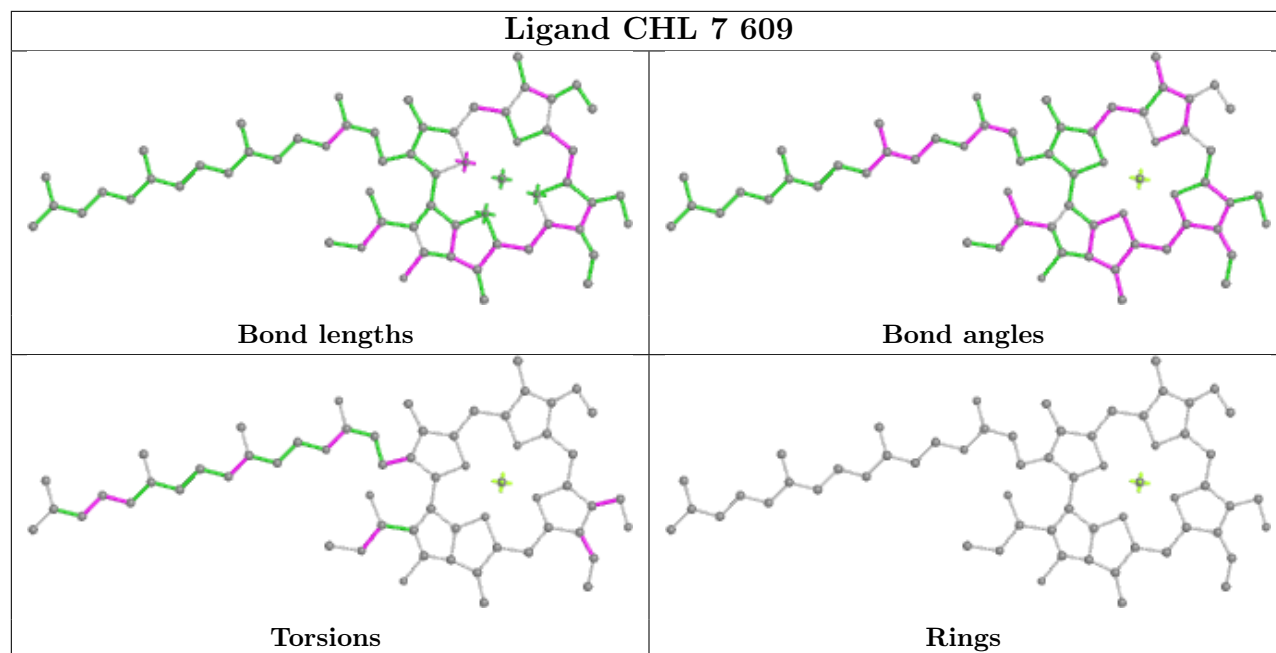
Rings



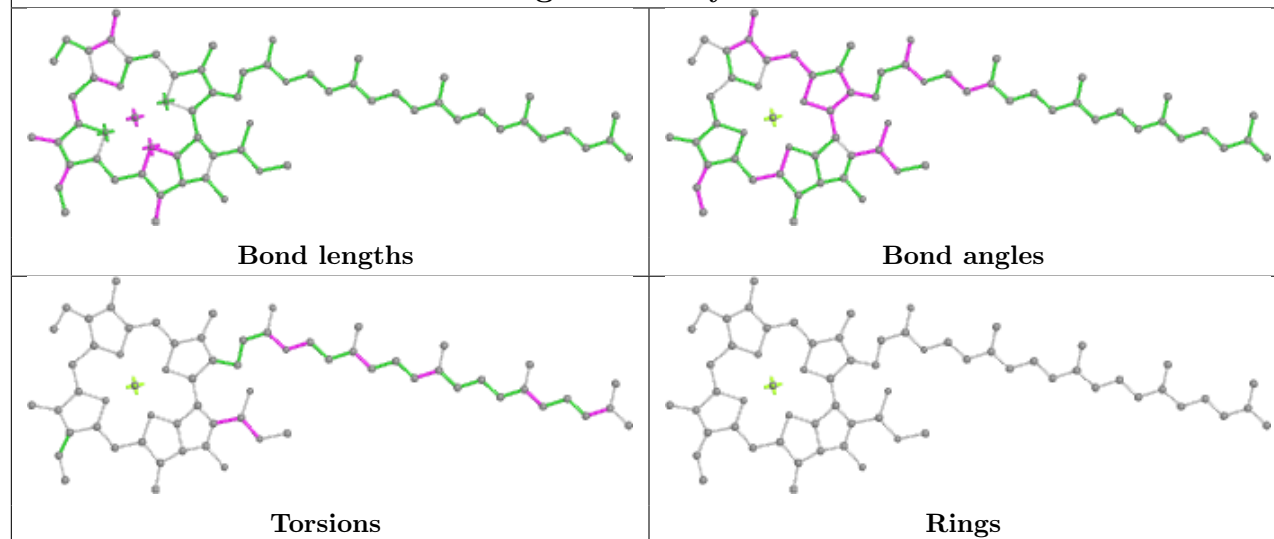




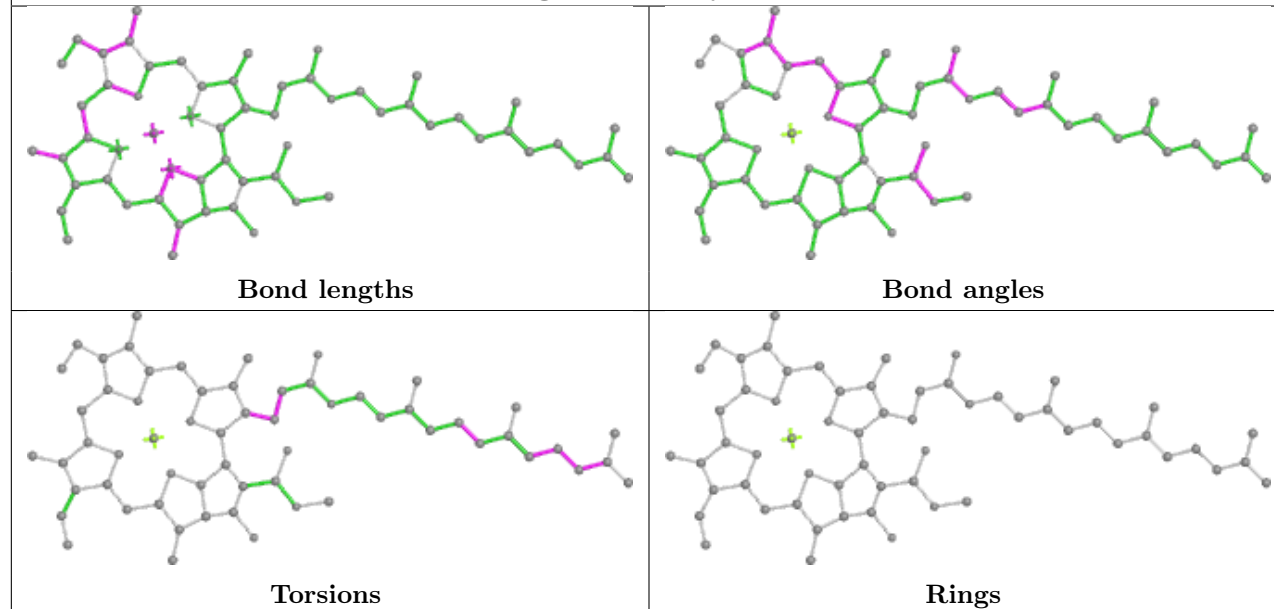




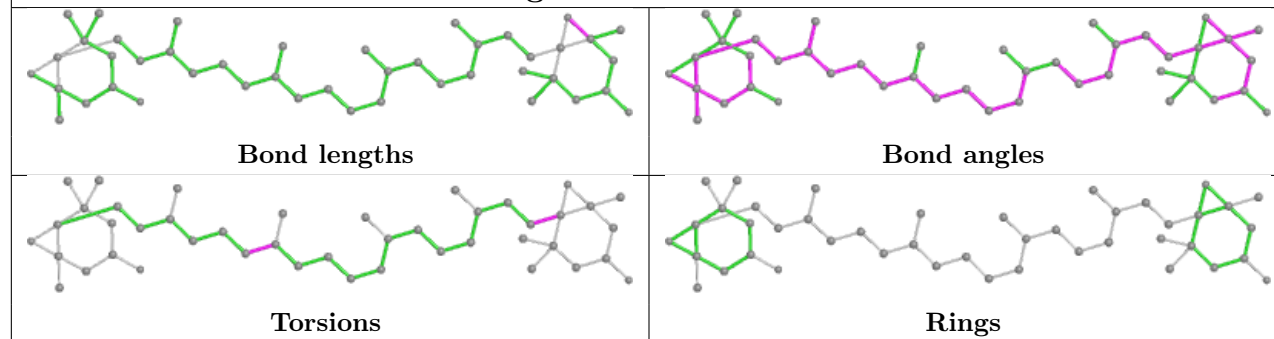
Ligand CLA y 603

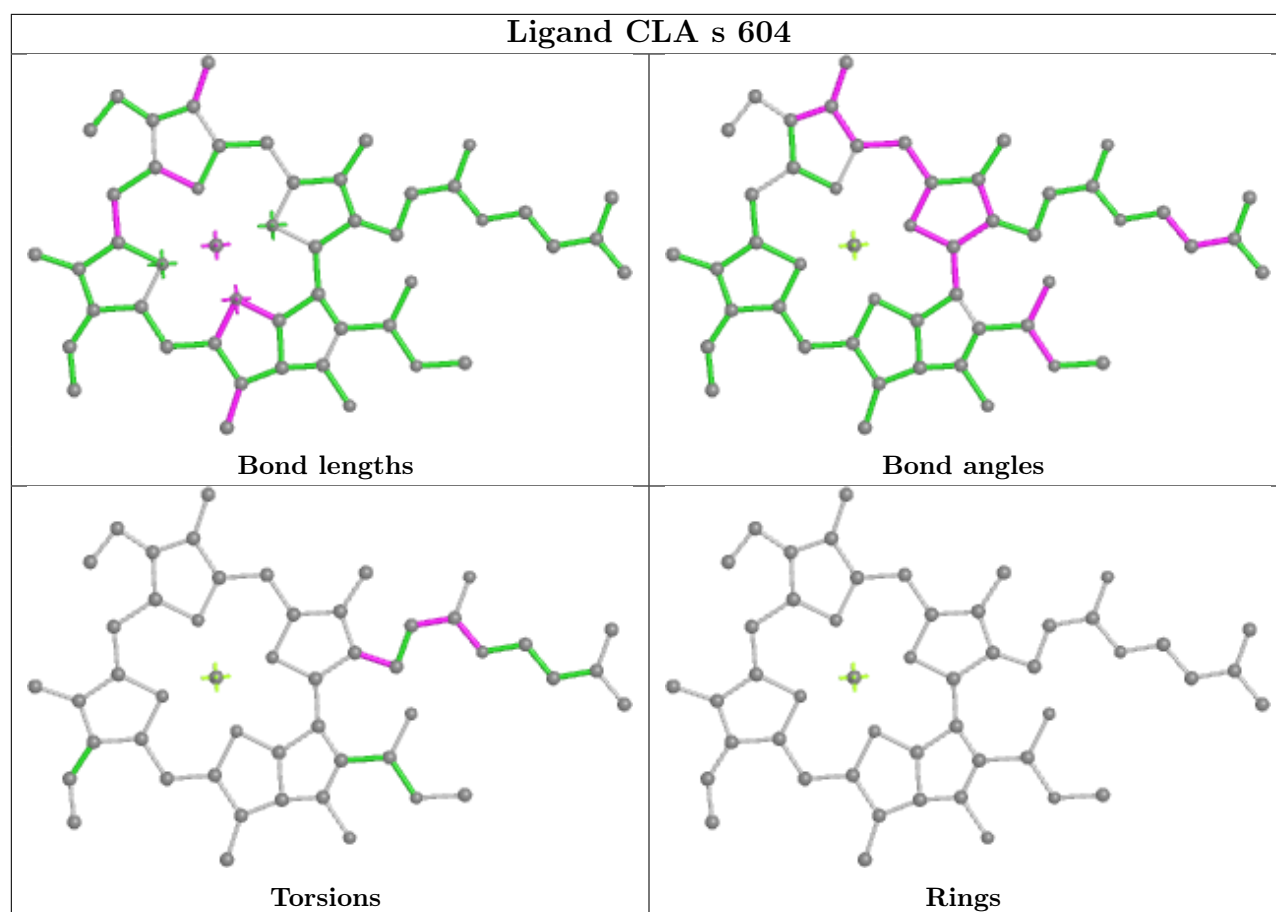


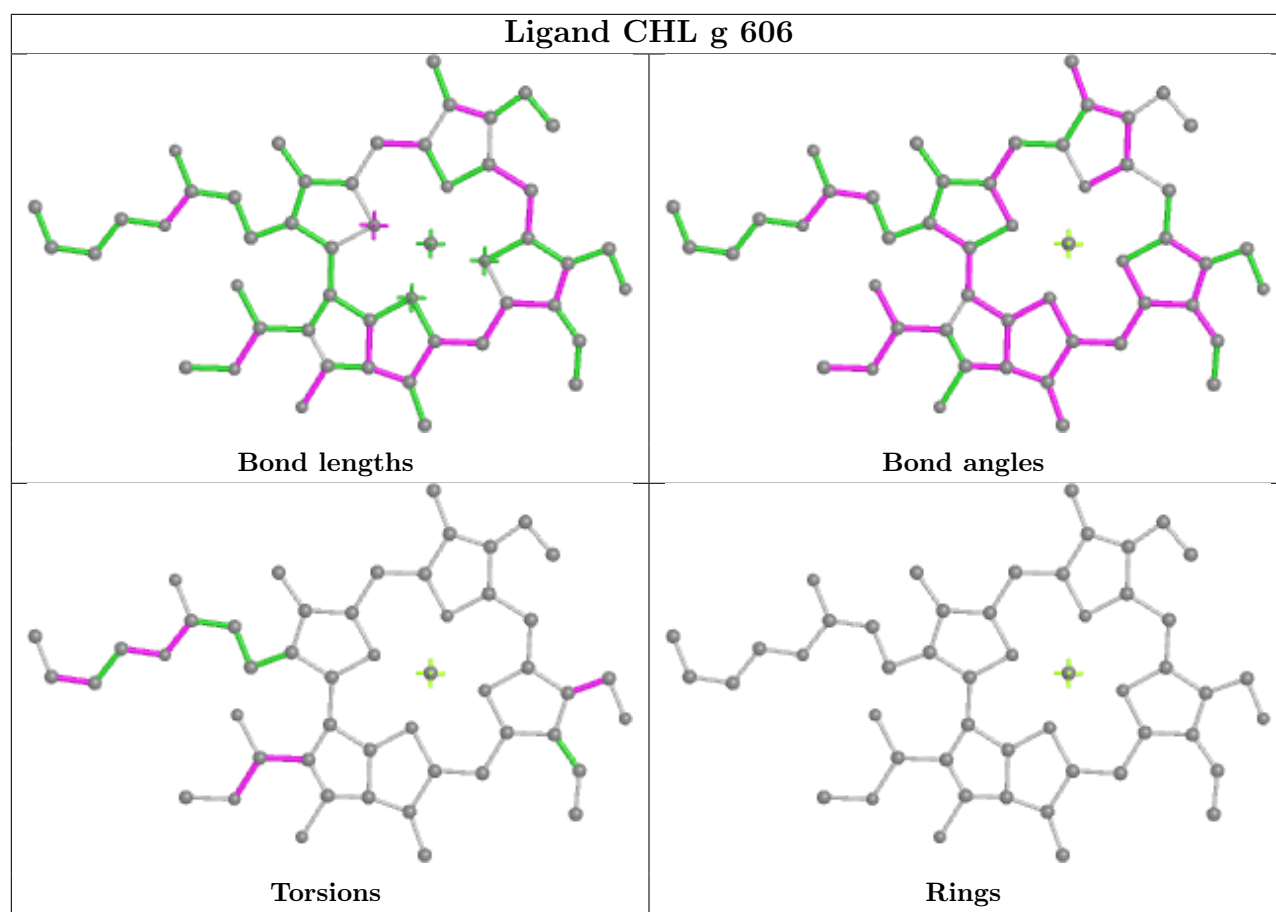
Ligand CLA y 610



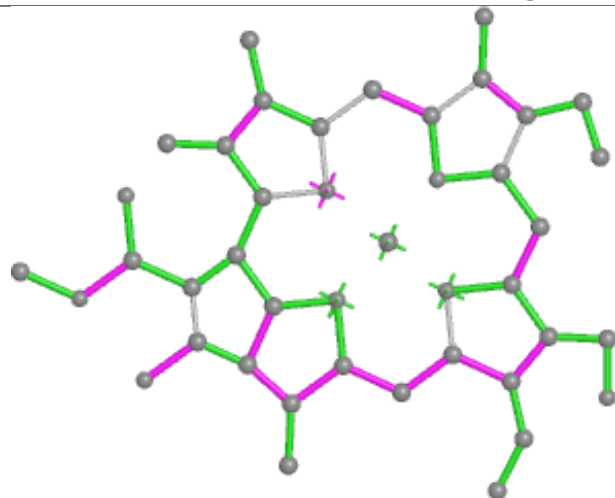
Ligand XAT 6 1622



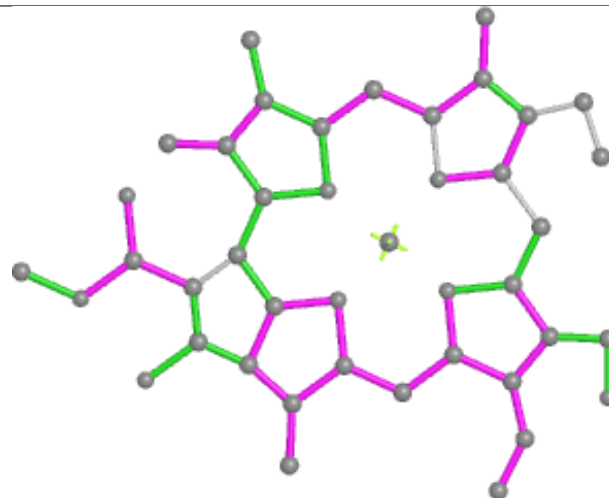




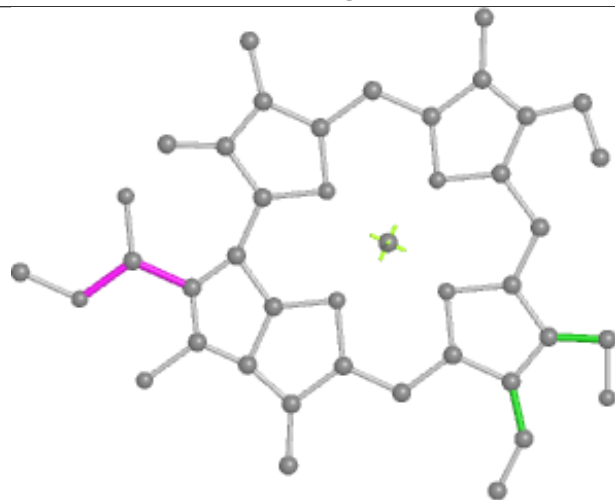
Ligand CHL r 614



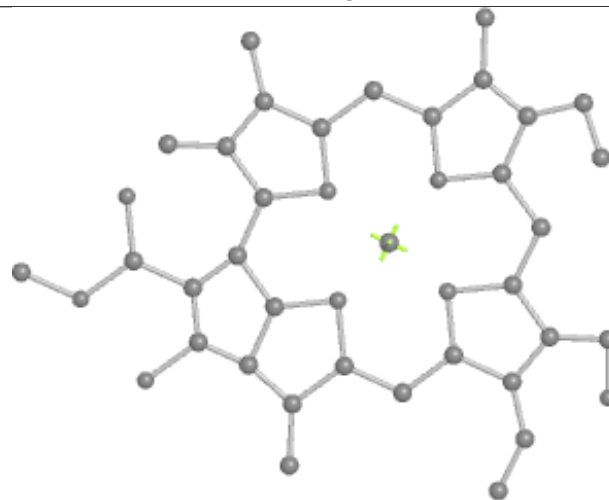
Bond lengths



Bond angles

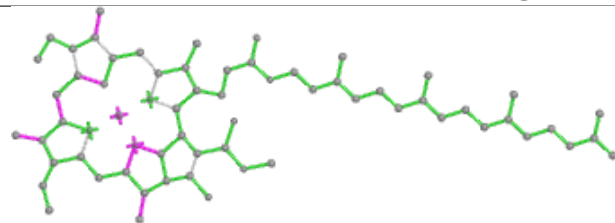


Torsions

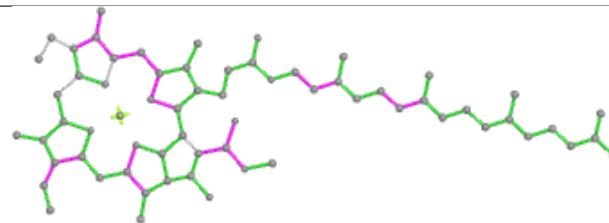


Rings

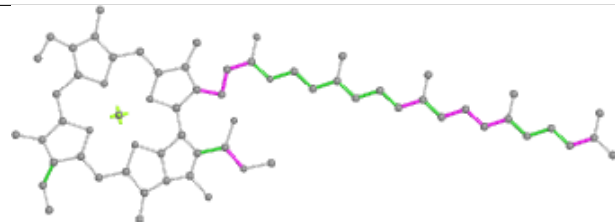
Ligand CLA N 602



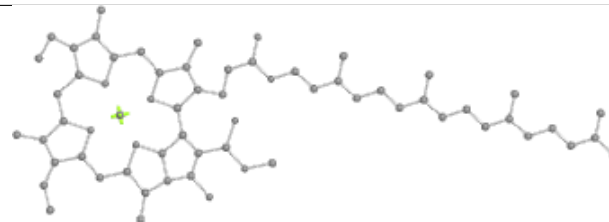
Bond lengths



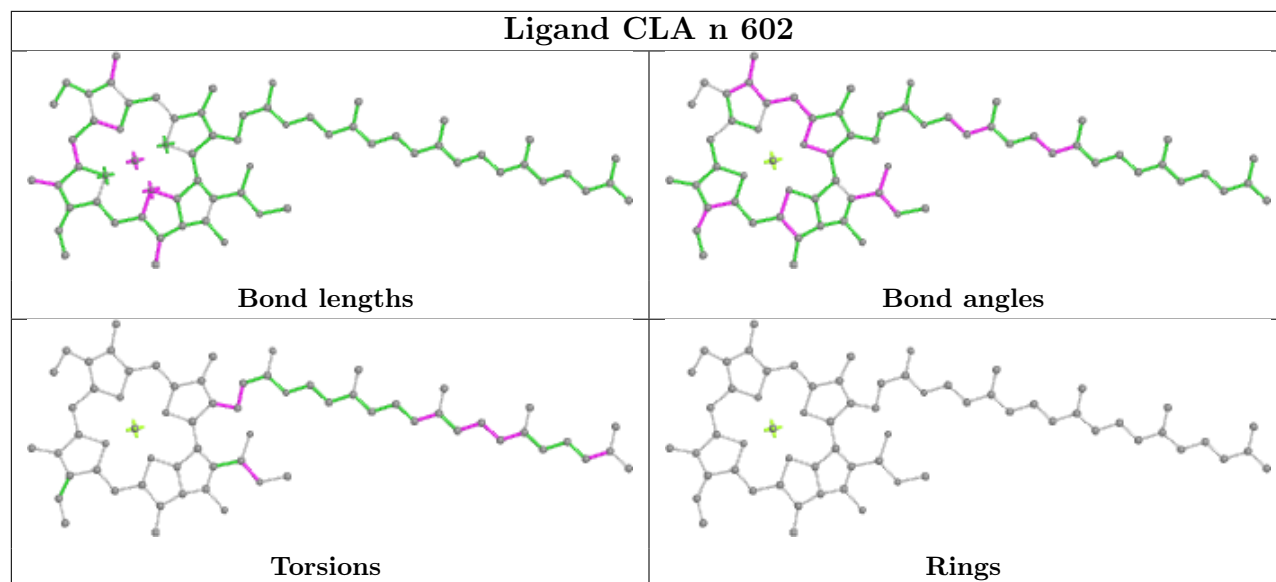
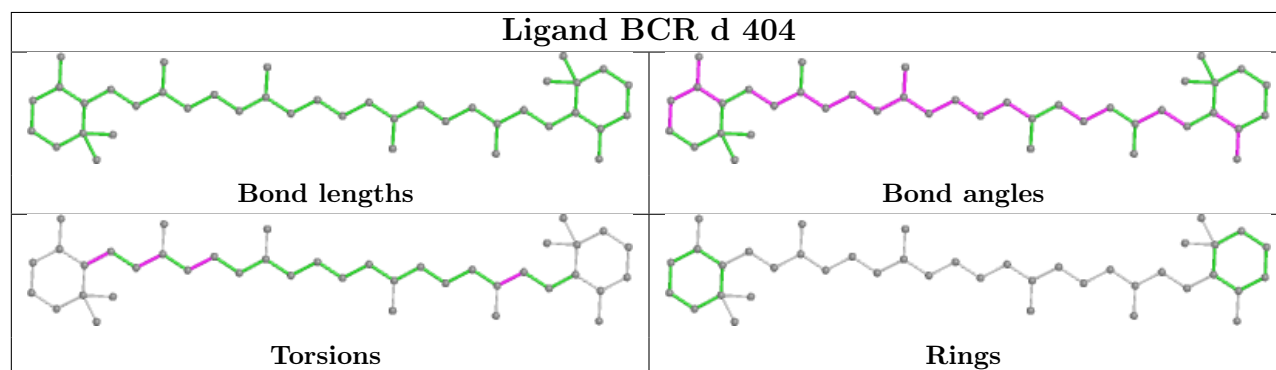
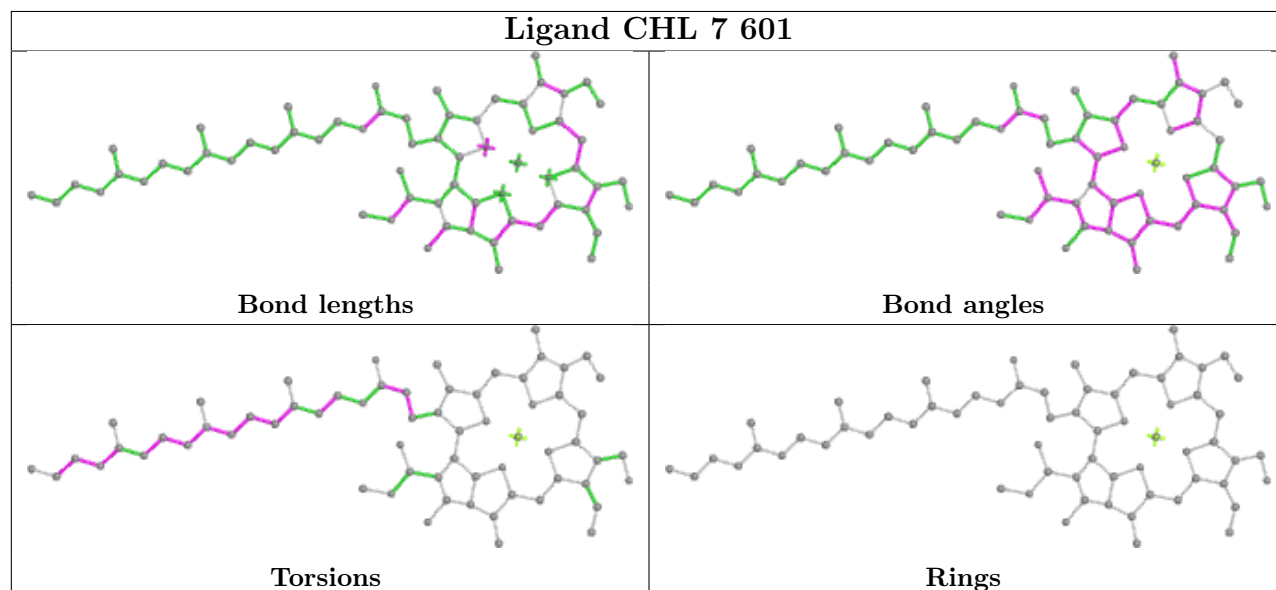
Bond angles

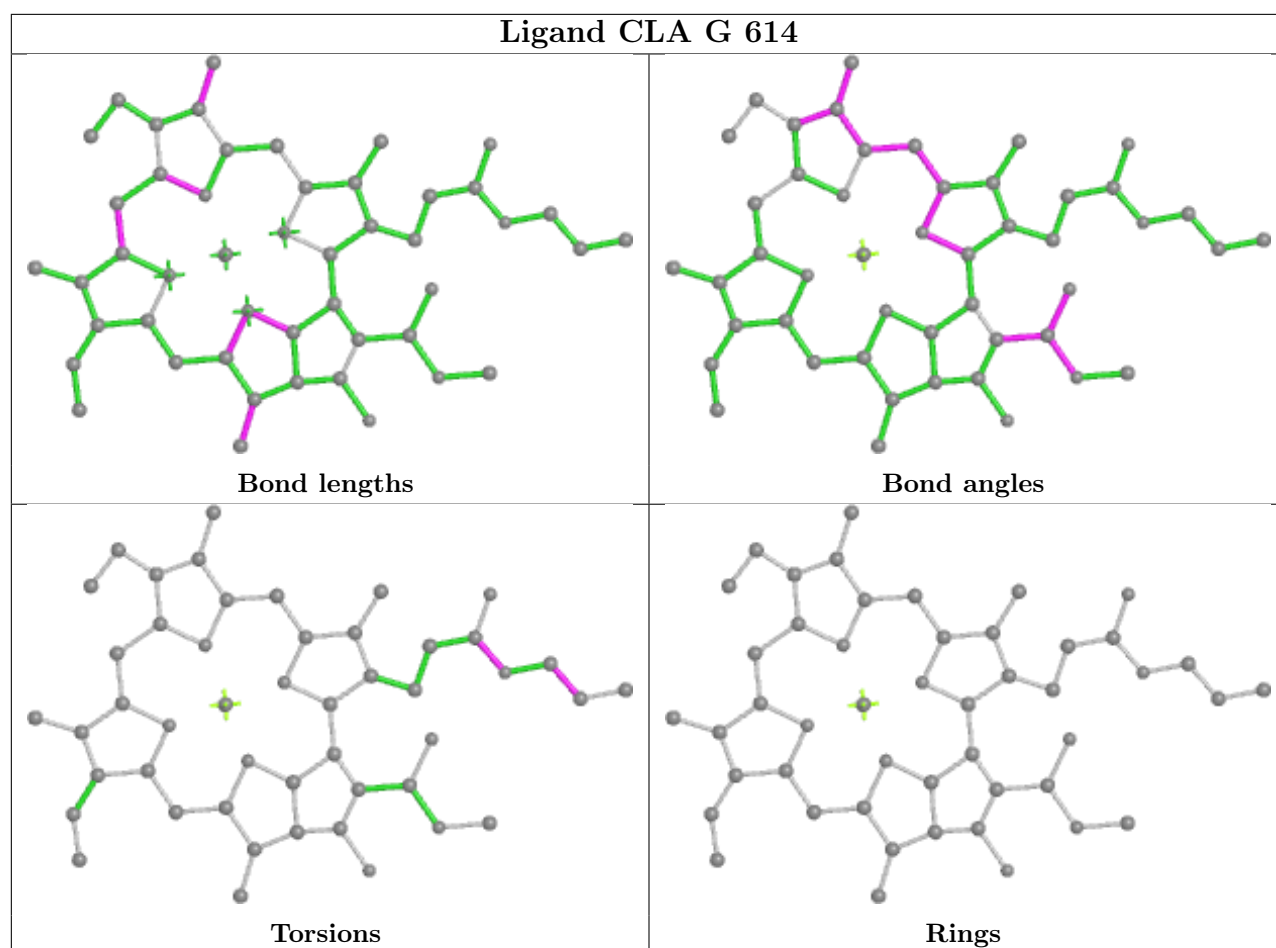


Torsions

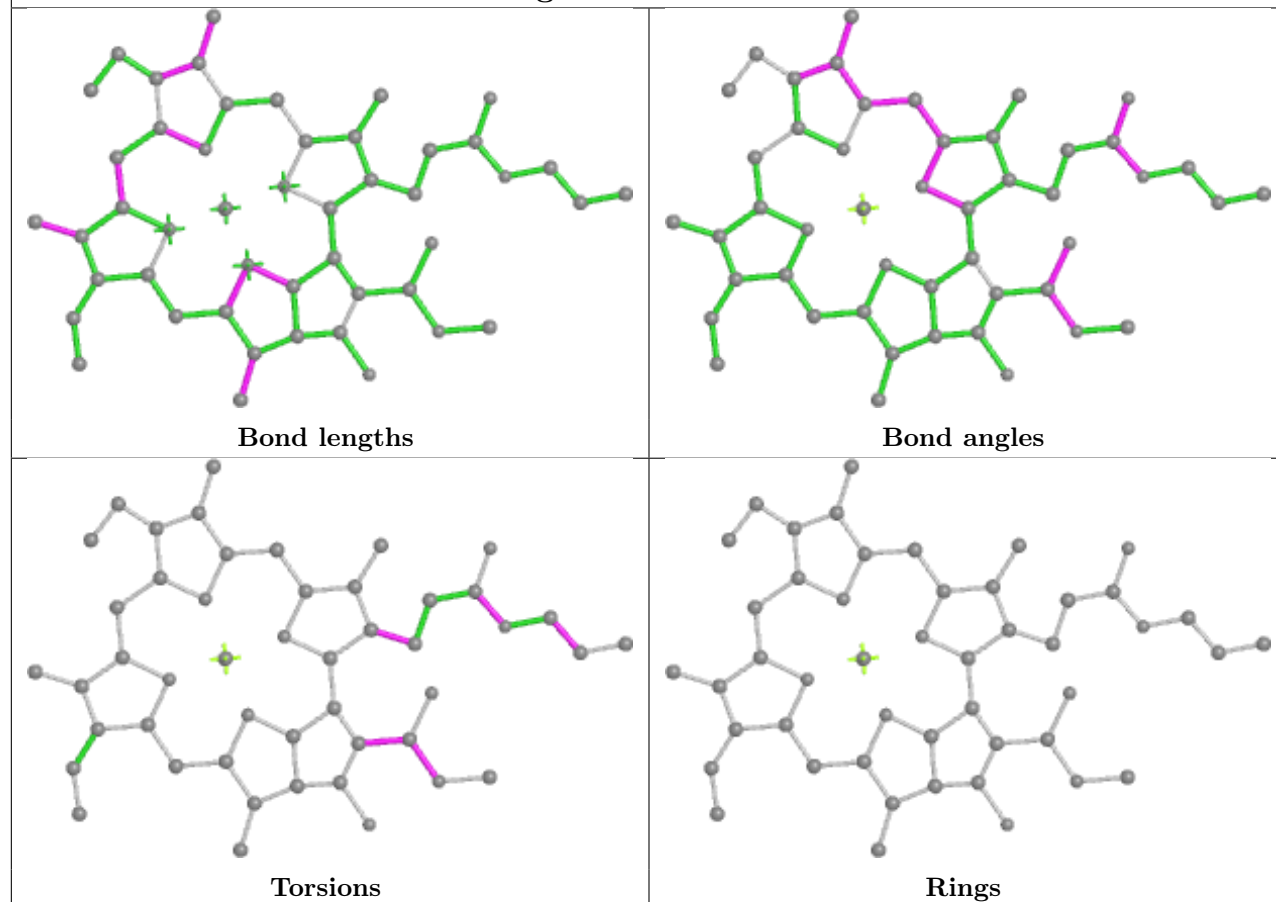


Rings

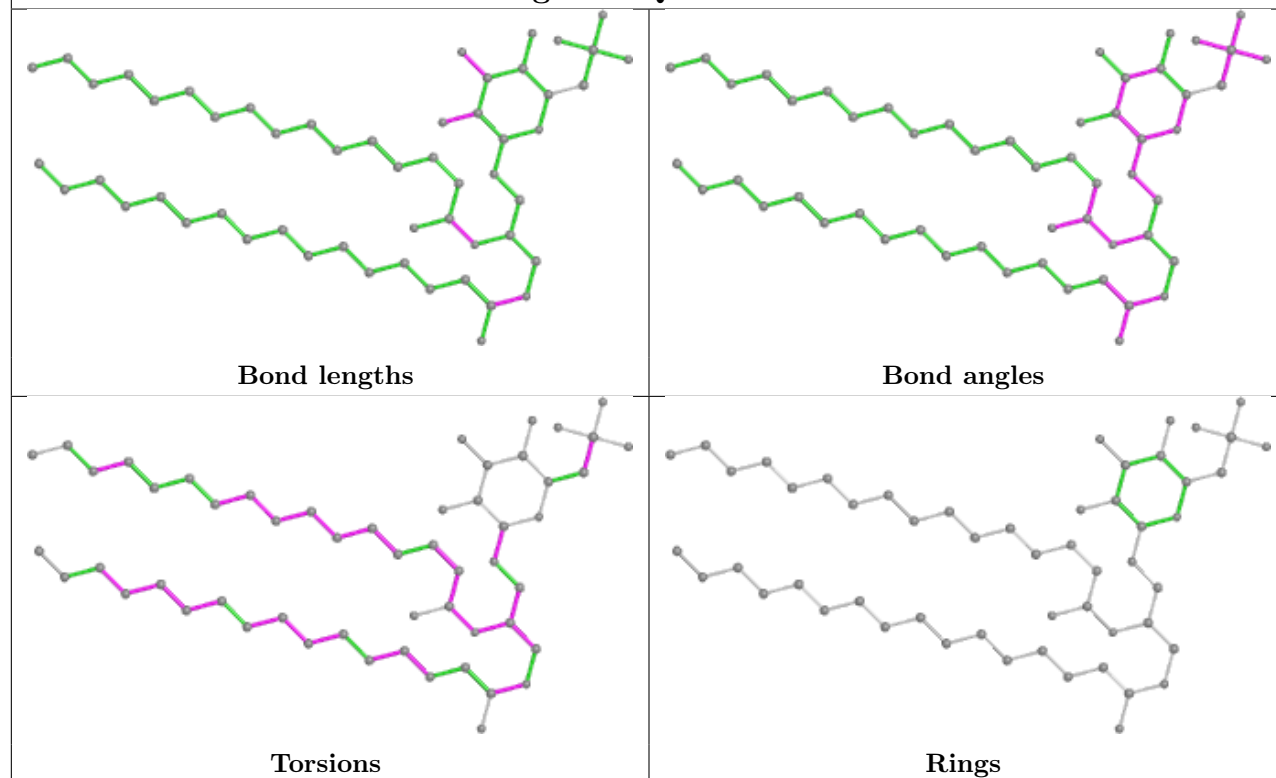
Ligand CLA n 602**Ligand BCR d 404****Ligand CHL 7 601**



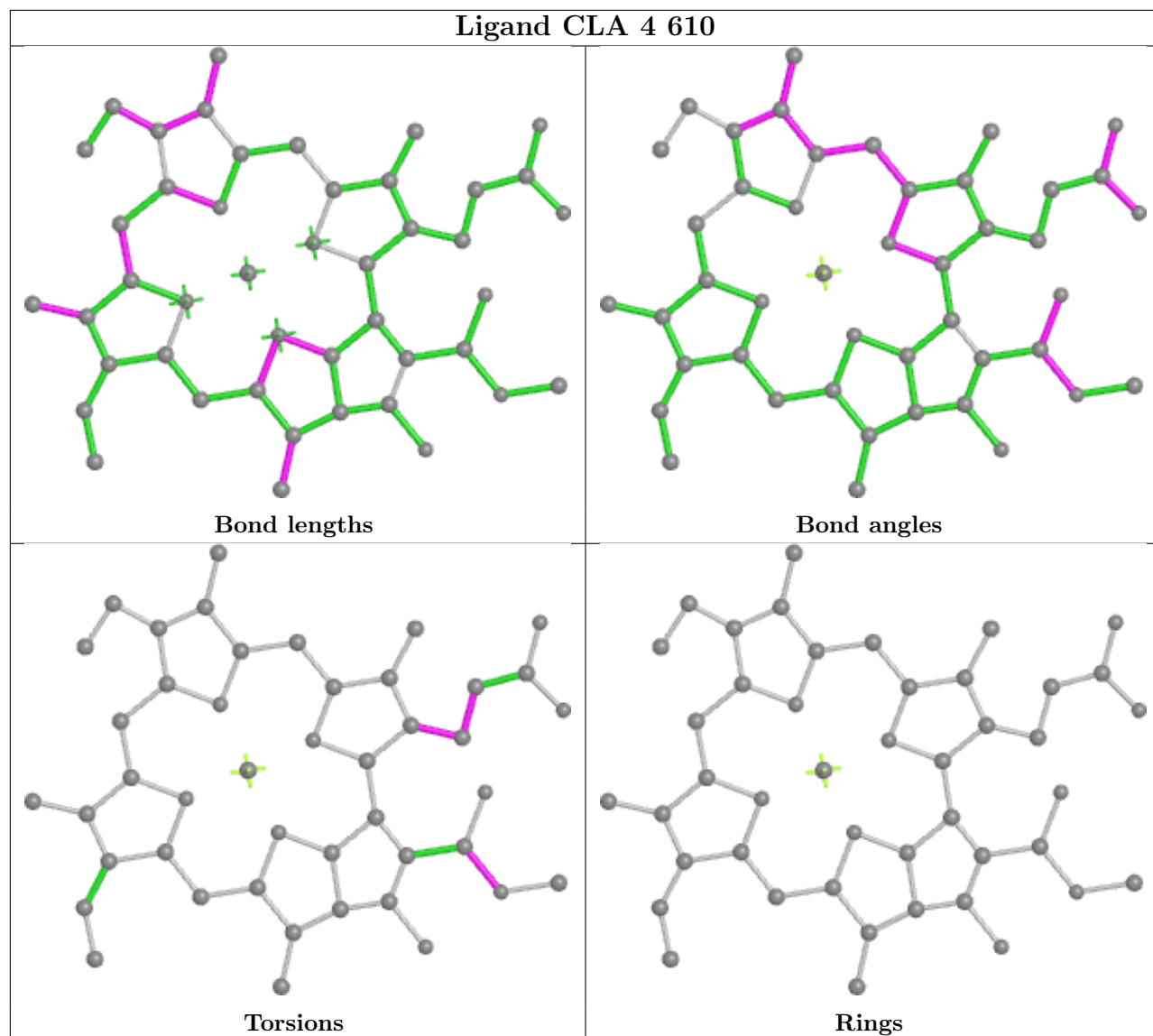
Ligand CLA 7 614



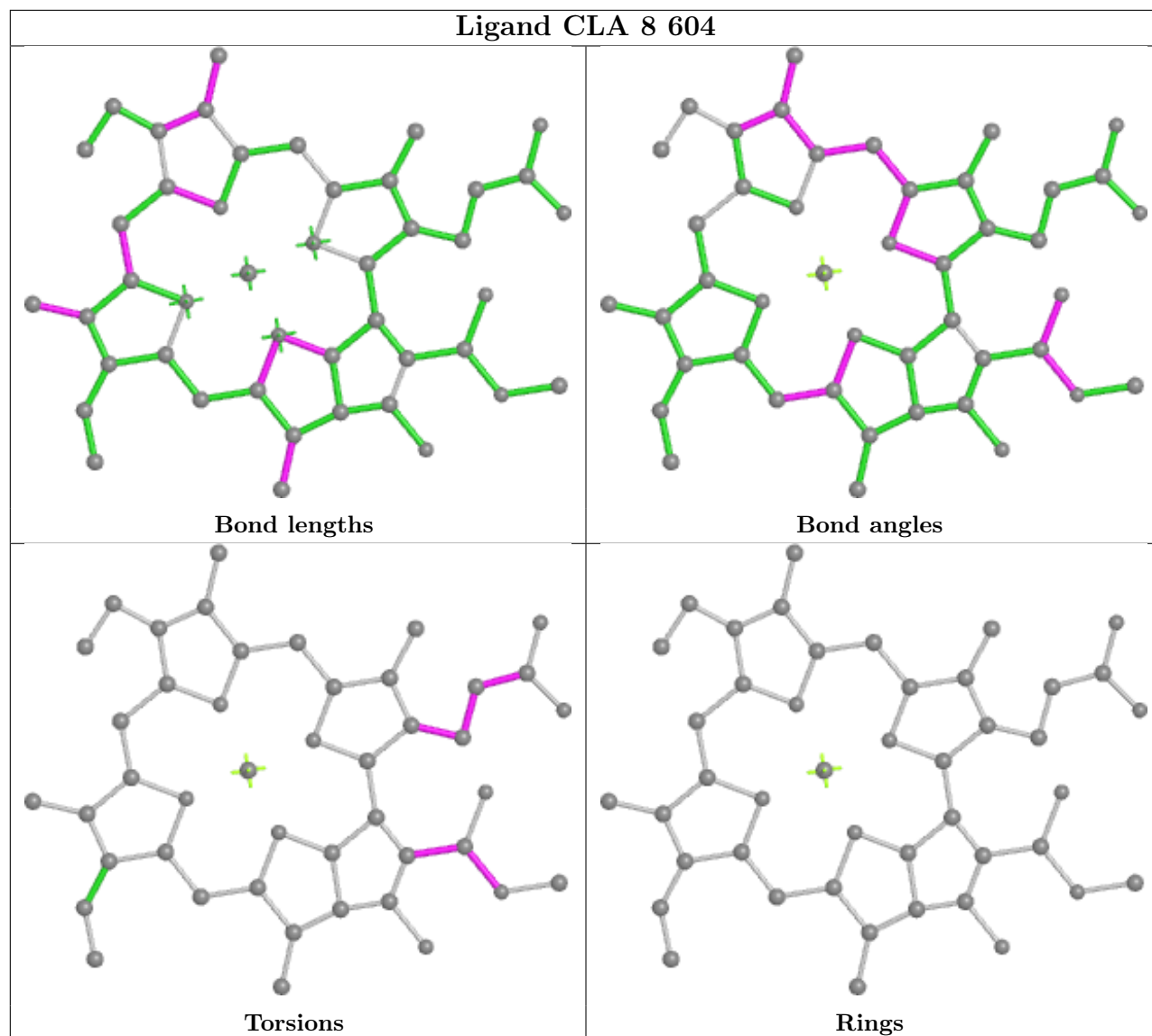
Ligand SQD B 621

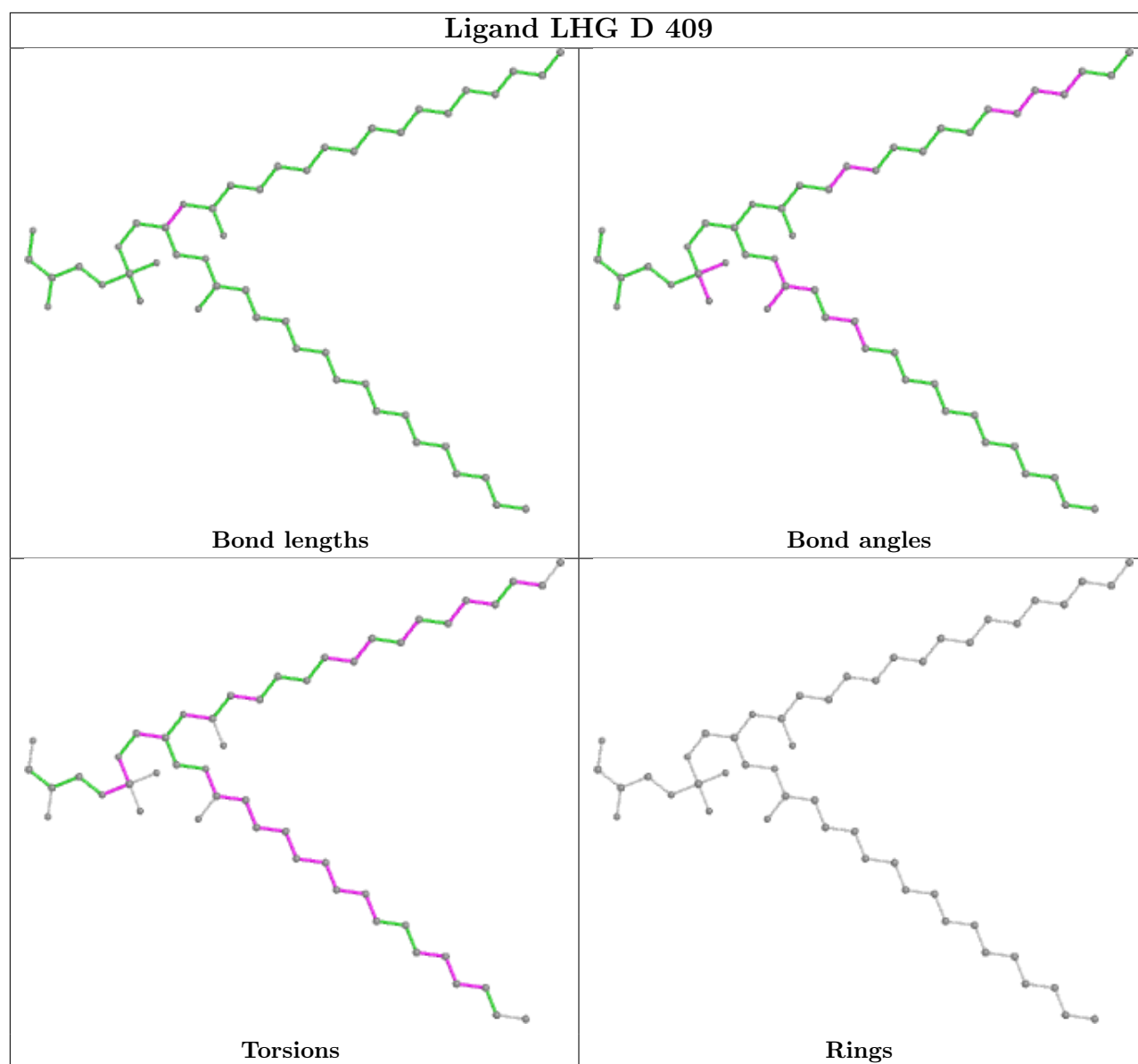


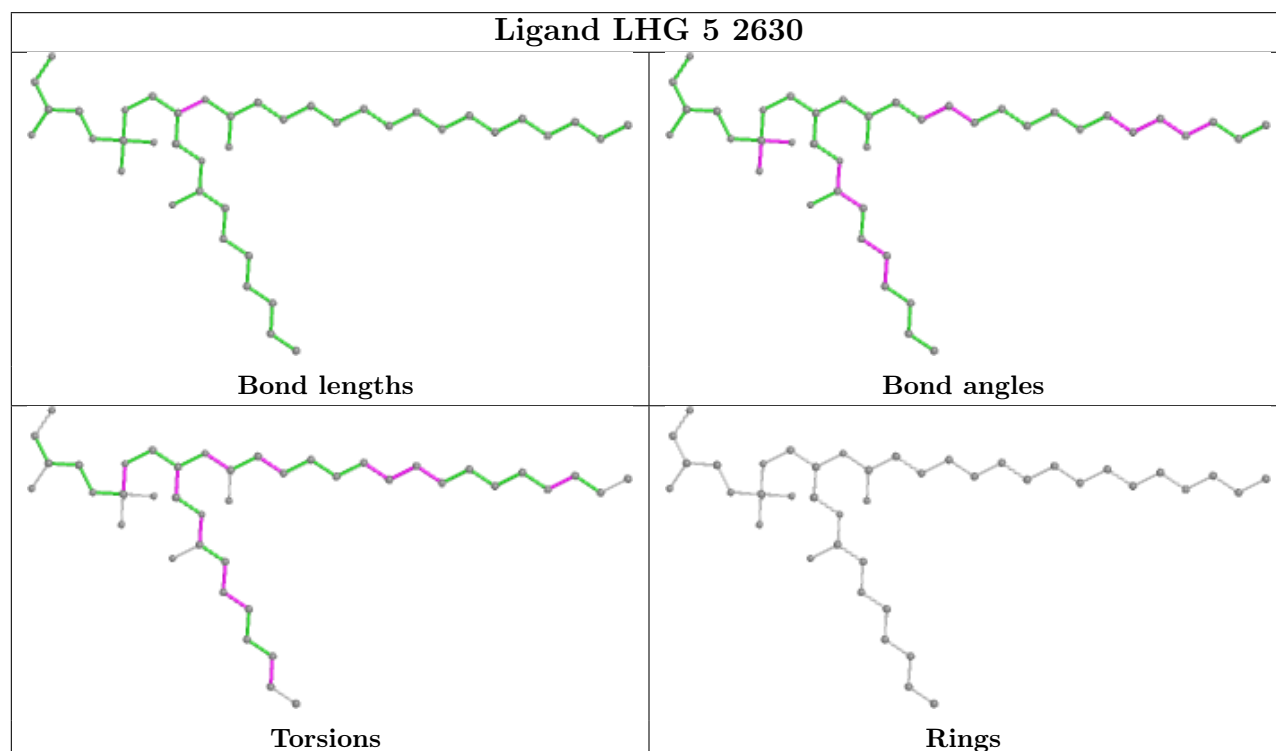
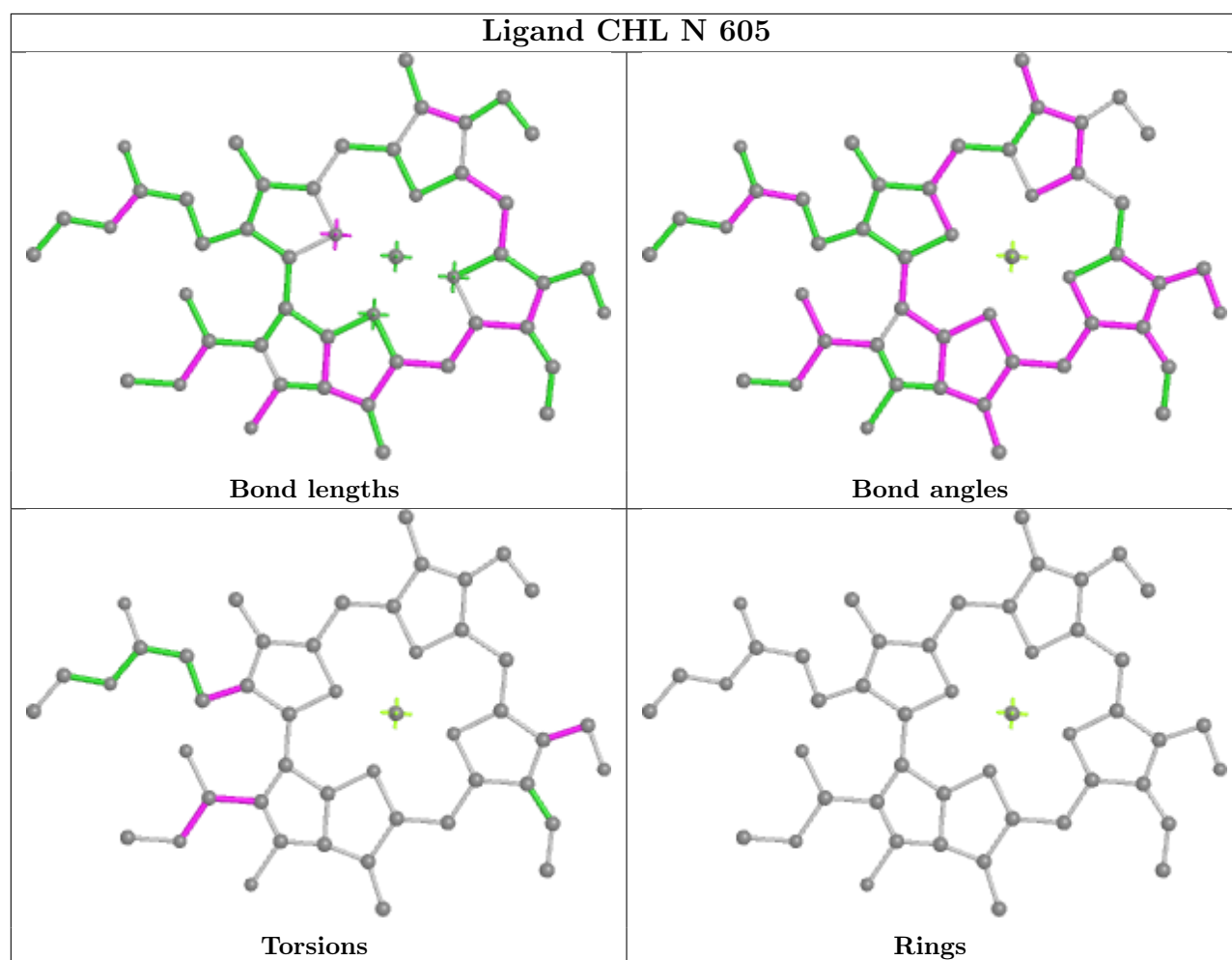
Ligand CLA 4 610

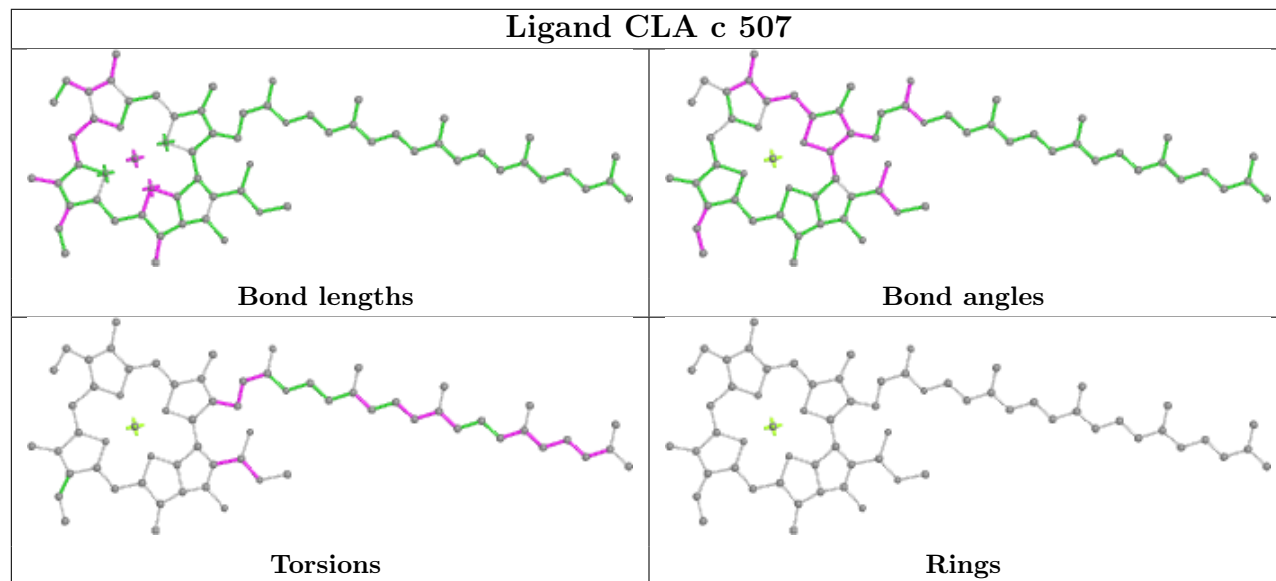
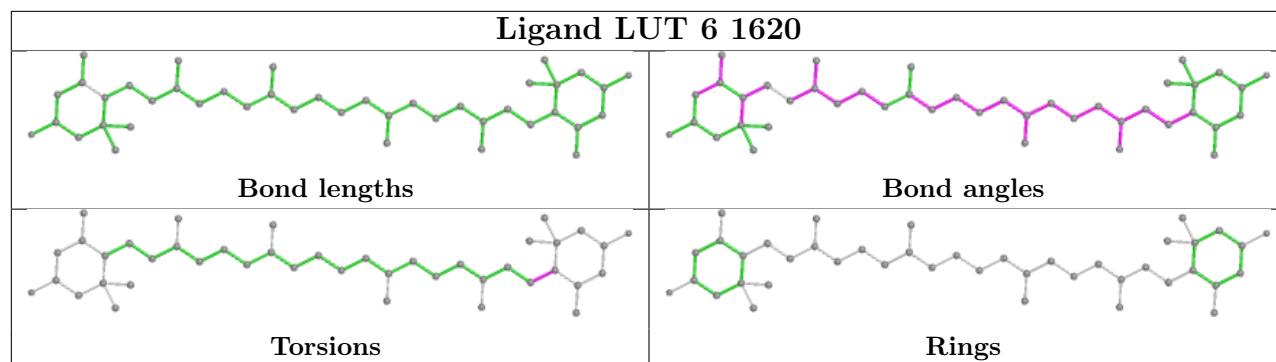


Ligand CLA 8 604

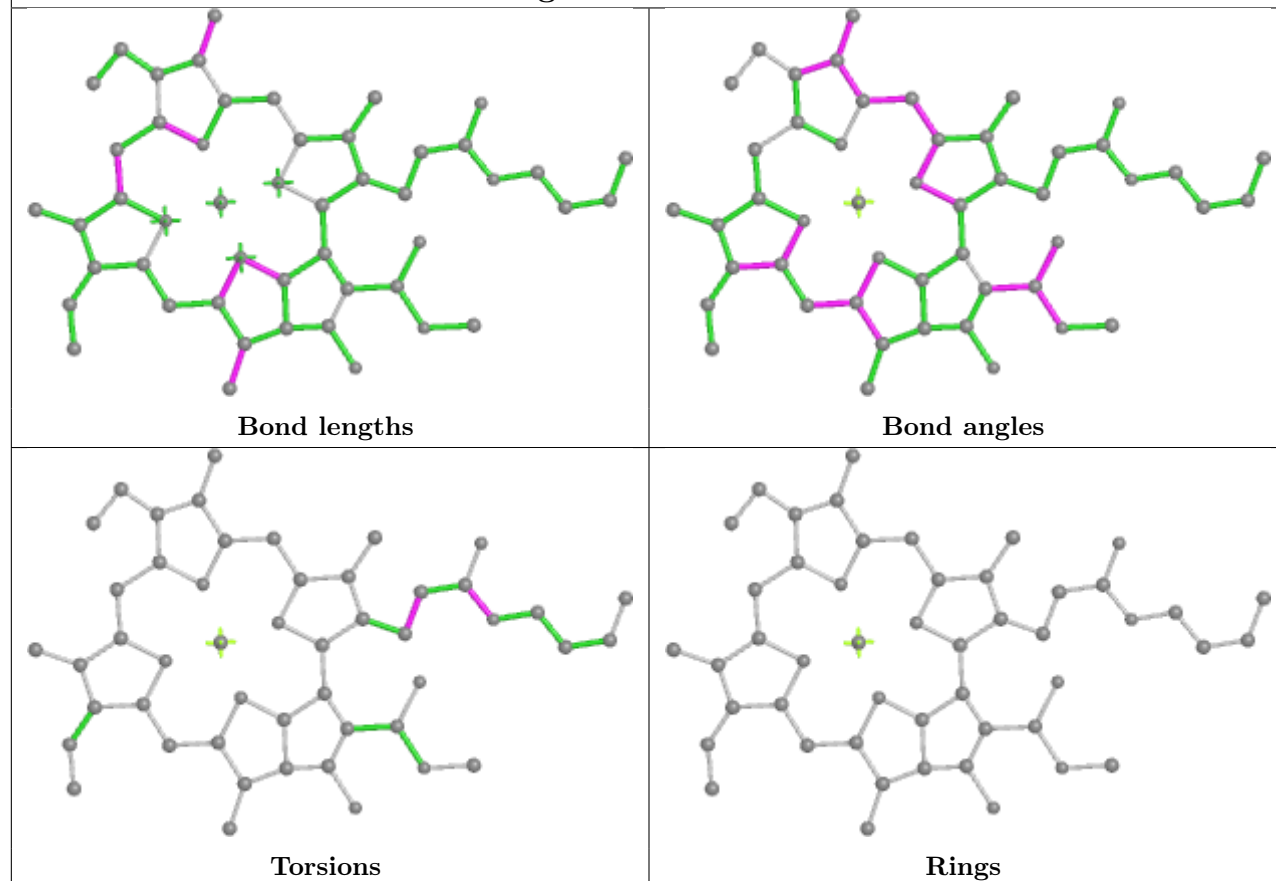




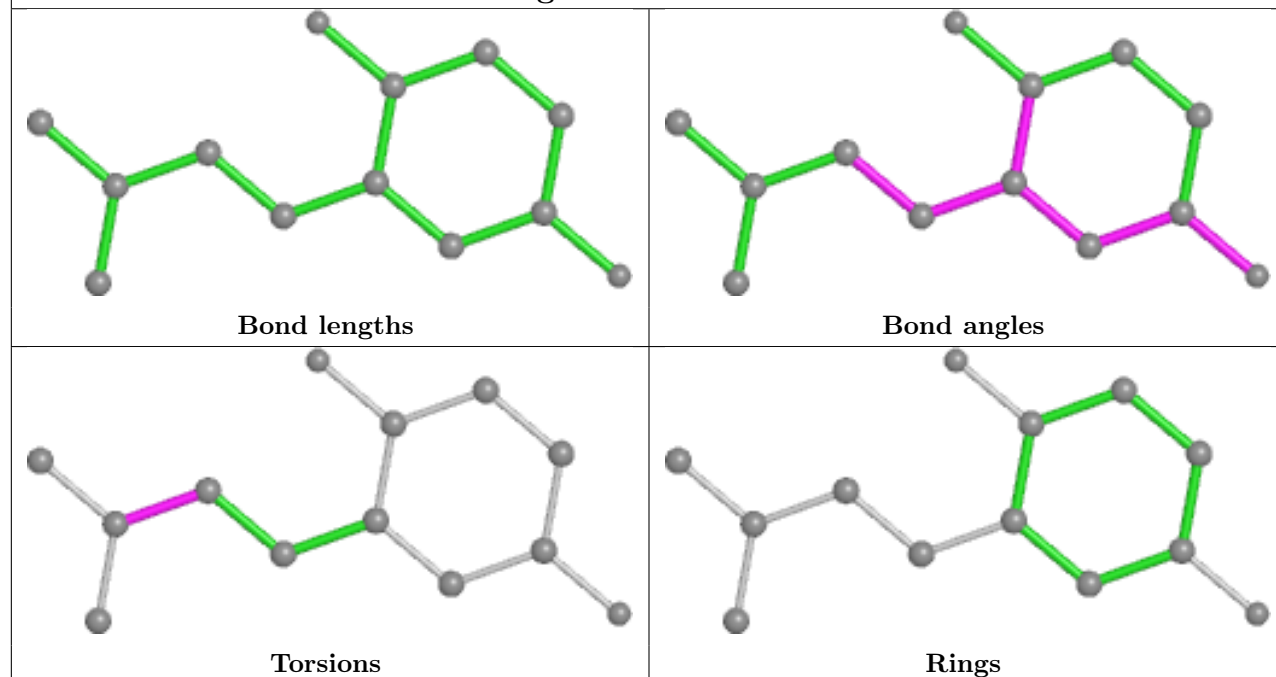




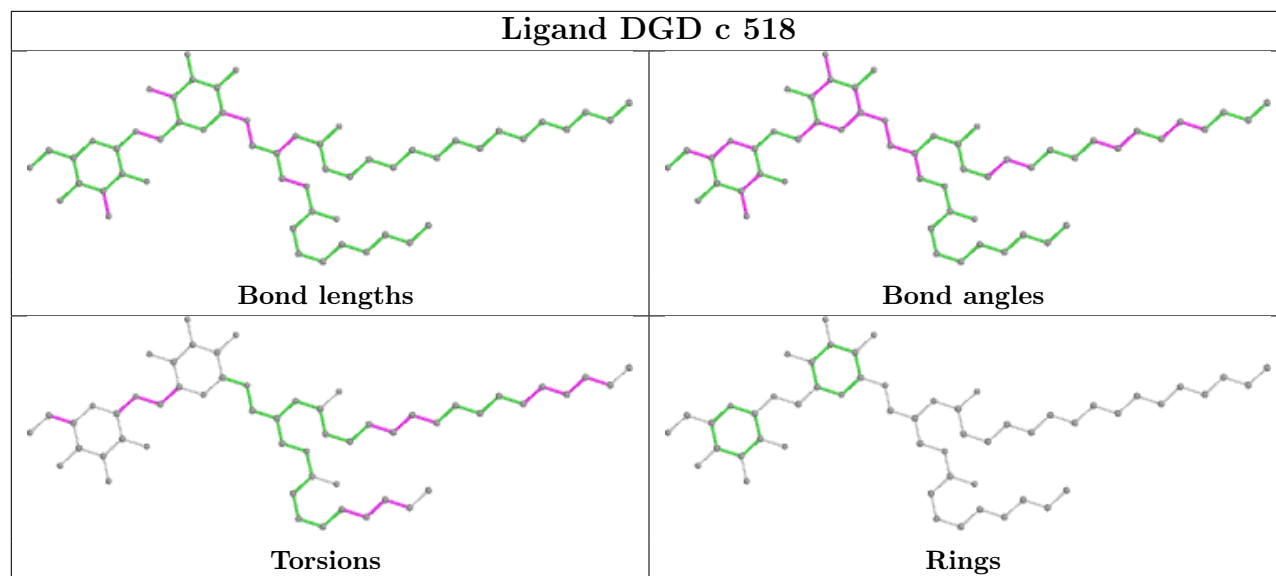
Ligand CLA s 614



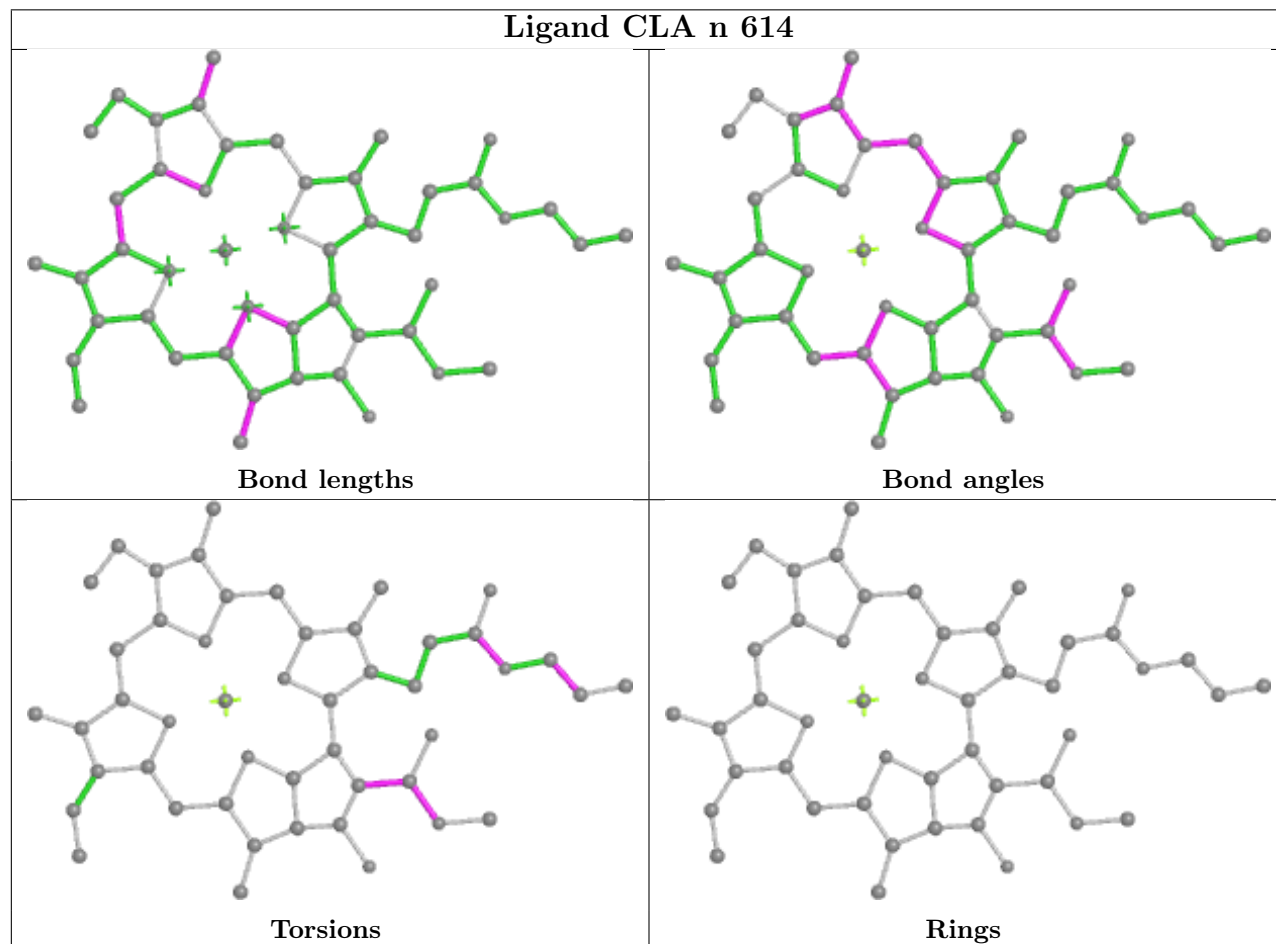
Ligand PL9 A 414

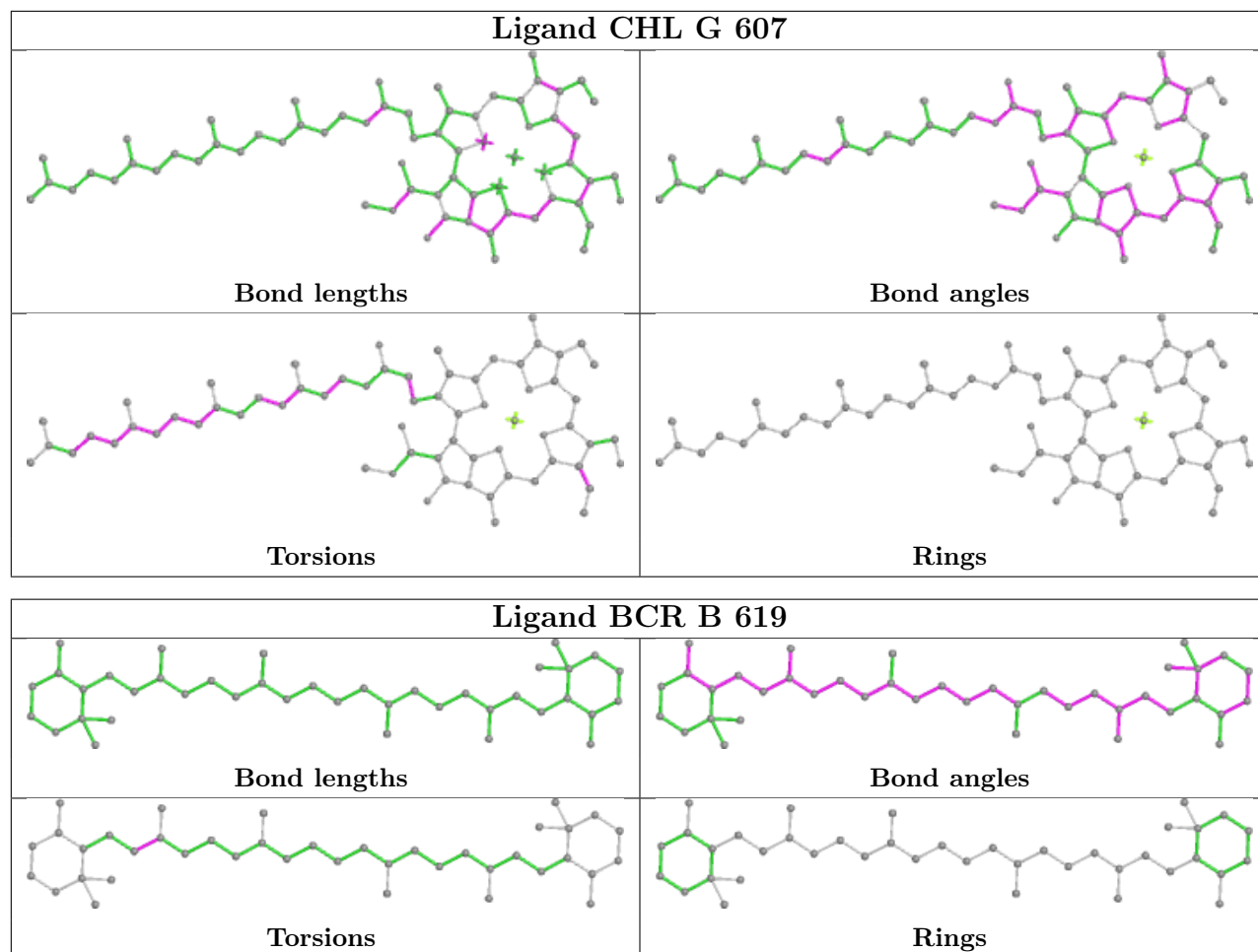


Ligand DGD c 518

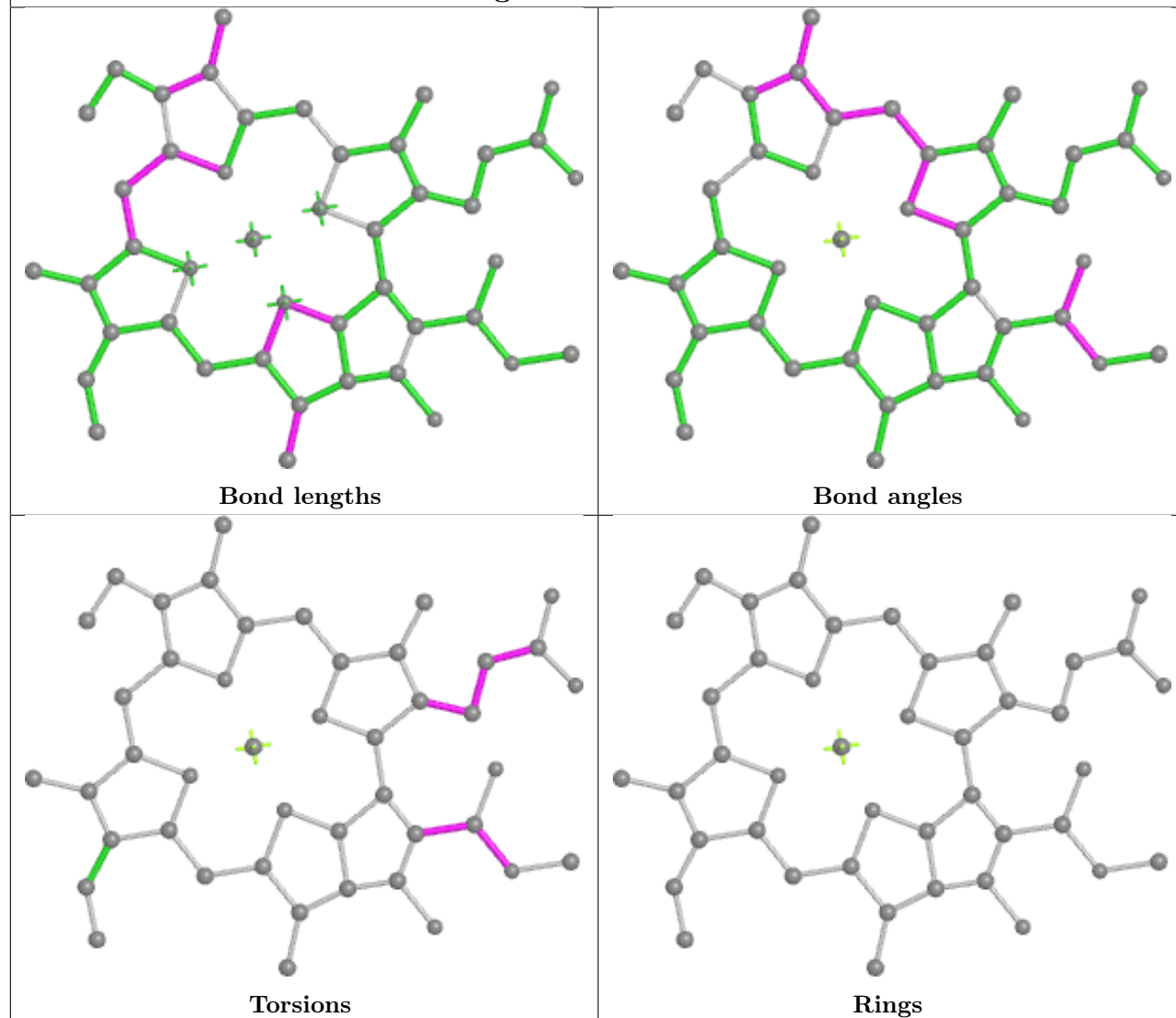


Ligand CLA n 614

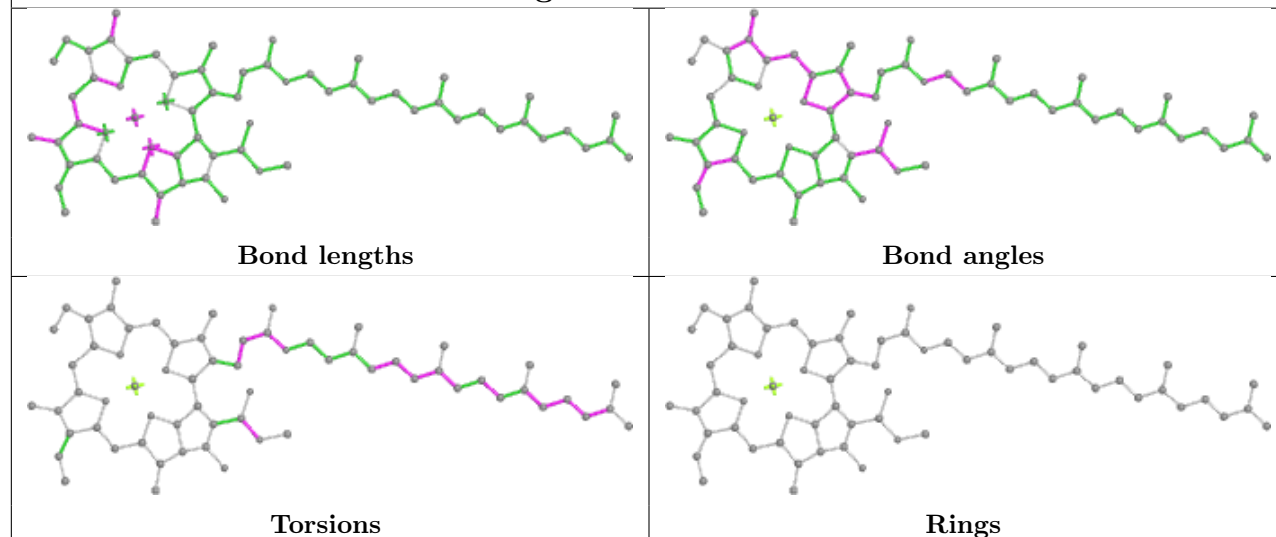




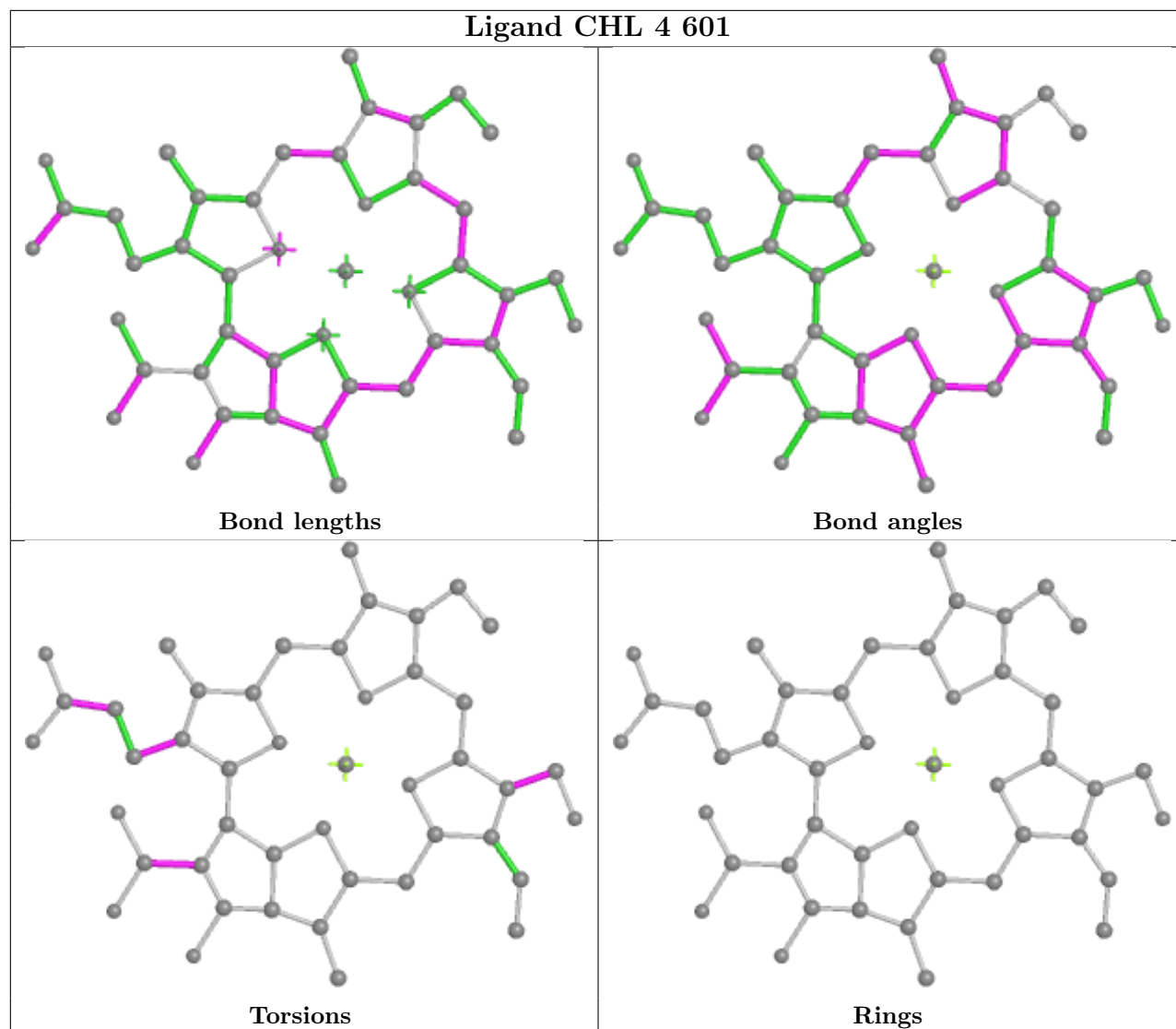
Ligand CLA 2 604

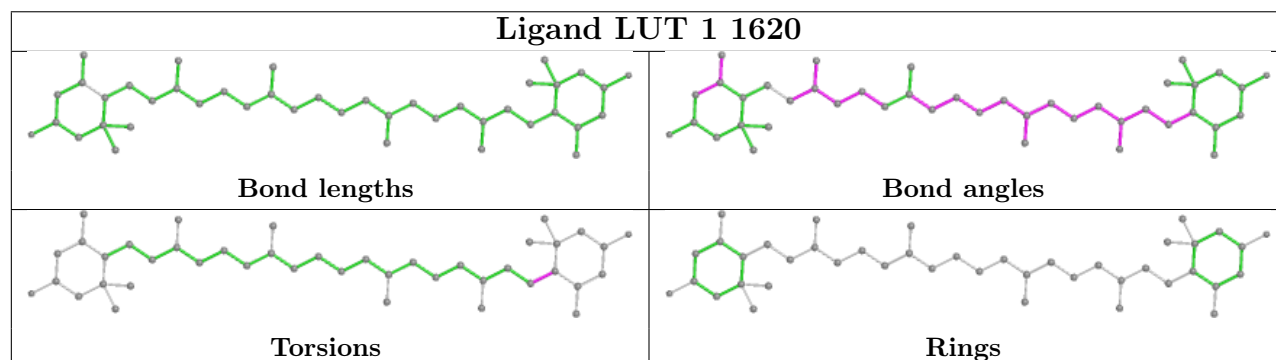
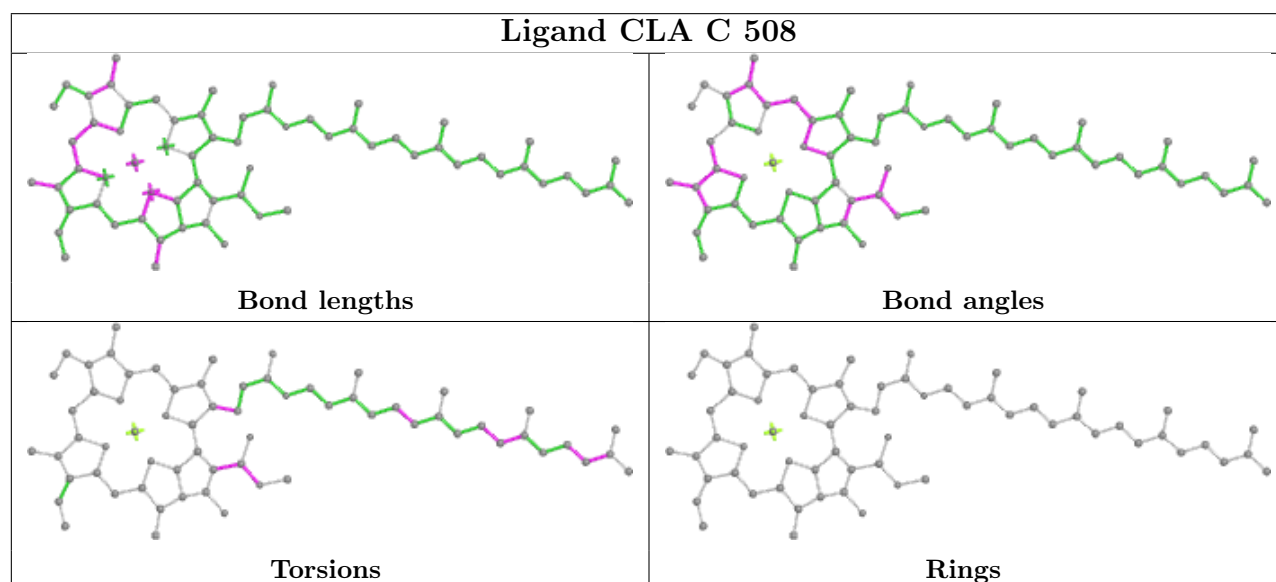
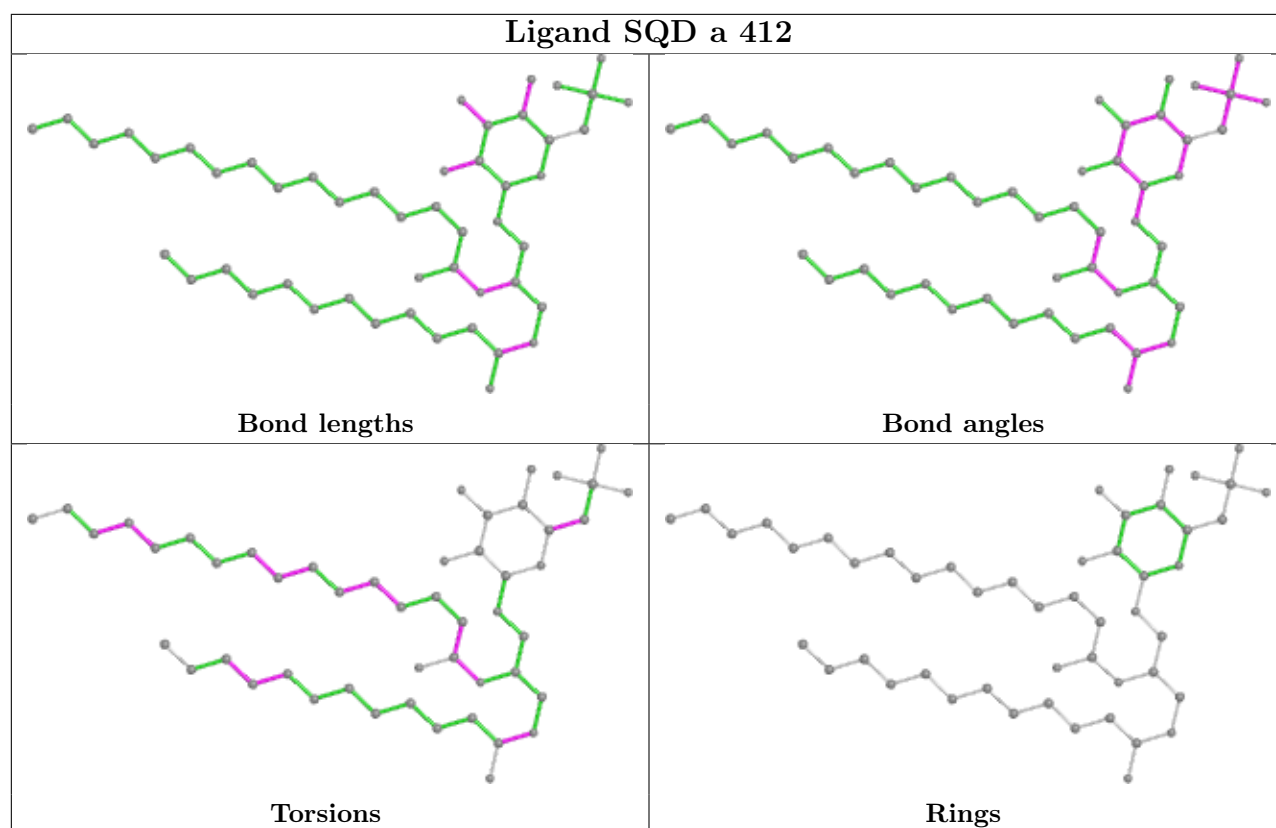


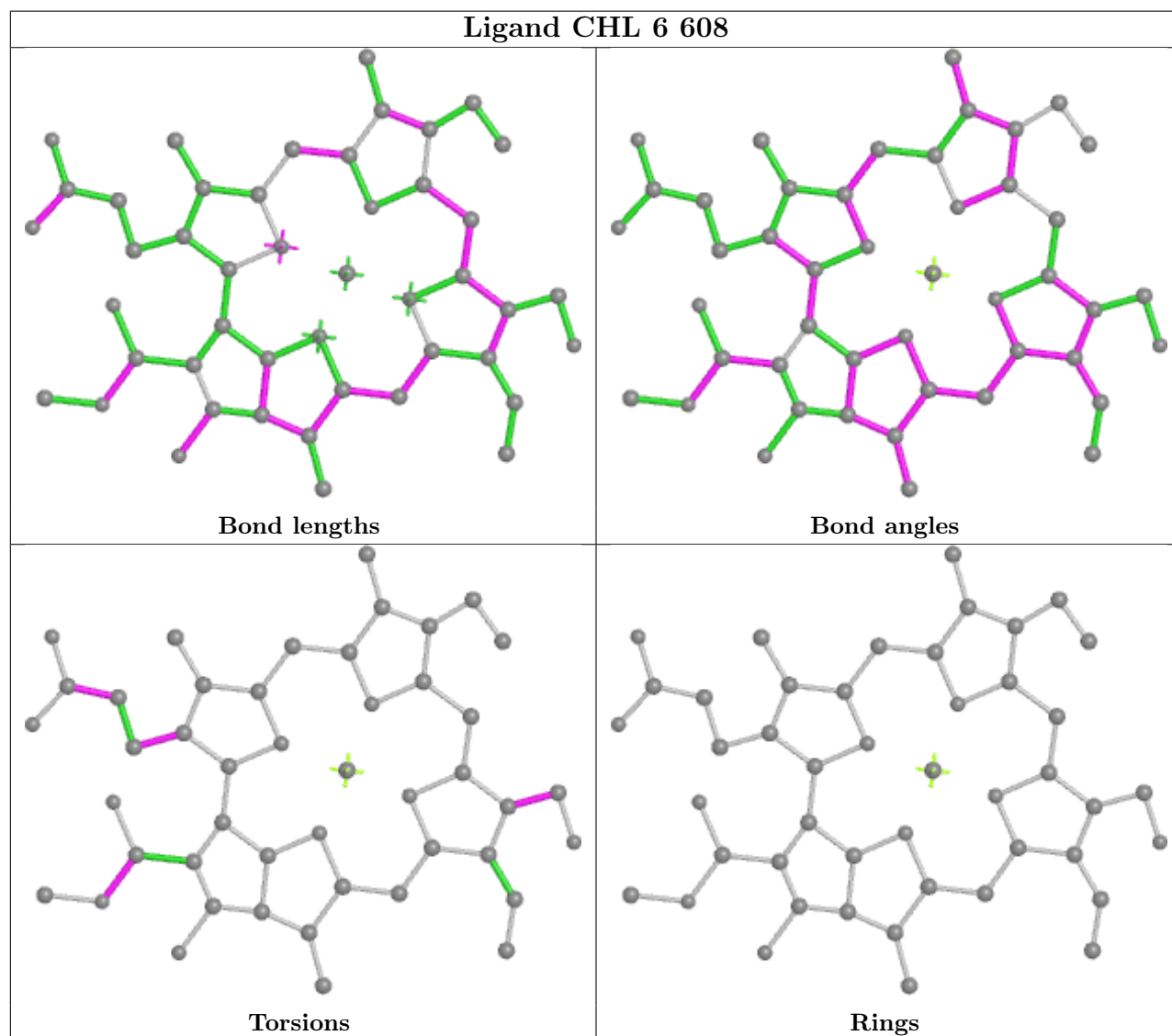
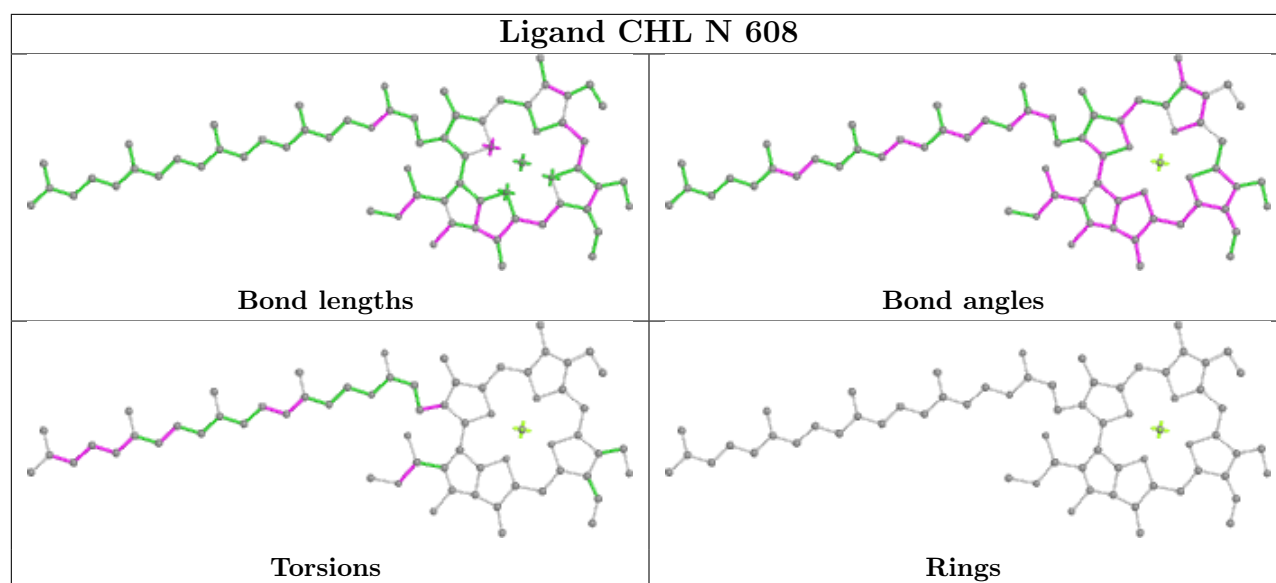
Ligand CLA b 617



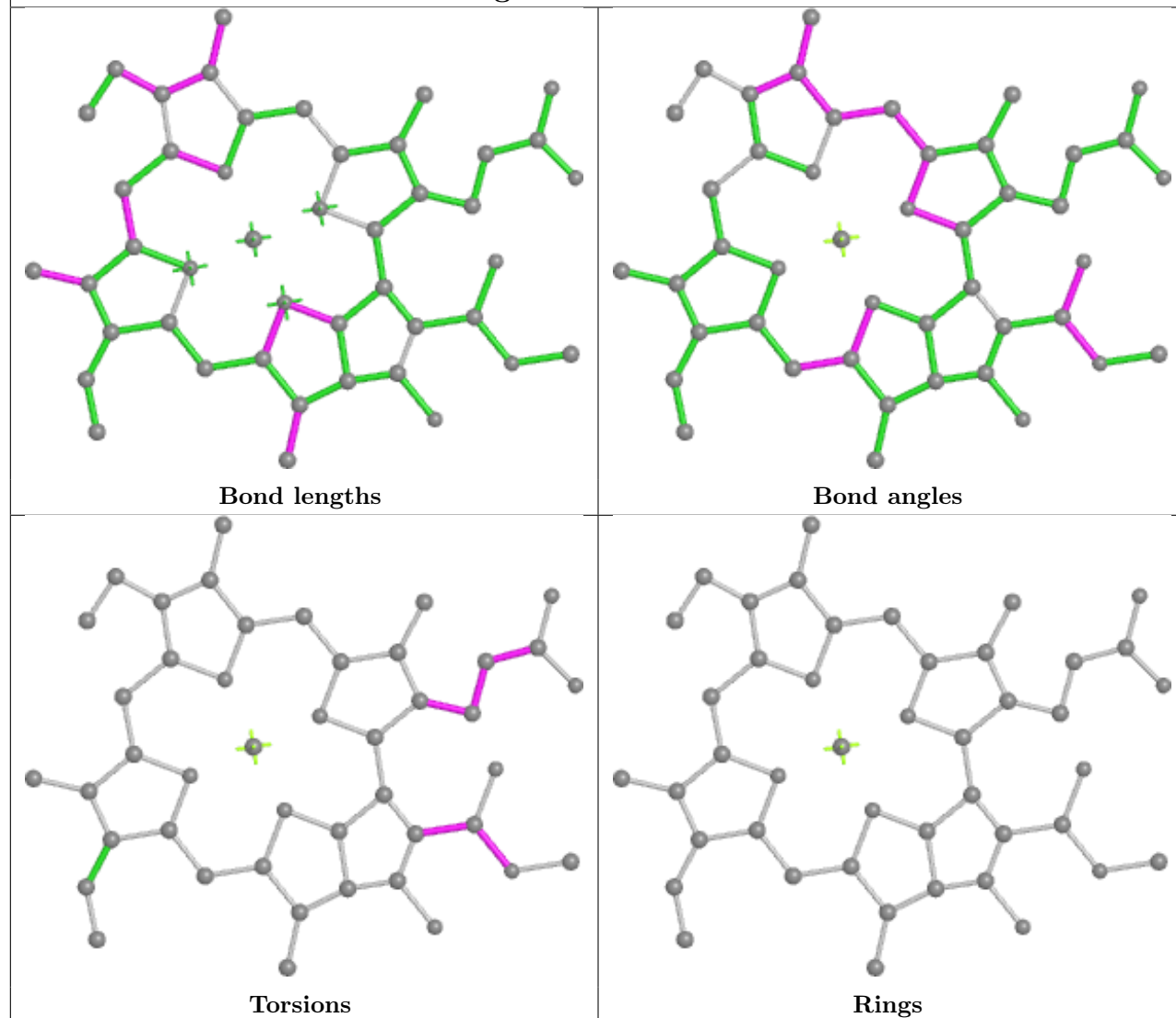
Ligand CHL 4 601



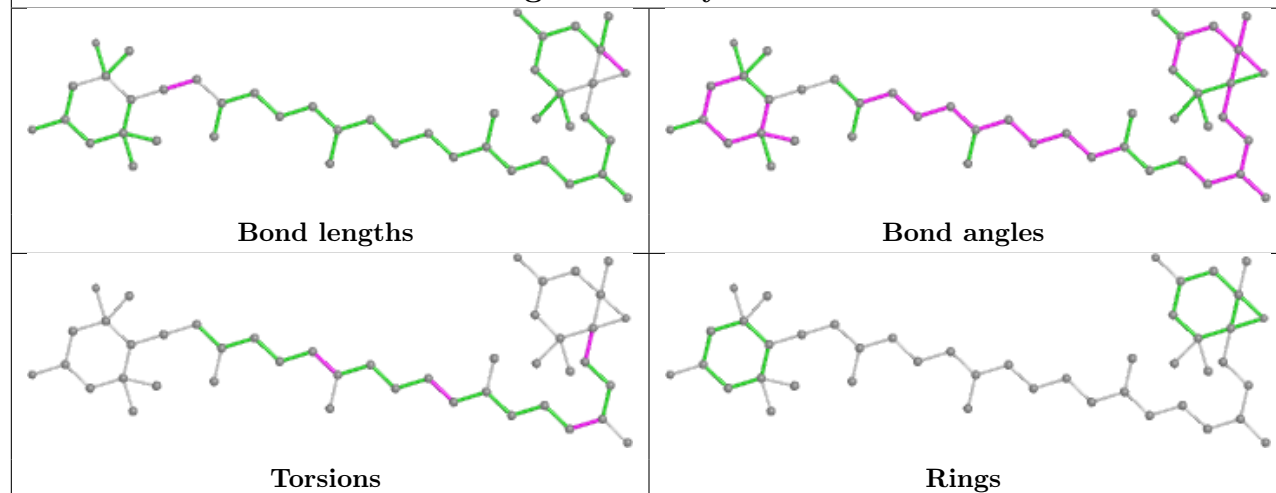




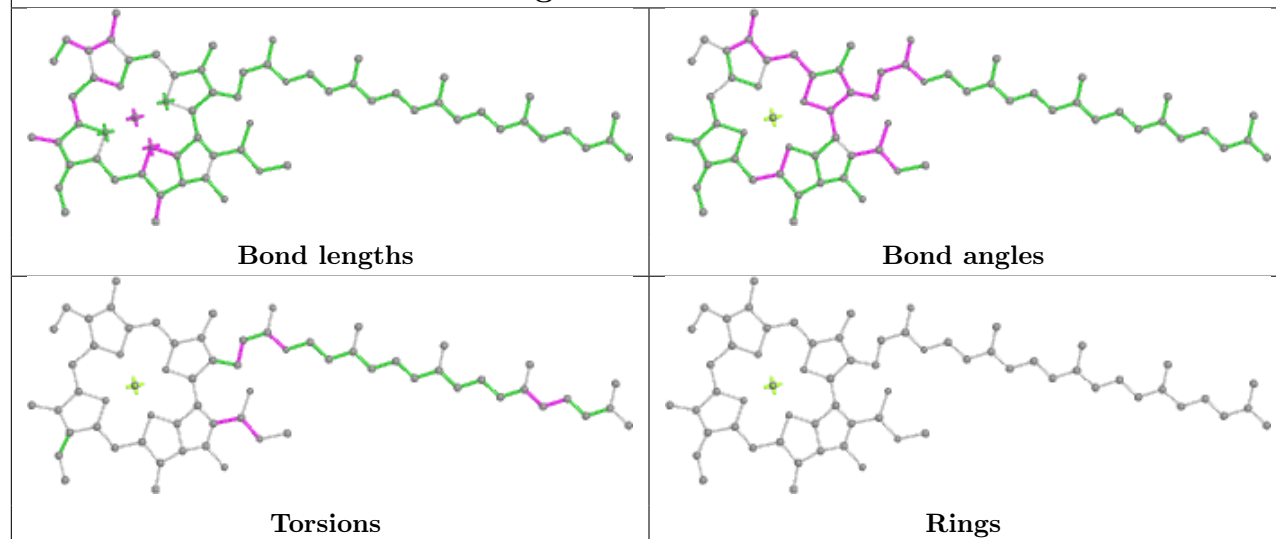
Ligand CLA 7 604



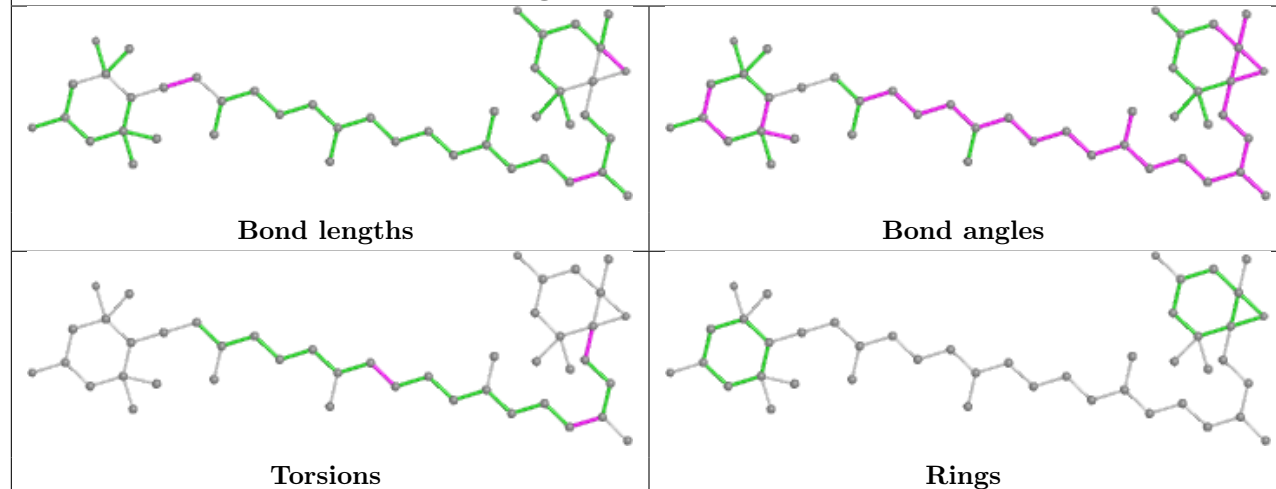
Ligand NEX y 1623



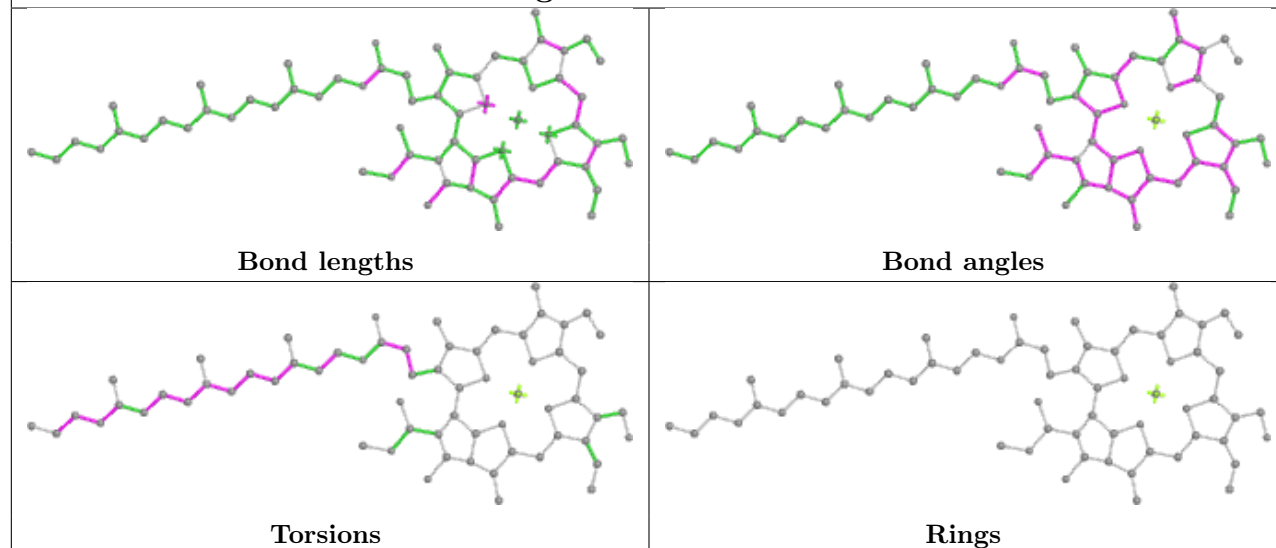
Ligand CLA b 611



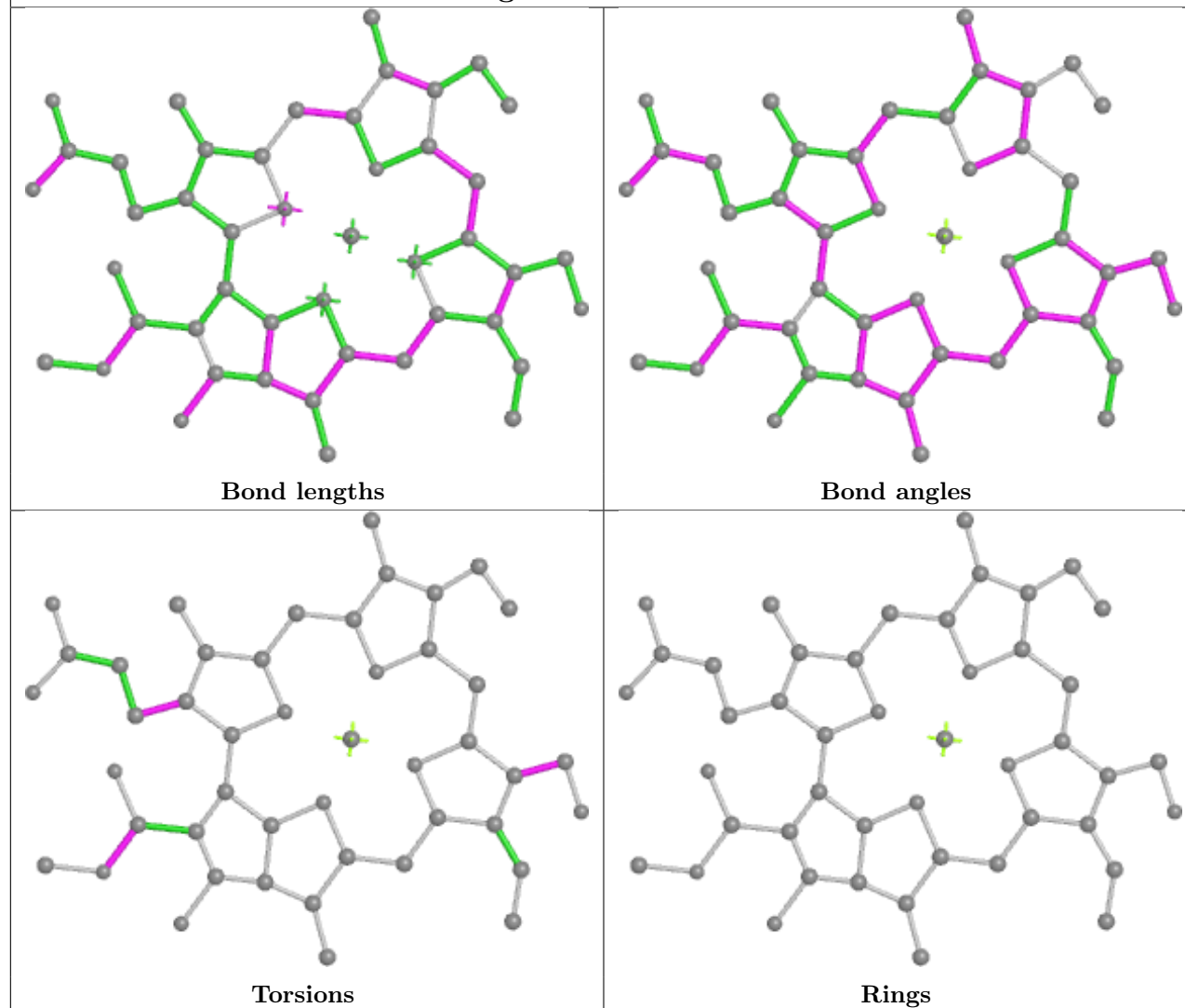
Ligand NEX r 623



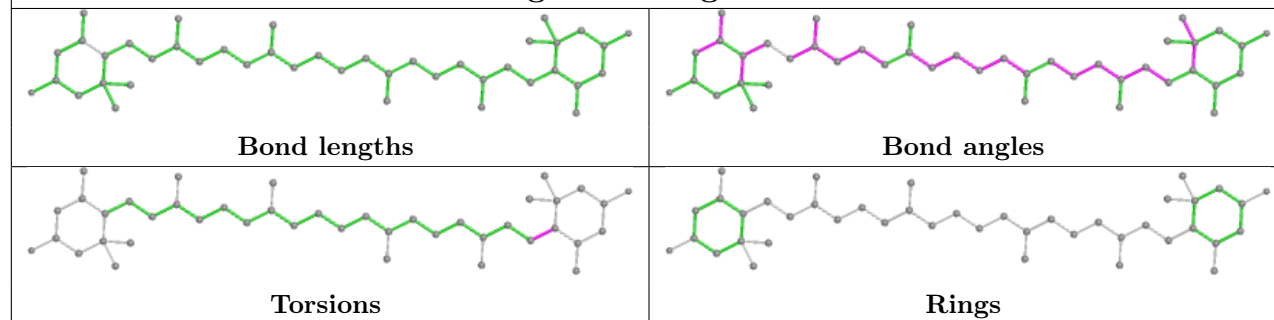
Ligand CHL 3 601

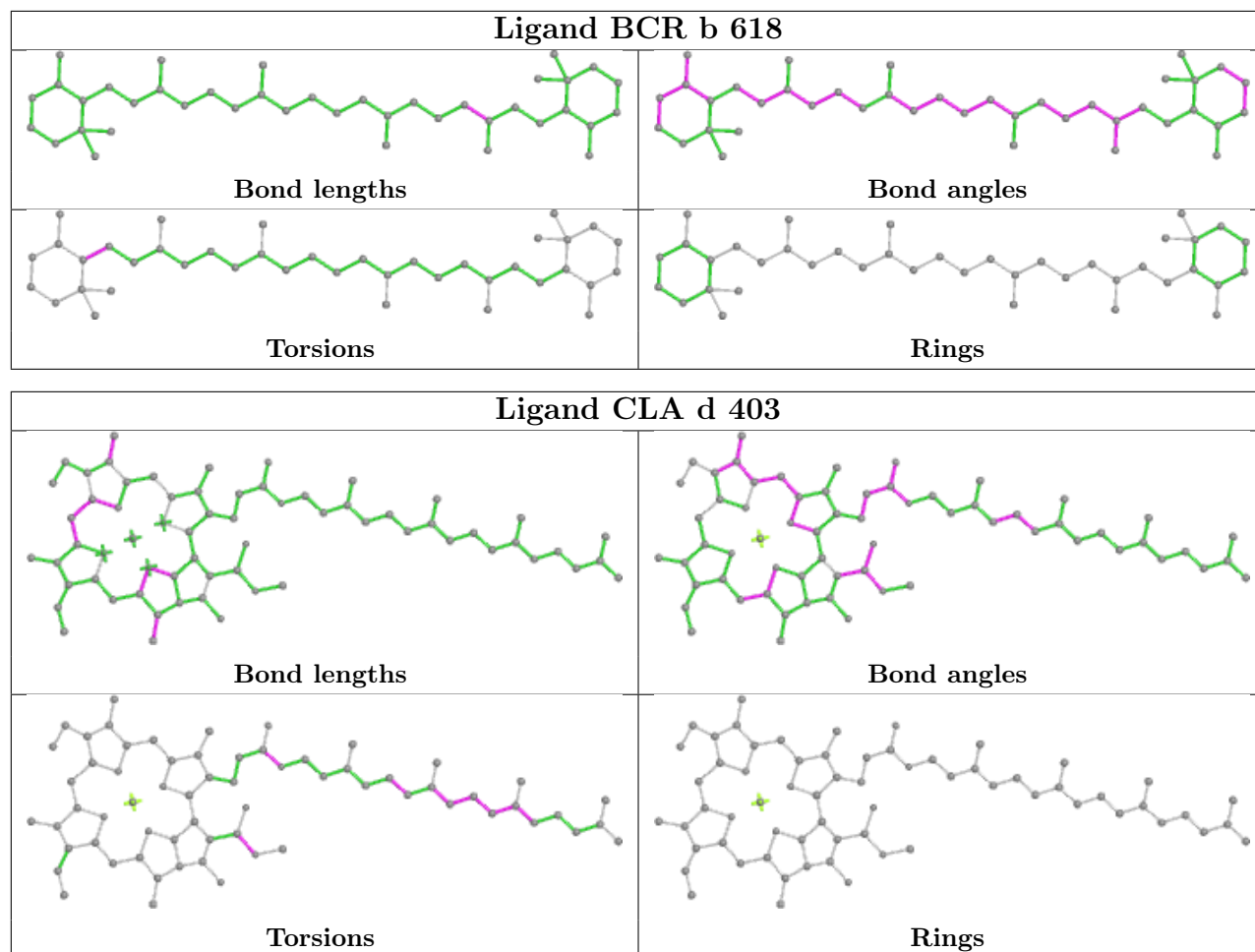


Ligand CHL 8 608

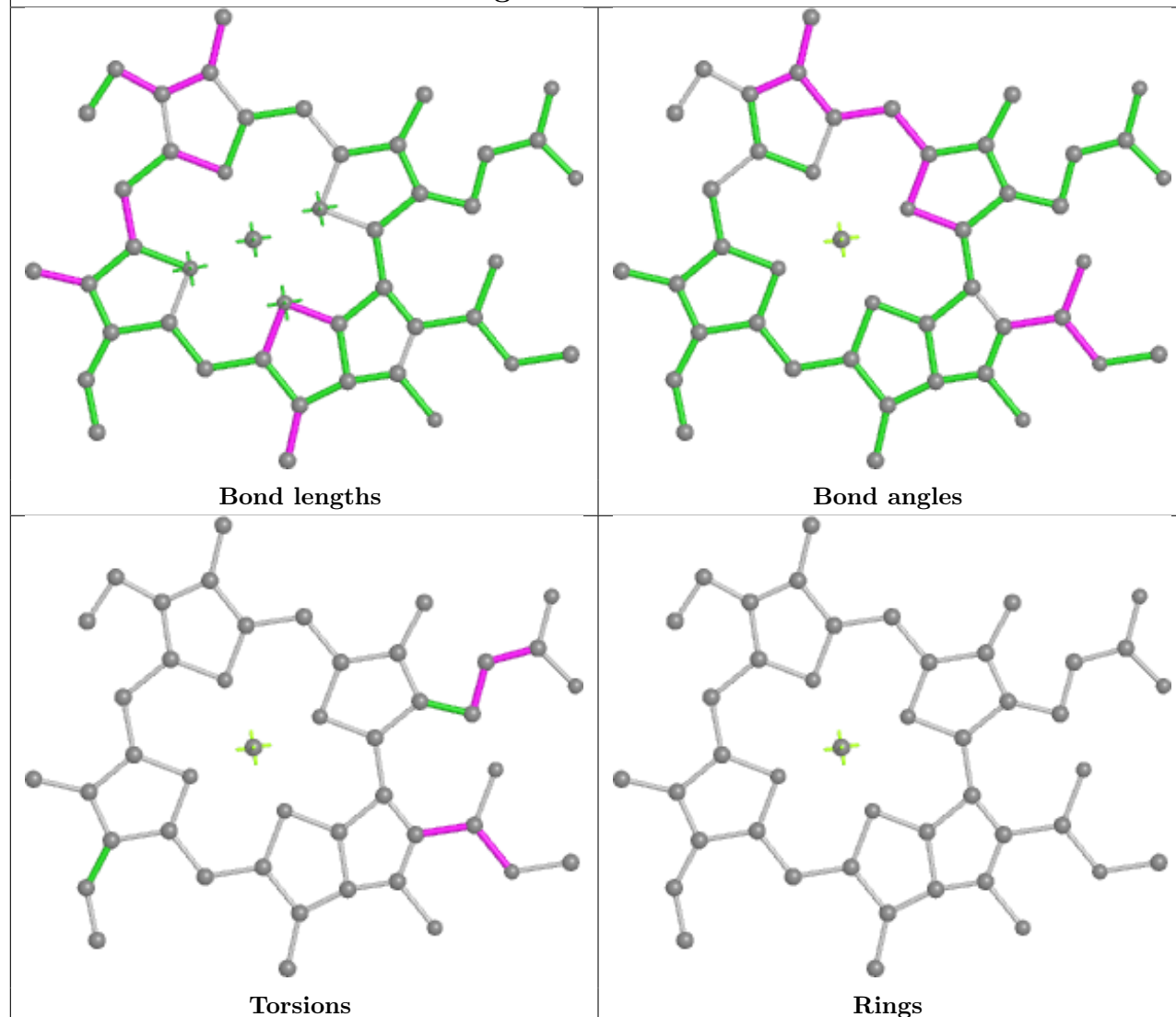


Ligand LUT g 1620

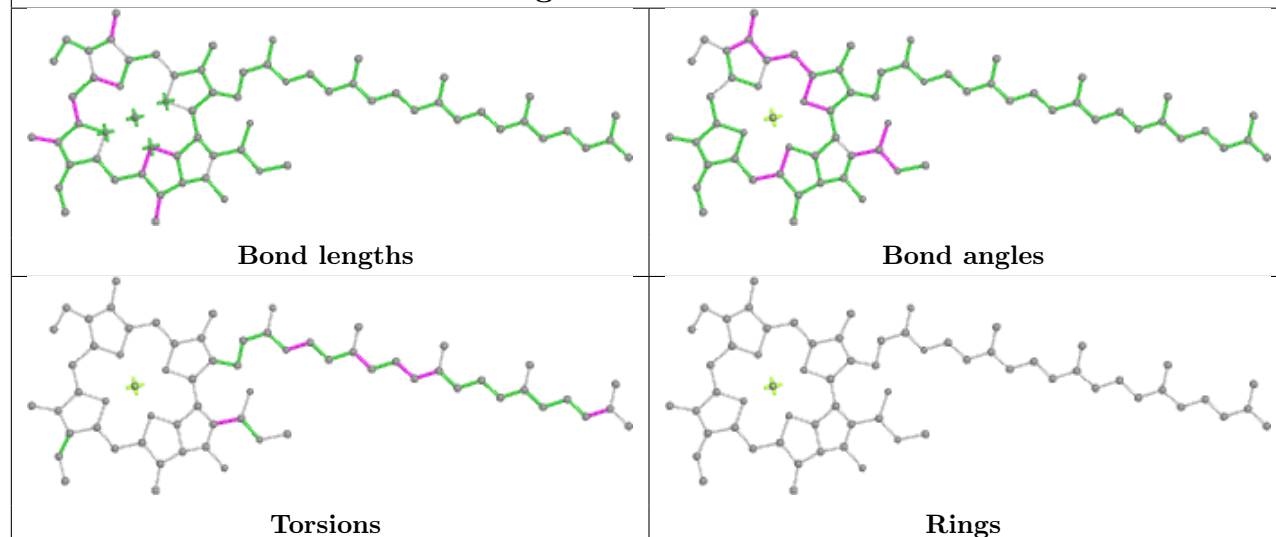


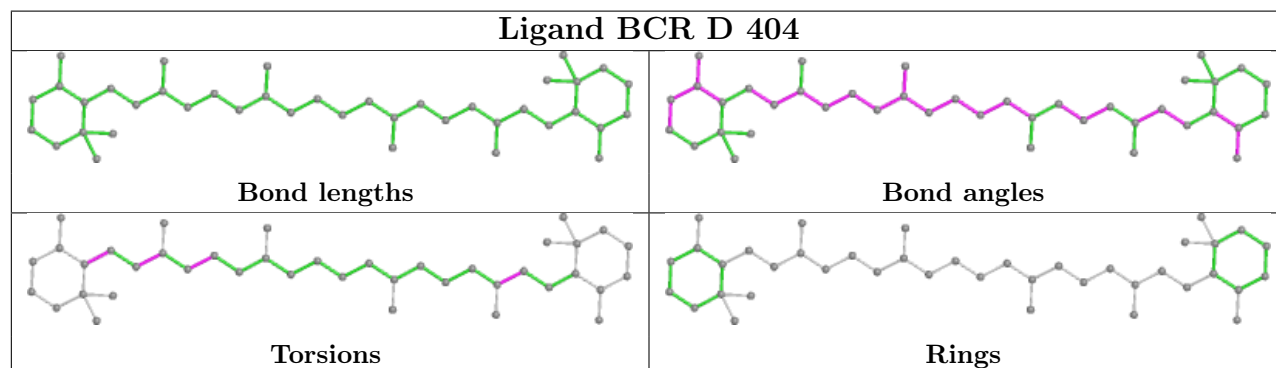
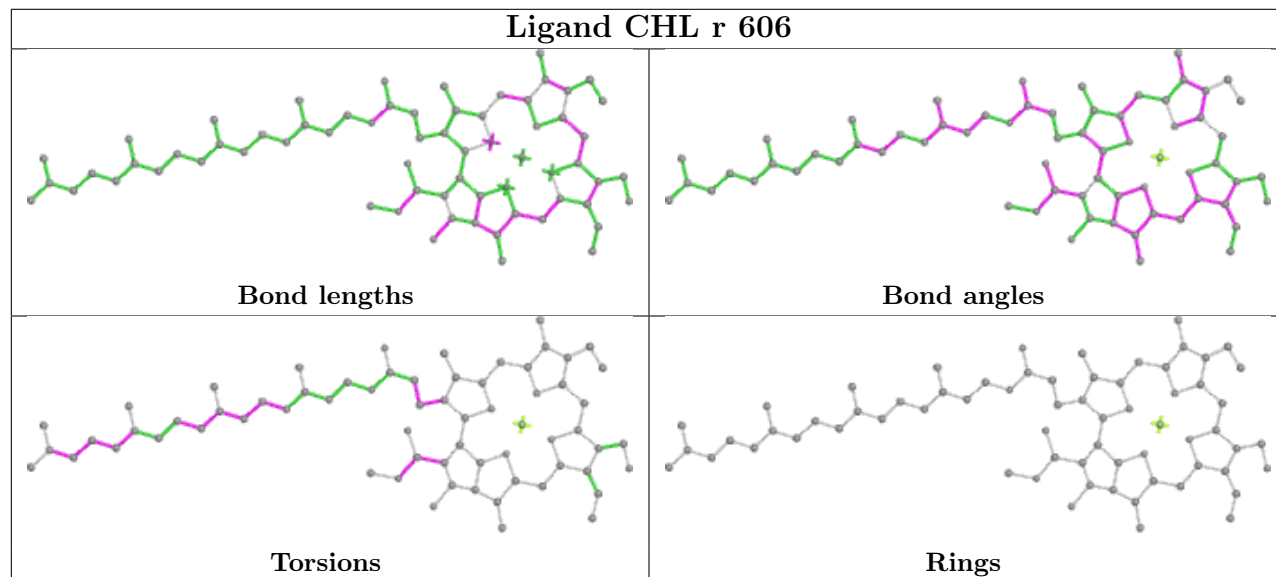
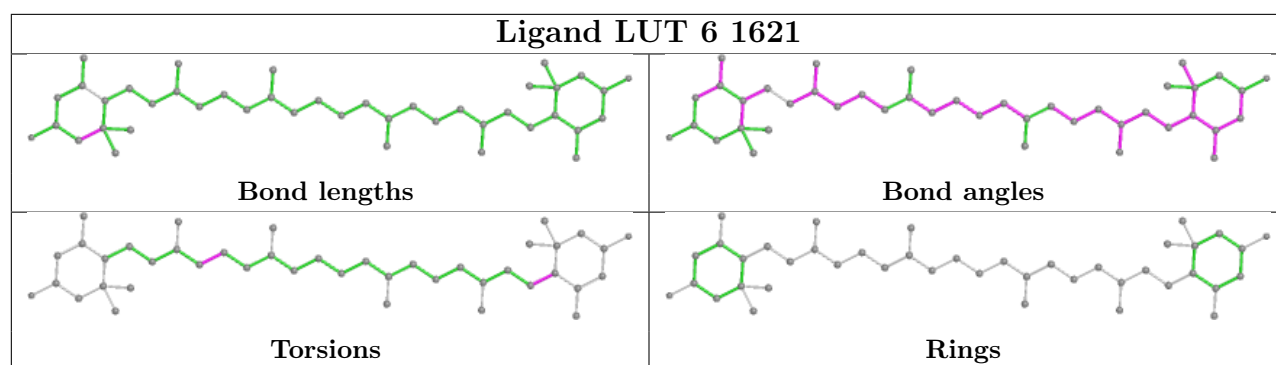


Ligand CLA 4 602

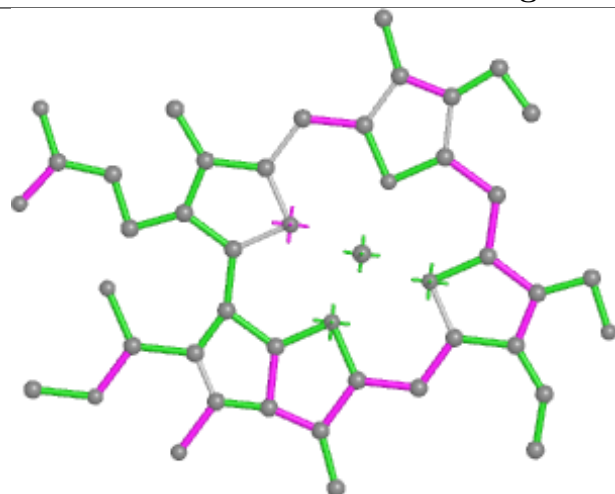


Ligand CLA b 603

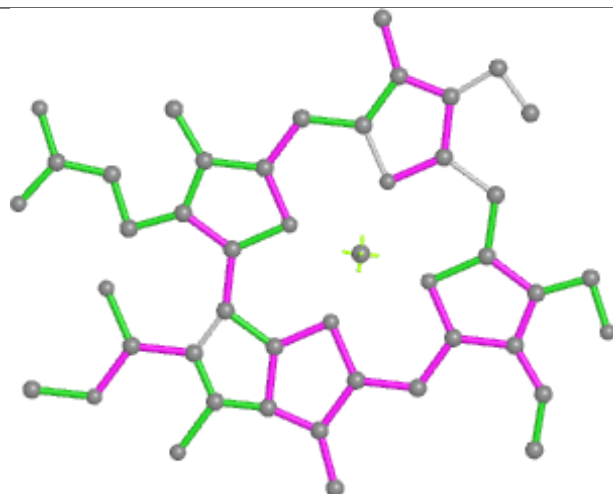




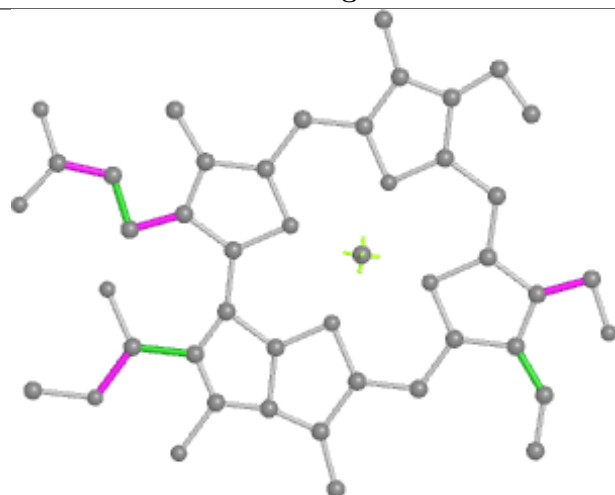
Ligand CHL 2 608



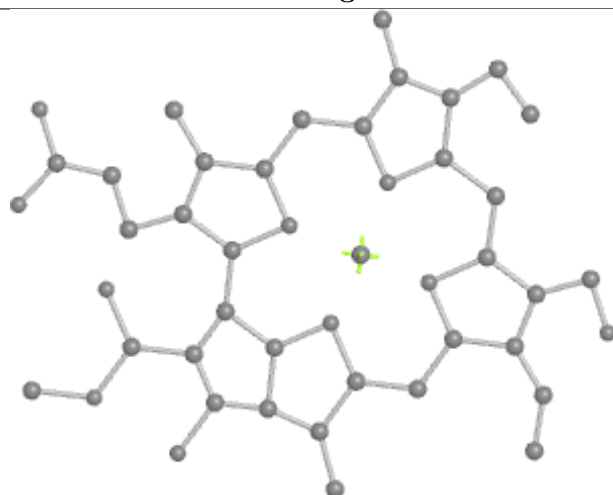
Bond lengths



Bond angles

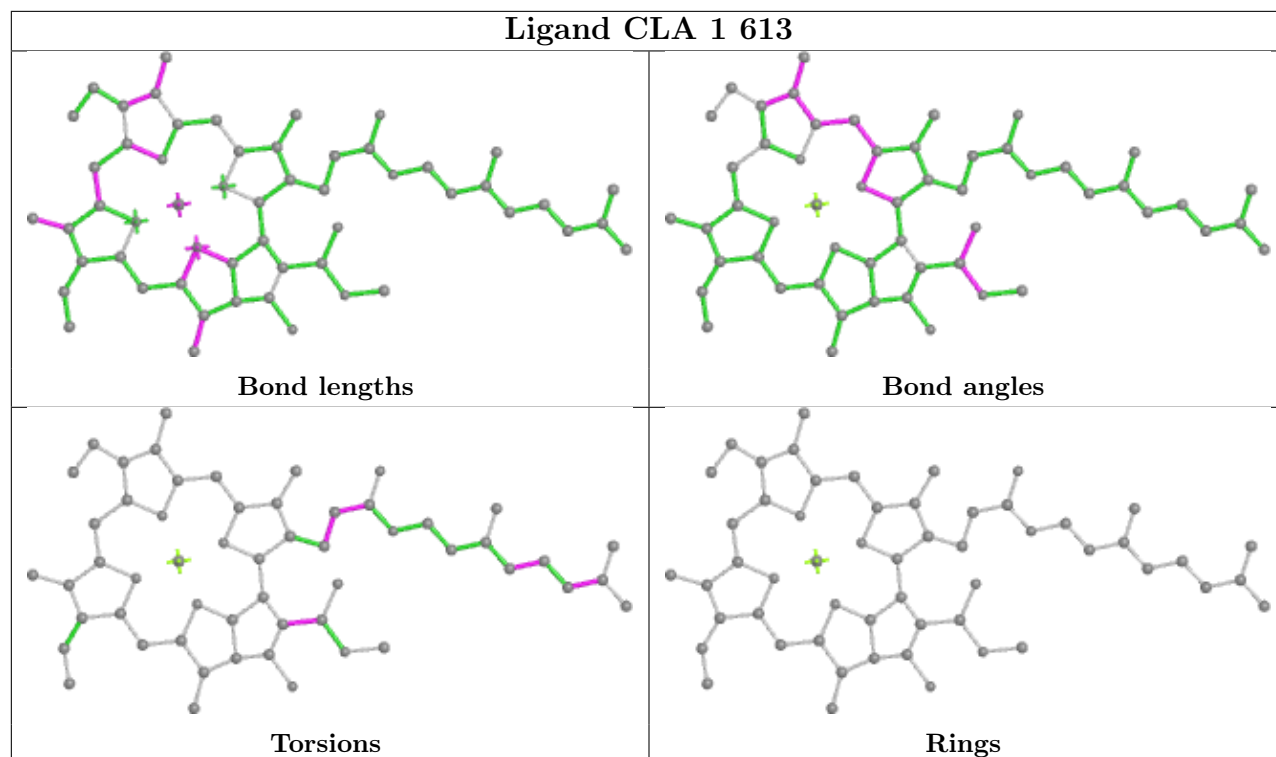


Torsions

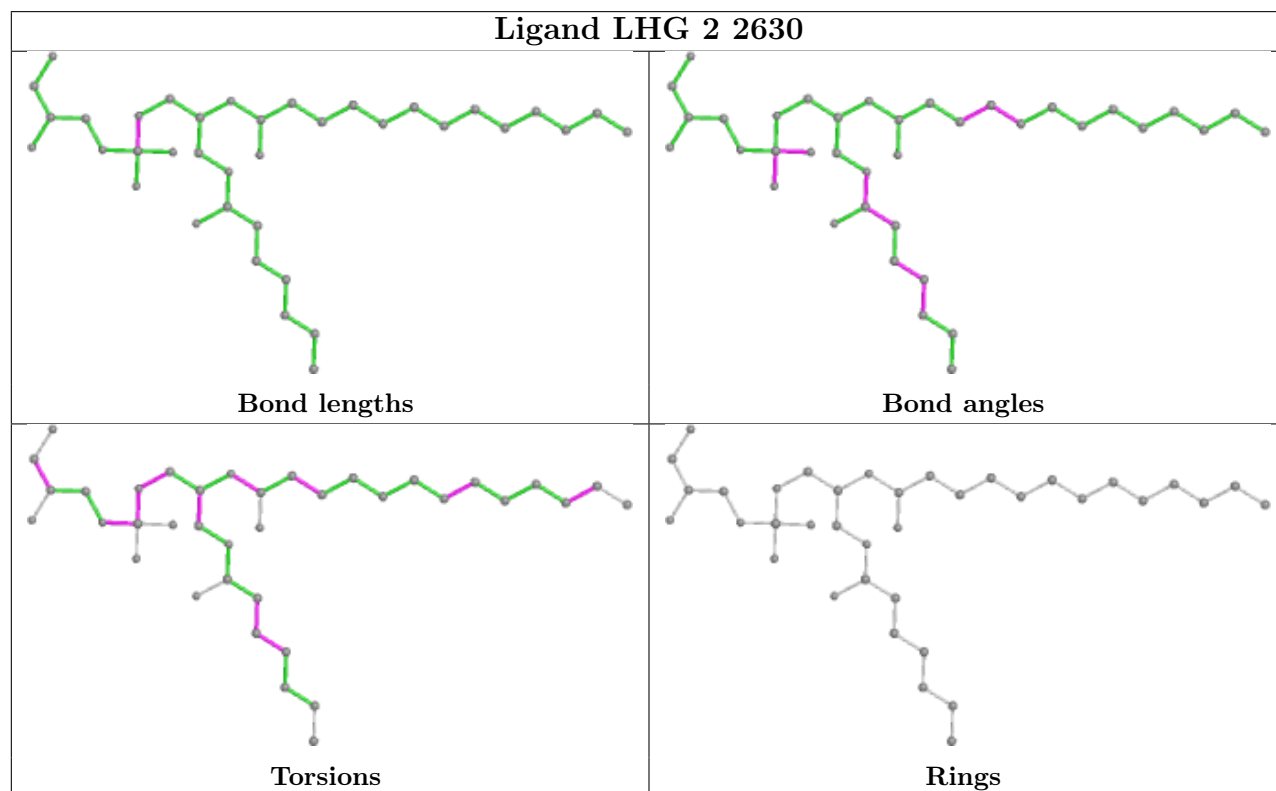


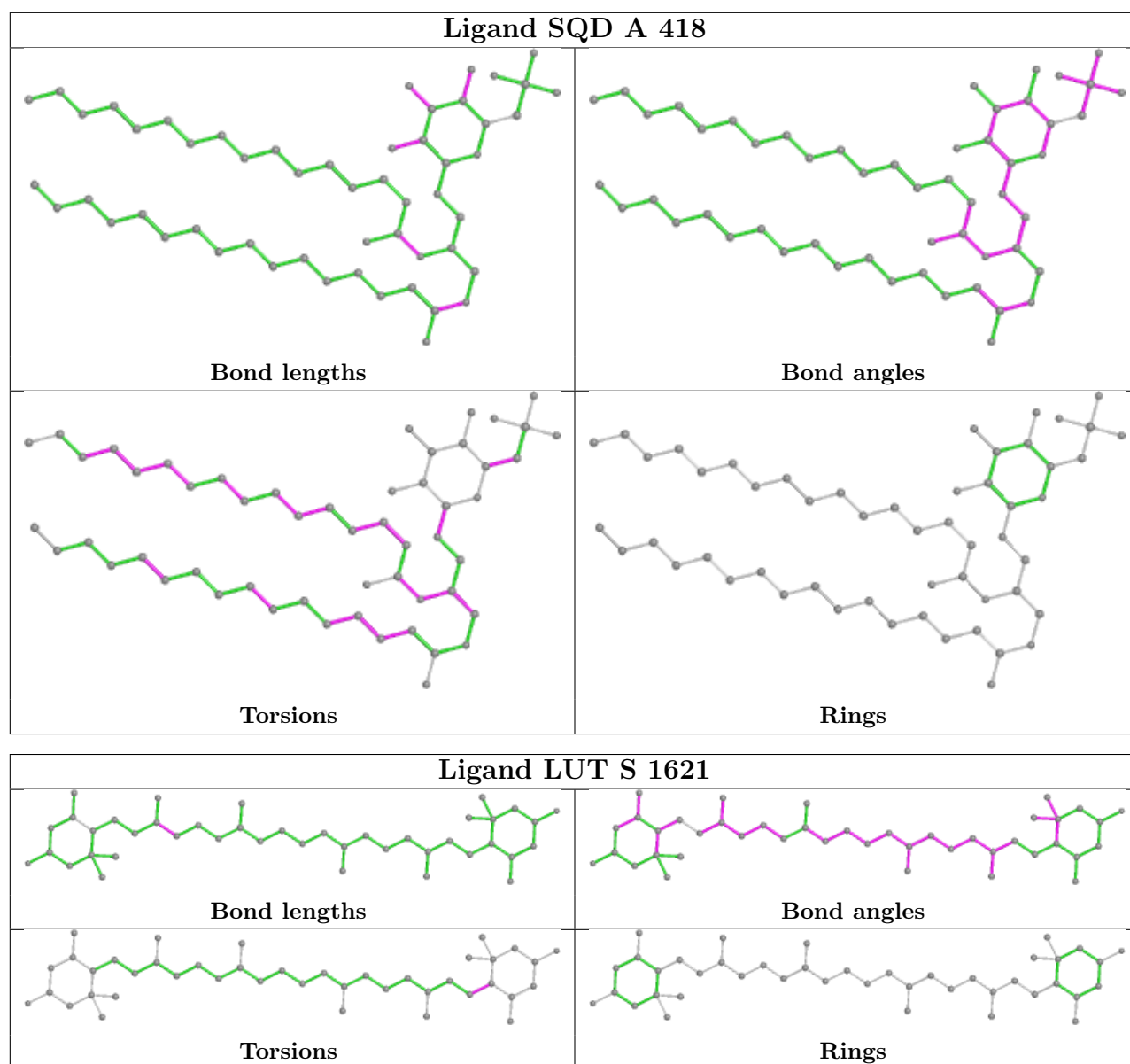
Rings

Ligand CLA 1 613

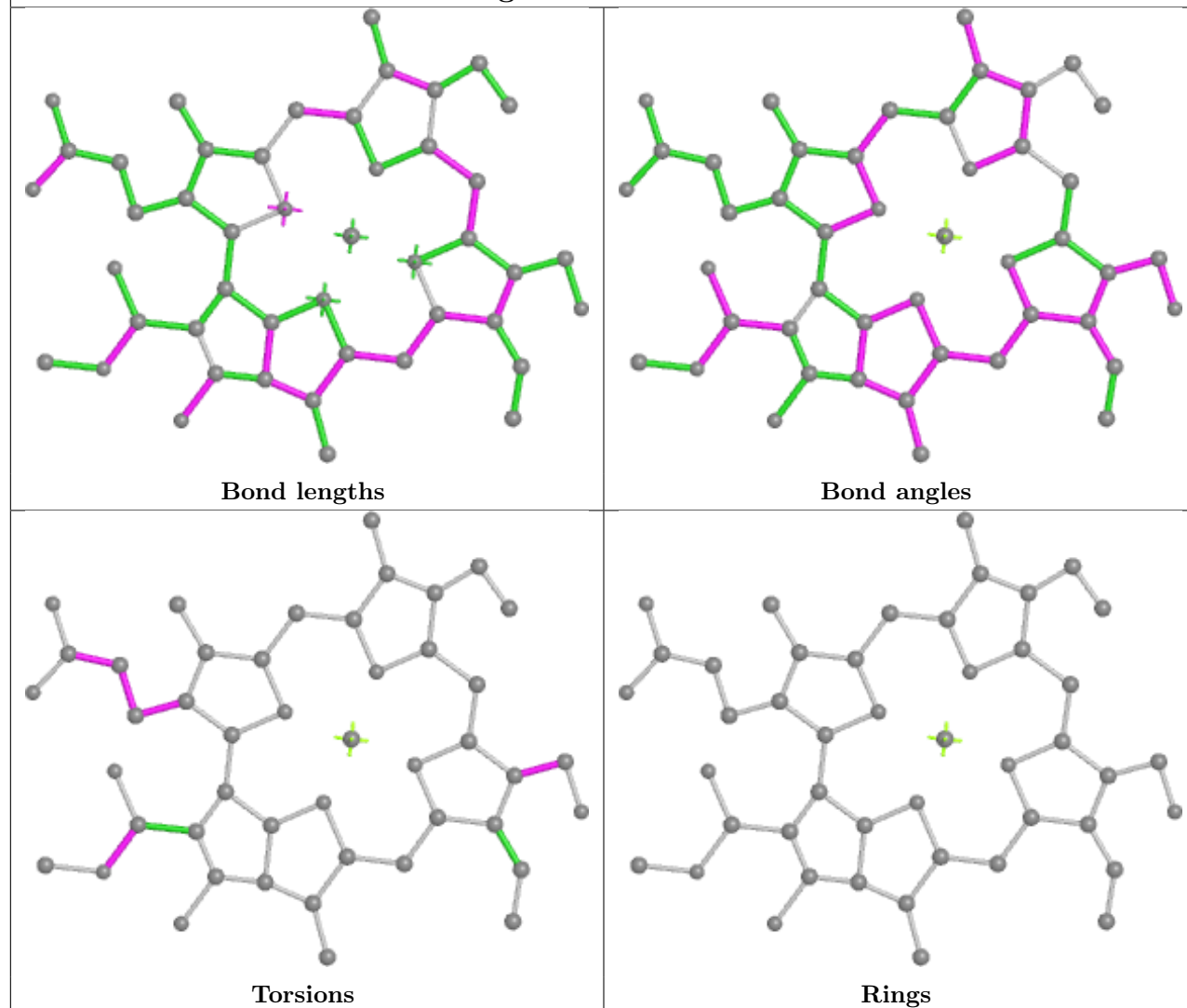


Ligand LHG 2 2630

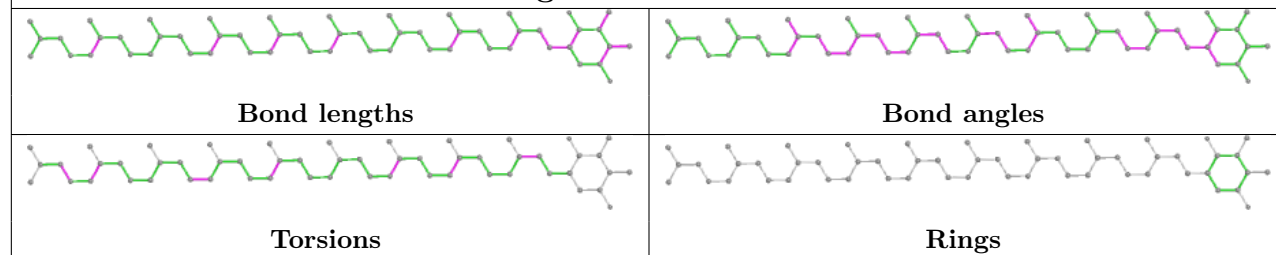




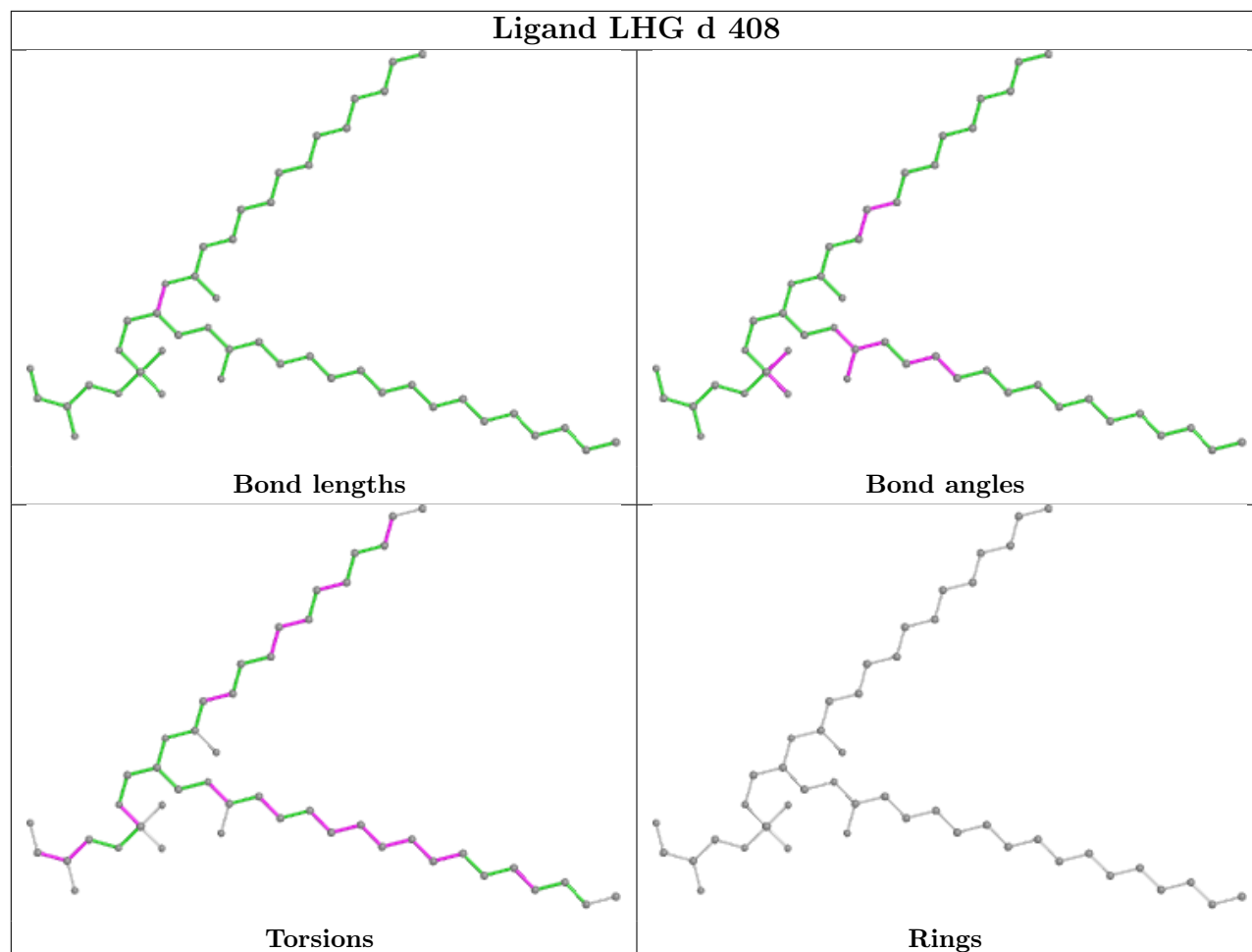
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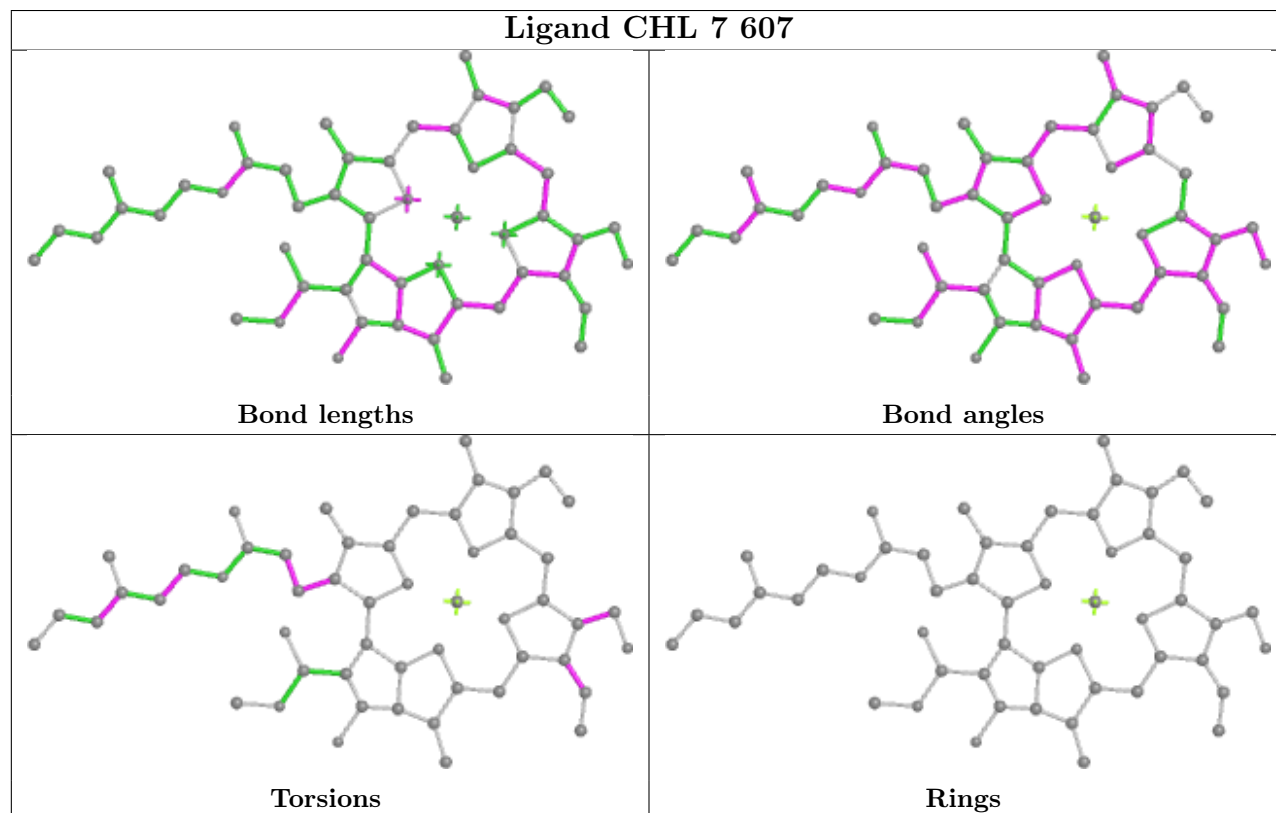
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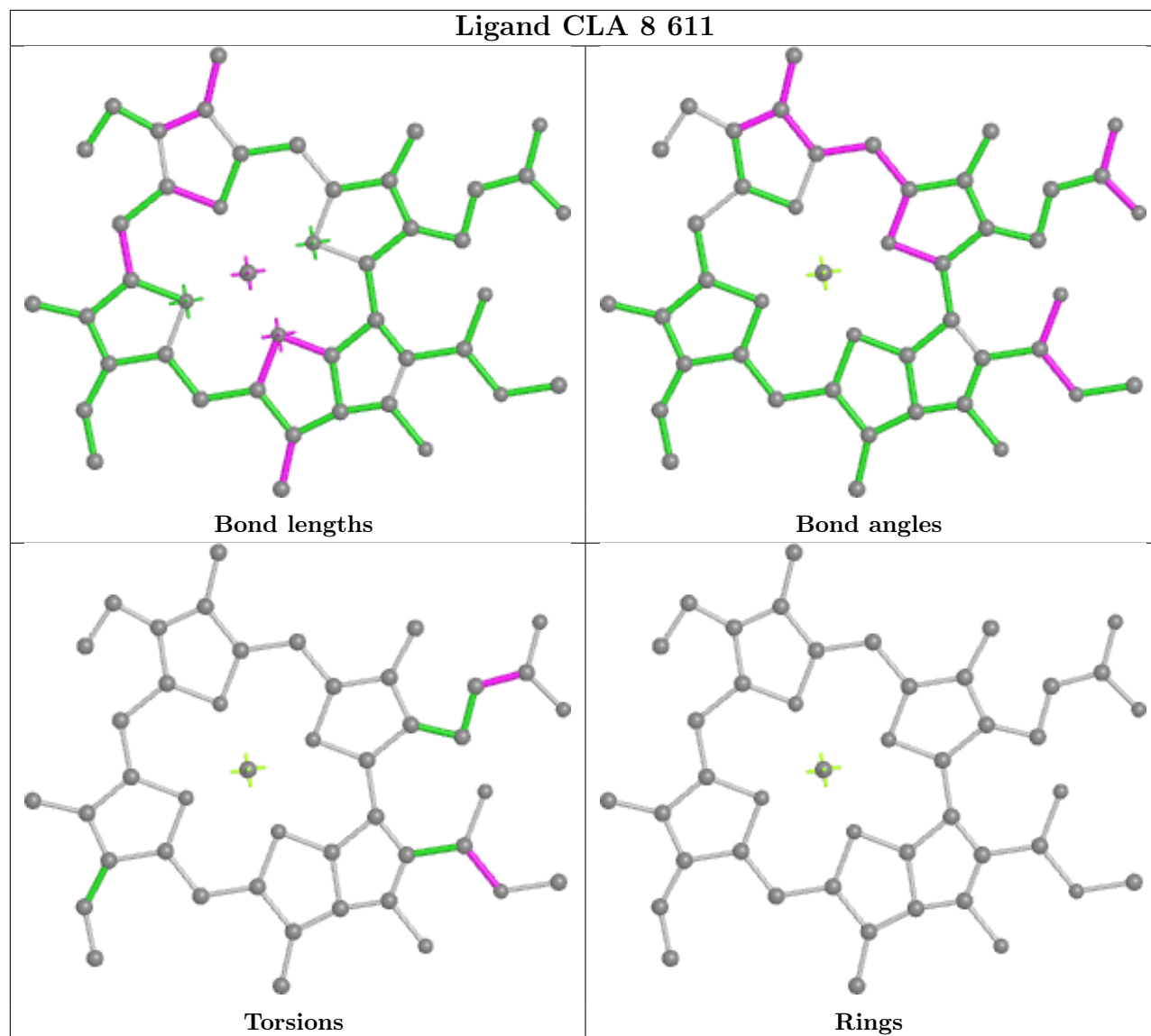
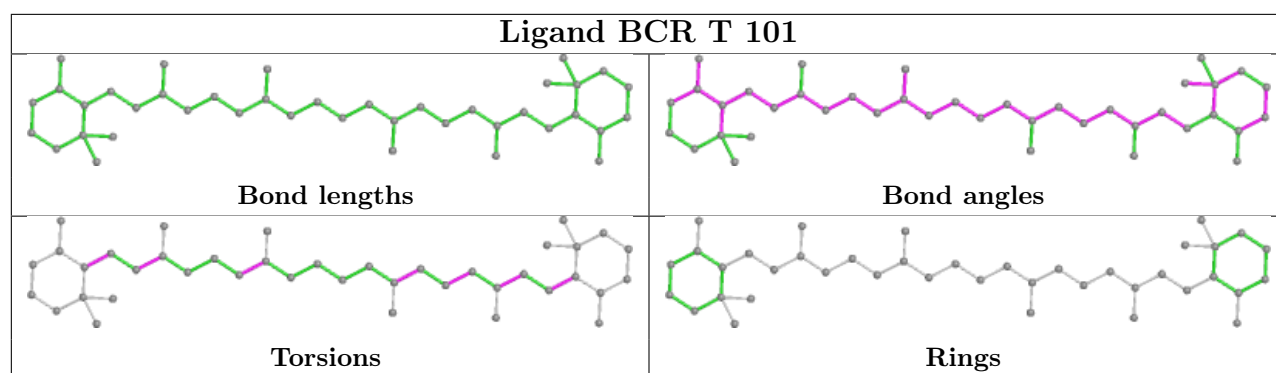


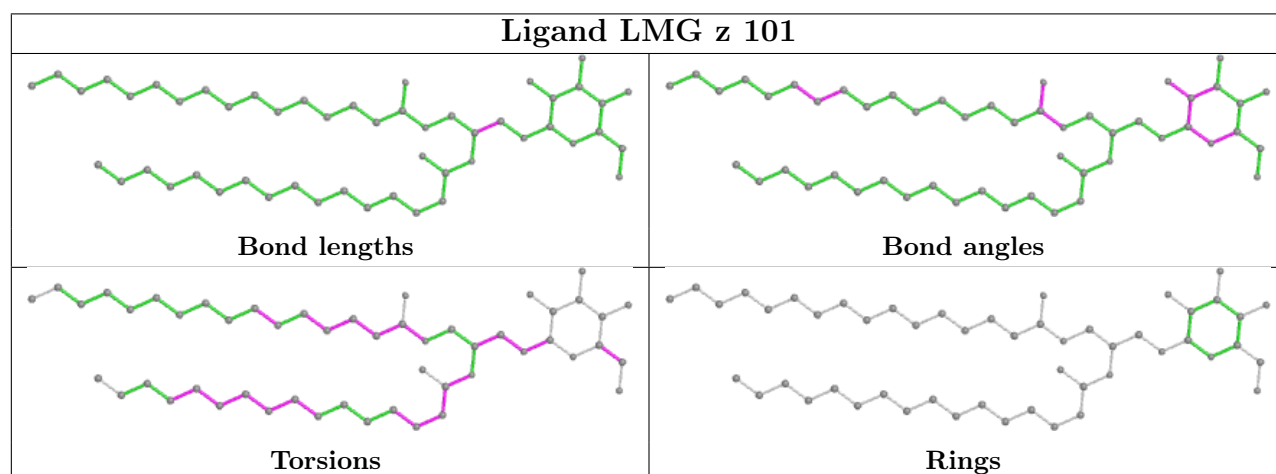
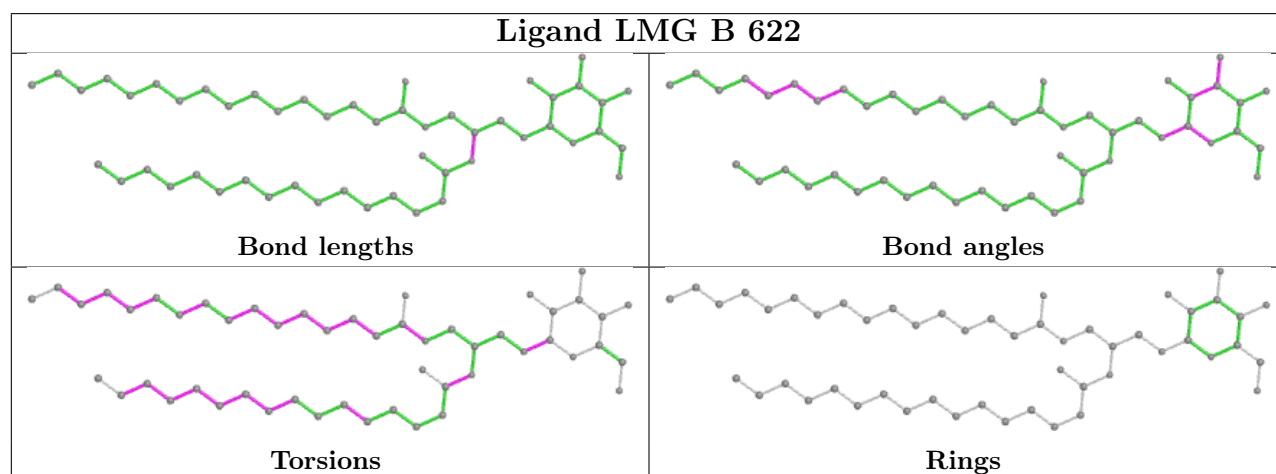
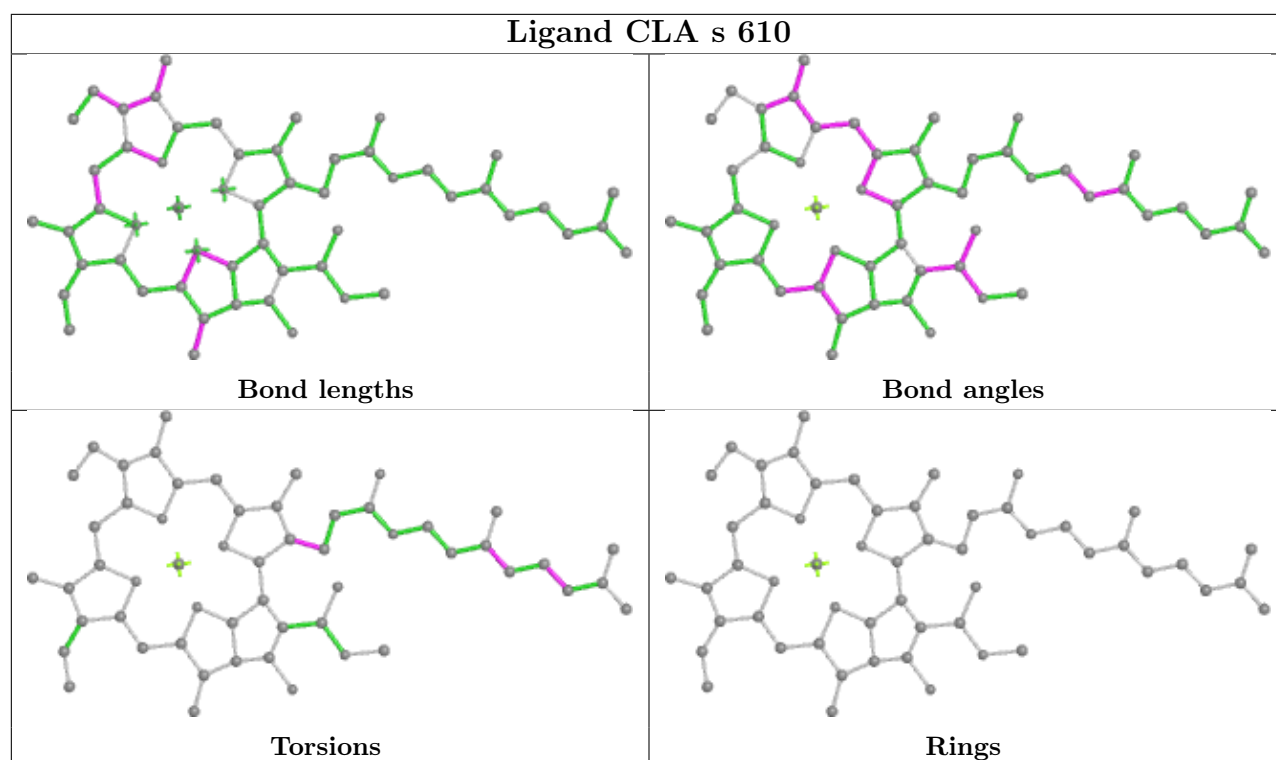
Ligand LHG d 408



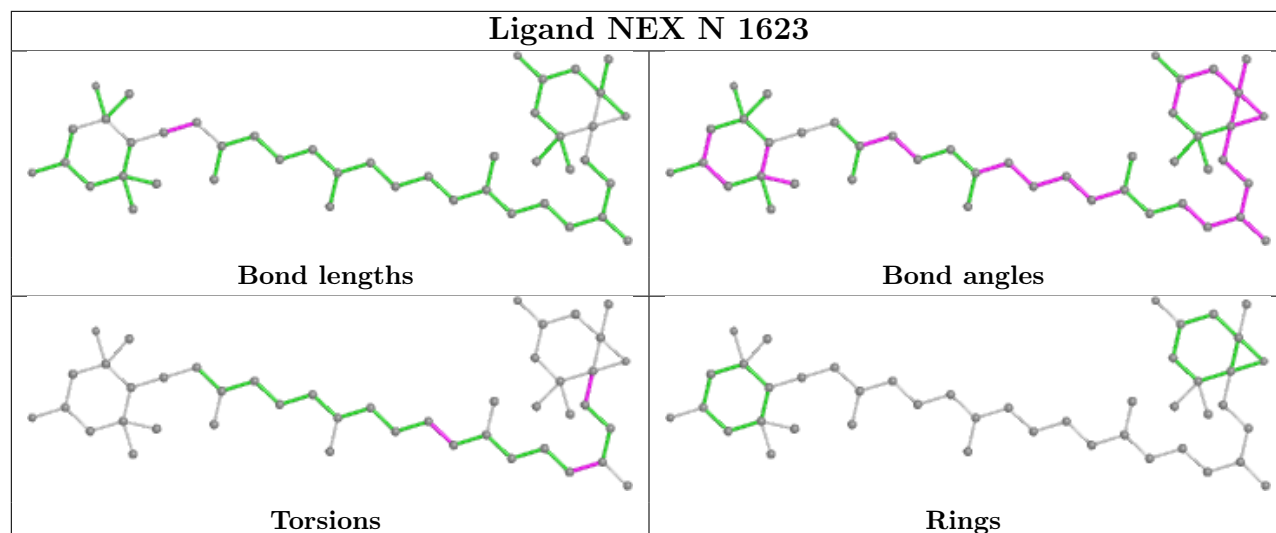
Ligand CHL 7 607



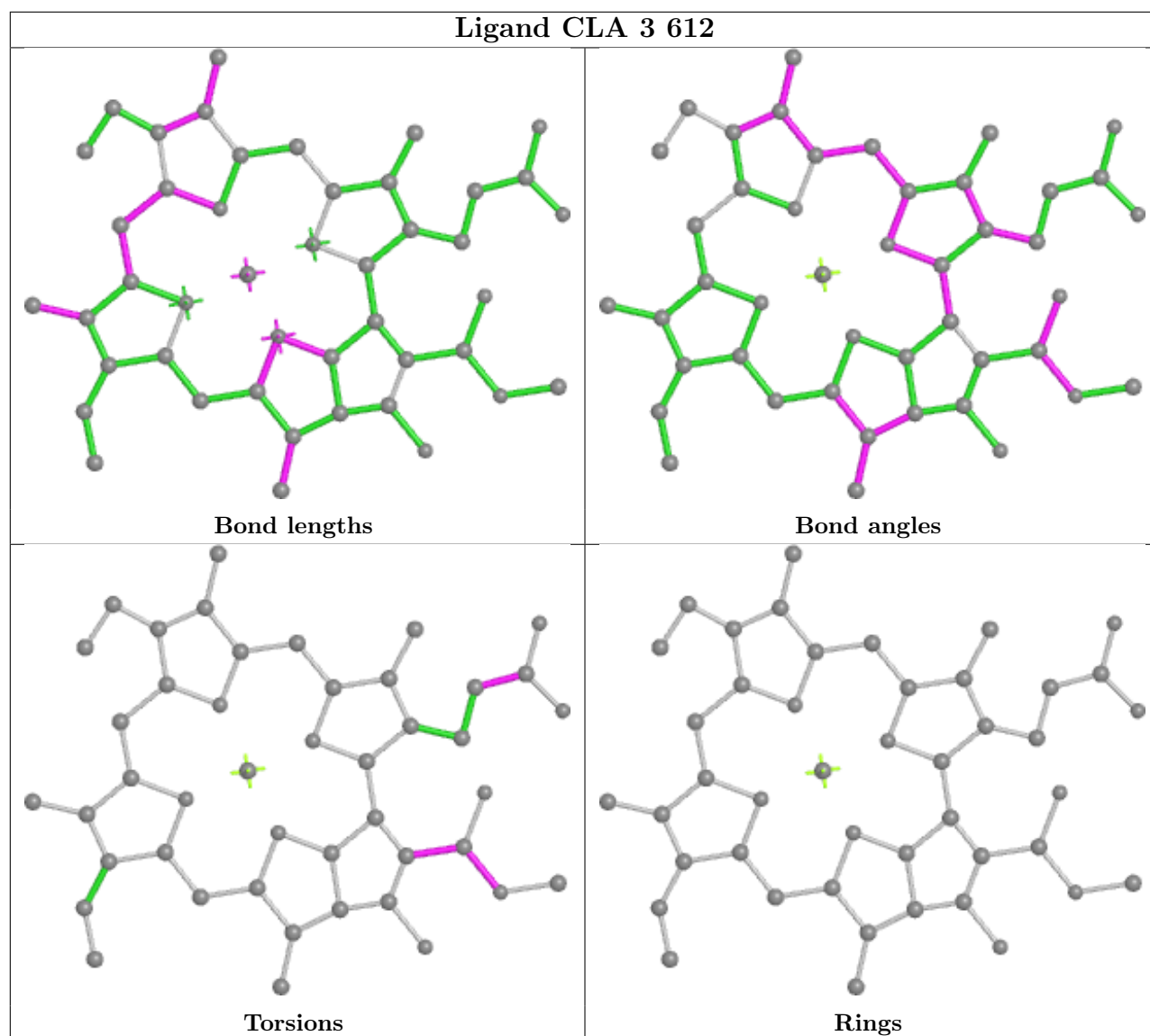


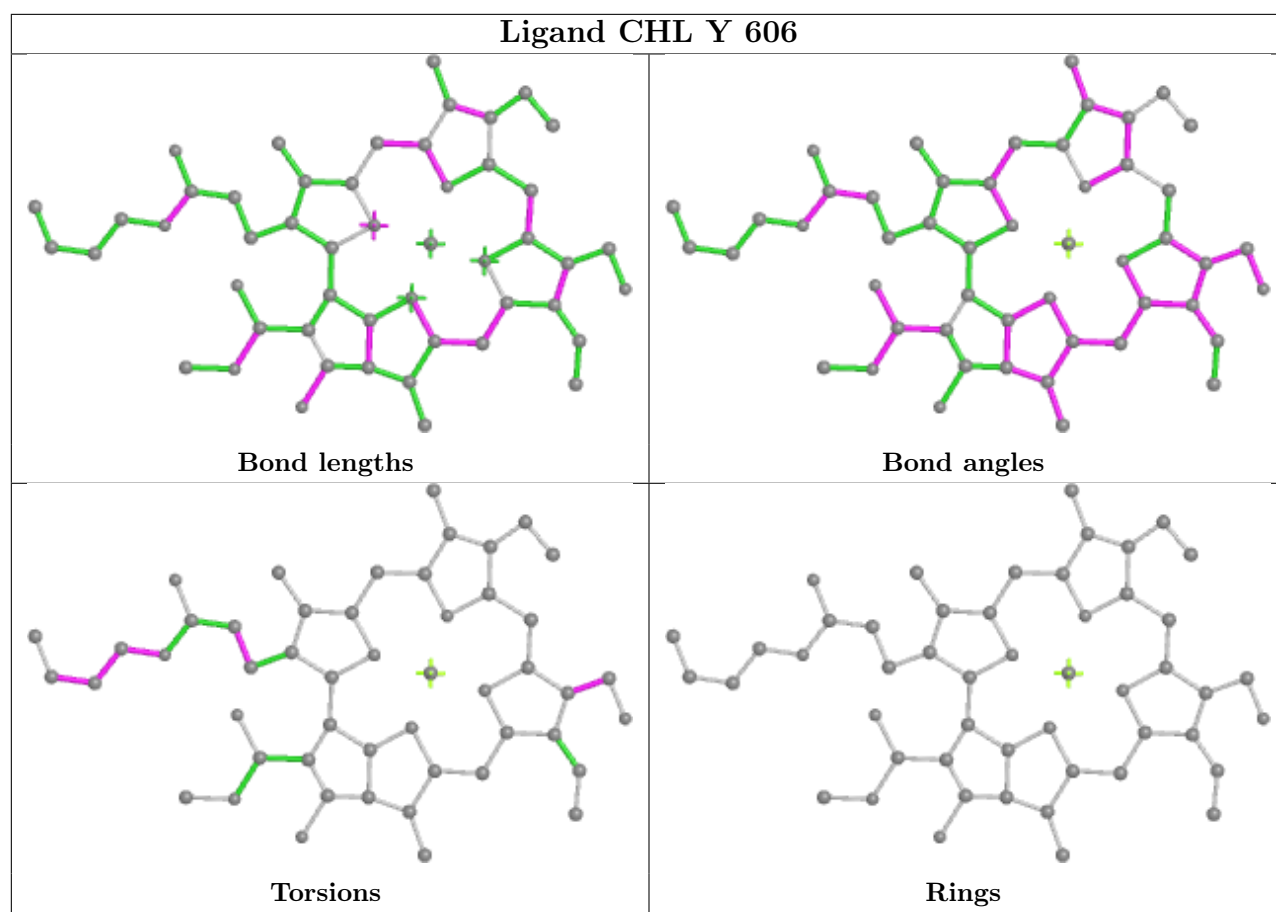


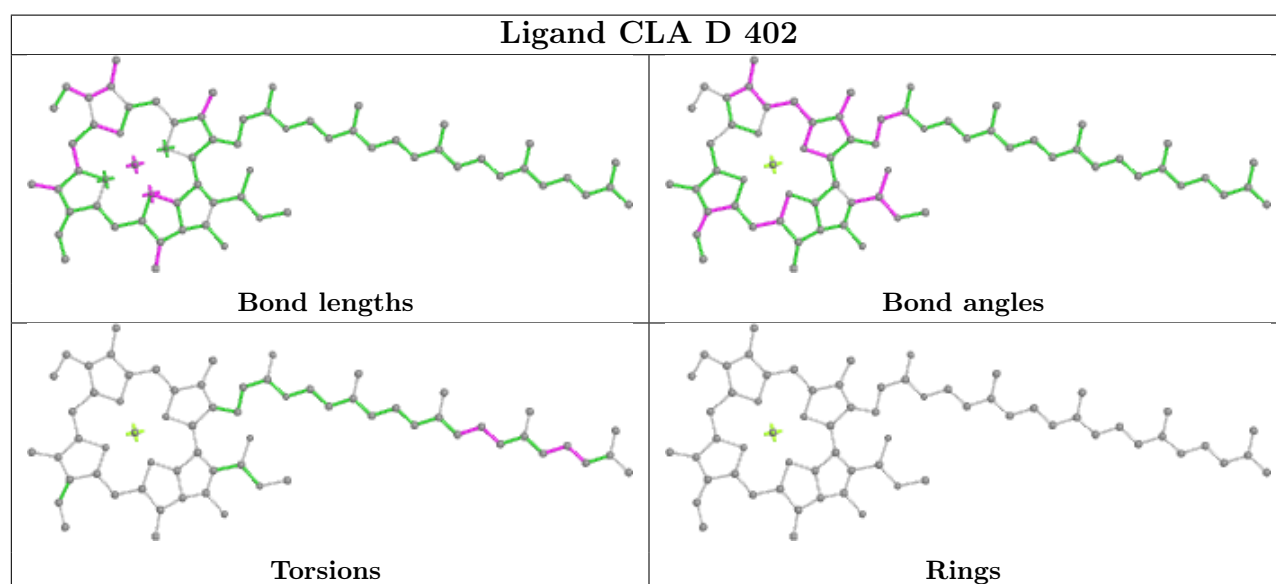
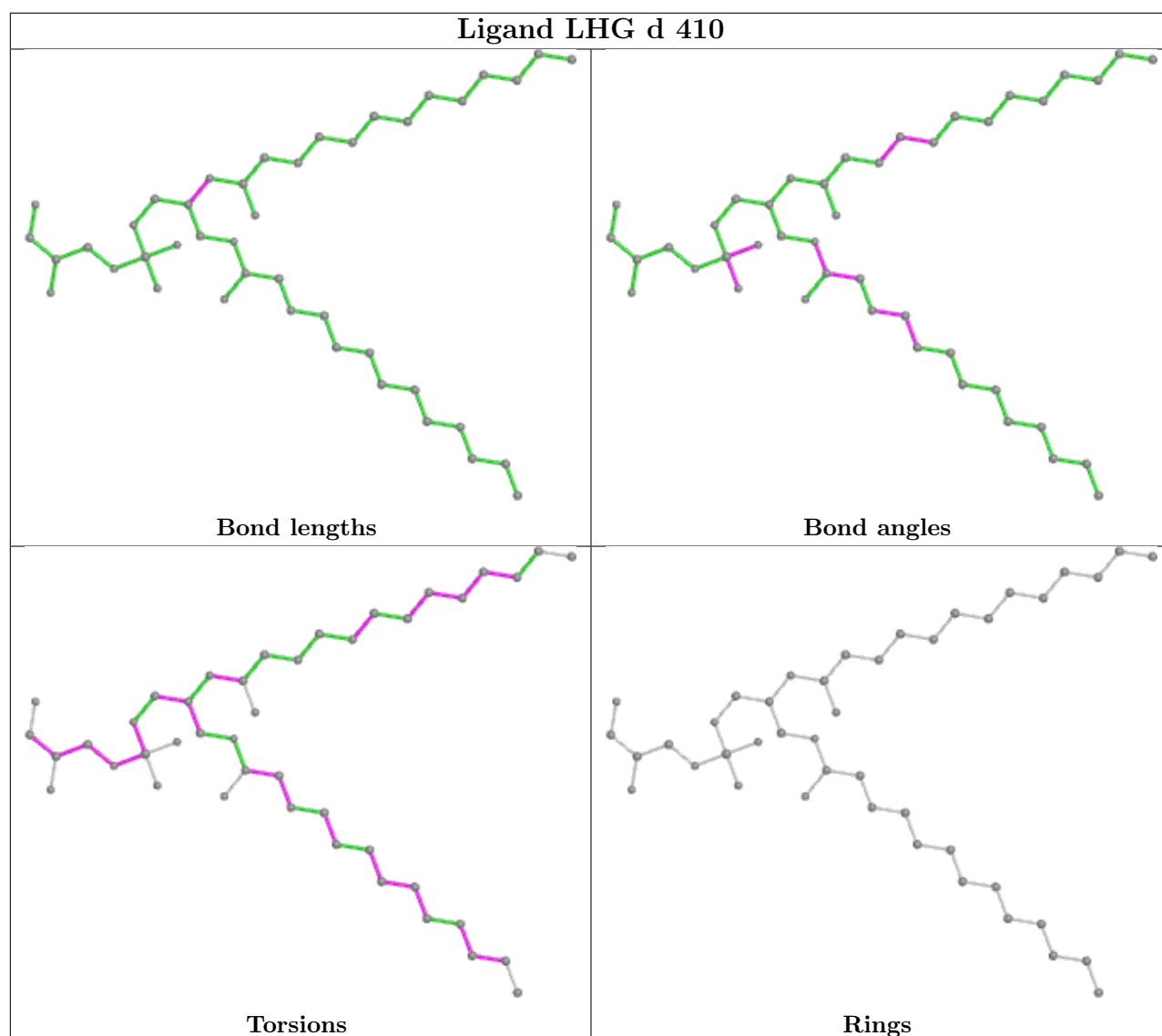
Ligand NEX N 1623

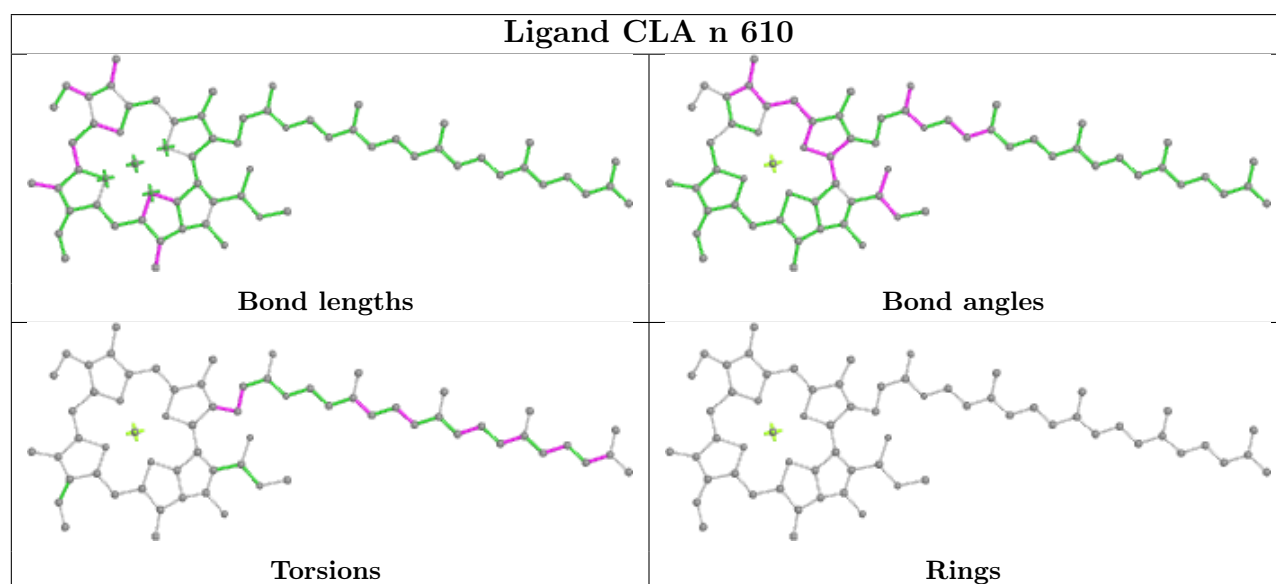
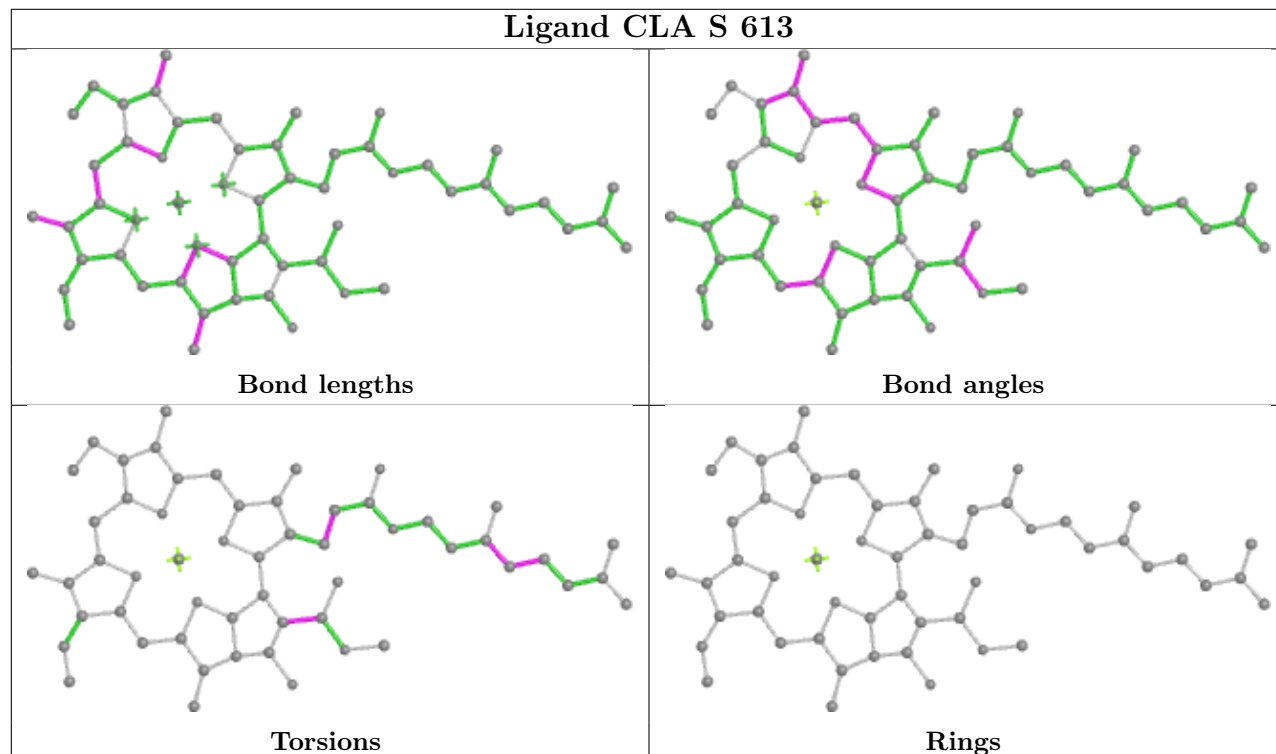
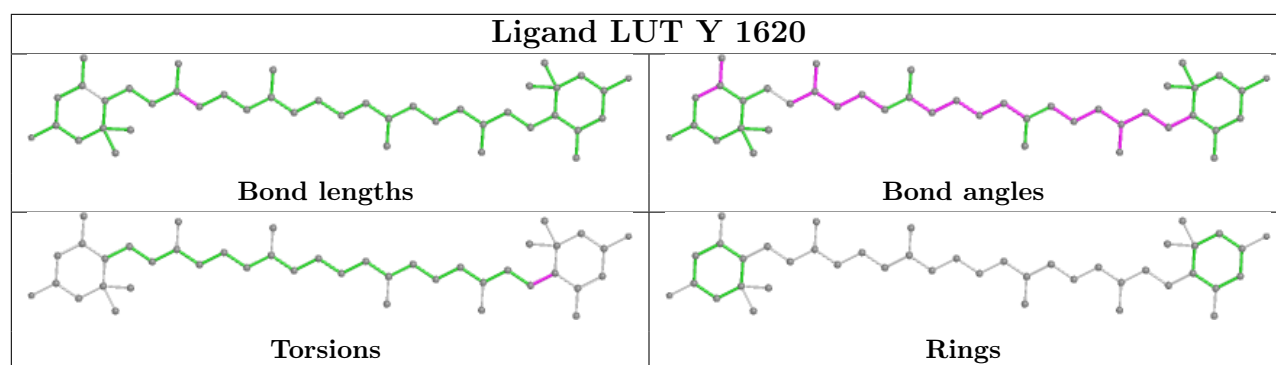


Ligand CLA 3 612

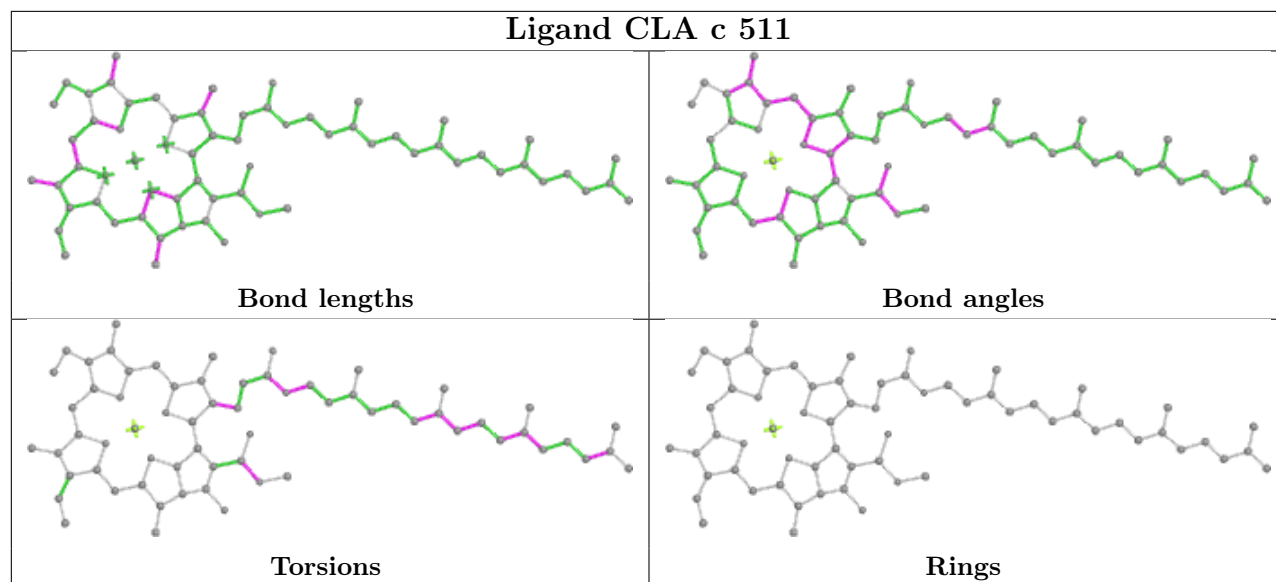




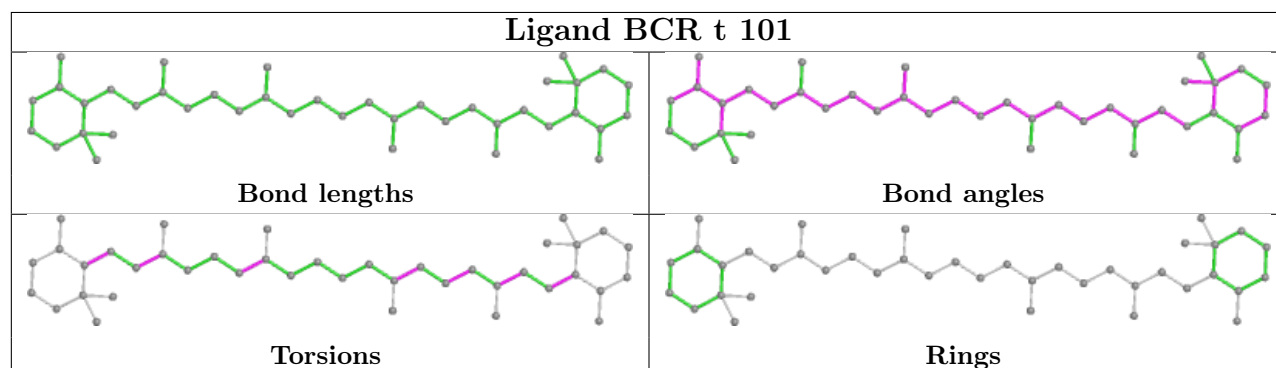




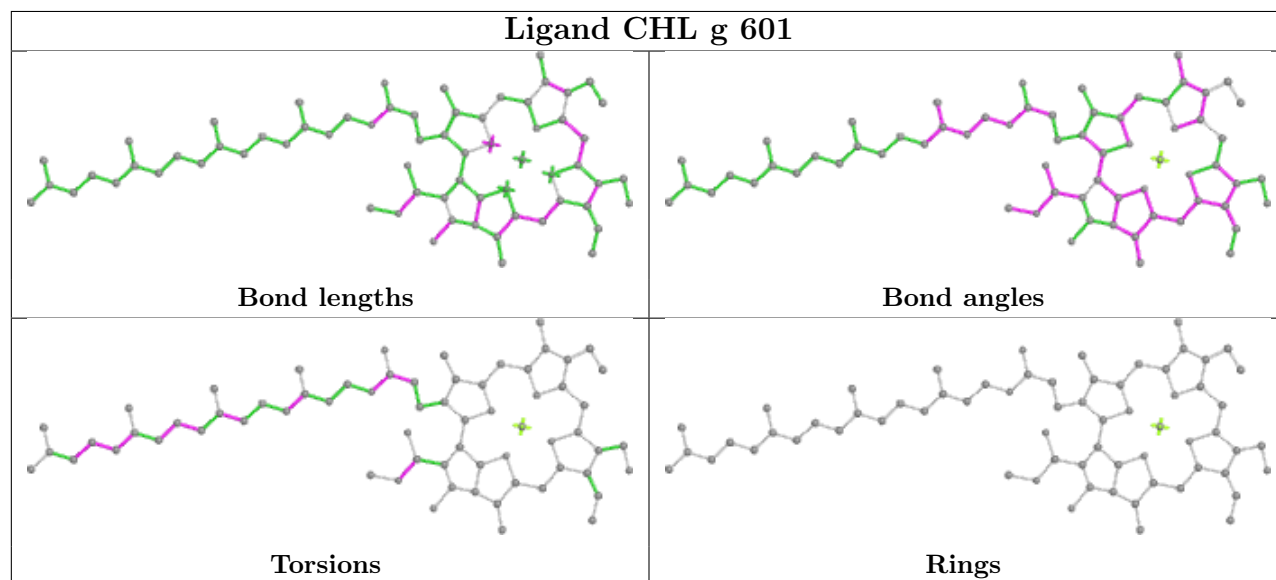
Ligand CLA c 511



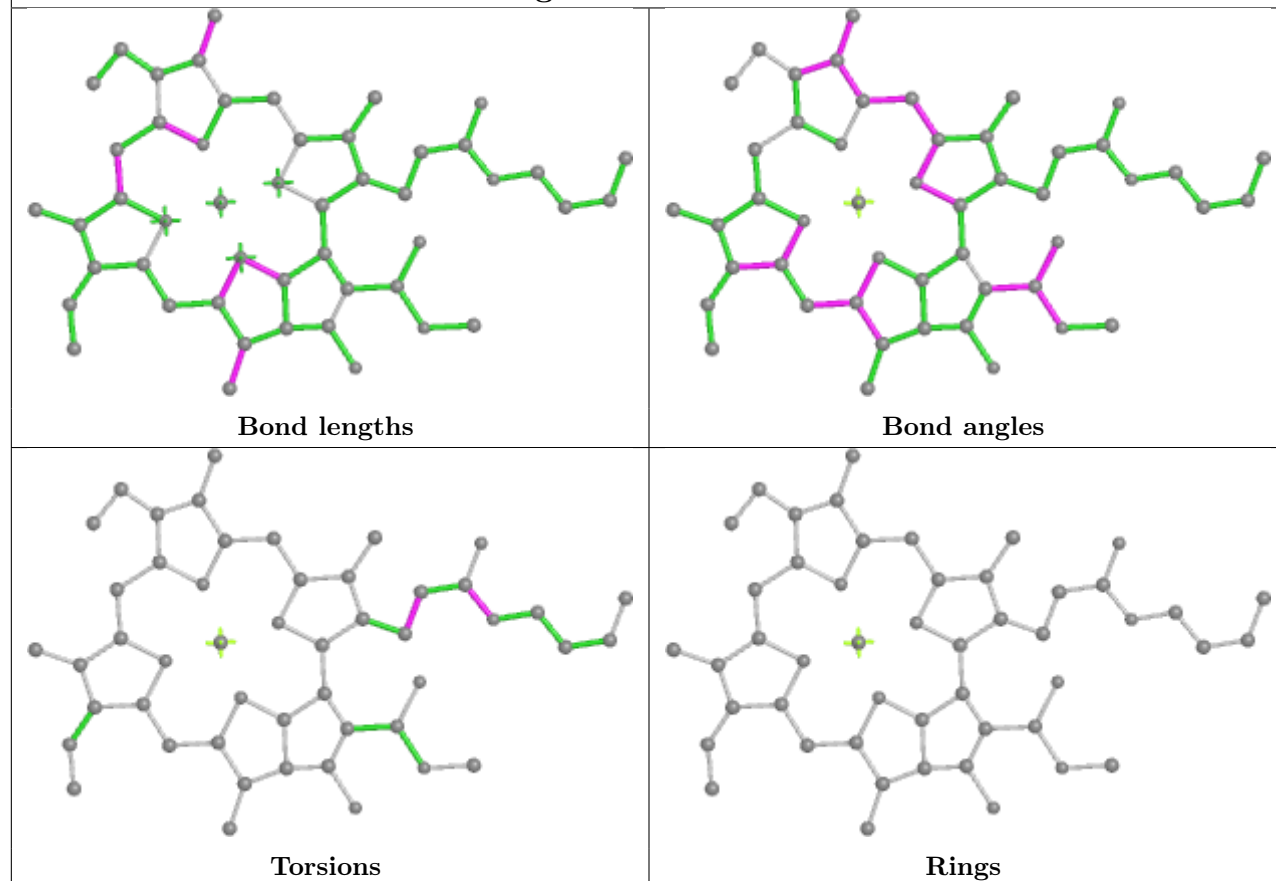
Ligand BCR t 101



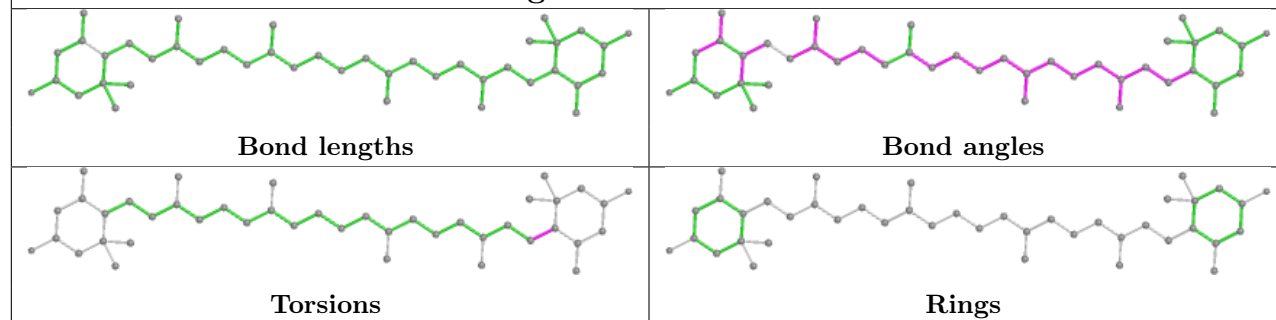
Ligand CHL g 601

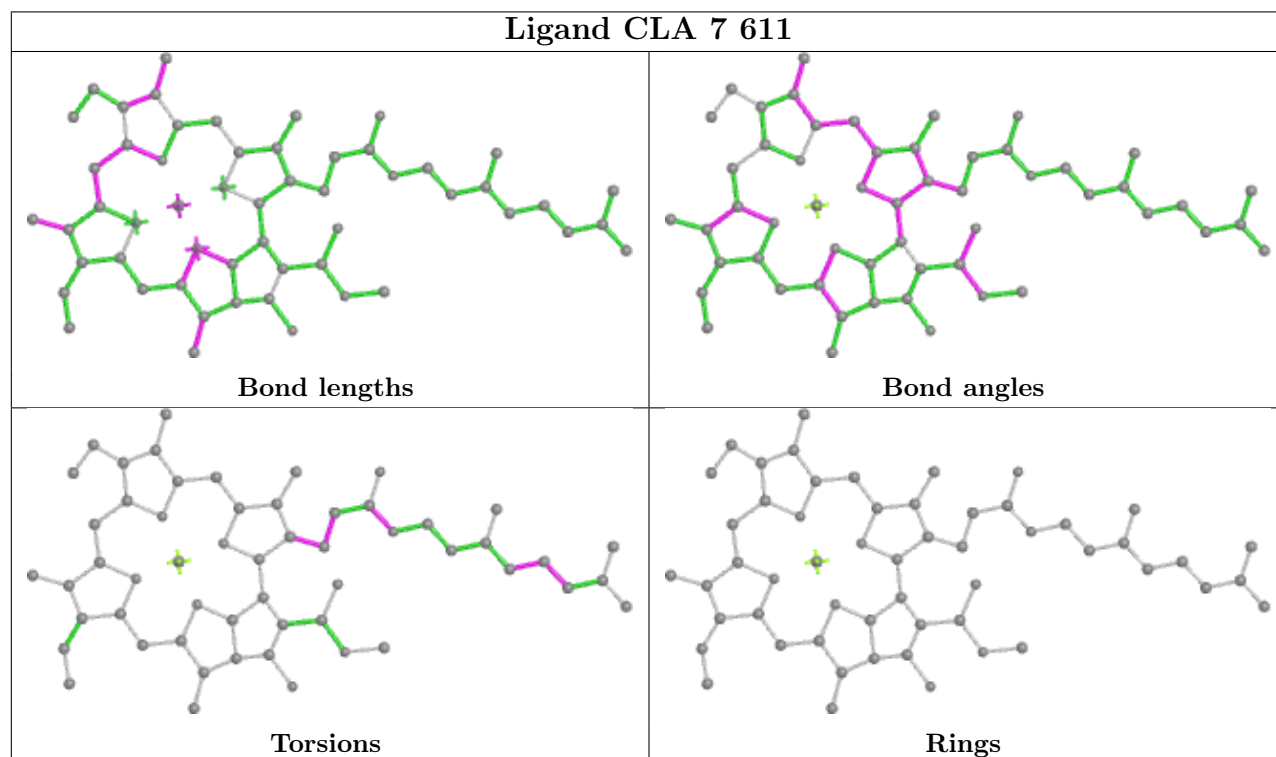
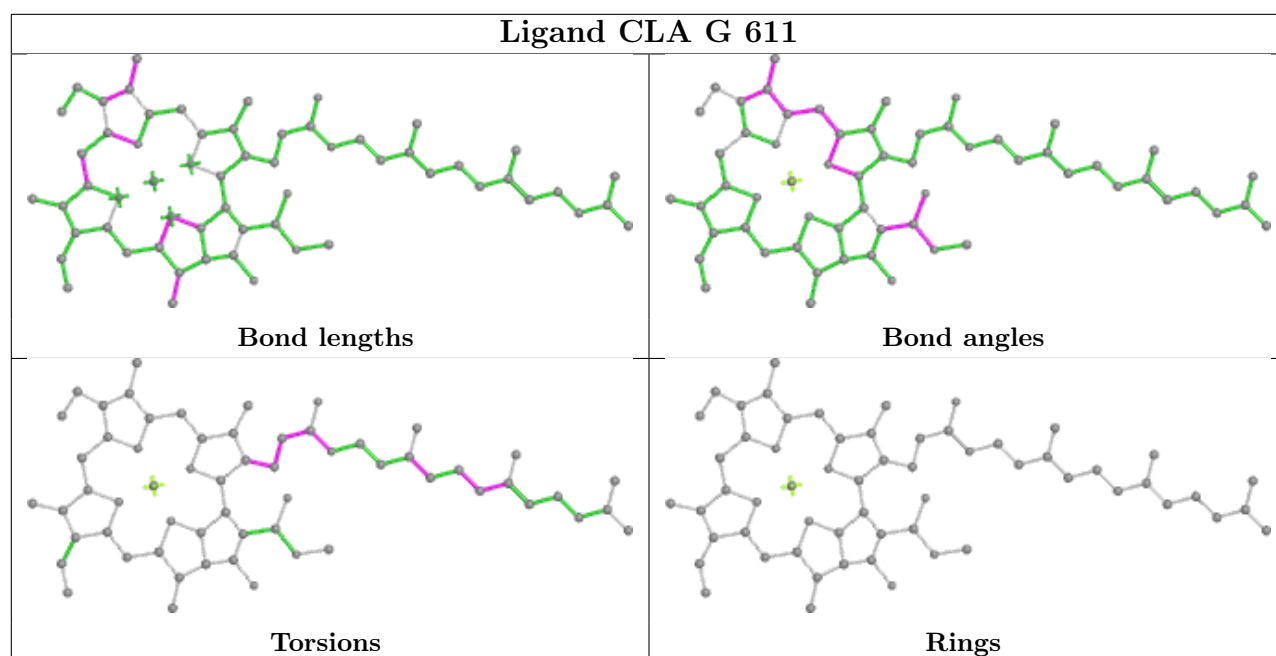


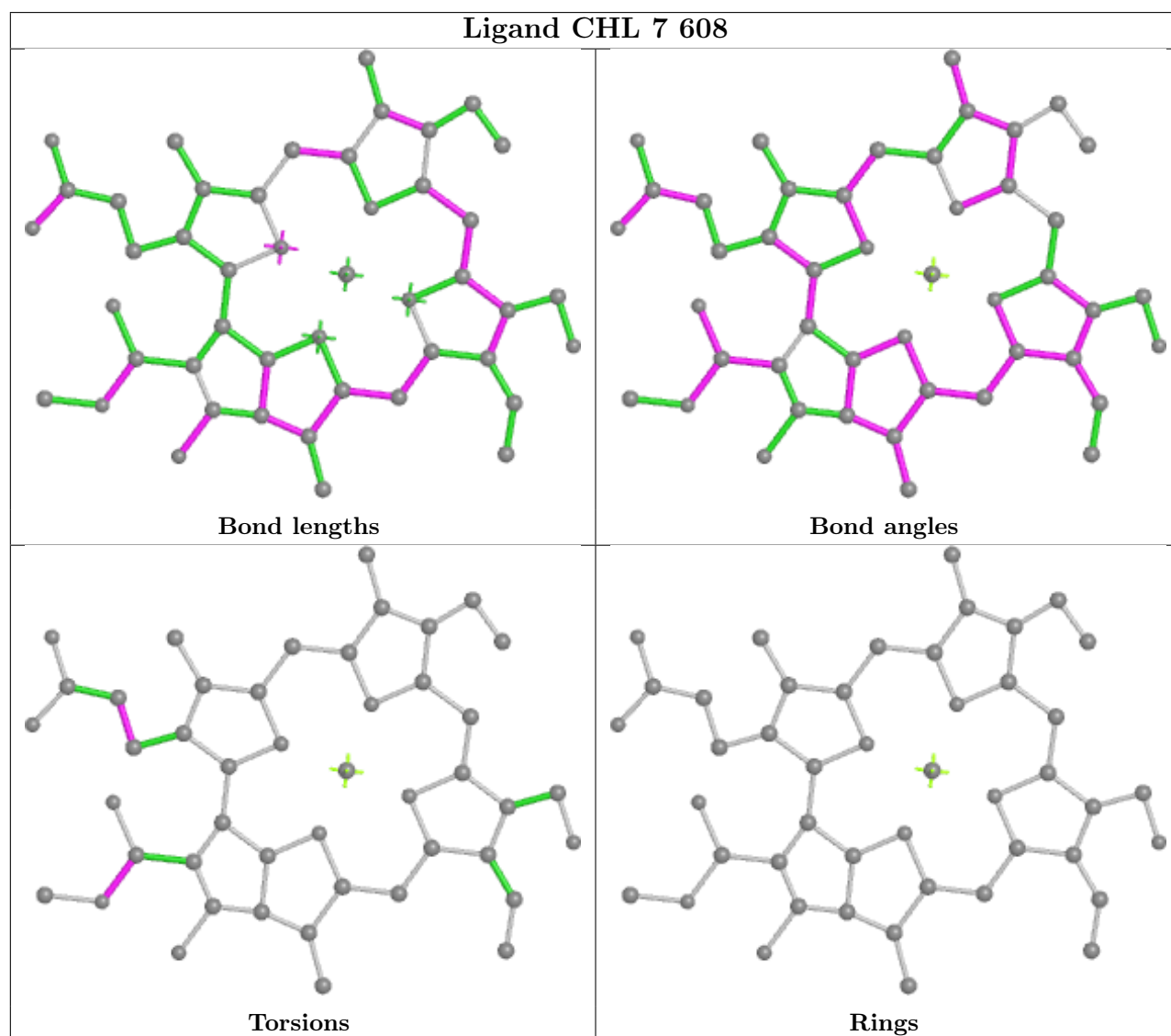
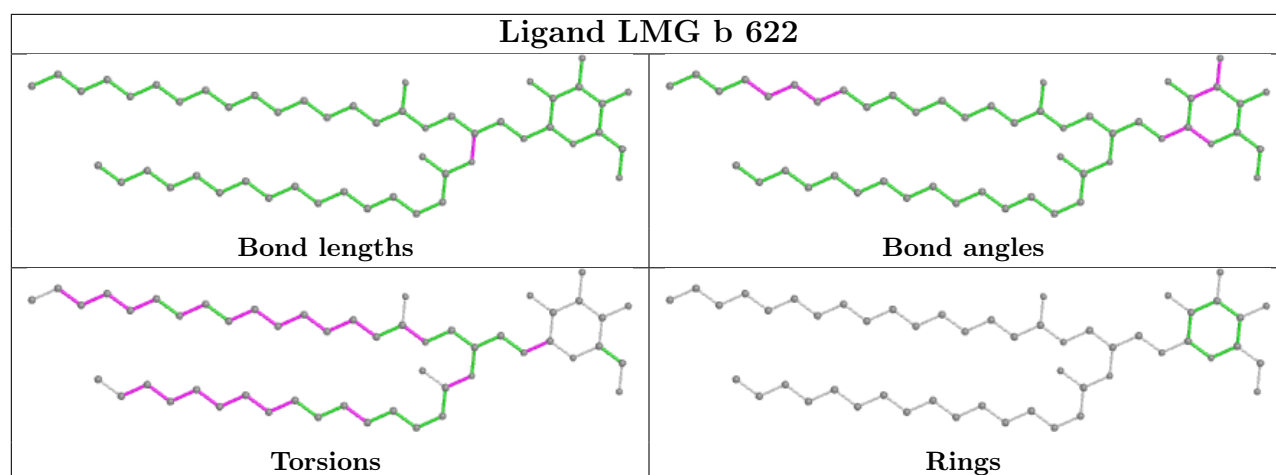
Ligand CLA S 614

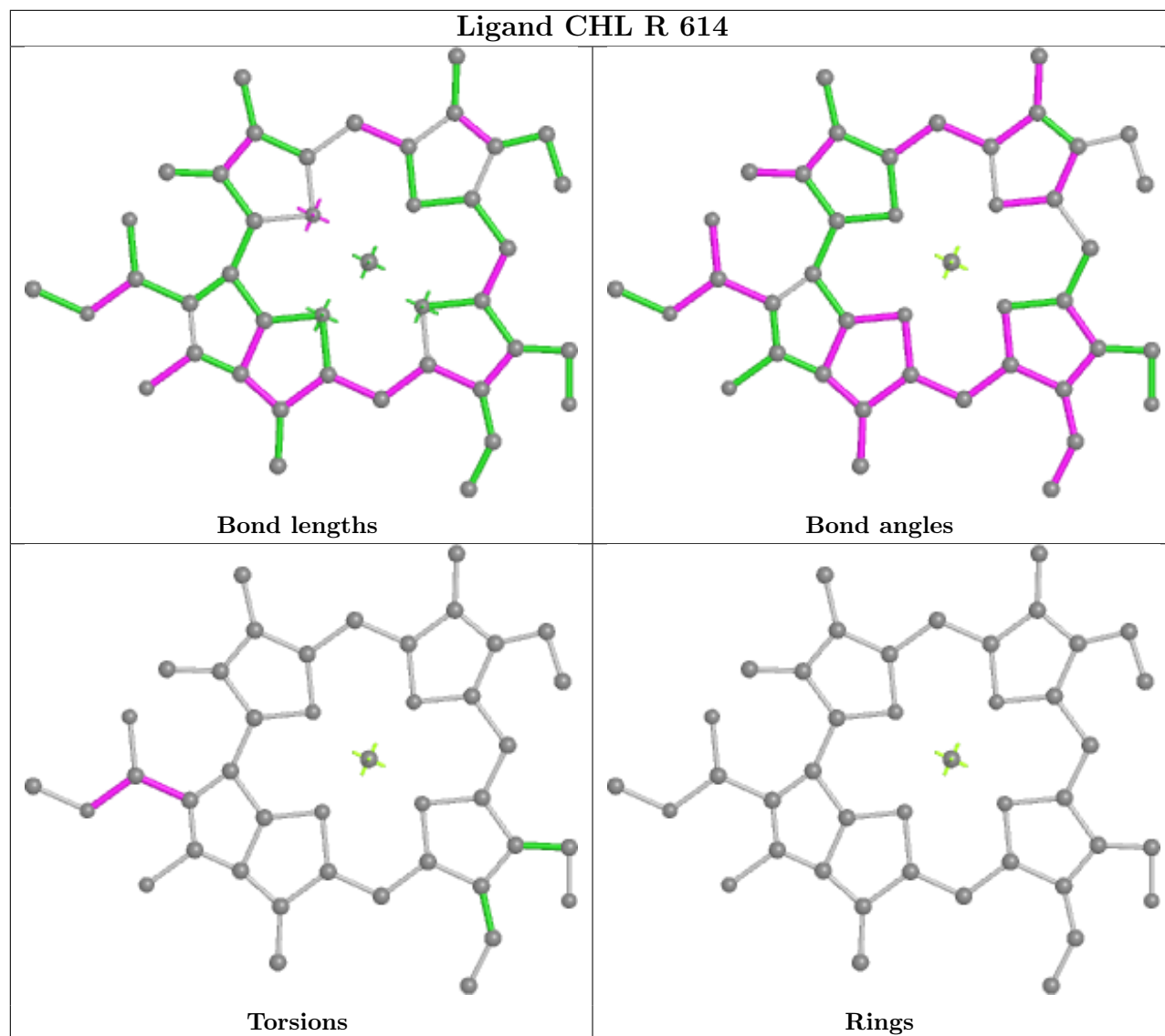
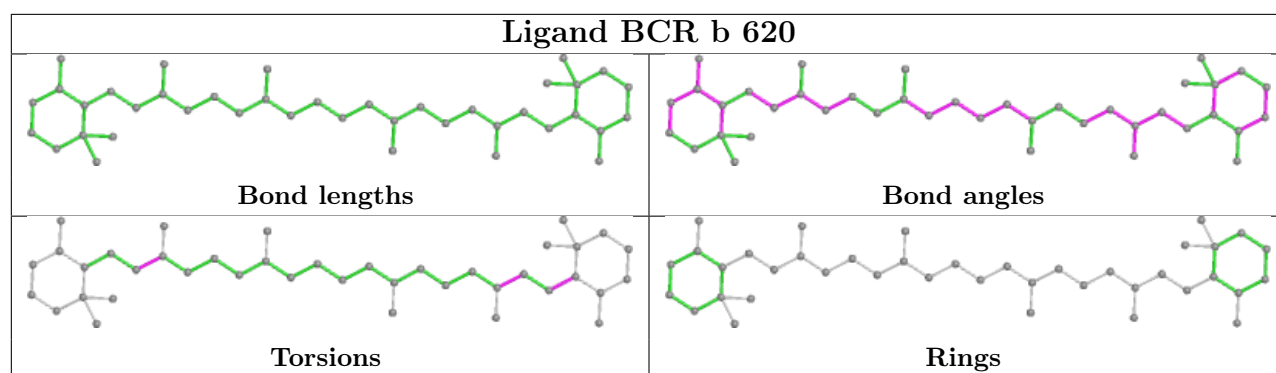


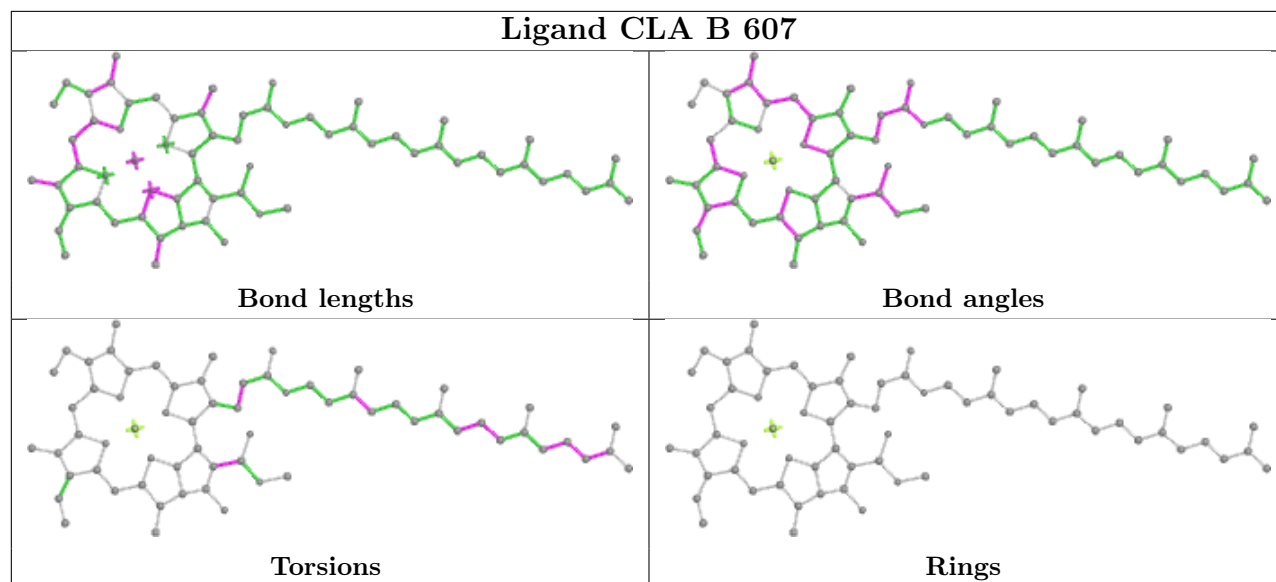
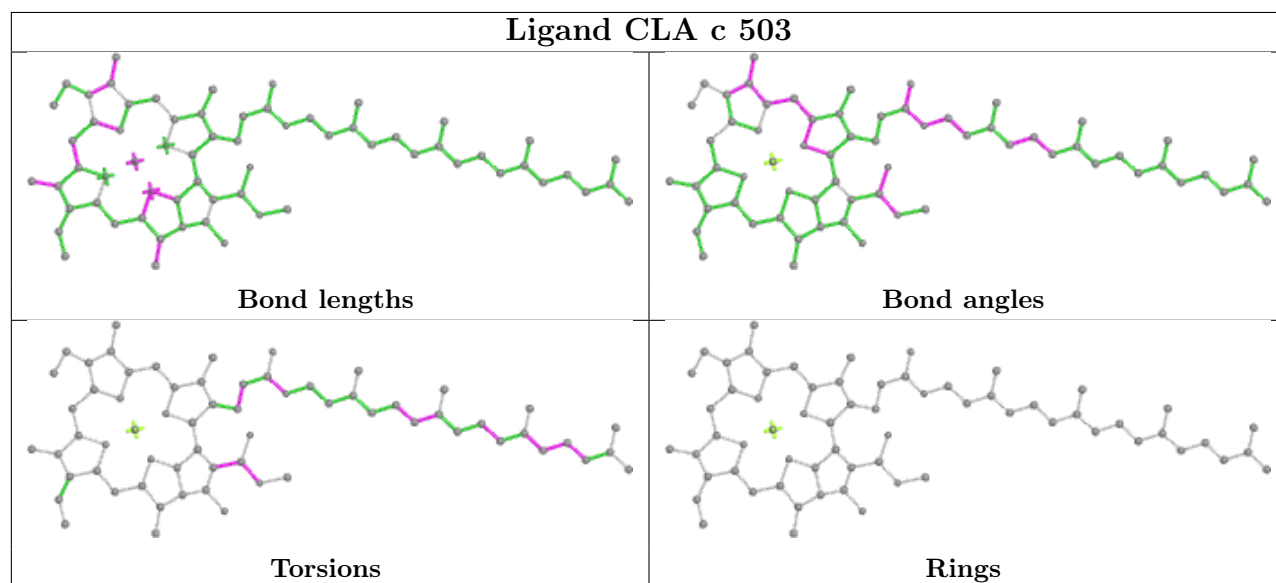
Ligand LUT 5 1620

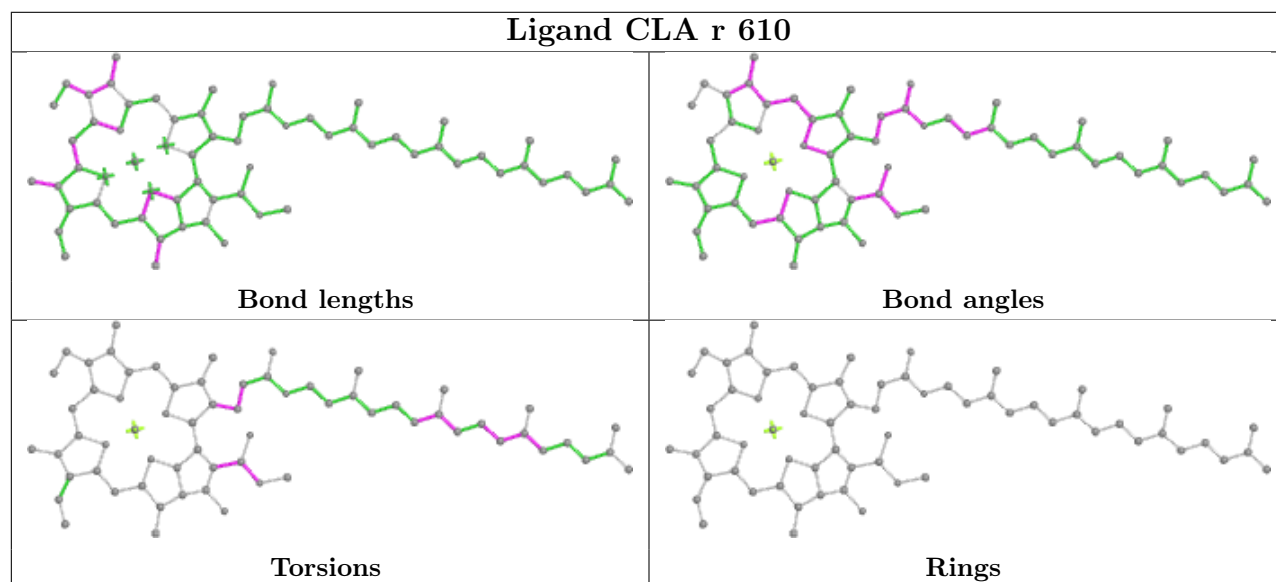
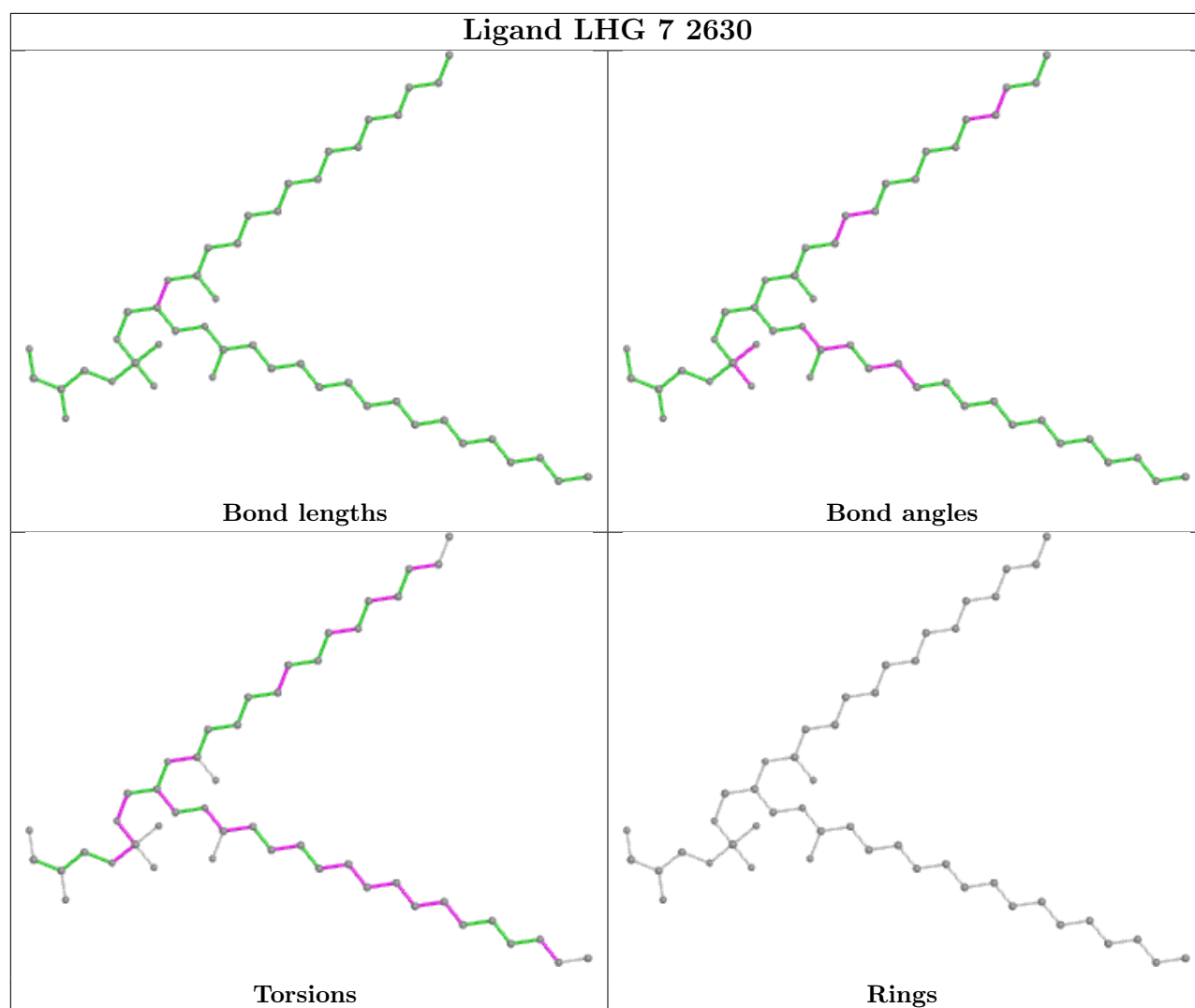


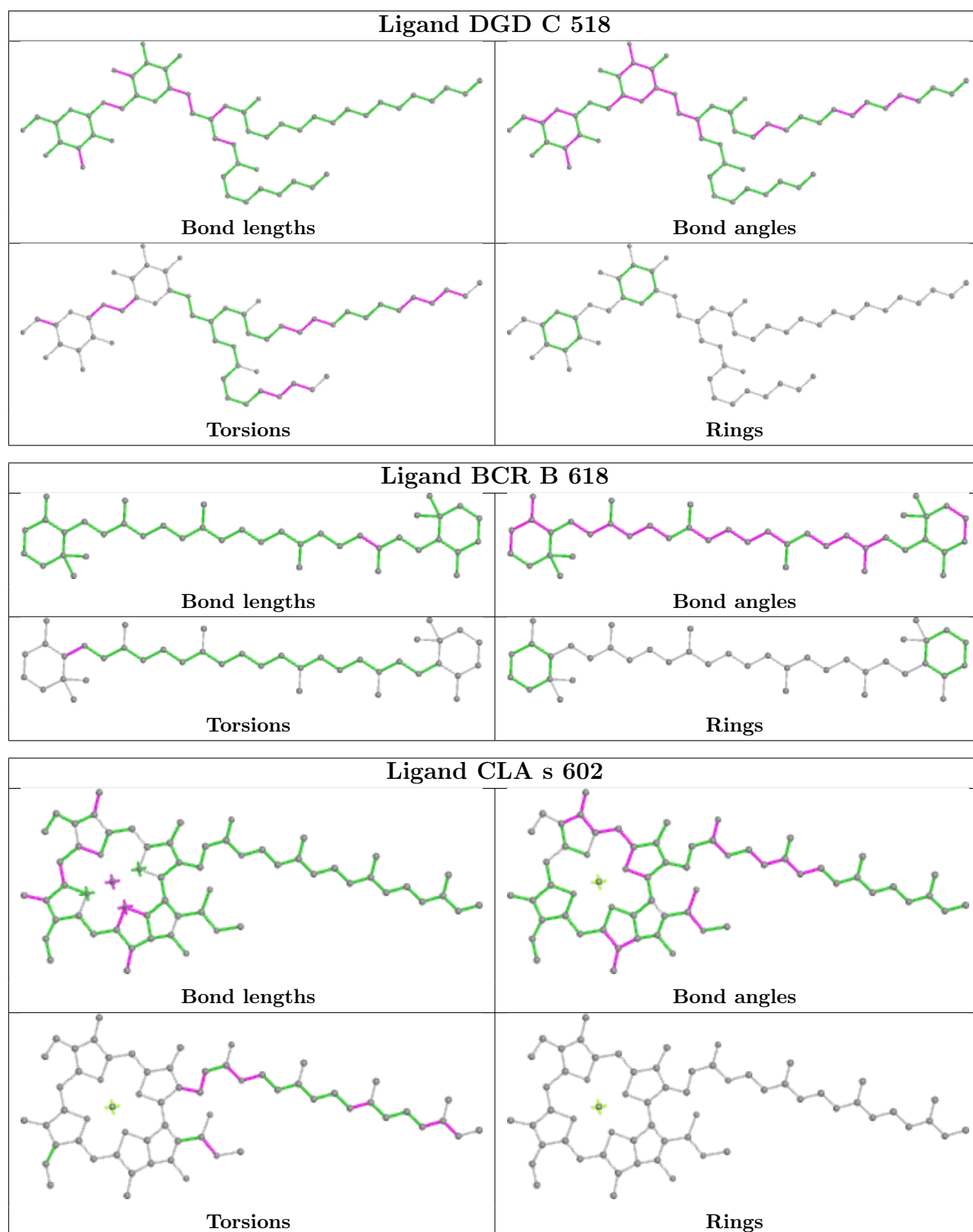


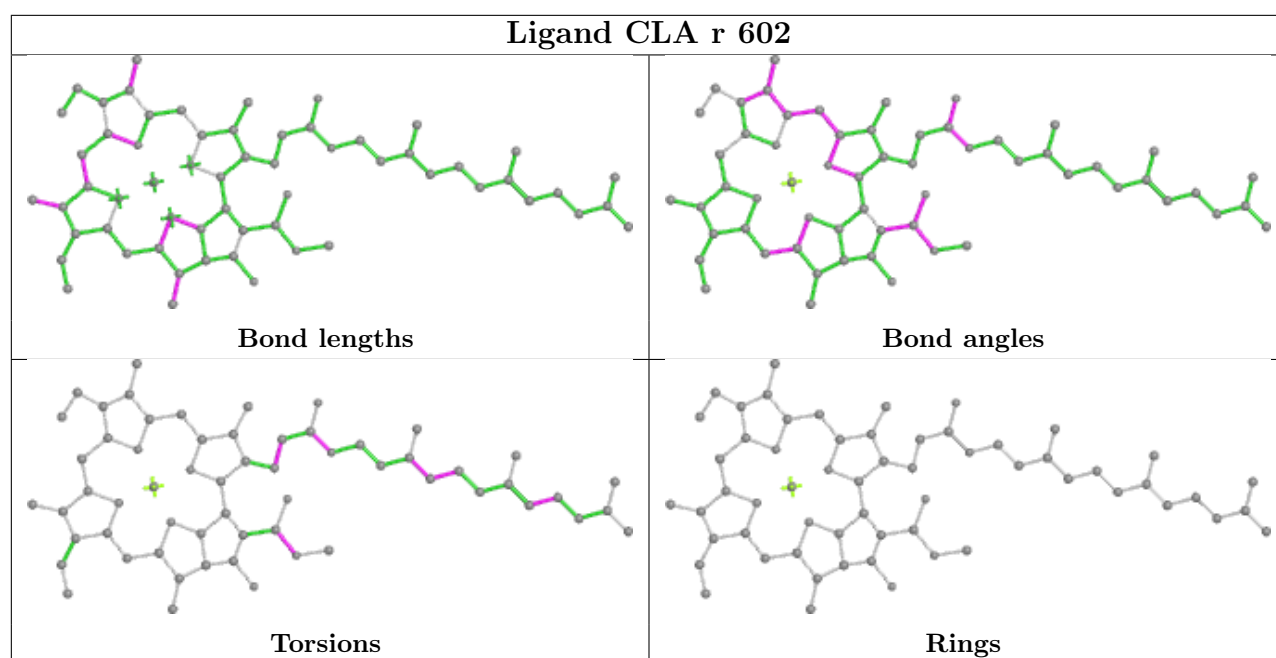
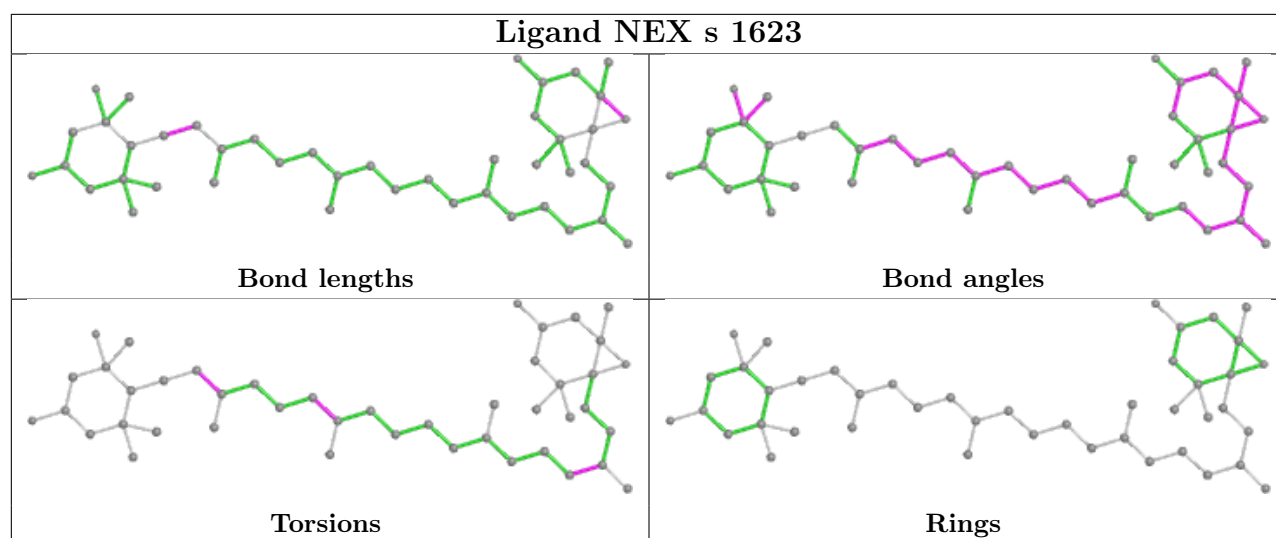


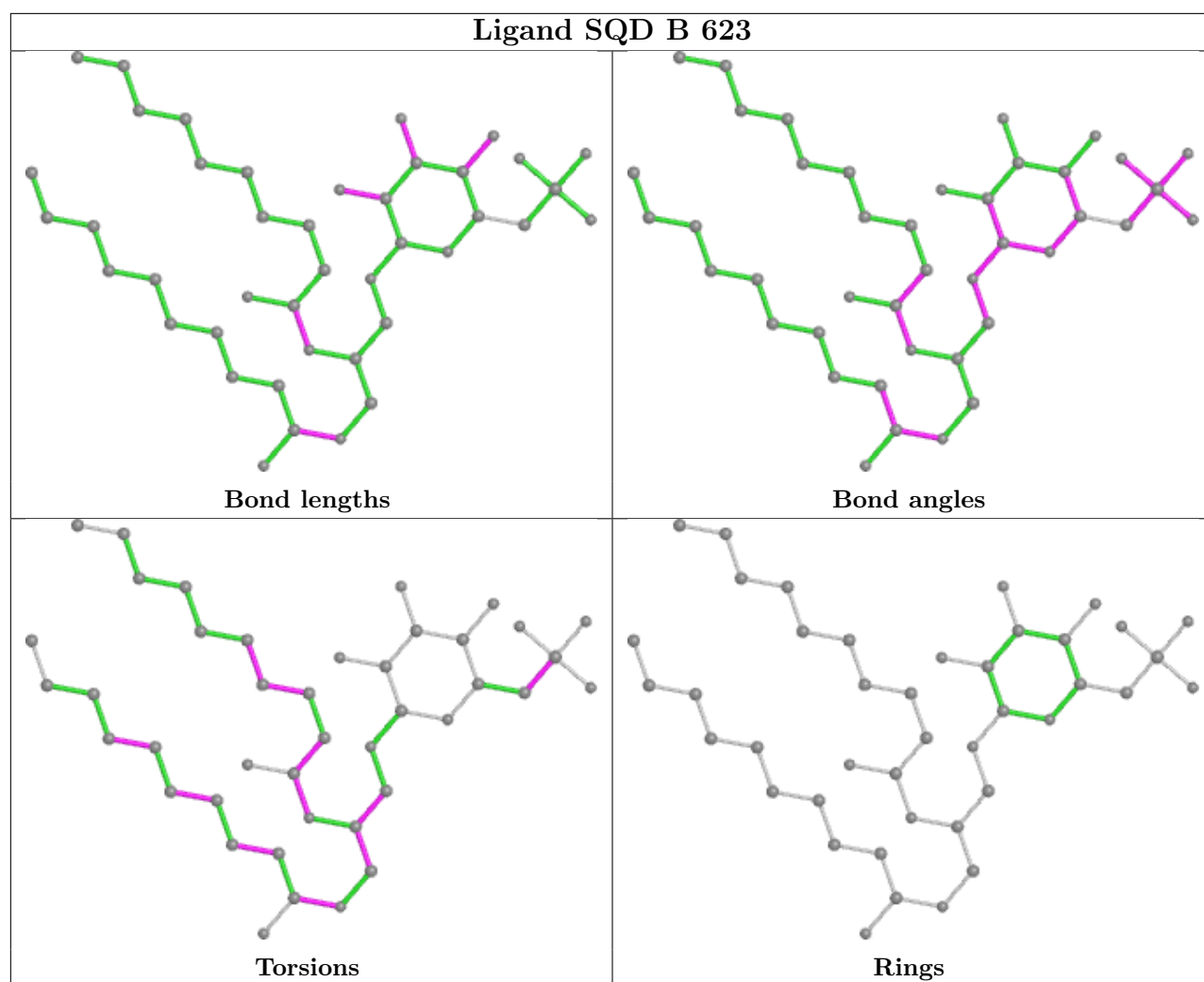


Ligand CLA B 607**Ligand CLA c 503**

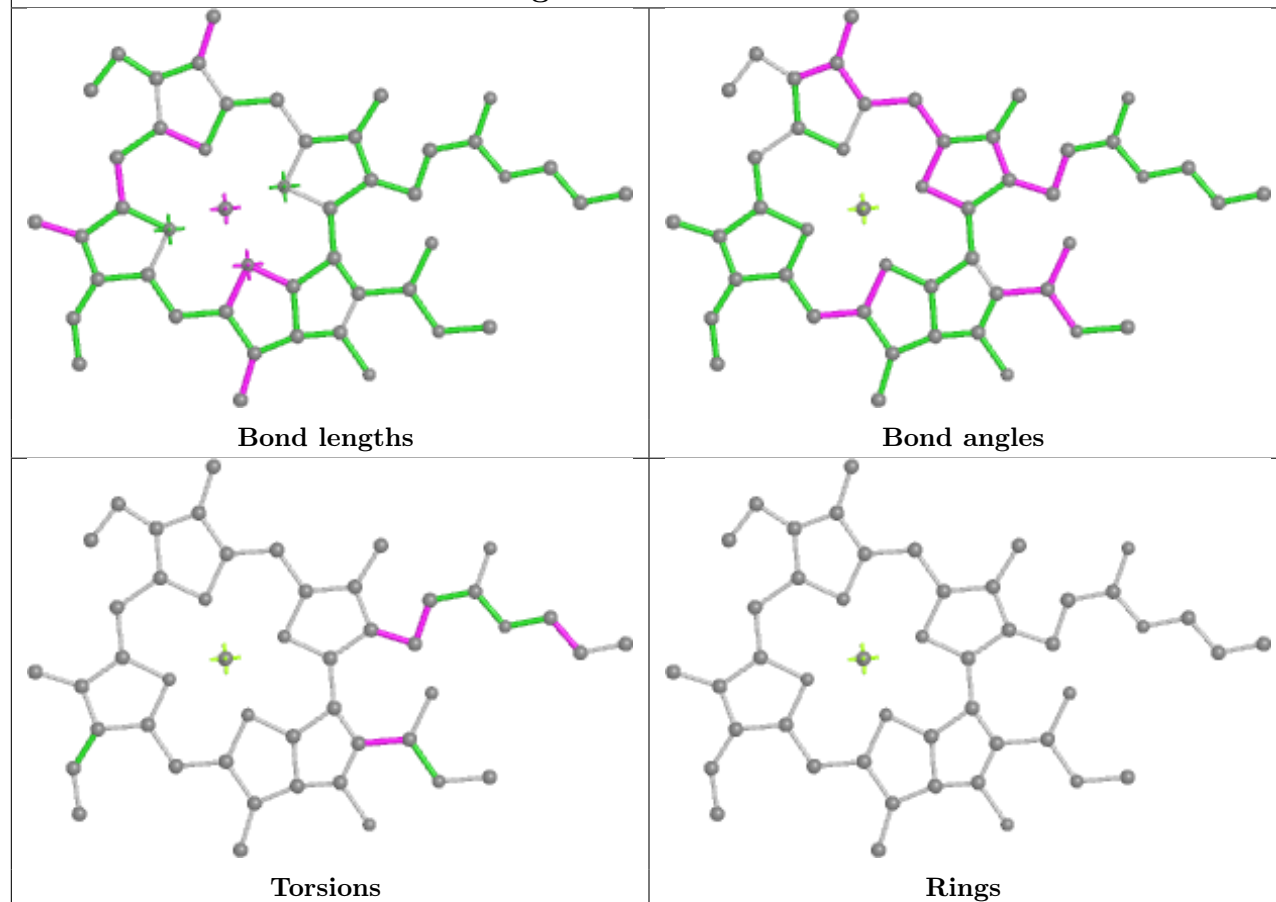




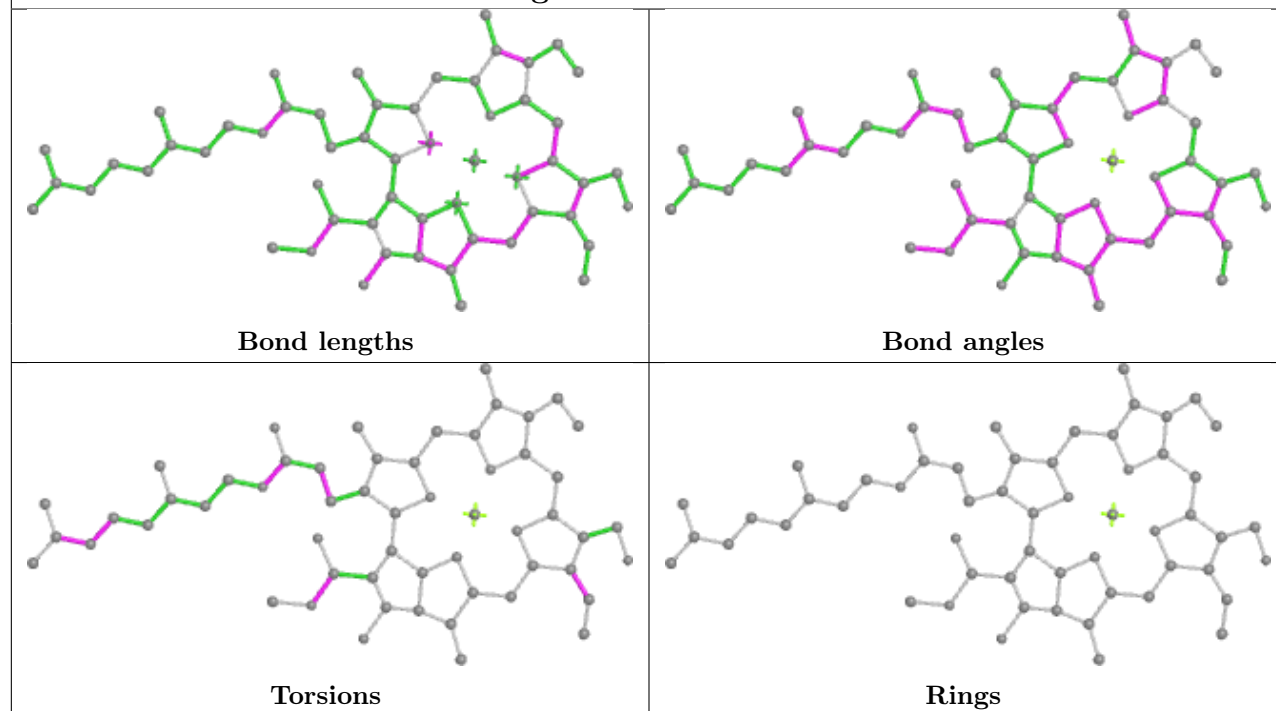




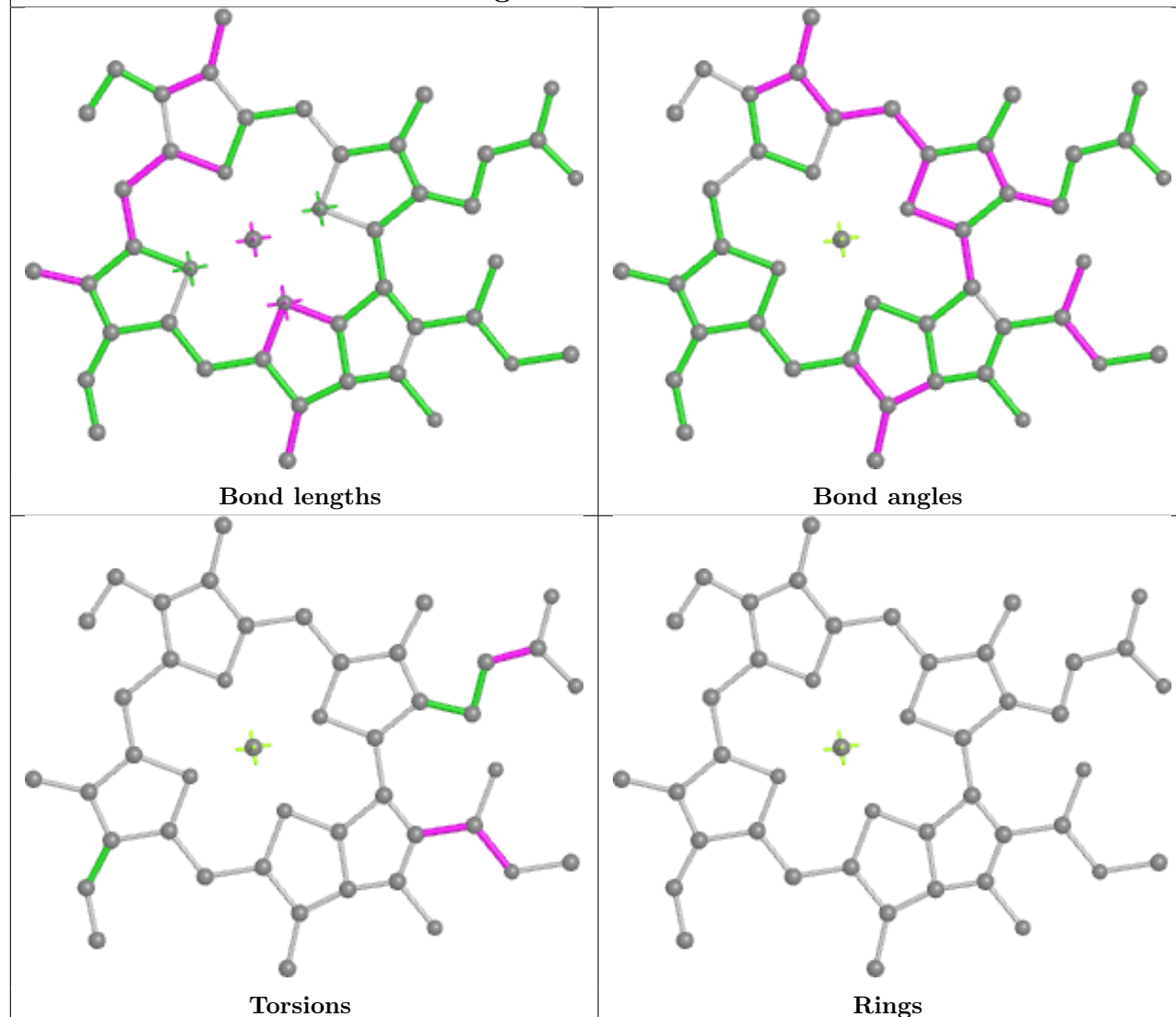
Ligand CLA R 604



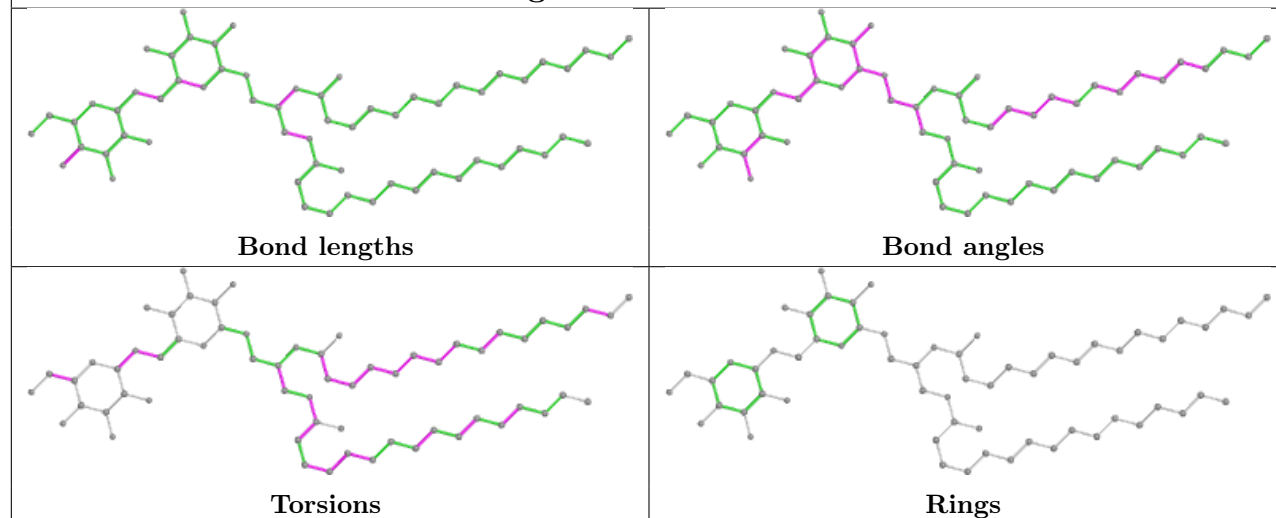
Ligand CHL R 607



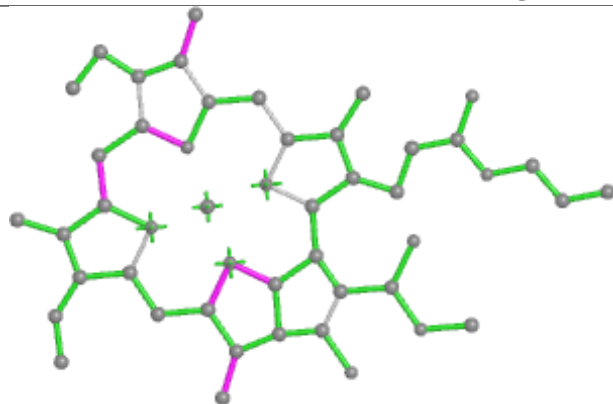
Ligand CLA 7 612



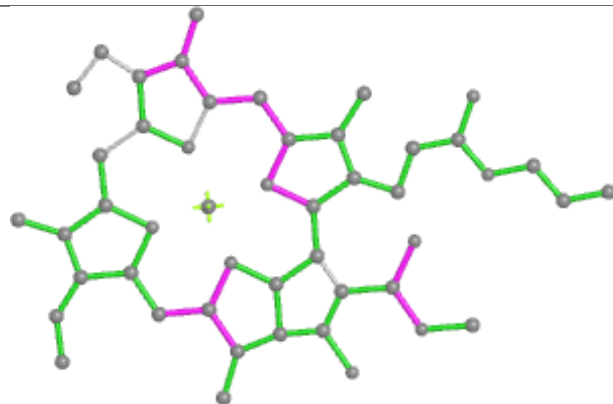
Ligand DGD C 519



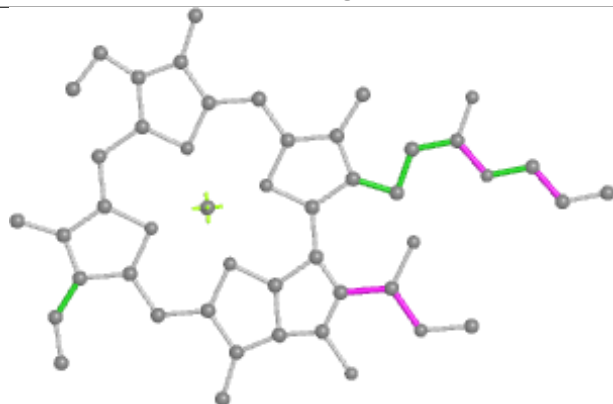
Ligand CLA N 614



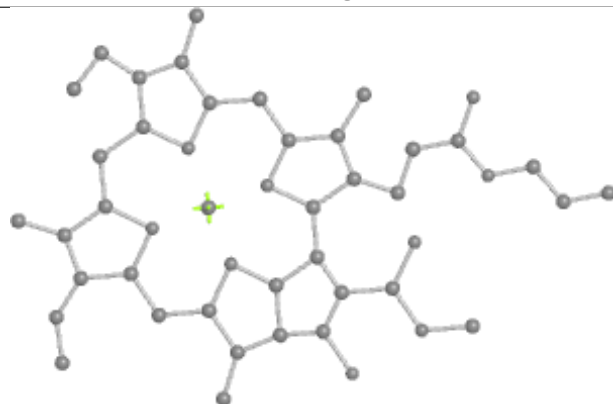
Bond lengths



Bond angles

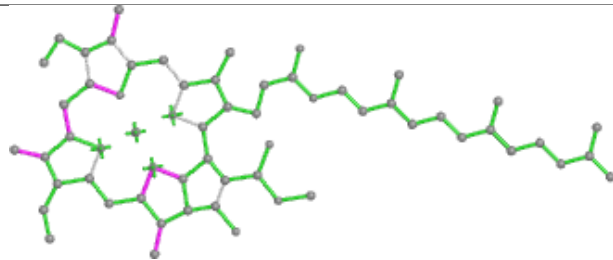


Torsions

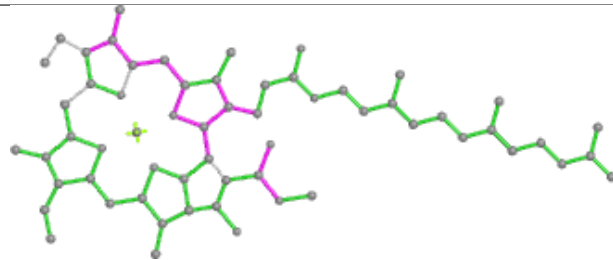


Rings

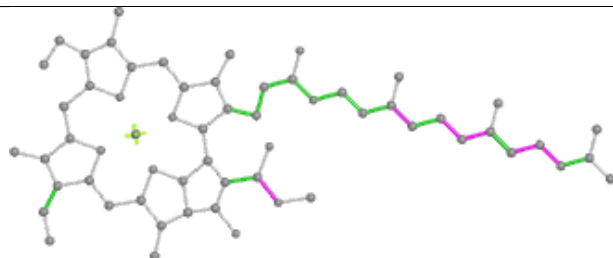
Ligand CLA N 612



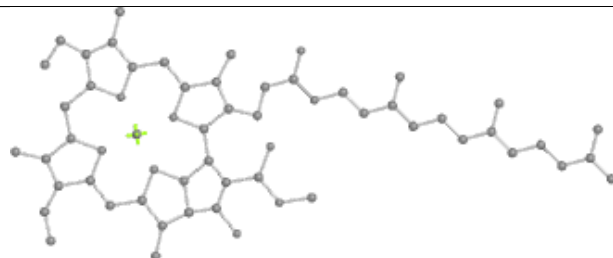
Bond lengths



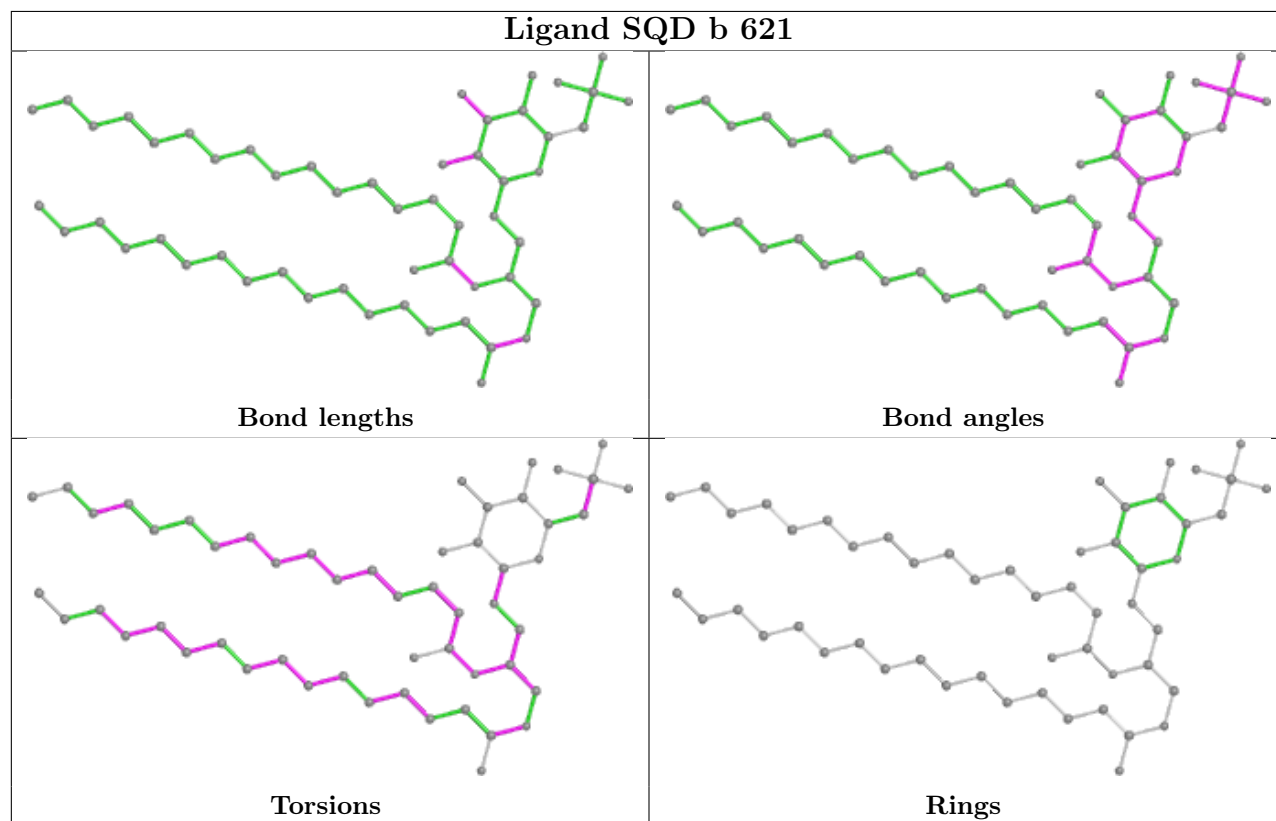
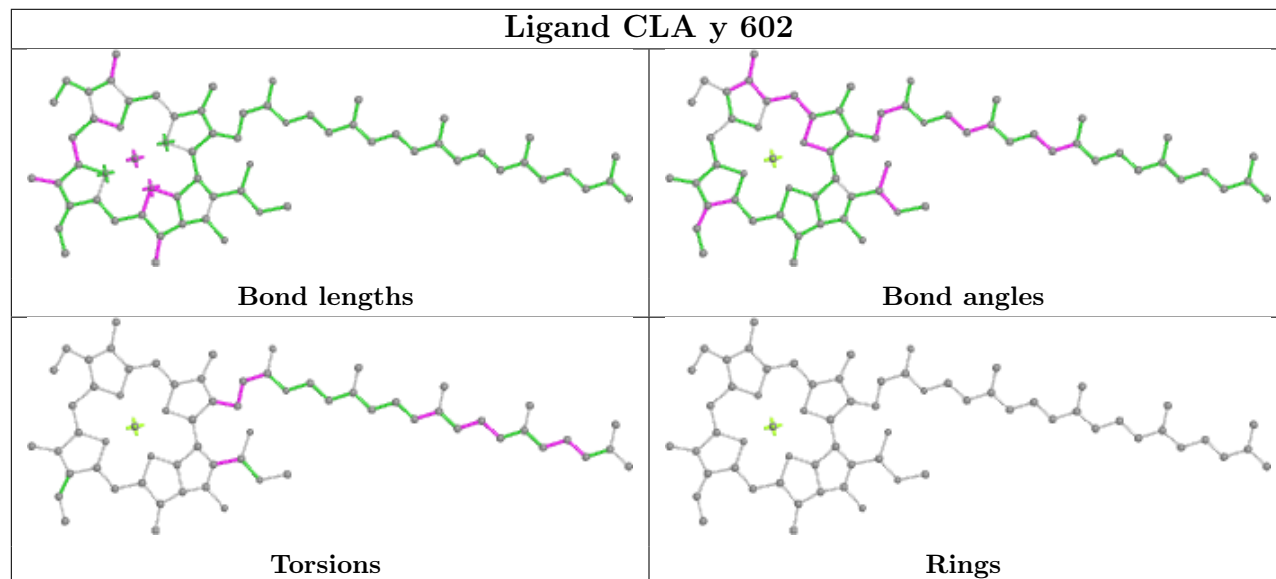
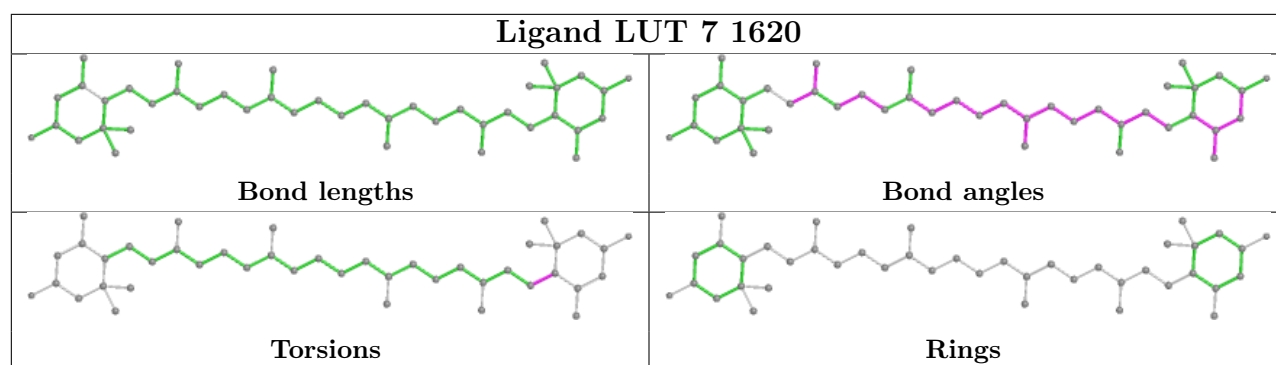
Bond angles



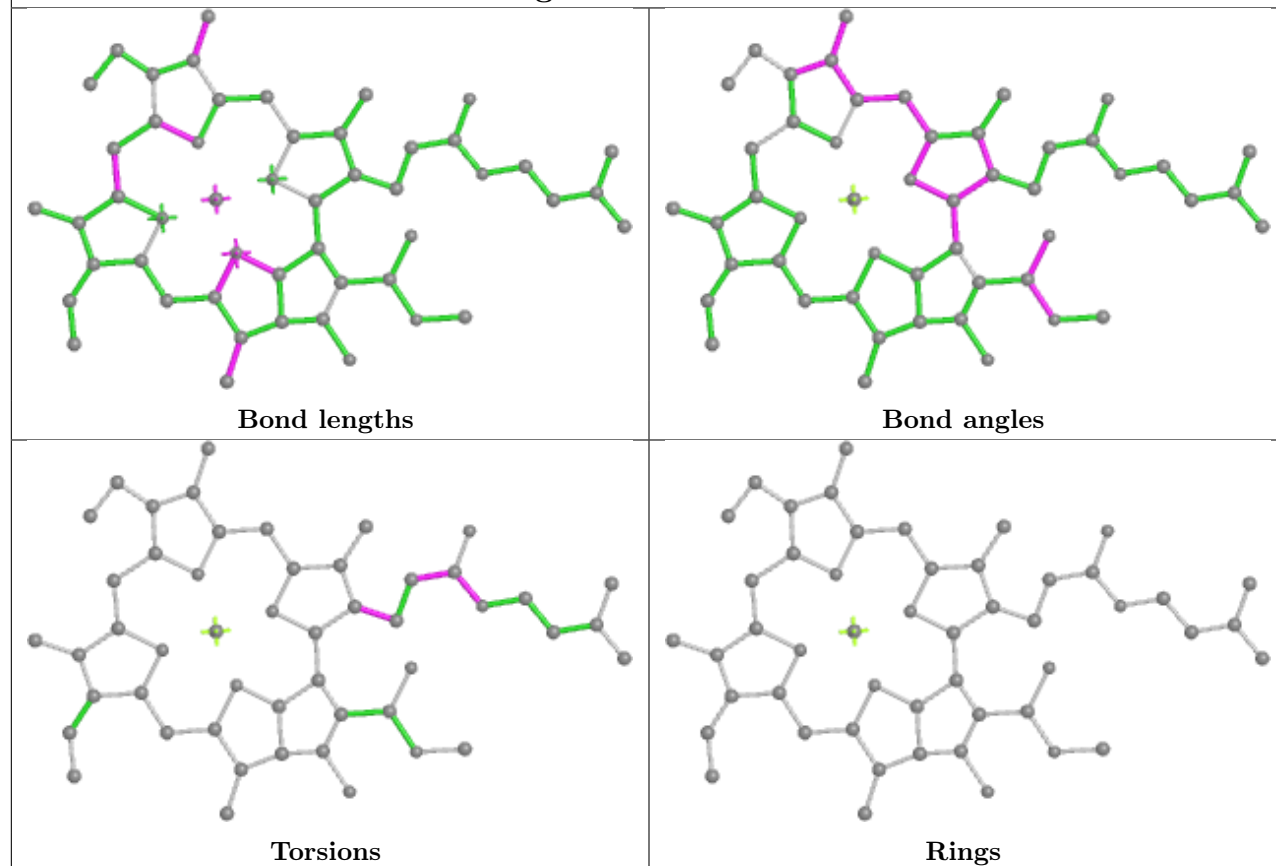
Torsions



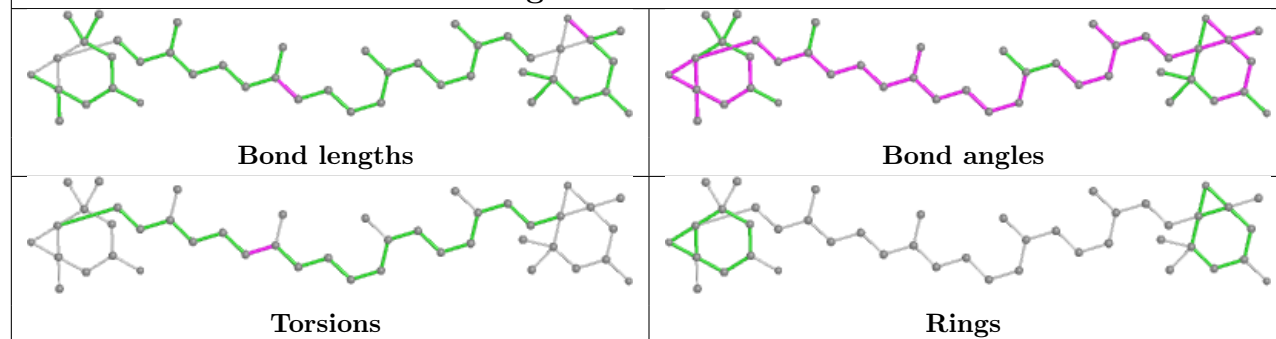
Rings



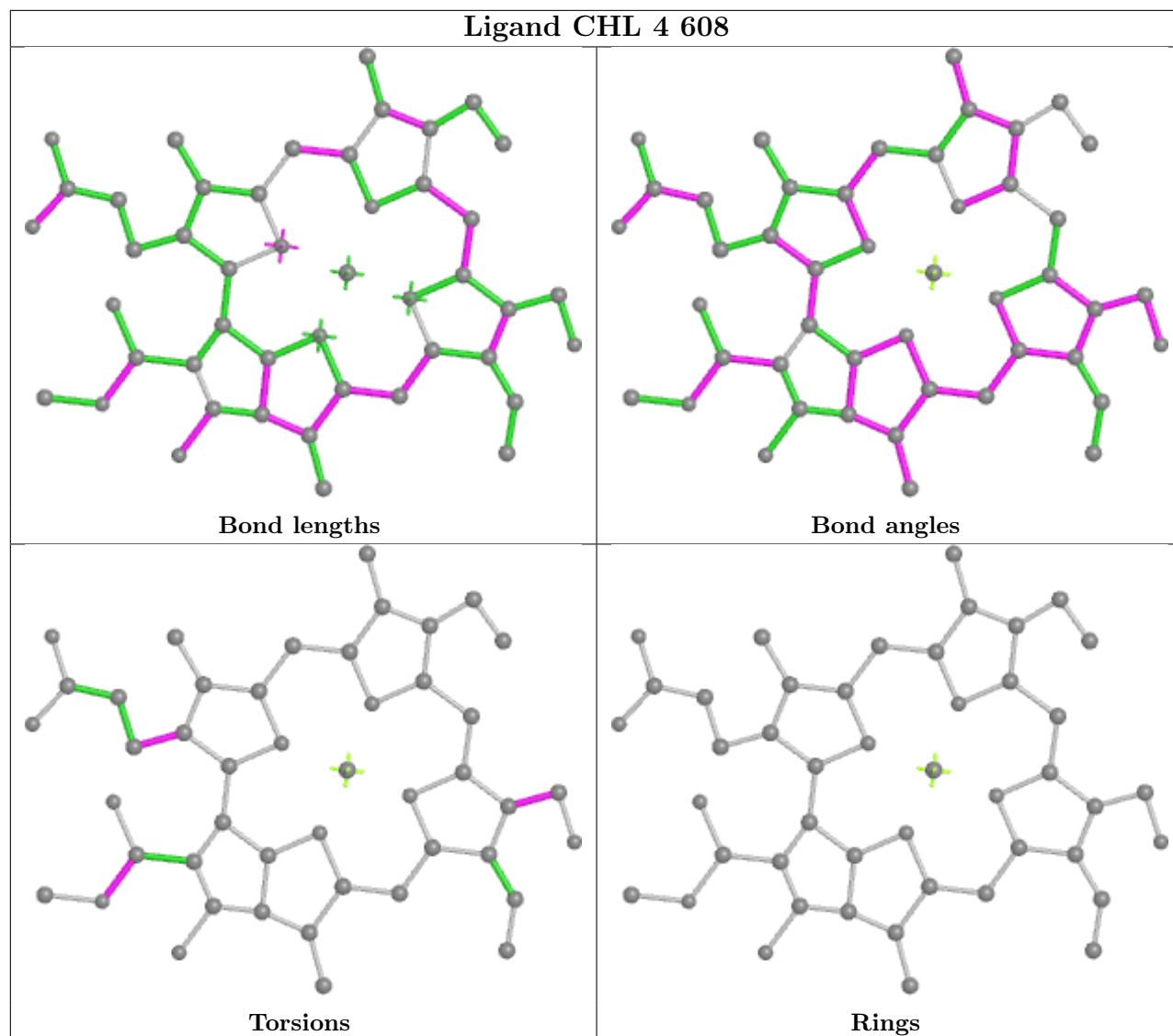
Ligand CLA S 604

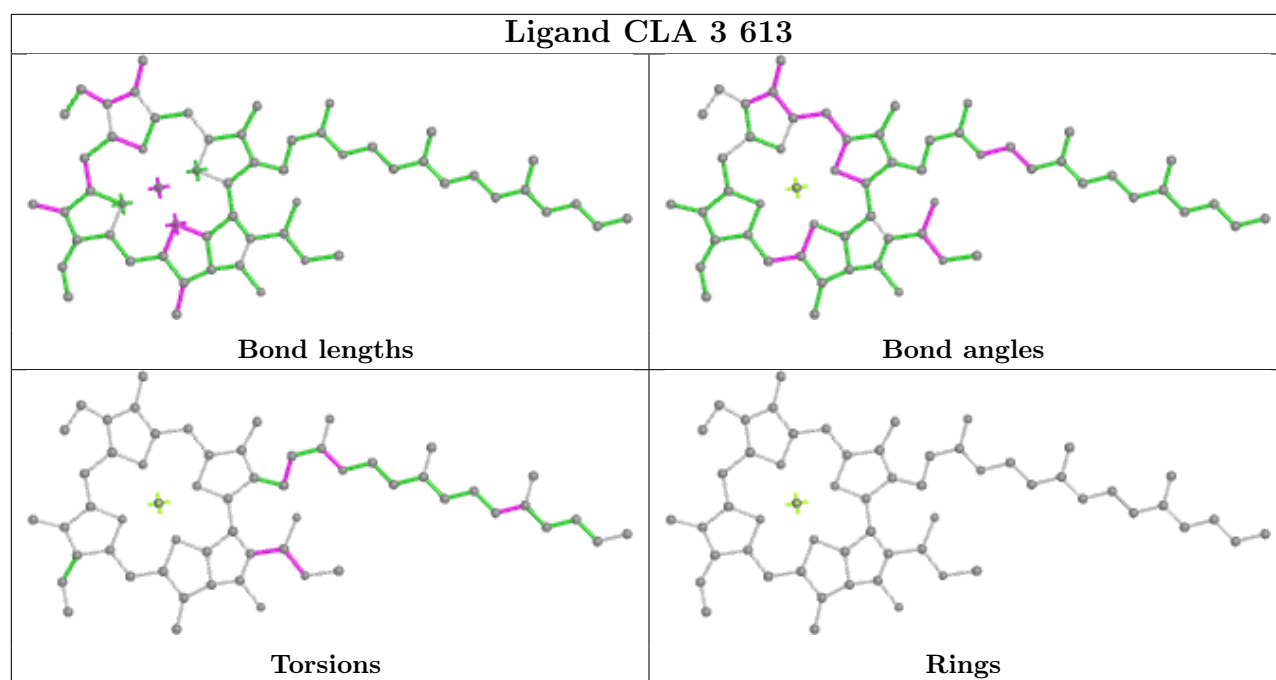


Ligand XAT 7 1622

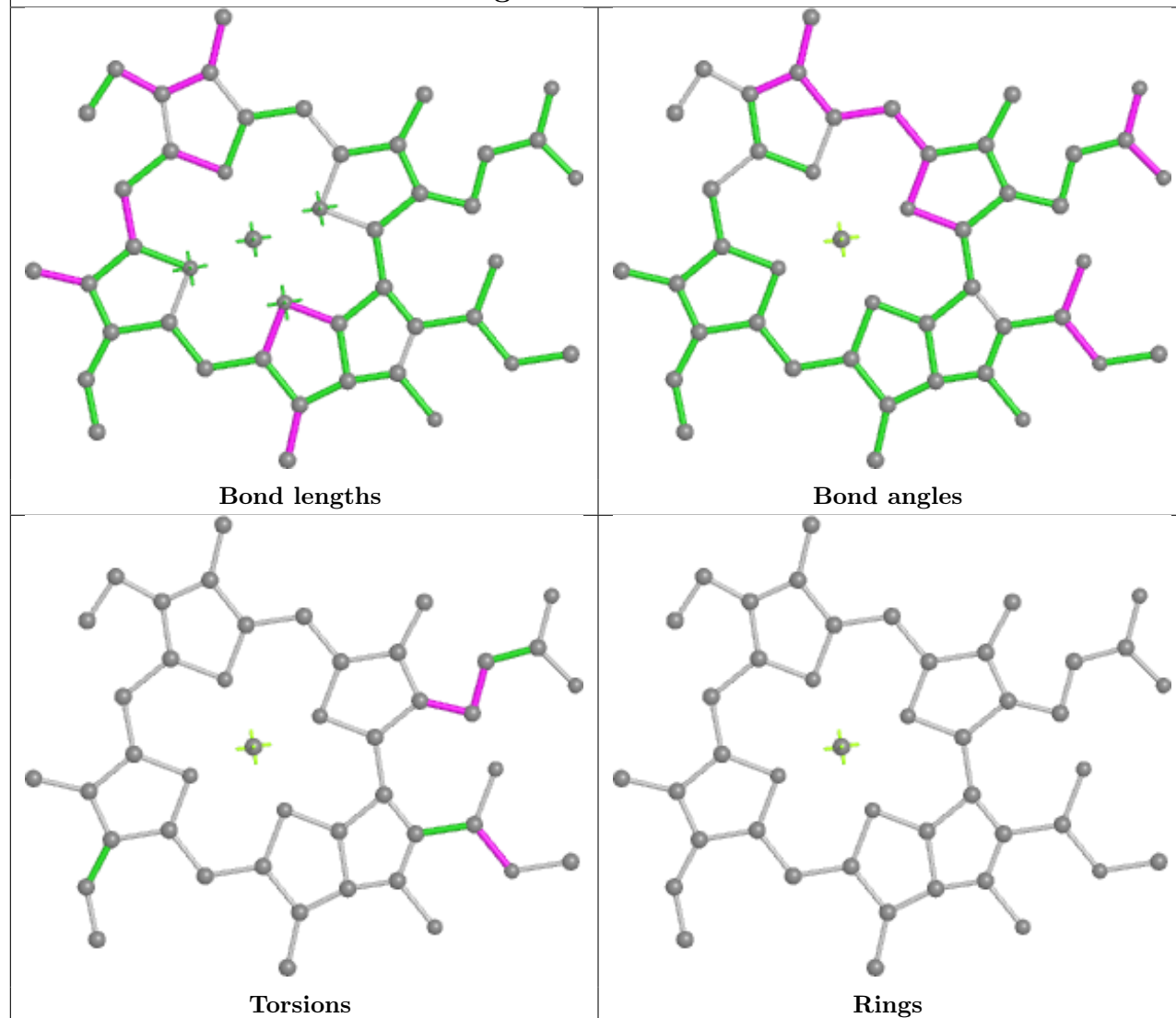


Ligand CHL 4 608

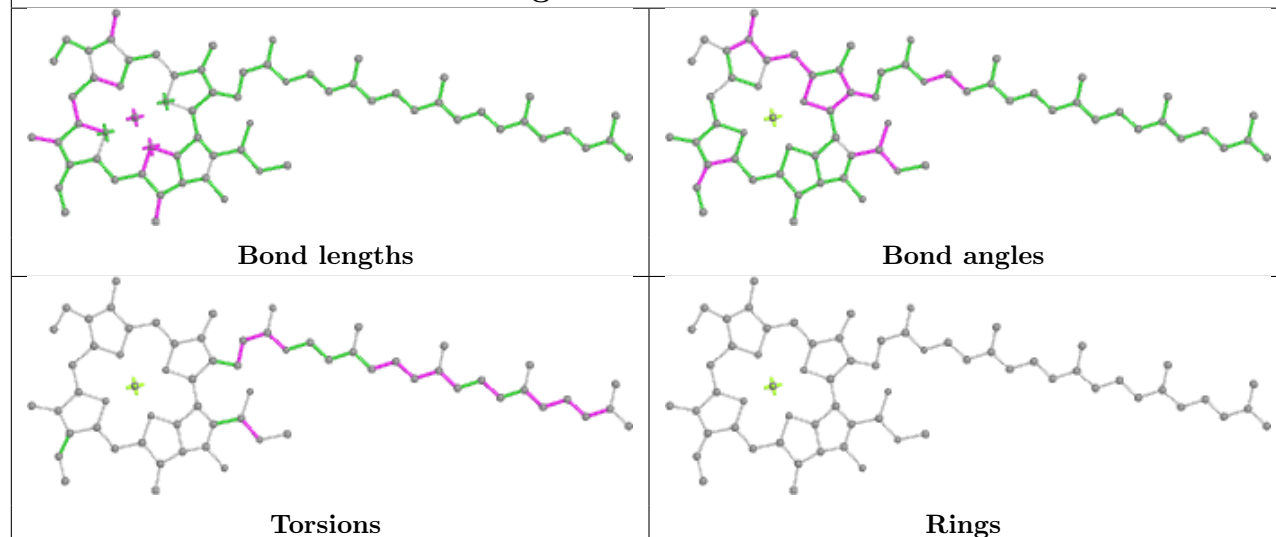


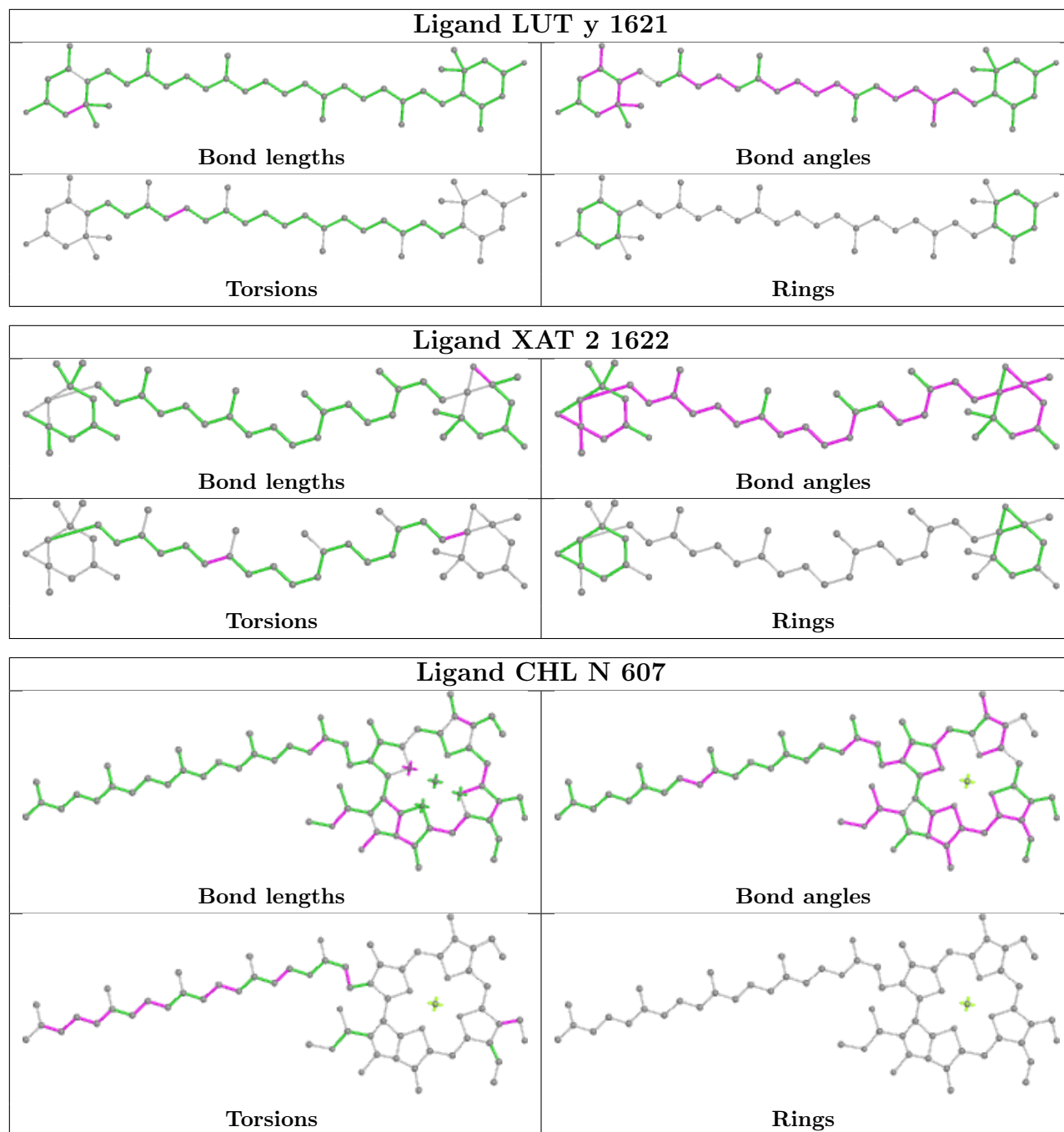


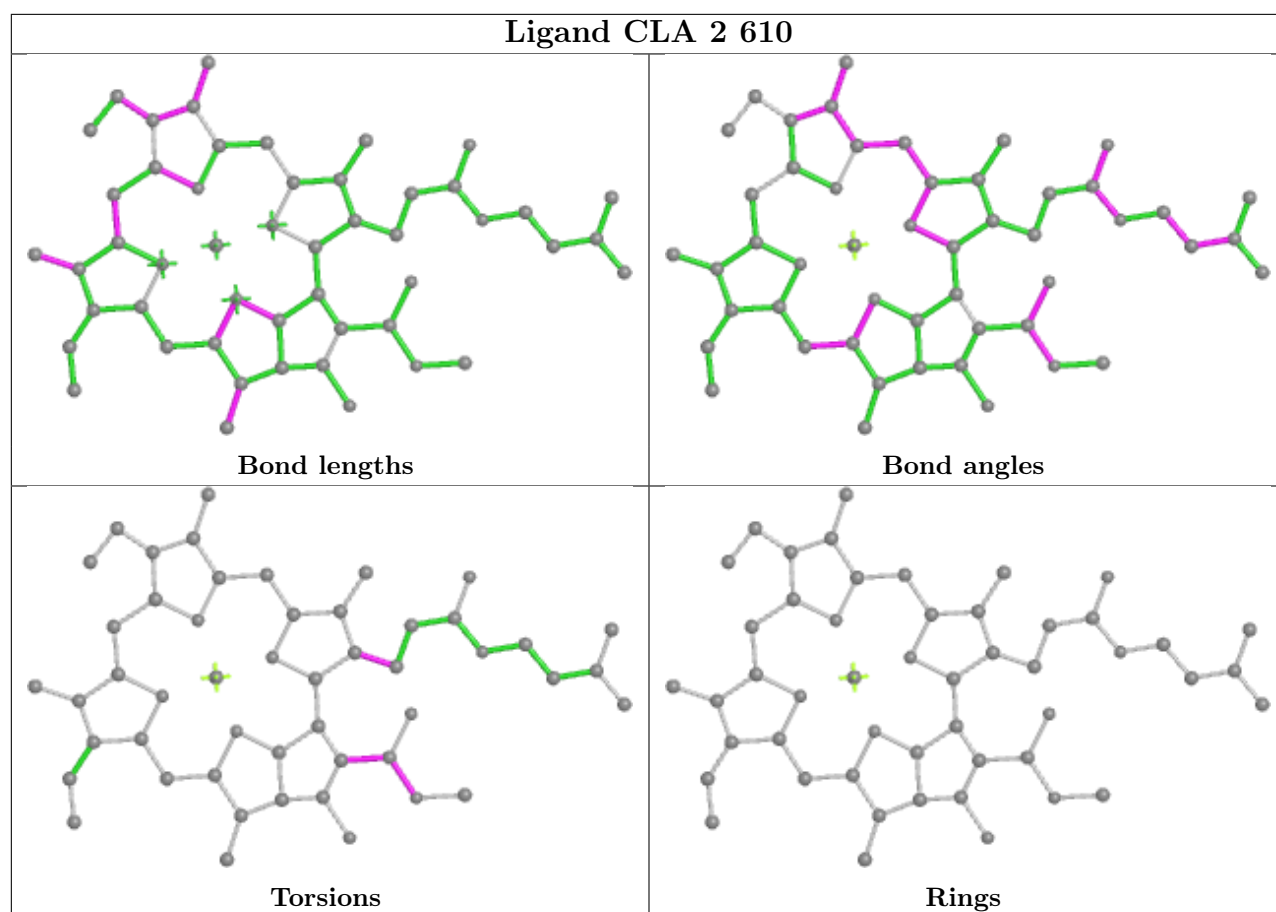
Ligand CLA 8 610



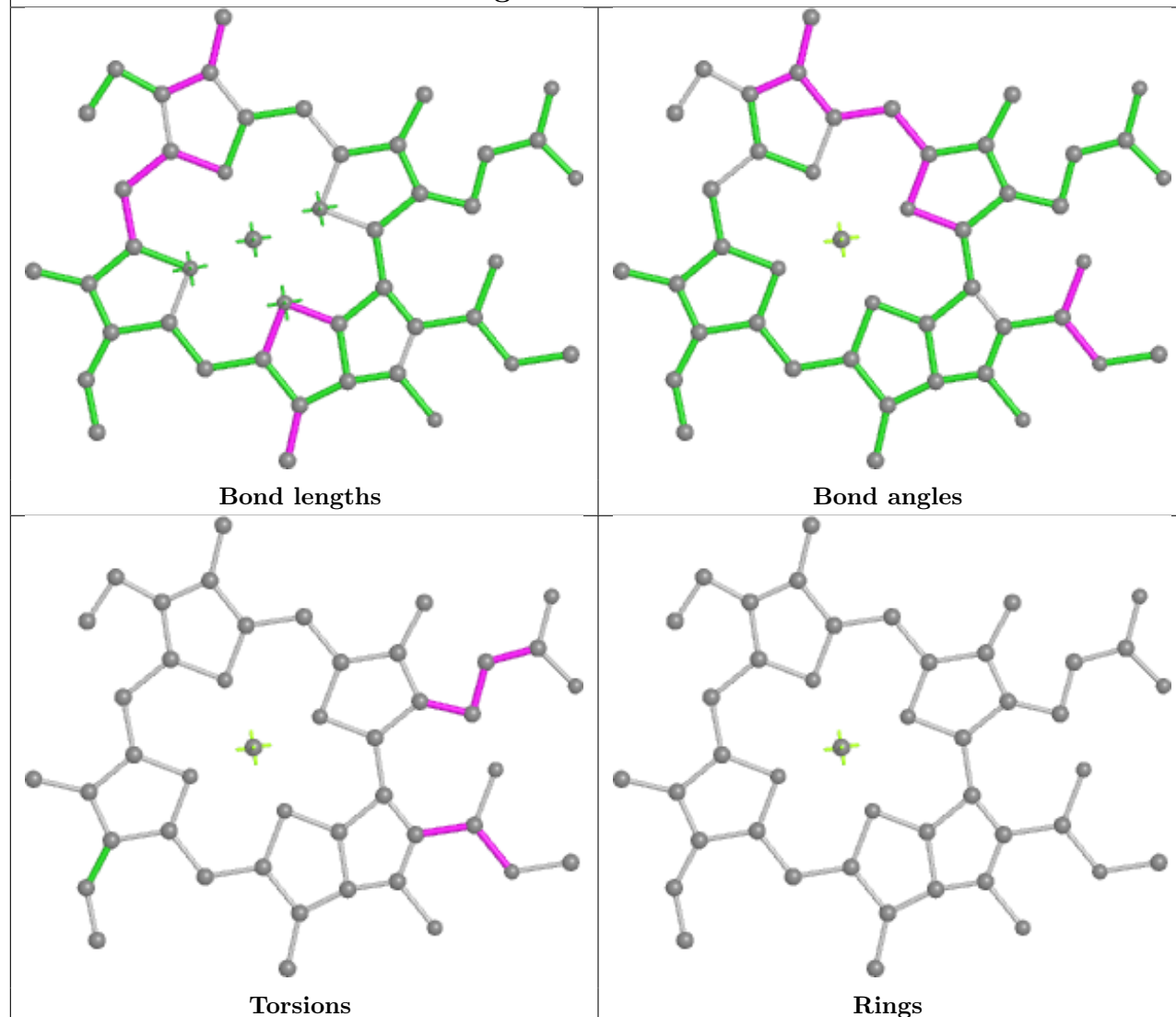
Ligand CLA B 617



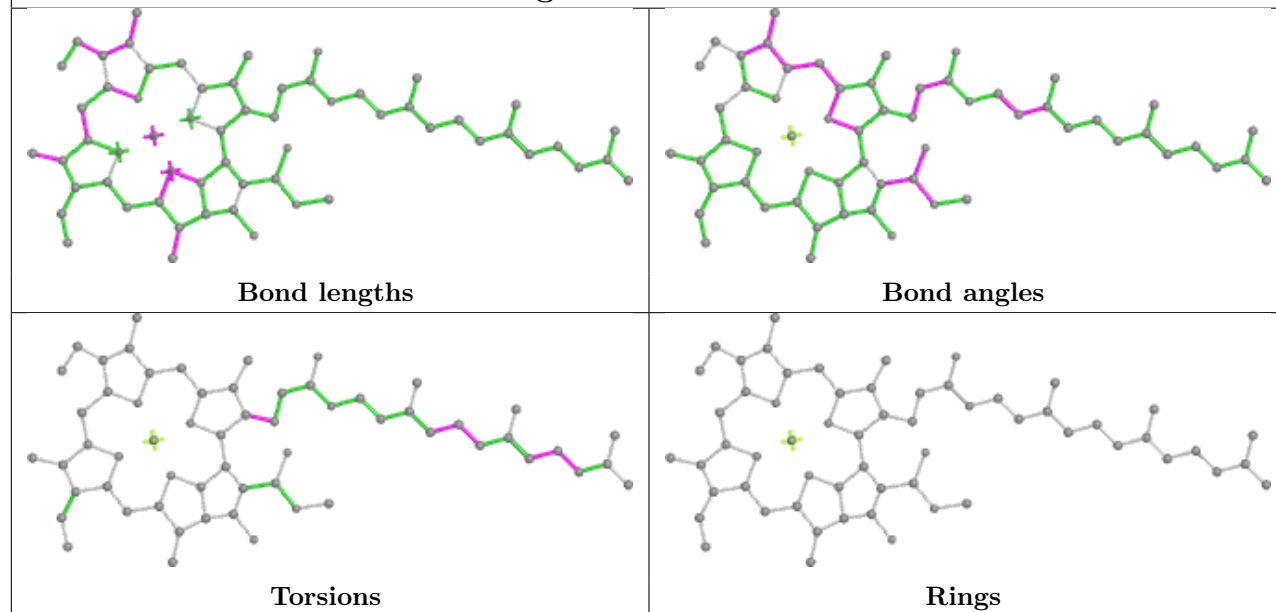


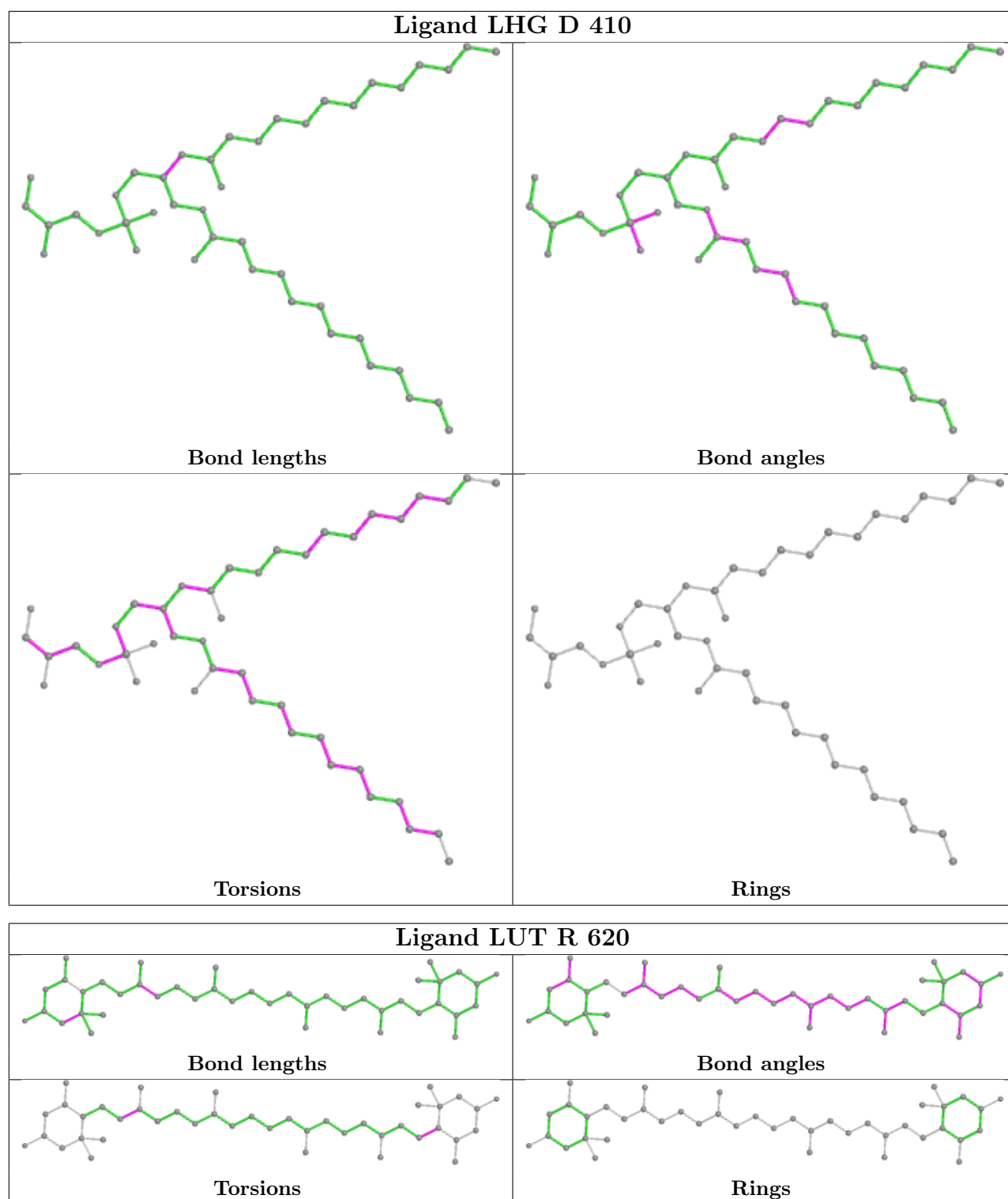


Ligand CLA 6 604

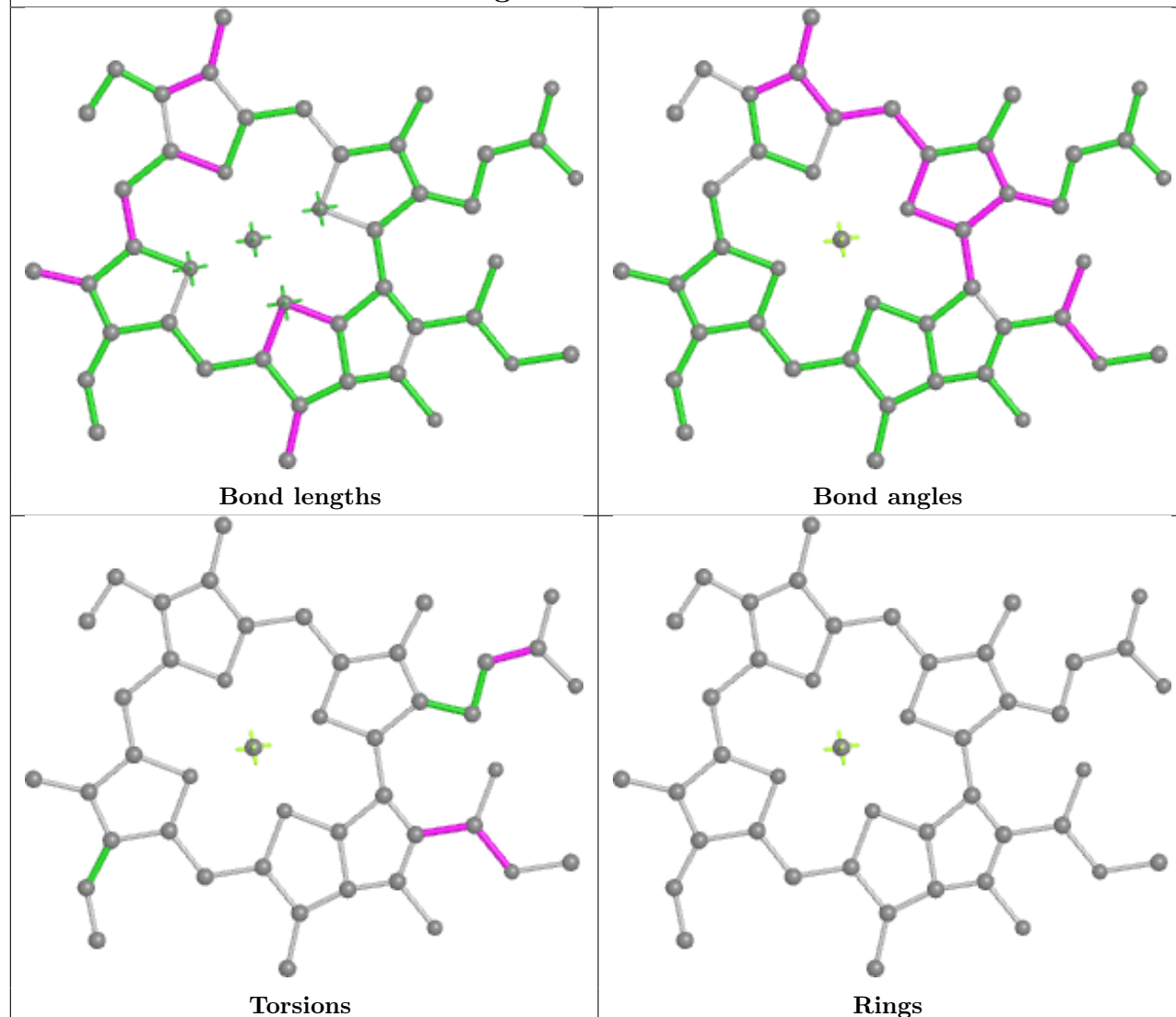


Ligand CLA a 410

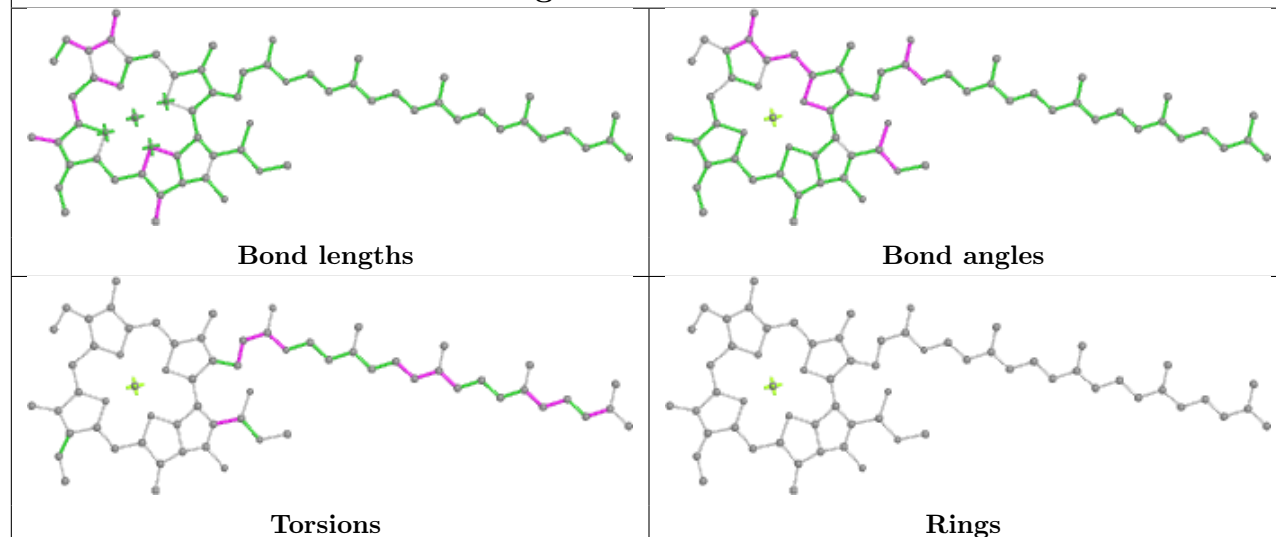


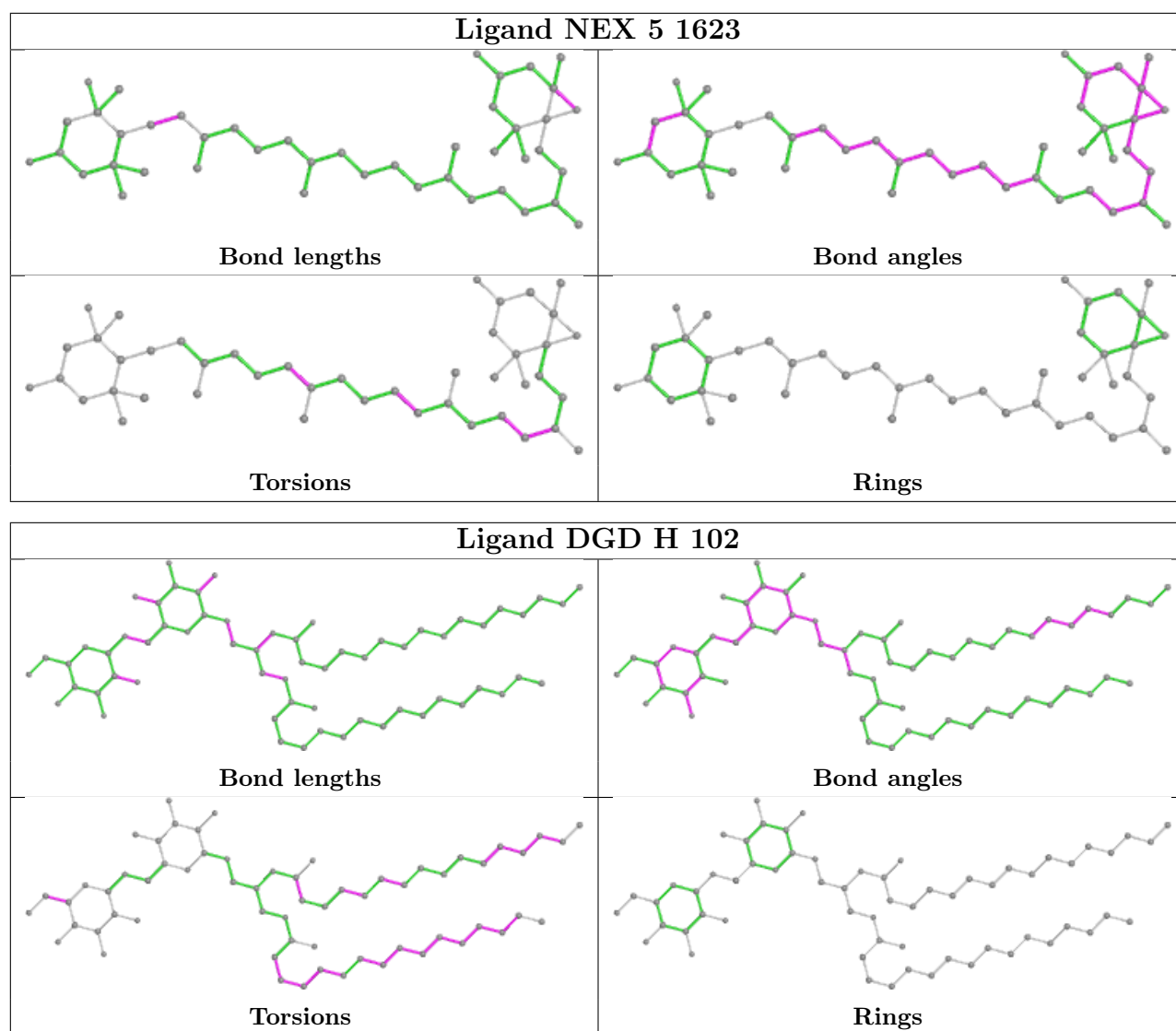


Ligand CLA 6 612



Ligand CLA b 602





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.

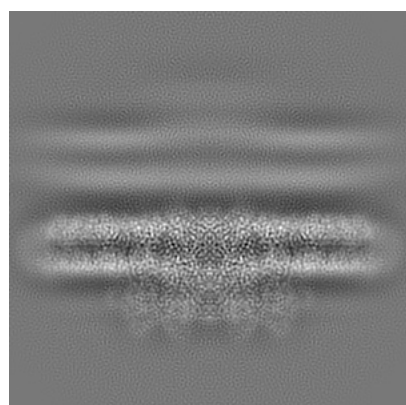
6 Map visualisation [i](#)

This section contains visualisations of the EMDB entry EMD-6741. These allow visual inspection of the internal detail of the map and identification of artifacts.

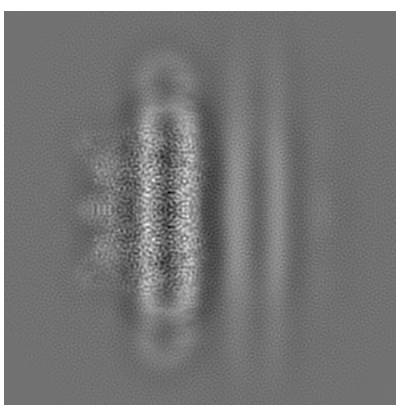
No raw map or half-maps were deposited for this entry and therefore no images, graphs, etc. pertaining to the raw map can be shown.

6.1 Orthogonal projections [i](#)

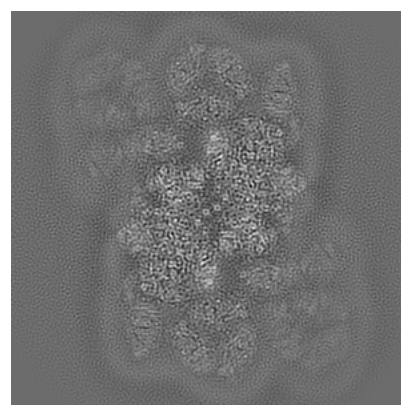
6.1.1 Primary map



X



Y

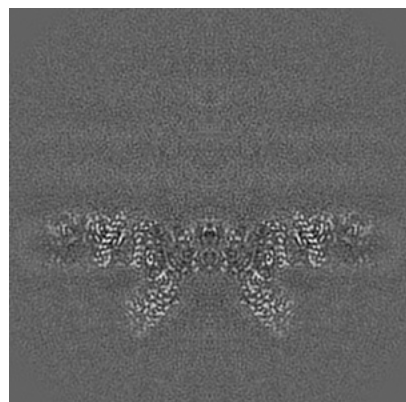


Z

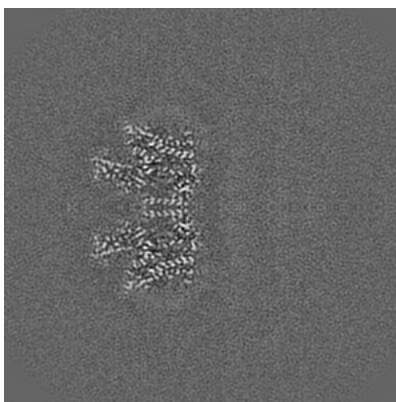
The images above show the map projected in three orthogonal directions.

6.2 Central slices [i](#)

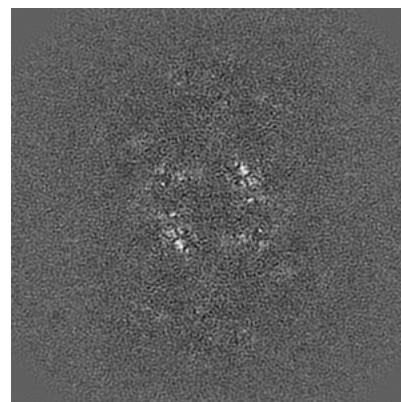
6.2.1 Primary map



X Index: 150



Y Index: 150

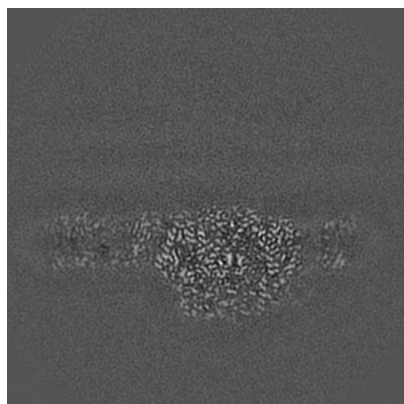


Z Index: 150

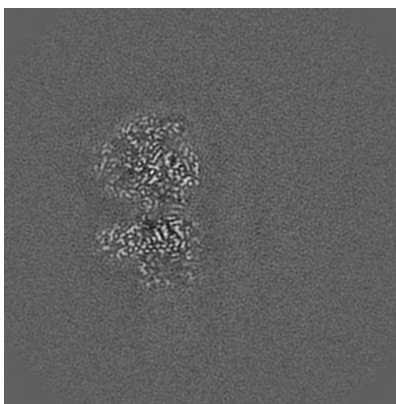
The images above show central slices of the map in three orthogonal directions.

6.3 Largest variance slices [i](#)

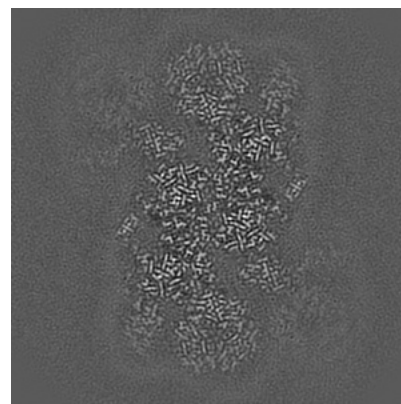
6.3.1 Primary map



X Index: 178



Y Index: 162

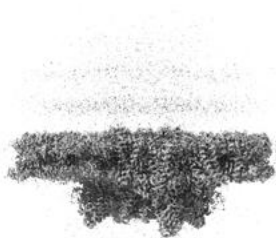


Z Index: 130

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

6.4 Orthogonal surface views [i](#)

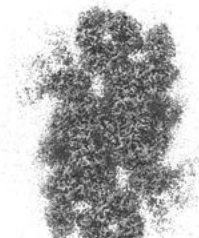
6.4.1 Primary map



X



Y



Z

The images above show the 3D surface view of the map at the recommended contour level 17.5. These images, in conjunction with the slice images, may facilitate assessment of whether an appropriate contour level has been provided.

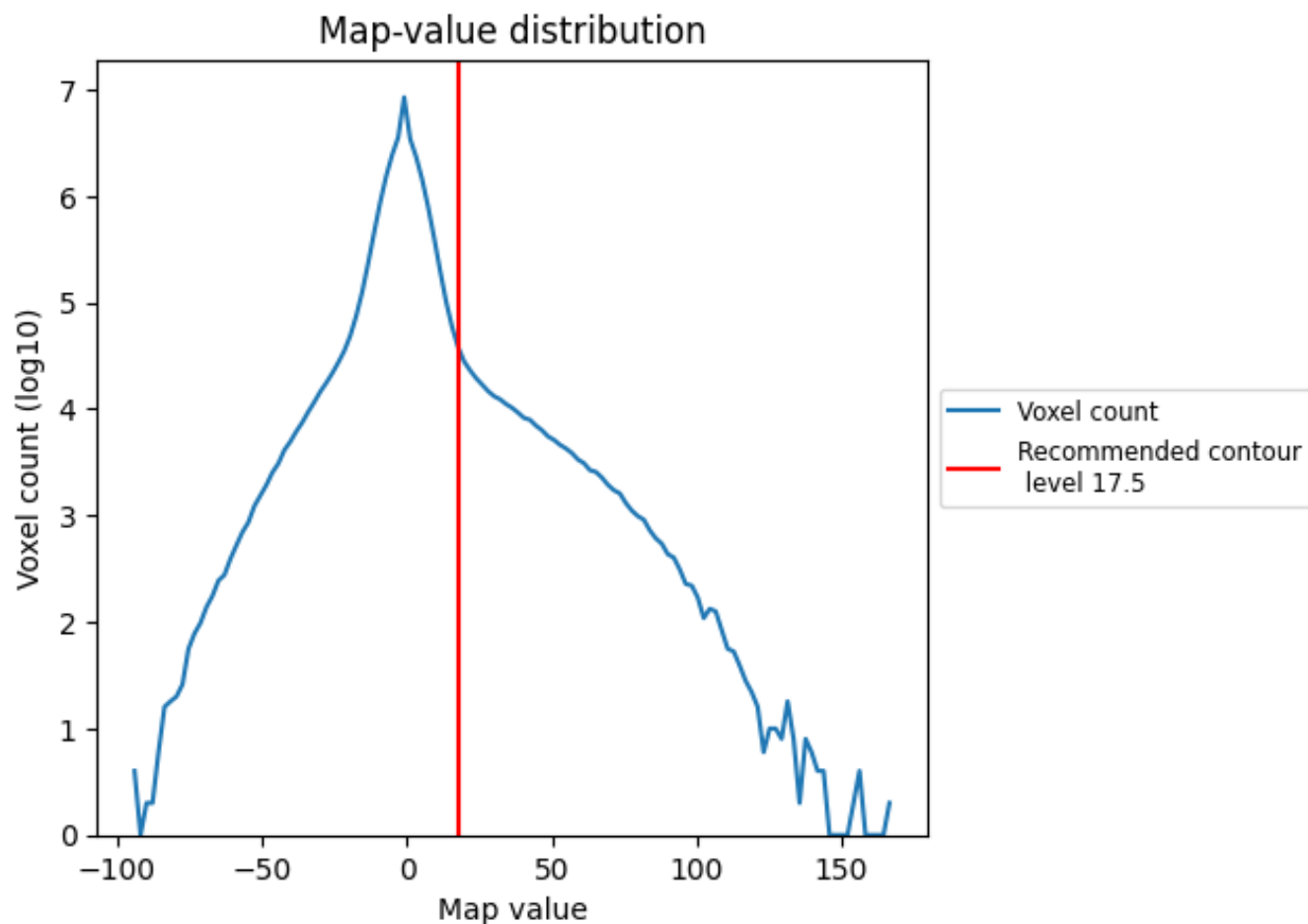
6.5 Mask visualisation

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

7 Map analysis [i](#)

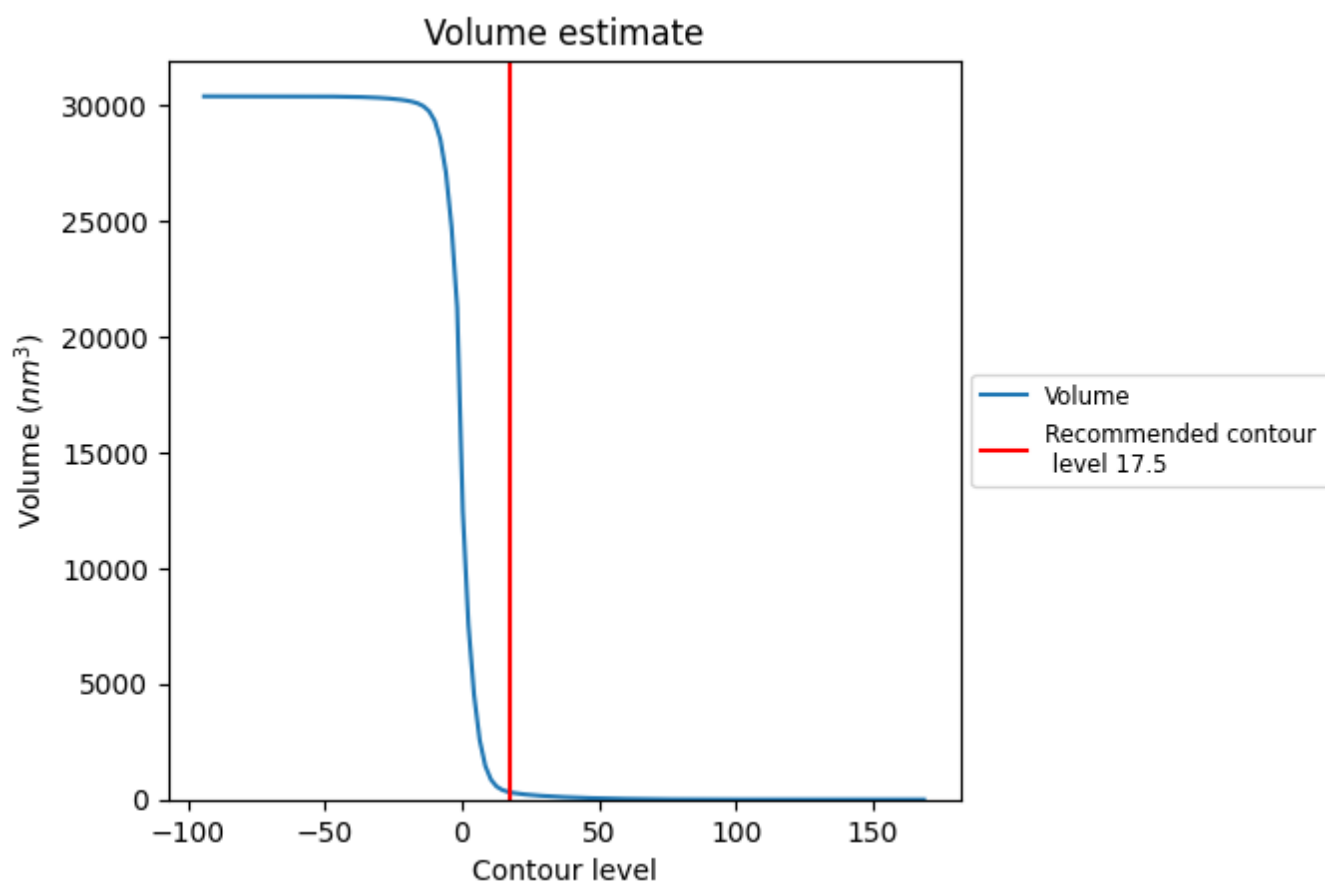
This section contains the results of statistical analysis of the map.

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.

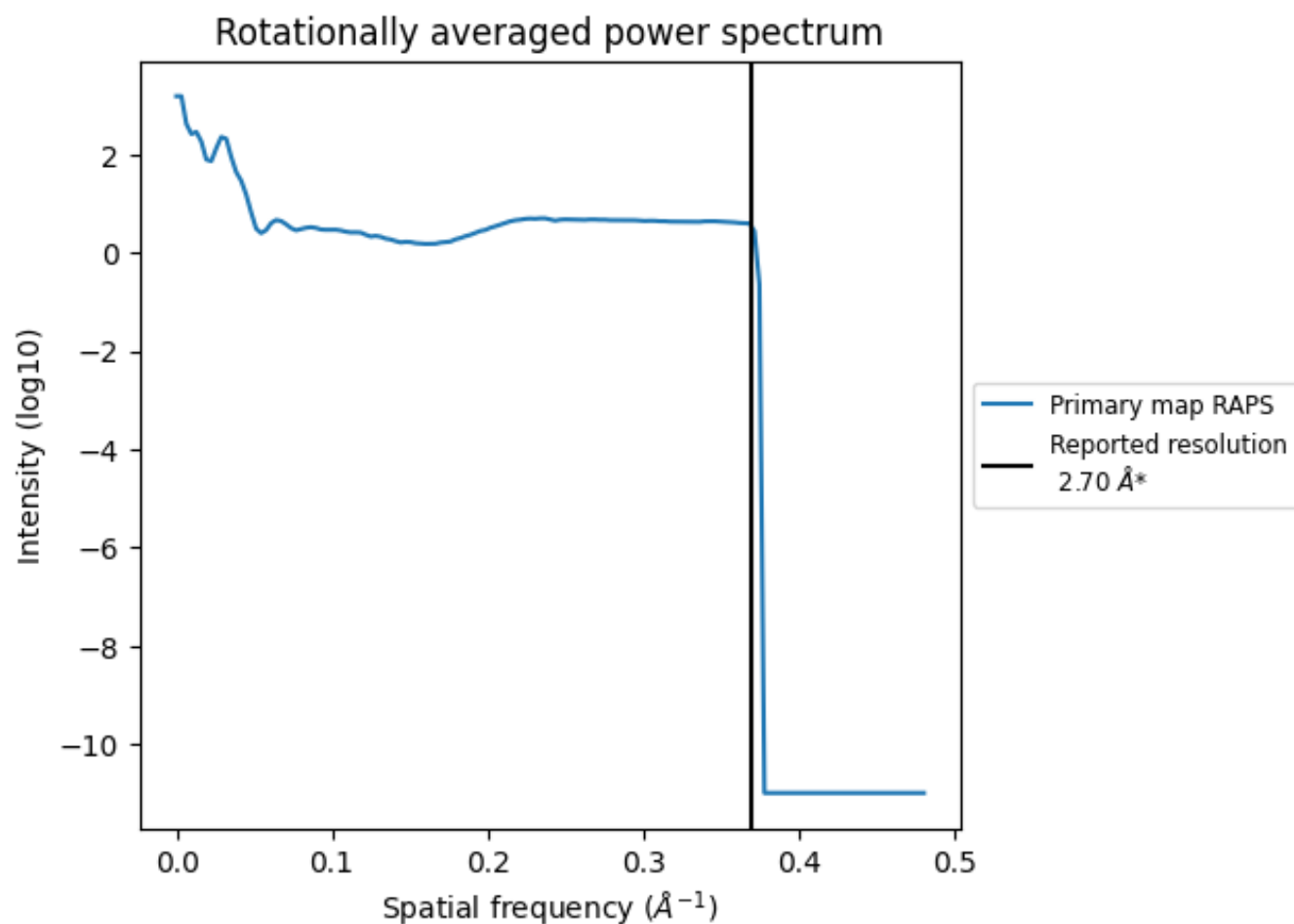
7.2 Volume estimate [i](#)



The volume at the recommended contour level is 319 nm³; this corresponds to an approximate mass of 288 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 0.370 Å⁻¹

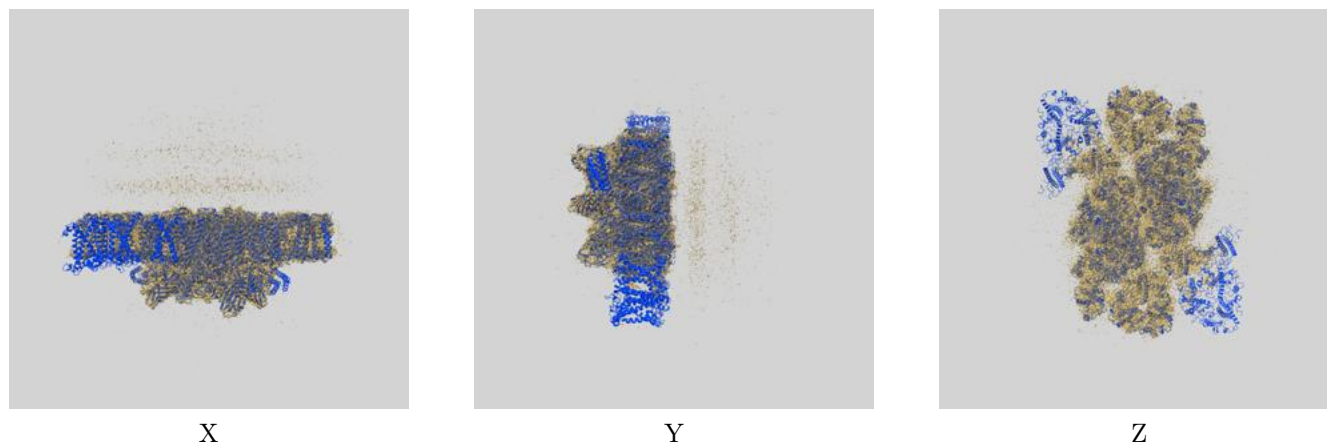
8 Fourier-Shell correlation

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

9 Map-model fit [i](#)

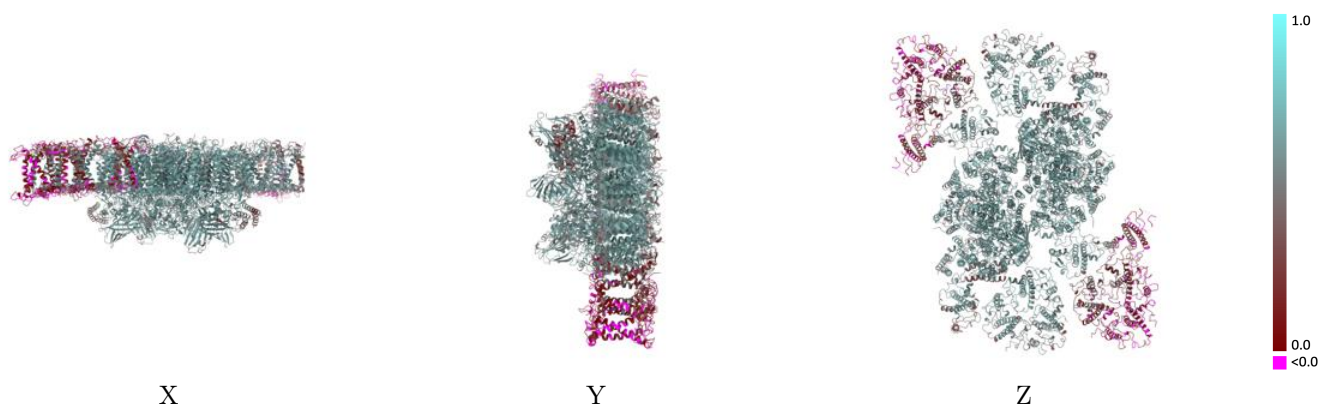
This section contains information regarding the fit between EMDB map EMD-6741 and PDB model 5XNL. Per-residue inclusion information can be found in section 3 on page 51.

9.1 Map-model overlay [i](#)



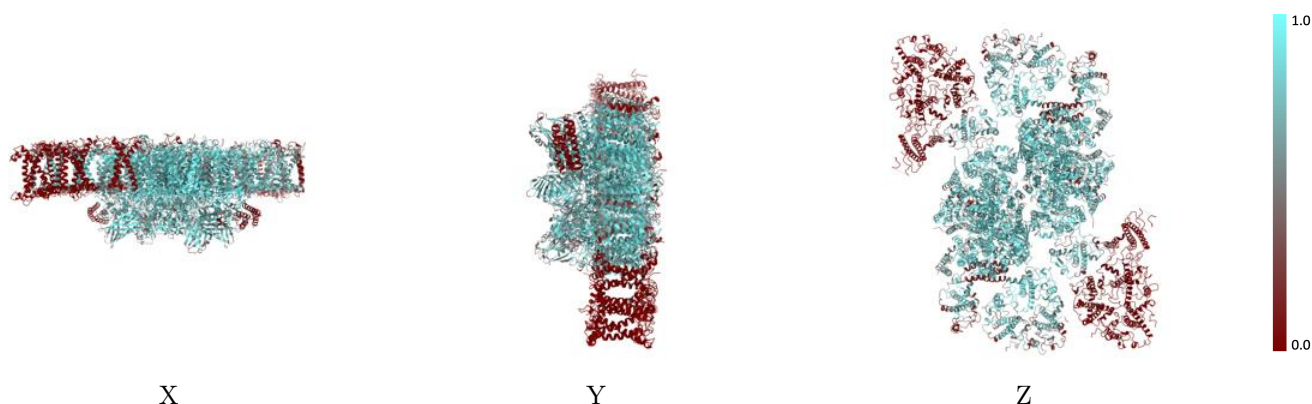
The images above show the 3D surface view of the map at the recommended contour level 17.5 at 50% transparency in yellow overlaid with a ribbon representation of the model coloured in blue. These images allow for the visual assessment of the quality of fit between the atomic model and the map.

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



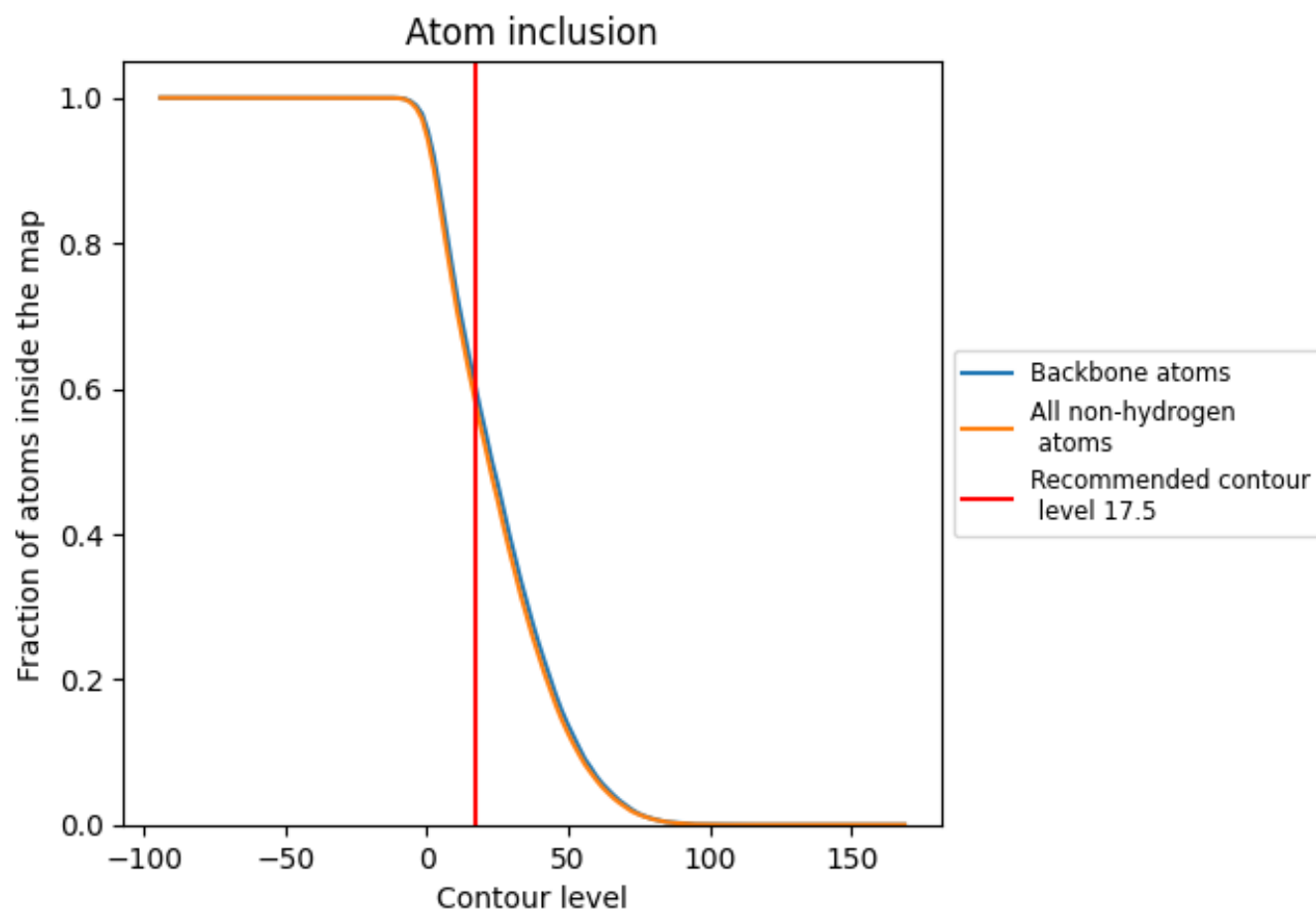
The images above show the model with each residue coloured according to its Q-score. This shows their resolvability in the map with higher Q-score values reflecting better resolvability. Please note: Q-score is calculating the resolvability of atoms, and thus high values are only expected at resolutions 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 (17.5).







































































9.4 Atom inclusion [i](#)



At the recommended contour level, 60% of all backbone atoms, 57% 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 (17.5) and Q-score for the entire model and for each chain.

Chain	Atom inclusion	Q-score
All	 0.5743	 0.5080
1	 0.0440	 0.2350
2	 0.0004	 0.0900
3	 0.0193	 0.2140
4	 0.0374	 0.1910
5	 0.0444	 0.2370
6	 0.0000	 0.0880
7	 0.0193	 0.2130
8	 0.0369	 0.1890
A	 0.8729	 0.6430
B	 0.8093	 0.6200
C	 0.8211	 0.6290
D	 0.8650	 0.6370
E	 0.7798	 0.6010
F	 0.7891	 0.6140
G	 0.5388	 0.5460
H	 0.8026	 0.6150
I	 0.8755	 0.6340
J	 0.6813	 0.5830
K	 0.7318	 0.5880
L	 0.8085	 0.6190
M	 0.6745	 0.5720
N	 0.6003	 0.5620
O	 0.7227	 0.5810
P	 0.6242	 0.5760
Q	 0.0757	 0.4090
R	 0.6353	 0.5630
S	 0.5200	 0.5220
T	 0.7013	 0.6000
W	 0.6925	 0.5860
X	 0.5876	 0.5550
Y	 0.7971	 0.6100
Z	 0.5575	 0.5360
a	 0.8719	 0.6420
b	 0.8082	 0.6200



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Chain	Atom inclusion	Q-score
c	 0.8196	 0.6300
d	 0.8643	 0.6370
e	 0.7798	 0.6010
f	 0.7927	 0.6130
g	 0.5411	 0.5450
h	 0.8007	 0.6110
i	 0.8755	 0.6330
j	 0.6773	 0.5810
k	 0.7318	 0.5800
l	 0.8056	 0.6240
m	 0.6667	 0.5710
n	 0.5988	 0.5610
o	 0.7211	 0.5820
p	 0.6256	 0.5770
q	 0.0767	 0.4070
r	 0.6361	 0.5650
s	 0.5220	 0.5210
t	 0.6879	 0.6000
w	 0.6925	 0.5880
x	 0.5876	 0.5590
y	 0.7967	 0.6110
z	 0.5536	 0.5340